Classification of ten-dimensional kinematical groups with space isotropy

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All the abstract ten-dimensional real Lie algebras that contain as a subalgebra the algebra of the three-dimensional rotation group (generators **J**) and decompose under the rotation group into three three-vector representation spaces (**J** itself, **K**, and **P**) and a scalar (generator H) are classified. In all cases, the existence of a homogeneous space of dimension 4 is shown.

I. INTRODUCTION

In this short note we want to present results that were obtained almost 20 years ago and that extend the classification of all kinematical groups obtained by one of the authors (H. B.) in collaboration with Lévy-Leblond.[1]

A kinematical group is a ten-parameter group preserving the isotropy of space. The physical interpretation of the transformations is rotations (three generators **J**), inertial transformations (three generators **K**), space translations (three generators **P**), and time translations (generator H). Space isotropy, a quite natural hypothesis, implies that the generators transform correctly under rotations, i.e., H must be a scalar and **J**, **K**, and **P** must be vectors, a property expressed by the commutation relations

$$\begin{aligned} &[\mathbf{J},\mathbf{J}]=\mathbf{J}, \quad [\mathbf{J},\mathbf{P}]=\mathbf{P}, \\ &[\mathbf{J},\mathbf{K}]=\mathbf{K}, \quad [\mathbf{J},H]=0, \end{aligned} \tag{1.1}$$

where $[\mathbf{A},\mathbf{B}]=\mathbf{C}$ is a shorthand for

$$[A_i,B_j]=\epsilon_{ijk}C_k \tag{1.2}$$

and ϵ_{ijk} is the antisymmetric Kronecker product.

Here we classify all the abstract ten-dimensional Lie algebras satisfying (1.1). This problem is more general than the one solved in Ref. 1. Indeed Eqs. (1.1) are invariant under the involutions

$$\begin{aligned} &\mathbf{J}'=\alpha\mathbf{J}, \quad \mathbf{K}'=\epsilon\mathbf{K}, \\ &\mathbf{P}'=\sigma\mathbf{P}, \quad H'=\delta H, \end{aligned} \tag{1.3}$$

where ϵ, σ, and δ are arbitrary signs[2] and $\alpha=1$.

In Ref. 1 the two following conditions were imposed.

(i) Parity π and time reversal τ defined by

$$\pi\colon\ \epsilon=-1, \quad \sigma=-1, \quad \delta=1, \tag{1.4}$$

$$\tau\colon\ \epsilon=-1, \quad \sigma=1, \quad \delta=-1, \tag{1.5}$$

were supposed to be (involutory) automorphisms of the algebras.

(ii) The K's generate noncompact subgroups.

The first condition defines the three vector spaces corresponding to **J**, **K**, and **P** uniquely since they behave differently under parity and time reversal. Unambiguous physical interpretations of the corresponding kinematical algebras followed. All the Lie algebras obtained were the two de Sitter Lie algebras [so(3,2) and so(4,1)] and all their isotropic contractions.[3]

Since, in the present work, we do not impose parity and time reversal invariance, the subspaces spanned by **P** and **K** are no longer uniquely defined. Transformations of the type

$$\begin{aligned} &\mathbf{P}'=x\mathbf{P}+y\mathbf{K}+z\mathbf{J}, \\ &\mathbf{K}'=x'\mathbf{K}+y'\mathbf{P}+z'\mathbf{J}, \end{aligned} \tag{1.6}$$

where x, y, z, x', y', and z' are real and

$$xx'-yy'\neq 0 \tag{1.7}$$

are allowed. We also use

$$H'=wH, \quad w\neq 0, \tag{1.8}$$

to put each algebra in a simple form (w real).

Because our classification only deals with Lie algebras, no condition concerning global transformations [like condition (ii) above] is made.

II. METHOD

Let us sketch in a few words the straightforward method we have used to obtain the classification.

(a) First we have looked for the complex algebras satisfying Eq. (1.1), defined up to transformations of the form given in Eqs. (1.6)–(1.8) with complex coefficients.

Denoting K_i, P_i, and J_i by $X_i^{(1)}$, $X_i^{(2)}$, and $X_i^{(3)}$, respectively, it is then easy to see that, following (1.1),

$$\mathrm{Ad}_H(X_i^{(A)}) \overset{\text{def}}{=} [H,X_i^{(A)}]$$

$$=\sum_{(B)} M^{(A)}_{(B)}\, X_i^{(B)}, \tag{2.1}$$

where the (3×3)-matrix M has its third row entries equal to zero. With the aid of transformations (1.6)–(1.8) the matrix M can be put in one of the following Jordan forms:

α = diagonal (with zero as an eigenvalue),
β = one of the five nondiagonal matrices,

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$$M_1=\begin{pmatrix}1&1&0\\0&1&0\\0&0&0\end{pmatrix},\quad M_2=\begin{pmatrix}0&1&0\\0&0&0\\0&0&0\end{pmatrix},$$
$$M_3=\begin{pmatrix}0&1&0\\0&0&1\\0&0&0\end{pmatrix},\quad M_4=\begin{pmatrix}0&0&0\\0&0&1\\0&0&0\end{pmatrix},\qquad (2.2)$$
$$M_5=\begin{pmatrix}1&0&0\\0&0&1\\0&0&0\end{pmatrix}.$$

(b) In order to obtain a Lie algebra we have to impose all the Jacobi identities. The ones involving the J's are satisfied identically as a result of (1.1).

It is easy to verify that there is no Lie algebra for the cases corresponding to M_3, M_4, and M_5.

In the case M_1 we obtain a unique complex algebra, the commutators of which are

$$[H,\mathbf{P}]=\mathbf{P}+\mathbf{K},\quad [H,\mathbf{K}]=\mathbf{K},\qquad (2.3)$$

$[\mathbf{P},\mathbf{P}]$, $[\mathbf{P},\mathbf{K}]$, and $[\mathbf{K},\mathbf{K}]$ being zero.

The matrix M_2 leads to two distinct complex Lie algebras, the Galilei and the Poincaré ones.

When the matrix M is diagonal, as a result of the Jacobi identities, we have to distinguish between the following sets of eigenvalues of M:

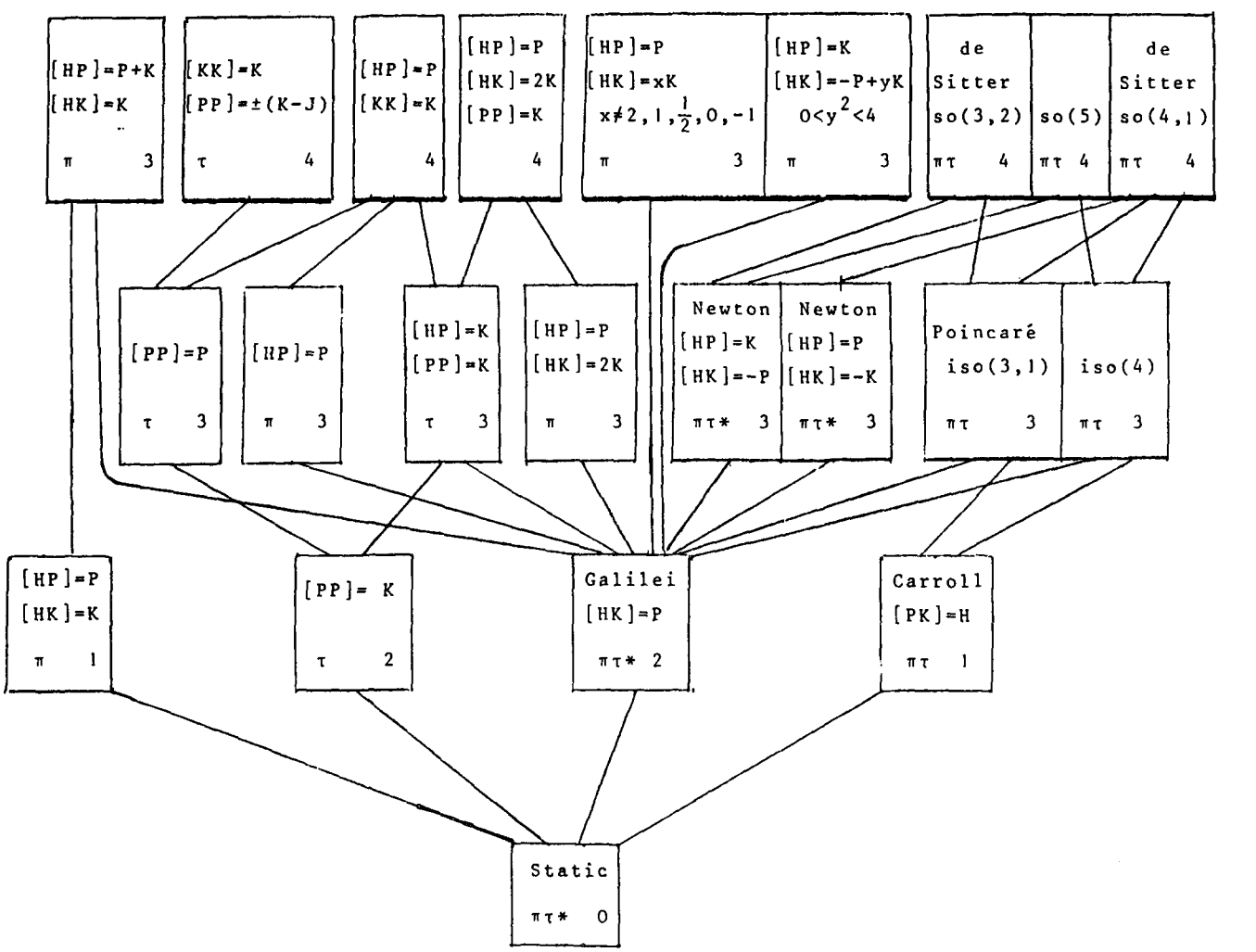
$$\lambda^{(1)}=\{0,0,0\},$$
$$\lambda^{(2)}=\{1,0,0\},$$
$$\lambda^{(3)}=\{1,1,0\},$$
$$\lambda^{(4)}=\{1,2,0\}\ \text{or}\ \{1,\tfrac{1}{2},0\},$$
$$\lambda^{(5)}=\{1,-1,0\},$$
$$\lambda^{(6)}=\{1,\theta,0\},\quad \theta\neq 2,1,\tfrac{1}{2},0,-1,$$

where θ can be complex. The first set of eigenvalues corresponds to the static and Carroll–Lie algebras,[1] the fifth set to the de Sitter and Newton–Lie algebras.

The procedure just defined leads us to 16 complex nonisomorphic algebras together with an infinite family of nonisomorphic algebras parametrized by θ in the sixth set of eigenvalues.

(c) It is then a simple matter to derive the real forms of those complex Lie algebras. The results are given in Table I and discussed in the next section. If we discard the well-known cases of de Sitter (three real forms), Poincaré (two

TABLE I. Deformations of the static algebra.



real forms), and Newton (two real forms), all the other complex algebras have only one real form except: (i) the ones associated with the sixth set for which two real forms depend on a continuous parameter and (ii) one Lie algebra associated with the first set which has two real forms.

III. RESULTS AND CONCLUSIONS

In Table I each box represents a Lie algebra except three boxes representing one discrete and two continuous families of algebras. The commutators (1.1) are valid for all of them. The different algebras are described by their nonvanishing other commutators except for so(5), de Sitter, Poincaré, and the inhomogeneous so(4) for which the commutation relations are not given but are well known. Adjacent boxes correspond to real forms of the same complex algebra. Lines describe all possible contractions[3] between these algebras.

Defining the static Lie algebra as that one for which all the commutators are zero but the ones of (1.1), the listed algebras represent all possible isotropic deformations (the inverse of contractions) of the static algebra.

The symbol * means that there exists a nontrivial central extension,[4] π means that there exists an involutory automorphism of the parity form (1.4), and τ means that there exists an involutory antiautomorphism of the time reversal form (1.5). Clearly those for which π and τ appear together are the ones which were classified in Ref. 1. By a regular change of basis (1.6)–(1.8) with real coefficients, each algebra can be written in the form

$$\begin{aligned}
&[\mathbf{P},\mathbf{P}] = \alpha\mathbf{P} + \beta\,\mathbf{K} + \gamma\mathbf{J}\,,\\
&[\mathbf{K},\mathbf{K}] = \alpha'\mathbf{K} + \beta'\mathbf{P} + \gamma'\mathbf{J}\,,\\
&[H,\mathbf{P}] = a\mathbf{P} + b\,\mathbf{K} + c\mathbf{J}\,,\\
&[H,\mathbf{K}] = a'\mathbf{K} + b'\mathbf{P} + c'\mathbf{J}\,,\\
&[\mathbf{P},\mathbf{K}] = \mu\mathbf{J} + \rho H\,,
\end{aligned} \tag{3.1}$$

where, in the last commutator, ρ is written for $\rho\delta_{ij}$. The coefficients $\{\alpha,\ldots,\rho\}$ depend on n arbitrary, independent, and continuous parameters. This number n is given for each algebra. In particular it should be noted that through a regular change of basis the roles of **K** and **P** can be interchanged.

It is one of the surprising results that every Lie algebra has at least one subalgebra of dimension 6 (generated by **J** and some combination of **K** and **P**), a fact which allows the construction of homogeneous space of dimension 4, the "space-time" associated with that algebra.

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[1] H. Bacry and J. M. Lévy-Leblond, J. Math. Phys. **9**, 1605 (1968).

[2] To every involutory automorphism of the algebra of the form (1.3), there corresponds an involutory antiautomorphism given by (1.3) with all the signs reversed and $[A,B]$ replaced by $[B',A']$. When an i is factorized for every generator, this antiautomorphism is related to complex conjugation. As is well known, time reversal is an antiautomorphism of that type.

[3] Contractions have been defined in E. Inonu and E. P. Wigner, Proc. Natl. Acad. Sci. USA **39**, 510 (1953).

[4] There exists a central extension of an algebra when a new generator M, which commutes with all the generators, can be added to the algebra to form a new Lie algebra. To induce a nontrivial central extension, that new generator must appear in the right-hand side of the commutators. By this operation a "mass operator" can be introduced in the Galilei group.

Nahm's equations, singular point analysis, and integrability

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A singular point analysis (Painlevé test) for certain special cases of Nahm's equations is performed. It is shown that there are cases in which the equations do not pass the test. The Laurent expansion does not contain the right number of arbitrary expansion coefficients. Nevertheless the systems under consideration are completely integrable.

I. INTRODUCTION

The Nahm equations arise in Nahm's construction of monopole solutions in Yang–Mills theory.[1–6] Let T_1, T_2, and T_3 be $n \times n$ matrices of complex-valued functions of the variable t. The Nahm equations are given by

$$\frac{dT_1}{dt} = [T_2, T_3], \tag{1a}$$

$$\frac{dT_2}{dt} = [T_3, T_1], \tag{1b}$$

$$\frac{dT_3}{dt} = [T_1, T_2], \tag{1c}$$

where [,] denotes the commutator. Thus we have an autonomous system of $3n^2$ ordinary differential equations. The system is scale invariant under $t \to \alpha^{-1}t$, $T_{j,nm} \to \alpha T_{j,nm}$. The Lax representation can be found as follows[7,8]: Let U and V be two vectors ($U = (U_1, U_2, U_3)$, $V = (V_1, V_2, V_3)$) with $UU^T = 1$ and $V = V \times U$ ($\times$ cross product). Then the system (1) can be written as (Lax representation)

$$\frac{d(V \cdot T)}{dt} = [V \cdot T, U \cdot T], \tag{2}$$

where $V \cdot T = V_1 T_1 + V_2 T_2 + V_3 T_3$. Consequently, $\mathrm{Tr}((V \cdot T)^k)$ are the constants of motion.

In the present paper we study the connection with the Painlevé test (compare Ref. 9 and references therein). Four special cases are discussed. In two of the cases the system passes the test, whereas in the remaining two the test will not be passed. In all cases the connection with (algebraic) integrability is discussed, where we apply Yoshida's theorems.[10,11]

II. YOSHIDA'S THEOREMS

For our discussion we use the theorems of Yoshida.[10,11] These theorems can be applied since the system (1) is scale invariant (that is, similarity invariant).

Theorem 1: In order that a given similarity-invariant system $dx_i/dt = F_i(x)$, $(i = 1,...,N)$ be algebraically integrable, it is necessary that every possible resonance (that is, Kowalewski's exponent) becomes a rational number.

In other words, if there exists at least one irrational or imaginary Kowalewski's exponent, the similarity-invariant system is not algebraically integrable. For $n = 2$ and $n = 3$ we find for the Nahm's equations (1) that the resonances are all integers. We conjecture that also for higher n's the resonances are integers. Since the system is similarity invariant there is a set of rational numbers $m_1,...,m_N$ such that the system is invariant under the similarity transformation $t \to \alpha^{-1}t$, $x_1 \to \alpha^{m_1}x_1,...,x_N \to \alpha^{m_N}x_N$, for a constant α. In the present case we have $m_1 = \cdots = m_N = 1$. Any similarity-invariant system $dx_i/dt = F_i(x)$ has, in general, a special type of particular solution $x_1(t) = c_1(t - t_1)^{-m_1},...,x_N(t) = c_N(t - t_1)^{-m_N}$ with constants $c_1,...,c_N$ to be determined. Suppose that the similarity-invariant system has a polynomial first integral $h(x_1,...,x_N)$. Consequently, $h(\alpha^{m_1}x_1,...,\alpha^{m_N}x_N)$ is again a first integral. We define that a polynomial $\phi(x_1,...,x_N)$ is a weighted homogeneous polynomial of weighted degree r when ϕ is multiplied α^r by the similarity transformation or the identity $\phi(\alpha^{m_1}x_1,...,\alpha^{m_N}x_N) = \alpha^r\phi(x_1,...,x_N)$ holds for arbitrary x and α.

Let us now give two theorems[10,11] which are helpful to find the first integrals (if any exist).

Theorem 2: Let h be a weighted homogeneous first integral of weighted degree r for the similarity invariant system $dx_i/dt = F_i(x)$. Assume that the elements of the vector grad $h(c)$ are finite and not identically zero for a fixed choice of the set $c_1,...,c_N$ in $F_i(c_1,...,c_N) = -m_i c_i$, $(i = 1,...,N)$. Then r is a resonance.

Theorem 3: Let h_1 and h_2 be two independent weighted homogeneous first integrals of the same weighted degree r. Suppose that the two vectors grad $h_1(c)$ and grad $h_2(c)$ are both finite, not identically zero, and these two vectors are linearly independent for a fixed choice of $c_1,...,c_N$. Then r is a resonance with multiplicity at least 2.

It is obvious that Theorem 3 can be extended to three (and more) independent weighted homogeneous first integrals of the same weighted degree r.

Let us emphasize that the algebraic first integrals correspond to resonances which are rational numbers. On the other hand not all resonances are related with first integrals in completely integrable systems. This demonstrates the following example. Let

$$H(p,q) = p_1^2/2 + p_2^2/2 + V(q),$$

where

$$V(q) = q_1^5/5 + 2q_1^3q_2^2 + q_1q_2^4.$$

Then, besides H, we find the first integral $h(p,q) = p_1p_2 + q_1^4q_2 + 2q_1^2q_2^3 + q_2^5/5$. From Theorem 2 we find that H and h correspond to the resonance $r = \frac{10}{3}$. The other resonances (besides $r = -1$) are $r = \frac{2}{3}$ and $r = \frac{5}{3}$. Moreover we see that the resonances need not be integers in order that a system be completely integrable.

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III. EXAMPLES

Let us now study our special cases of the Nahm equation (1). In our first example we put $T_j(t) = if_j(t)\sigma_j$, where σ_1, σ_2, and σ_3 are the Pauli matrices. Then we find

$$\dot{f}_1 = -2f_2f_3, \quad \dot{f}_2 = -2f_1f_3, \quad \dot{f}_3 = -2f_1f_2. \tag{3}$$

The Painlevé test for this system has been already performed in literature.[12] The system passes the test. The dominant behavior is given by $f_1(t) \propto \tau^{-1}$, $f_2(t) \propto \tau^{-1}$, $f_3(t) \propto \tau^{-1}$, where $\tau = t - t_0$. Since the system is scale invariant it follows that $f_1(t) = a\tau^{-1}$, $f_2(t) = b\tau^{-1}$, $f_3(t) = c\tau^{-1}$ is a solution to the system (3) where $a = 2bc$, $b = 2ac$, $c = 2ab$. The resonances are given by $r_1 = -1, r_2 = 2$ (twofold). The resonance $r = 2$ (twofold) is related to first integrals given by $h_1(f) = f_1^2 - f_2^2$ and $h_2(f) = f_1^2 - f_3^2$. Since the equations of motion are scale invariant under $t \to \alpha^{-1}t$, $f_i \to \alpha f_i$, we have $h_1(\alpha f_1, \alpha f_2) = \alpha^2 h_1(f_1, f_2)$ and $h_2(\alpha f_1, \alpha f_2) = \alpha^2 h_2(f_1, f_2)$ (Theorem 3).

Consider now system (1) with $n = 2$ and assume that the $T_{i,jk}$'s are real-valued functions. Then the first integrals are given by

$$h_1(T) = T_{1,11} + T_{1,22}, \tag{4a}$$

$$h_2(T) = T_{2,11} + T_{2,22}, \tag{4b}$$

$$h_3(T) = T_{3,11} + T_{3,22}, \tag{4c}$$

$$h_4(T) = \sum_{j=1}^{3} T_{j,12}^2, \tag{4d}$$

$$h_5(T) = \sum_{j=1}^{3} T_{j,21}^2, \tag{4e}$$

$$h_6(T) = T_{1,12}T_{1,21} - T_{1,11}T_{1,22} + \sum_{j=1}^{3} T_{j,11}T_{j,22}, \tag{4f}$$

$$h_7(T) = T_{2,12}T_{2,21} - T_{2,11}T_{2,22} + \sum_{j=1}^{3} T_{j,11}T_{j,22}, \tag{4g}$$

$$h_8(T) = T_{3,12}T_{3,21} - T_{3,11}T_{3,22} + \sum_{j=1}^{3} T_{j,11}T_{j,22}. \tag{4h}$$

The system (1) ($n = 2$) can be solved by quadrature with the help of these eight first integrals. For the singular point analysis we consider the system in the complex domain. The dominant behavior is given by

$$T_i(t) = \begin{pmatrix} C_{i,11}\tau^{-1} & C_{i,12}\tau^{-1} \\ C_{i,21}\tau^{-1} & C_{i,22}\tau^{-1} \end{pmatrix}, \tag{5}$$

where

$$C_i = -\frac{1}{2}\sum_{j=1}^{3}\sum_{k=1}^{3} \epsilon_{ijk}[C_j, C_k]. \tag{6}$$

For the resonances we find $r_1 = -1$, $r_2 = 0$ (threefold), $r_3 = 1$ (threefold), and $r_4 = 2$ (fivefold). The resonance $r_3 = 1$ (threefold) corresponds to the three first integrals given by Eqs. (4a)–(4c). The resonance $r_4 = 2$ (fivefold) corresponds to the five first integrals given by Eqs. (4d)–(4h).

Our third and fourth special cases are as follows. Let $\{H_\alpha, \alpha = 1,\ldots,n-1\}$ be generators of the Cartan subalgebra of $\mathrm{sl}(n) = A_{n-1}$, and $\{E_\alpha, E_{-\alpha}\}$ be step operators satisfying

$$[H_\alpha, E_{\pm\beta}] = \pm K_{\alpha\beta}E_{\pm\beta}, \quad [E_\alpha, E_{-\beta}] = \delta_{\alpha\beta}H_\beta, \tag{7}$$

where $(K_{\alpha\beta})$ is the $(n-1)\times(n-1)$ Cartan matrix of $\mathrm{sl}(n)$. Assume that

$$T_1(t) = \frac{i}{2}\sum_{\alpha=1}^{n-1} q_\alpha(t)(E_\alpha + E_{-\alpha}), \tag{8a}$$

$$T_2(t) = -\frac{1}{2}\sum_{\alpha=1}^{n-1} q_\alpha(t)(E_\alpha - E_{-\alpha}), \tag{8b}$$

$$T_3(t) = \frac{i}{2}\sum_{\alpha=1}^{n-1} p_\alpha(t)H_\alpha. \tag{8c}$$

Then the Nahm equations take the form

$$\dot{p}_\alpha = q_\alpha^2, \quad \dot{q}_\alpha = \frac{1}{2}\sum_{\beta=1}^{n-1} p_\beta K_{\alpha\beta}q_\alpha. \tag{9}$$

Setting $f_\alpha = 2\ln q_\alpha$ yields

$$\ddot{f}_\alpha = \sum_{\beta=1}^{n-1} K_{\alpha\beta}\exp(f_\beta). \tag{10}$$

These are Toda molecule equations. Now let $n = 2$. The Cartan matrix of $\mathrm{sl}(2) = A_1$ is given by $(K_{\alpha\beta}) = 2$. Then system (9) takes the form $\dot{p} = q^2$, $\dot{q} = pq$. This system passes the Painlevé test and the resonances are given by -1 and 2. The first integral is given by $h(q,p) = q^2 - p^2$. Consequently, $h(\alpha q, \alpha p) = \alpha^2 h(q,p)$ which indicates that $r = 2$ has to be a resonance. Now let $n = 3$. The Cartan matrix is given by

$$(K_{\alpha\beta}) = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \tag{11}$$

and therefore we obtain

$$\dot{p}_1 = q_1^2, \quad \dot{p}_2 = q_2^2, \tag{12a}$$

$$\dot{q}_1 = q_1(p_1 - p_2/2), \quad \dot{q}_2 = q_2(p_2 - p_1/2). \tag{12b}$$

Inserting the ansatz $p_1 \propto a_0(t-t_1)^{-m_1}$, $p_2 \propto b_0(t-t_1)^{-m_2}$, $q_1 \propto c_0(t-t_1)^{-m_3}$, and $q_2 \propto d_0(t-t_1)^{-m_4}$ we find $m_1 = m_2 = m_3 = m_4 = 1$ and $a_0 = b_0 = -2, c_0^2 = d_0^2 = 2$. Only one branch arises with $a_0, b_0, c_0, d_0 \neq 0$. The resonances are given by $-1, 2, 3$, and -2. We obtain a Laurent expansion of the form

$$p_1(t) = \sum_{j=0}^{\infty} a_j(t-t_1)^{j-1}, \tag{13a}$$

$$p_2(t) = \sum_{j=0}^{\infty} b_j(t-t_1)^{j-1}, \tag{13b}$$

$$q_1(t) = \sum_{j=0}^{\infty} c_j(t-t_1)^{j-1}, \tag{13c}$$

$$q_2(t) = \sum_{j=0}^{\infty} d_j(t-t_1)^{j-1}, \tag{13d}$$

where two expansion coefficients can be chosen arbitrarily. The resonance -1 corresponds to the arbitrariness of the pole position in Eqs. (13a) through (13d). Thus the system (12) does not pass the Painlevé test, since in order to pass the test three expansion coefficients have to be chosen arbitrarily. That this is not the case is due to the resonance -2. Now the resonances 2 and 3 are related to polynomial first integrals. In fact we find the first integrals

$$h_1(p,q) = p_1^2 + p_2^2 - p_1p_2 - q_1^2 - q_2^2 \tag{14a}$$

and

$$h_2(p,q) = p_1^2 p_2 - p_1 p_2^2 + p_1 q_2^2 - p_2 q_1^2, \tag{14b}$$

where $h_1(\alpha p,\alpha q) = \alpha^2 h_1(p,q)$ and $h_2(\alpha p,\alpha q) = \alpha^3 h(p,q)$ (Theorem 2). Solution (13) is a Laurent expansion in the neighborhood of t_1. In literature we sometimes find the remark that negative resonances (like -2 in the case given above) are purely formal. However, the connection is as follows. Instead of looking for an expansion of the form (13) in the neighborhood of t_1 we consider an expansion of the form

$$p_1(t) = \sum_{j=0}^{\infty} a_{-j} t^{-j-1}, \tag{15a}$$

$$p_2(t) = \sum_{j=0}^{\infty} b_{-j} t^{-j-1}, \tag{15b}$$

$$q_1(t) = \sum_{j=0}^{\infty} c_{-j} t^{-j-1}, \tag{15c}$$

$$q_2(t) = \sum_{j=0}^{\infty} d_{-j} t^{-j-1}. \tag{15d}$$

This means we study an expansion around infinity. Inserting ansatz (13) into system (12) we find that d_{-1} and d_{-2} can be chosen arbitrarily. Therefore, expansion (15) contains two arbitrary expansion coefficients.

IV. CONCLUSIONS

Let $dx_i/dt = F_i(x)$ be a similarity-invariant system and let the F_i's be polynomial ($F_i: \mathbb{R}^n \to \mathbb{R}$). Then the polynomial first integrals can be found using the ansatz

$$h(x) = \sum_{j_1,\ldots,j_n=0}^{M} C_{j_1 \cdots j_n} x_1^{j_1} \cdots x_n^{j_n}, \tag{16}$$

where $M = j_1 + \cdots + j_n$. The coefficients $C_{j_1 \cdots j_n}$ *are determined by* $dh/dt = 0$ [modulo $dx_i/dt = F_i(x)$]. Now the Painlevé test gives us a restriction on M if we know the dominant behavior and the resonances. In our first example the dominant behavior is -1 and the highest resonance is 2. Consequently, M can be restricted to $M = 2$. In our fourth example we find $M = 3$.

System (12) does not pass the Painlevé test in the sense that the Laurent expansion (13) does not contain the right number of arbitrary expansion coefficients. On the other hand the system (12) is completely integrable in the sense that it can be solved by quadrature using the first integrals (14a) and (14b). We find this behavior for $n = 4$, too. We should recall the problem of the motion of a heavy rigid body near a fixed point treated by Kovalevskaya.[13] The system is described by an autonomous system of six first-order ordinary differential equations. To integrate the system completely we only need four first integrals. The fourth first integral imposes conditions on the constants which the system enter.

Finally, we mention that the field theoretical extension

$$\frac{\partial^2 u_j}{\partial r^2} - \frac{\partial^2 u_j}{\partial t^2} = \exp\left(\sum_{i=1}^{l} k_{ji} u_i\right) \tag{17}$$

of Eq. (10) has been discussed extensively by Ganoulis *et al.*[6] Steeb *et al.*[14] have shown that the equations $u_{rr} - u_{tt} = e^u$ and $u_{rr} - u_{tt} = ae^u + be^{-2u}$ pass the Painlevé test (after the transformation $v = e^u$) in the sense of Weiss *et al.*[15]

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On the integration of the self-similar equations, and the meaning of the Cole–Hopf transformation

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The existence of a first integral of the self-similar equations associated with a given partial differential system, in one space dimension, is shown, whenever there exists a conserved quantity Q whose scale remains time independent. That result is most conveniently derived through the introduction of $Y \equiv \exp Q$ as a new unknown. In the case of the Burgers equation, the velocity potential Φ has the required property, and the transformation to the new variable $\exp \Phi$ is precisely the Cole–Hopf transform. The latter, as is well known, linearizes the Burgers equation.

I. INTRODUCTION

Much work has been done recently in the field of nonlinear dynamics to elucidate the connection between the property of integrability of a partial differential system, the presence of a Lie group of symmetry of infinite order, and the Painlevé property.[1–4] The nonlinear equations that exhibit solitons have been found to possess the Painlevé property, and their associated self-similar equations are Painlevé equations as well.[3]

The Burgers equation

$$v_t + vv_x = v_{xx} \tag{1.1}$$

is a well-known example, but it is also very special, as it is reducible to a purely *linear equation*, by a transformation known as the Cole–Hopf transform:

$$2Y_x + vY = 0. \tag{1.2}$$

The result is the heat equation, as is well known:

$$Y_t = Y_{xx}. \tag{1.3}$$

It can be shown that the Burgers equation possesses the Painlevé property, in the generalized sense of partial differential equations, as defined by Weiss *et al.*[4]; the associated self-similar equations [i.e., the equations giving the homogeneous solutions of (1.1)] are second-order ordinary differential equations (ODE's), which are the fifth canonical type, among the 50 types of Painlevé equations (Ince, see Ref. 5). That type is known to be semi-integrable (i.e., integrable once),[5] and is reducible to a Riccati equation for the unknown, $z(x)$. The latter may be linearized by the well-known transformation $y = \exp \int z\, dx$, that is, the self-similar analog of the Cole–Hopf transformation.

In the present paper we show that the semi-integrability of these self-similar equations (hereafter, SSE's) is not accidental: it can be predicted in a systematic way in more general cases, and it is related to the existence of a conserved quantity Q, which has the property that its typical scale remains *time independent* for the self-similar equations considered. The semi-integrability becomes manifest through the introduction of

$$Y = \exp Q \tag{1.4}$$

as a new unknown.

The Cole–Hopf transform is precisely of the type (1.4), where Q represents the *velocity potential.*

II. THE FORMULATION OF CONSERVATION LAWS

In one dimension, a conservation law of the general form

$$J_{0t} + J_{1x} = 0 \tag{2.1}$$

is equivalent to the condition of integrability of a potential Q, defined by the pair of equations

$$Q_x = J_0, \quad Q_t = -J_1, \tag{2.2}$$

where it is assumed that the conserved current's components J_0 and J_1 are given functions of the physical variables and of their partial derivatives. In physically meaningful situations, J_0 and J_1 have given dimensions; as a result they are power-law functions of time in the case of self-similar solutions (hereafter, SSS's).

We now consider the case where the dimension of J_1 is such that the power-law index is -1 for the SSE considered, i.e.,

$$J_1 = j_1(\xi)/t, \tag{2.3}$$

where $\xi = xt^{\lambda}$ is the self-similar coordinate, and the exponent λ is a constant, namely, the power-law index of J_0:

$$J_0 = \xi j_0(\xi)/x \equiv t^{\lambda} j_0(\xi). \tag{2.4}$$

In terms of the variables t,ξ, Eqs. (2.2) read

$$Q_{\xi} = j_0(\xi), \quad Q_t|_{\xi} = -[j_1(\xi) + \lambda \xi j_0(\xi)]/t. \tag{2.5}$$

The integration is straightforward:

$$Q = q(\xi) + r(t), \tag{2.6}$$

with

$$q(\xi) = \int j_0(\xi) d\xi, \quad r(t) = \alpha \ln t \quad (\alpha \text{ constant}),$$

and the condition of compatibility (which is automatically fulfilled since, by hypothesis, Q is a conserved quantity) reads

$$j_1(\xi) + \lambda \xi j_0(\xi) + \alpha = 0. \tag{2.7}$$

In the process *an integration constant α has emerged.* Equation (2.7) is a first integral of the differential system.

Another form, which is equivalent to (2.7), may be obtained by choosing as the new unknown

$$Y = \exp Q = t^{\alpha} y,$$

with $y = \exp q(\xi)$. The SSE system becomes an ordinary

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differential equation for the unknown $y(\xi)$, and it contains an explicit dependence on the integration constant α. The equation is manifestly homogeneous in y, and accordingly its order can be reduced, which produces the required first integral.

III. THE BURGERS AND THE NAVIER–STOKES EQUATIONS

A. Burgers equation

The relevant conserved quantity is the velocity potential Φ, defined as

$$\Phi_x = v, \quad \Phi_t = v_x - v^2/2; \tag{3.1}$$

the condition of compatibility is the Burgers equation itself. Dimensional analysis of Eq. (1.1) indicates that self-similar solutions exist only for the value $\lambda = -\frac{1}{2}$ of the exponent, i.e., the self-similar variable ξ is

$$\xi = x/\sqrt{t}. \tag{3.2}$$

Thus in the self-similar case the scale of the conserved quantity Φ has the property of being *time independent.*

With the notation of Sec. II, we have

$$j_0 = \xi z, \quad j_1 = \xi^2 z^2/2 - z - \xi z'(\xi), \tag{3.3}$$

where we have introduced a dimensionless variable z:

$$z = vt/x. \tag{3.4}$$

Thus the first integral (2.7) is a first-order ODE for the unknown z:

$$\xi \frac{dz}{d\xi} + \frac{\xi^2 z(1-z)}{2} + z - \alpha = 0, \tag{3.5}$$

which is a Riccati equation, as expected.

If we choose $Y = \exp(-\Phi/2) = t^{\alpha} y(\xi)$ instead of z as the unknown, we have

$$y'(\xi)/y = -\xi z/2, \tag{3.6}$$

and the Riccati equation (3.5) is turned into a *linear* second-order equation for y,

$$2y'' + \xi y' + \alpha y = 0, \tag{3.7}$$

in agreement with the known result for the Cole–Hopf transformation.

Equation (3.7) is the self-similar form of the heat equation (1.3).

B. The Navier–Stokes equations

For a barotropic fluid of index γ the Navier–Stokes equations read, in one dimension

$$c_t + vc_x + \frac{(\gamma-1)}{2} c v_x = 0 \quad \text{(continuity equation)}, \tag{3.8a}$$

$$v_t + vv_x + \frac{2}{(\gamma-1)} c c_x - v_{xx} = 0 \quad \text{(Euler's equation)}, \tag{3.8b}$$

where v represents the fluid's velocity and c the sound speed. It is worth noticing that, for the class of solutions characterized by a vanishing pressure (i.e., $c = 0$), the above system reduces to the Burgers equation. We assume for simplicity the value $\gamma = 3$ in what follows. The velocity potential still exists, and it is given by the following pair of equations:

$$\Phi_x = v, \quad \Phi_t = v_x - (v^2 + c^2)/2. \tag{3.9}$$

The condition of integrability of Φ precisely coincides with the Euler equation (3.8b).

In order to perform the self-similar analysis, we introduce, as usual, dimensionless variables z and $\tilde{z}$:

$$z = vt/x, \quad \tilde{z} = ct/x. \tag{3.10}$$

Substitution into the Navier–Stokes equations yields the following system:

$$\xi \tilde{z} z' + \xi(z - \tfrac{1}{2})\tilde{z}' + \tilde{z}(2z - 1) = 0, \tag{3.11a}$$

$$2z'' + z'[4/\xi + \xi(1 - 2z)] + 2z(1 - z) = 2\tilde{z}(\xi \tilde{z}' + \tilde{z}). \tag{3.11b}$$

As is well known [see, e.g., Ref. 6, Eq. (4.16)], the continuity equation (3.11a) admits of a first integral, expressing the law of mass conservation, namely

$$\xi^2 \tilde{z}(2z - 1) = C \quad (C \text{ constant}); \tag{3.12}$$

thus $\tilde{z}$ can be eliminated, and we obtain a second-order ODE for the unknown function $z(\xi)$.

Applying the method described in the preceding sections, we have

$$j_0 = \xi z, \quad j_1 = \xi^2(z^2 + \tilde{z}^2)/2 - (\xi z' + z), \tag{3.13}$$

and the general result (2.7) becomes

$$\xi \frac{dz}{d\xi} + \frac{1}{2}\xi^2[z(1 - z) - \tilde{z}^2] + z - \alpha = 0 \quad (\alpha \text{ constant}). \tag{3.14}$$

Thus the second-order SSE admits of a first integral, as predicted, which is the above equation (3.14).

The latter is not a Riccati equation, and it cannot be turned into linear form, unless the constant C vanishes. When $C \neq 0$, movable branch points appear on the horizontal axis ($z = 0$).

Finally, as a "generalization" of the Cole–Hopf transform, we may choose $Y = t^{\alpha} y(\xi) = \exp(-\Phi/2)$ as a new unknown. In the same way as in Sec. II A, this yields a second-order equation for y, which, however, remains nonlinear in the general case ($C \neq 0$). Substitution of $y'/y = -\xi z/2$ [Eq. (3.6)] produces, instead of the linear equation (3.7),

$$2y'' + \xi y' + \alpha y = -\xi^2 y \tilde{z}^2/2 \equiv -C^2 y^3/[2(4y' + \xi y)^2]. \tag{3.15}$$

IV. CONCLUSION

We have shown the existence of *a new type of first integral* of the self-similar equations associated with a given partial differential system, which occurs whenever there exists a conserved quantity Q, whose typical scale remains time independent. In particular, in the case of the Burgers and the Navier–Stokes equations in one dimension, the *velocity potential* plays the role of the conserved quantity Q; the corresponding self-similar equations *can accordingly be reduced to the first order.*

Unlike Q itself, the quantity $Y = \exp Q$ exhibits the characteristic self-similar behavior

$Y = t^{\alpha} y(xt^{\lambda})$.

The first integral arises as a consequence of the separable form of Y and of the *homogeneity* of the self-similar equation for y; and the integration constant may be interpreted as the exponent α.

It is remarkable that it is precisely the same potential Y that linearizes the Burgers equation; the choice of Y as the new unknown is known as the Cole–Hopf transformation.[7]

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On the Bäcklund transformation and Hamiltonian properties of superevaluation equations

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Bäcklund and Darboux–Bäcklund transformations are deduced for the superevaluation equations recently deduced by Kupershmidt [B. Kuperschmidt, "A super-K–dV equation—An integrable system," preprint UTSI-Tullahoma, 1984; Phys. Lett. A **102**, 213 (1983); J. Phys. A **17**, L863 (1984)] and Gürses [H. Gürses and O. Oguz, Phys. Lett. A **108**, 437 (1985)]. By a extension of the technique of BPT [M. Boiti, F. Pempinelli, and G. Z. Tu, Nuovo Cimento B **79**, 231 (1984)] to anticommuting variables the bi-Hamiltonian structure and hence the form of the recursion operator for the Lie–Bäcklund symmetry for such equations are deduced. Incidentally some explicit forms of the Lie–Bäcklund symmetry are also deduced.

I. INTRODUCTION

Extension of an integrable class of evolution equations to include anticommuting field variables has recently been done by Gürses and Oguz[1] and also by Kupershmidt.[2] While the approach of Kupershmidt is based on a generalization of the pseudodifferential calculus of Gelfand and Dikii,[3] that of Gürses and Oguz is a straightforward generalization of the matrix structure of the AKNS[4] problem to include super Lie algebras. Below we first recapitulate the work of Gürses and Oguz and then develop a generalization of methodology of BPT[5] to deduce the Bäcklund and Darboux–Bäcklund transformations for such equations. Last we deduce the Hamiltonian structure associated with such equations.

II. FORMULATION

In Ref. 1 the authors start from a linear problem

$$\Psi_x = U\Psi, \tag{1a}$$

where U is a matrix belonging to the Lie superalgebra $b(0,1)$ having the form

$$U = qE_2 + i\lambda E_0 + rE_1 + \epsilon E_3 + \beta E_4, \tag{1b}$$

where (ϵ, β) are anticommuting variables, (r,q) are commuting fields, and λ is the eigenvalue of the problem. They now adjoin a temporal evolution ψ given by the equation

$$\psi_t = V\psi, \tag{2}$$

V again belonging to $b(0,1)$ but with nine arbitrary elements all depending functionally on (q, r, β, ϵ, and λ). In Eq. (1a), the E_i's are the generators of the superalgebra[6] $b(0,1)$ satisfying the following commutation rules:

$$[E_0,E_1] = -2E_2, \quad [E_0,E_2] = 2E_1, \quad [E_1,E_2] = E_0,$$
$$[E_0,E_3] = E_3, \quad [E_0,E_4] = -E_4, \quad [E_1,E_3] = 0,$$
$$[E_1,E_4] = E_3, \quad [E_2,E_3] = E_4, \quad [E_2,E_4] = 0,$$
$$\{E_3,E_4\} = E_0, \quad \{E_3,E_3\} = -2E_1, \quad \{E_4,E_4\} = 2E_2,$$

where $[E_j,E_k]$ is a commutator and $\{E_j,E_k\}$ denotes an anticommutator.

In (1) it was seen that by expansion of each element of V in λ and keeping terms up to λ^3, it is possible to generate the superversions of KdV, NLSE, etc. Here we first generalize this result by expanding V up to nth order in λ.

Let us assume

$$V = \begin{pmatrix} A & C & \alpha \\ B & -A & \rho \\ \rho & -\alpha & 0 \end{pmatrix}. \tag{3}$$

If we assume $R = \sum_{j=1}^{N} R_j \lambda^{n-j}$, where $R = (A,C,\alpha,\beta,\rho)$, with A,B,C commuting, α,ρ anticommuting, then from the consistency condition $\Psi_{xt} = \Psi_{tx}$ we deduce

$$2i \begin{pmatrix} B_{j+1} \\ C_{j+1} \\ \rho_{j+1} \\ \alpha_{j+1} \end{pmatrix} = \pounds \begin{pmatrix} B_j \\ C_j \\ \rho_j \\ \alpha_j \end{pmatrix}, \tag{4}$$

where £ is the superrecursion operator written as

$$\pounds = \begin{pmatrix} \frac{\partial}{\partial x} - 2q\partial^{-1}r & 2q\partial^{-1}q & 2\epsilon - 2q\partial^{-1}\beta & -2q\partial^{-1}\epsilon \\ -2r\partial^{-1}r & \frac{\partial}{\partial x} + 2r\partial^{-1}Q & -2r\partial^{-1}\beta & -2\beta - 2r\partial^{-1}\epsilon \\ -2\beta - 2\epsilon\partial^{-1}r & 2\epsilon\partial^{-1}q & 2\frac{\partial}{\partial x} - 2\epsilon\partial^{-1}\beta & 2q - 2\epsilon\partial^{-1}\epsilon \\ -2\beta\partial^{-1}r & 2\epsilon + 2\beta\partial^{-1}q & -2r - 2\beta\partial^{-1}\beta & -2\frac{\partial}{\partial x} - 2\beta\partial^{-1}\epsilon \end{pmatrix}.$$

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So the class of equations are

$$\begin{pmatrix} q_t \\ r_t \\ \epsilon_t \\ \beta_t \end{pmatrix} = \left(\frac{\pounds}{2i}\right)^n \begin{pmatrix} b_0 \\ c_0 \\ \rho_0 \\ \alpha_0 \end{pmatrix}, \tag{5}$$

where $(b_0,c_0,\rho_0,\alpha_0)$ are arbitrary constants.

III. BÄCKLUND AND DARBOUX–BÄCKLUND TRANSFORMATIONS

One of the most important properties of these complete evolution equations is the existence of a class of transformations that takes one solution to another solution of the same or a different equation. The former class is known as an auto-Bäcklund transformation. Here we will derive a supersymmetric generalization of such an auto-Bäcklund transformation for the class of equations under consideration.

At present there exist various approaches for the deduction of the Bäcklund transformation. We will be adapting the technique of Darboux, which starts by connecting the two different eigenvalue problems pertaining to the two different solutions.

Let

$$\Psi_x = U(q,r,\epsilon,\beta)\Psi,\ \Psi_{x'} = U'(q',r',\epsilon',\beta')\Psi' \tag{6}$$

be the two linear problems, where the corresponding nonlinear fields are denoted by an unprimed and a primed set, which are assumed to be two different sets of solution of the same system of equations. Let us assume that it is possible to find a mapping between the old and new linear variables, Ψ and Ψ', as

$$\Psi' = Q\Psi = Q(\lambda,q,r,\epsilon,\beta,q',r',\epsilon',\beta')\Psi. \tag{7}$$

Then from Eqs. (6), we get

$$Q_x = U'Q - QU$$

or

$$Q_x = i\lambda\,[E_0,Q\,] + M'Q - QM, \tag{8}$$

where

$$\begin{aligned} M &= qE_2 + rE_1 + \epsilon E_4 + \beta E_3, \\ M' &= q'E_2 + r'E_1 + \epsilon' E_4 + \beta' E_3. \end{aligned} \tag{9}$$

In the following we will be using the following nomenclature. Every supermatrix is assumed to have the following structures:

$$Q = Q^e + Q^o = (Q^e_D + Q^e_F) + Q^o_F, \tag{10}$$

where the superscript "e" means even part and "o" means odd elements and the subscripts "D" and "F" refer to, respectively, the diagonal and off-diagonal elements of a matrix. Since the odd part is always off diagonal we set $Q^o = P$, $Q^e_D = D$, $Q^e_F = F$ and expand each in a series of λ:

$$\begin{aligned} P &= \sum_{j=0}^{n} \lambda^{n-j} P_j, \quad F = \sum_{j=0}^{n} \lambda^{n-j} F_j, \\ D &= \sum_{j=0}^{n} \lambda^{n-j} D, \end{aligned} \tag{11}$$

then Eqs. (8) and (9) yield

$$\begin{aligned} F_{jx} &= [e_0,F_{j+1}\,] + M'^e_F D_j - D_j M^e_F + M'^e_D F_j \\ &\quad - F_j M^e_D + (M'^o P_j - P_j M^o)F, \\ D_{jx} &= M'^e D_j - D_j M^e_D + M'^e_F F_j - F_j M^e_F \\ &\quad + (M'^o P_j - P_j M^o)_0, \\ P_{jx} &= [e_0,P_{j+1}\,] + M'^e_F P_j - P_j M^e_F + M'^o_D P_j \\ &\quad - P_j M^e_D + M'^o D^e_j - D^e_j M^o. \end{aligned} \tag{12}$$

Explicitly the matrices F_j, D_j, and P_j are of the form

$$F_j = \begin{pmatrix} 0 & c_j & 0 \\ g_j & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad D_j = \begin{pmatrix} a_j & 0 & 0 \\ 0 & h_j & 0 \\ 0 & 0 & p_j \end{pmatrix},$$

$$P_j = \begin{pmatrix} 0 & 0 & e_j \\ 0 & 0 & k_j \\ m_j & n_j & 0 \end{pmatrix}.$$

Then we can deduce the following equations for the determination of the Darboux matrix:

$$\begin{aligned} c_{jx} &= 2ic_{j+1} + r'h_j - ra_j + \beta' n_j - \beta e_j, \\ g_{jx} &= -2ig_{j+1} + q'a_j - qh_j + \epsilon' m_j - \epsilon k_j, \\ a_{jx} &= r'g_j - qc_j + \beta' m_j - \epsilon e_j, \\ h_{jx} &= q'c_j - rg_j + \epsilon' n_j + \beta k_j, \\ p_{jx} &= \epsilon' e_j - \beta' k_j - \beta m_j - \epsilon n_j, \\ e_{jx} &= ie_{j+1} + r'k_j + \beta' p_j - \beta a_j - \epsilon e_j, \\ k_{jx} &= -ik_{j+1} + q'e_j + \epsilon' p_j - \beta g_j - \epsilon h_j, \\ m_{jx} &= -im_{j+1} - qn_j - \epsilon p_j, \\ n_{jx} &= in_{j+1} - rm_j + \beta p_j. \end{aligned} \tag{13}$$

These recursion relations can be solved in stages. To make an explicit calculation we consider the expansion (11) only up to second order in λ. Then we obtain

$$\begin{aligned} &e_1 = i\alpha(\beta' - \beta), \quad k_1 = i\alpha(\epsilon - \epsilon'), \\ &m_1 = i\epsilon\alpha, \quad n_1 = i\beta\alpha, \\ &c_1 = (i\alpha/2)(r' - r), \quad g_1 = (i\alpha/2)(q - q'). \end{aligned} \tag{14}$$

The whole computation becomes extremely laborious and unwieldy if all the four nonlinear fields are treated simultaneously, so we only display a few of the results of computation, and the final Bäcklund transformation is written for the special case $\beta = 0$, $r = r_0$.

Following the same line of computation we get

$$\begin{aligned} c_2 &= (\alpha/4)(r'_x - r_x + [r + r']\{\partial^{-1} rq - \partial^{-1} r'q\} \\ &\quad + (r - r')2\,\partial^{-1}\epsilon\beta - 4\{r'\partial^{-1}\epsilon'\beta + r\,\partial^{-1}\beta'\epsilon\}), \\ g_2 &= (\alpha/4)(q'_x - q_x + [q + q']\{\partial^{-1} rq - \partial^{-1} r'q'\} \\ &\quad + 2(q - q')\partial^{-1}\epsilon\beta - \{q\,\partial^{-1}\beta'\epsilon + q'\,\partial^{-1}\epsilon'\beta\}). \end{aligned} \tag{15}$$

Similarly for the others. The odd elements are obtained in the form

$$\begin{aligned} m_2 &= \alpha(-\epsilon_x - q\beta + \epsilon\,\partial^{-1}\epsilon'\beta \\ &\quad - \epsilon\,\partial^{-1}\beta'\epsilon - 2\epsilon\,\partial^{-1}\epsilon'\beta'), \end{aligned}$$

$$n_2 = \alpha(\beta_x + r\epsilon + \beta\partial^{-1}\epsilon'\beta - \beta\partial^{-1}\beta'\epsilon - 2\beta\partial^{-1}\epsilon'\beta'). \tag{16}$$

After the determination of the Darboux matrix, the Bäcklund transformation (BT) is obtained by the condition that the coefficients of λ^3 in (8) are identically equal to zero, which yields the direct relation between the old and new sets of nonlinear fields (q,r,ϵ,β) and (q',r',ϵ',β'). As said before, we write out the BT for the case $\beta = 0$, $r = r_0$ pertaining to the super-KdV case. Here we get

$$\begin{aligned}
&(q'-q)_x + r_0 D^{-1}(q-q')(q'_x - q_x) + r_0^2(q'-q)(\partial^{-1}q' - \partial^{-1}q)^2 + 4r_0(q'-q)\partial^{-1}\epsilon'\epsilon - 4(\epsilon'\epsilon_x + \epsilon\epsilon'_x + \epsilon\epsilon_x) = 0,\\
&(\epsilon-\epsilon')_{xx} + (r_0/2)\epsilon_x(\partial^{-1}q' - \partial^{-1}q) + (r_0\epsilon/4)(q-q') + r_0 q'\epsilon' - r_0\epsilon\partial^{-1}\epsilon'\epsilon + r_0^2\epsilon\partial^{-1}(q-q')(\partial^{-1}q' - \partial^{-1}q) = 0.
\end{aligned} \tag{17}$$

The same procedure can be followed to determine the time part of the BT.

For the time part of the BT we again start from the two equations

$$\Psi_t = V\Psi, \quad \Psi'_t = V'\Psi'.$$

Then we obtain immediately

$$Q_t = V'Q - QV,$$

and this equation can be solved for time dependence of Q in an identical manner.

IV. HAMILTONIAN STRUCTURE

The Hamiltonian structure of the superevolution equations can be determined via the usual technique of Riccati equations and by extending the variational approach of Gui-Zhang.[7]

From the IST equation (1) and (4) we first obtain Riccati equations for Ψ_1/Ψ_2 and Ψ_3/Ψ_4:

$$\gamma_x = 2i\lambda\gamma - r - \beta\eta + q\gamma^2 + \epsilon\gamma\eta, \quad \eta_x = i\lambda\eta + \beta - \epsilon\gamma + q\eta\gamma, \tag{18}$$

with

$$\gamma = \Psi_1/\Psi_2, \quad \eta = \Psi_3/\Psi_4.$$

If we now expand γ and η in inverse powers of λ, then we can determine the infinite set of conservation laws. The recurrence relations for such expansion coefficients are

$$2i\gamma_{n+1} = \gamma_{nx} - q\sum_{j+k=n}\gamma_j\gamma_k - \epsilon\sum_{j+k=n}\gamma_j\eta_k, \quad i\eta_{n+1} = \eta_{nx} + \epsilon\gamma_\eta - q\sum_{j+k=n}\eta_j\gamma_k, \tag{19}$$

along with

$$\gamma_1 = r/2i, \quad \eta_1 = 0.$$

In the following we note a few of these odd and even conserved quantities:

even	odd
$\gamma_1 = r/2i$	$\eta_1 = 0$
$\gamma_2 = -r_x/4$	$\eta_2 = -\epsilon r/2$
$\gamma_3 = -\frac{r_{xx}}{8i} + \frac{9\gamma}{8i} - \frac{qrr_x}{4}$	$\eta_3 = -\frac{\epsilon_x r}{2i} - \frac{3}{4i}\epsilon r_x$
$\gamma_4 = \frac{r_{xxx}}{16} - \frac{q_x r^2}{16} - \frac{qrr_x}{4}$	$\eta_4 = \frac{1}{2}\epsilon_{xx} r + \frac{5}{4}\epsilon_x r_x + \frac{7}{8}\epsilon r_{xx} - \frac{3}{8}\epsilon q r^2$

These integrals of motion are really making up the various Hamiltonians for which we define the analytic function (for the time being we have kept "r" variable)

$$H = -i\lambda - q\gamma - \epsilon\eta, \tag{20}$$

and assume

$$H = \sum \lambda^{-n} H_n.$$

So that upon equating different powers of λ we obtain, by use of the above table,

$$H_{-1} = -i, \quad H_0 = 0, \quad H_1 = -\frac{qr}{2i}, \quad H_2 = -\frac{qr_x}{4}, \quad H_3 = \frac{qr_{xx}}{8i} + \frac{q^2r^2}{2i} + \frac{\epsilon\epsilon_x r}{2i}. \tag{21}$$

To extend the formalism of Ref. 4, we set $\delta H/\delta q = N$, $\delta H/\delta r = M$, and $\delta H/\delta\epsilon$, and deduce, from the formulas for the chain rule of variational derivatives,

$$\begin{pmatrix} \delta/\delta H \\ \delta/\delta\gamma \\ \delta/\delta\eta \end{pmatrix} = \begin{pmatrix} -\gamma & -1/\gamma & -\eta/\gamma \\ D + 2i\lambda + q\gamma + \epsilon\eta & -q/\gamma + \epsilon\eta/\gamma^2 & -\epsilon/\gamma \\ 0 & -i\lambda\eta/\gamma^2 - q\eta/\gamma - \eta D/\gamma^2 + \epsilon/\gamma & -i\lambda/\gamma + q + D/\gamma + \epsilon\eta/\gamma \end{pmatrix} \begin{pmatrix} \delta/\delta r \\ \delta/\delta q \\ \delta/\delta\epsilon \end{pmatrix}. \tag{22}$$

Applying Eq. (22) on both sides of H, we obtain

$$\gamma = -\gamma^2 M - N - \eta Q, \tag{23}$$

$$2i\lambda\gamma M = -\gamma M_x - q\gamma^2 M + qN + \epsilon Q + \epsilon\eta, \tag{24}$$

$$2i\lambda N = N_x - r - 2r\gamma M - 2i\lambda\eta Q - q\gamma\eta Q - \epsilon\eta N, \tag{25}$$

which are the equations to be solved recursively for the variational derivatives of H.

We quote here a few results of such a computation:

	N_i	M_i
$i=0$	0	0
$i=1$	$-r/2i$	$-q/2i$
$i=2$	$r_x/4$	$-q_x/4$
$i=3$	$\frac{r_{xx}}{8i} - \frac{r^2 q}{4i}$	$\frac{q_{xx}}{4} - \frac{rq^2}{4i} + \frac{\epsilon\epsilon_x}{2i}$
$i=4$	$-\frac{r_{xxx}}{16} + \frac{3}{8} r r_x q$	$\frac{q_{xxx}}{16} - \frac{3}{8} q q_x r + \frac{3}{4}\epsilon\epsilon_{xx}$

Similar computations can also be done for Q. It is interesting to observe that we get the following structure in the Hamiltonian formalism for the super-KdV equation:

$$\begin{pmatrix} q_t \\ \epsilon_t \end{pmatrix} = \partial \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \delta H_4/\delta q \\ \delta H_4/\delta t \end{pmatrix}, \tag{26}$$

when we have reverted to the old case $r = r_0$.

V. THE LIE–BÄCKLUND SYMMETRIES

It is now almost an established fact that the completely solvable equations do possess an infinite number of Lie–Bäcklund (LB) symmetries. Here we show that even in the case of superevolution equations we can find out such LB symmetries, whose hierarchy is connected by a recursion operator. Let us consider the general transformation

$$\begin{aligned} q &\to q + \xi\eta_1'(q, q_1 \cdots q_n, \epsilon, \epsilon_1 \cdots \epsilon_n), \\ \epsilon &\to \epsilon + \xi\eta_2'(q, q_1 \cdots q_n, \epsilon, \epsilon_1 \cdots \epsilon_n), \end{aligned} \tag{27}$$

where

$$\epsilon_i = \frac{\partial^i \epsilon}{\partial x^i}, \quad q_j = \frac{\partial^j q}{\partial x^j},$$

and ξ is a small parameter. Then the condition of invariance of (11) leads to

$$\begin{aligned} \eta_{1t}' &= 6r_0\eta_{1x}' q + 6r_0 q_1\eta_1' - 12\eta_2'\epsilon_2 - 12\epsilon\eta_{2xx}' + \eta_{1xxx}', \\ \eta_{2t}' &= \eta_{2xxx}' + 6r_0\eta_1'\epsilon_x + 6r_0 q\eta_{2x}' + 3r_0 q_1\eta_2' + 3r_0\eta_{1x}'\epsilon, \end{aligned} \tag{28}$$

where the $\partial/\partial t, \partial/\partial x$ act according to the formulas

$$\frac{\partial}{\partial x} = \sum q_{i+1}\frac{\partial}{\partial q_i} + \sum \epsilon_{i+1}\frac{\partial}{\partial \epsilon_i}$$

and

$$\frac{\partial}{\partial t} = \sum q_{it}\frac{\partial}{\partial q_i} + \sum \epsilon_{it}\frac{\partial}{\partial \epsilon_i}.$$

The first two symmetries, which are quite evident and are solutions of (28), are the space and time translational symmetry, given as

$$\begin{pmatrix} \eta_1' \\ \eta_2' \end{pmatrix} = \begin{pmatrix} q_x \\ \epsilon_x \end{pmatrix}, \quad \begin{pmatrix} \eta_1' \\ \eta_2' \end{pmatrix} = \begin{pmatrix} -q_3 + 6qq_1 - 12\epsilon\epsilon_1 \\ -4\epsilon_3 + 6\epsilon_1 q + 3\epsilon q_1 \end{pmatrix}, \tag{29}$$

so we proceed to determine the next nontrivial symmetry by keeping q_i and ϵ_i up to $i = 5$. Since the whole calculation is much too cumbersome we only report the final result ($r_0 = 1$)

$$\begin{aligned} \eta_1' &= q_5 - 8qq_3 - 20q_2 q_1 + 18q^2 q_1 - 2\epsilon q_3 + 12(\epsilon_1\epsilon_1 + \epsilon\epsilon_3) \\ &\quad - 4\epsilon_1\epsilon_3 - 12\epsilon\epsilon_4 + 24\epsilon\epsilon_1 q_1 + 18\epsilon\epsilon_2 q + 12\epsilon q q_1, \\ \eta_2' &= 16\epsilon_5 - 27\epsilon q_3 - 24\epsilon_3 q - 60\epsilon_2 q_1 + 30\epsilon_1 q^2 \\ &\quad - 48\epsilon_1 q_2 + 30\epsilon q q_1. \end{aligned} \tag{30}$$

It is not very difficult to observe that the symmetries given by (29) and (30) can be connected by the operator R given as (where $r_0 = 1$)

$$R = \begin{pmatrix} 2\epsilon + 2\,\partial q\,\partial^{-1} - \partial^2 & 2\phi\,\partial + \partial\epsilon \\ 2\,\partial\epsilon\,\partial^{-1} + \epsilon & 4(q - \partial^2) \end{pmatrix} \tag{31}$$

and is

$$R = \begin{pmatrix} \eta_1'^{,i} \\ \eta_2'^{,i} \end{pmatrix} = \begin{pmatrix} \eta_1'^{,i+1} \\ \eta_2'^{,i+1} \end{pmatrix}, \tag{32}$$

which helps to generate the infinite class. Furthermore with a little observation it appears that we can write R in a factorized form:

$$R = \begin{pmatrix} 2(q\partial + \partial q) - \partial^3 & 2\epsilon\partial + \partial\epsilon \\ 2\partial\epsilon + \epsilon\partial & 4(q - \partial^2) \end{pmatrix} \begin{pmatrix} \partial^{-1} & 0 \\ 0 & 1 \end{pmatrix}. \tag{33}$$

Such a factorization of the recursion operator can give rise to the Lenard relation, bi-Hamiltonian structure, and so on.

VI. DISCUSSIONS

In our above computations we have deduced some symmetry properties of some supersymmetric evolution equations, and also deduced their Hamiltonian structure. Our computation suggests that it may be possible to consider a supersymmetric generalization of the Miura map and other special properties of these bosonic equations to their fermionic counterpart. It may be interesting to harness the connection between these properties through an extension of the deformation technique.[8] At present such problems are under study and will be communicated in future.

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Smoothness of the action of the gauge transformation group on connections

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The NLF–Lie group structure of the group $\mathcal{G}$ of the gauge transformations, defined as the group of sections of the bundle $P[G]$ associated to the principal bundle $P(M,G)$, is discussed. Other current definitions of the group of gauge transformations are shown to admit a nontrivial smooth structure only in the case of compact G. The space $\mathcal{C}$ of principal connections, as well, is given the structure of local affine NLF-manifold, after identifications of connections with sections of a convenient vector bundle on M. Finally, the smoothness of the action of $\mathcal{G}$ on $\mathcal{C}$ is proved in general. In the case of compact M, the group $\mathcal{G}$ becomes a tame Fréchet–Lie group and the action a tame smooth action.

I. INTRODUCTION

In gauge theories a first and important step is the study of the action of the group $\mathcal{G}$ of the gauge transformations of a principal bundle $P(M,G)$ on the set $\mathcal{C}$ of principal connections. In fact, according to the gauge principle, physical objects are the classes of gauge equivalent connections rather than connections themselves. In a natural way physicists are virtually forced to look at $\mathcal{G}$ as a smooth group acting on a smooth manifold $\mathcal{C}$.

The problem of endowing these objects with appropriate smoothness structures has been approached essentially on the basis of projective limit techniques (see Ref. 1 and references therein), making use of a rather indirect notion of smoothness and of very reductive assumptions like compactness of the base space M and of the structure group G. A new approach of the Japanese school[2] to infinite continuous groups introduces the "regular" Fréchet–Lie groups. Even in this approach one cannot avoid the compactness hypothesis for M in the treatment of the group $\mathcal{G}$ as a Lie group.

In a previous paper[3] the group $\mathcal{G}$, defined as the group of sections of the associated bundle $P[G]$, has been given the structure of the "Schwartz–Lie" group, i.e., of a Lie group modeled on a Schwartz space, without any assumption of compactness for M and G. In this paper we analyze two other current definitions of the gauge transformation group and show that they are not quite satisfactory from the point of view of smoothness properties, at least in the general case. However, assuming compactness of G we are able to show that the three definitions give isomorphic Lie groups (Sec. II).

In Sec. III we identify the principal connections with sections of a convenient vector bundle on M and again without any assumption of compactness we give $\mathcal{C}$ the structure of a local affine manifold model on a Schwartz space.

In Sec. IV we give the proof of the smoothness of the action of $\mathcal{G}$ on $\mathcal{C}$, in the case of compact M the group $\mathcal{G}$ becomes a tame Fréchet–Lie group and the action a tame smooth action.

The results of this paper, in our opinion interesting by themselves, are a necessary tool for the study of the orbit space $\mathcal{C}/\mathcal{G}$ and its stratification structure. This will be the content of a forthcoming paper.

II. THE GROUP OF GAUGE TRANSFORMATIONS

Our basic object is a principal bundle $P(M,G) \equiv (P,p,M;G)$, where M is an *ordinary* manifold (ordinary manifold means Hausdorff, second countable, and locally compact C^∞-manifold, hence finite-dimensional paracompact and metricizable) and G an *ordinary* Lie group. Throughout the paper we will denote by A the principal action, $A: P \times G \to P$, and by A^a and A_u the partial maps

$$A^a: P \to P, \quad A^a(u) = A(u,a), \quad a \in G,$$
$$A_u: G \to P, \quad A_u(a) = A(u,a), \quad u \in P.$$

We consider the associated bundles $P[G] \equiv (P \underset{G}{\times} G, p_G, M)$ (with fiber G and action of G on it given by inner automorphisms, $a \mapsto bab^{-1}$) and $P[\mathcal{g}] \equiv (P \underset{G}{\times} \mathcal{g}, p_{\mathcal{g}}, M)$ (with fiber the Lie algebra $\mathcal{g}$ of G and action of G on it given by the adjoint representation).

We recall that the total space $P \underset{G}{\times} F$ of an associated bundle $P[F]$ $(P \underset{G}{\times} F, p_F, M)$ with fiber F consists of equivalence classes on $P \times F$ relative to the joint action of G.

We will denote by $[(u,f)]_G$ the equivalence class of the point $(u,f) \in P \times F$. Thus, in the case of $P[G]$,

$$[(u,a)]_G := \{(u',a') \in P \times G \mid \exists b \in G:\ (u',a') = (ub, b^{-1}ab)\}$$

and similarly for $[(u,\alpha)]_G$ in the case of $P[\mathcal{g}]$.

The group $\mathcal{G}$ of gauge transformations of $P(M,G)$ is, by definition, the set Sec $P[G]$ of the (smooth) sections of $P[G]$ with pointwise defined composition law.

It has been proved in Ref. 3 that $\mathcal{G}$ is an NLF–Lie group, that is, a Lie group modeled on a complete locally convex nuclear space, strict inductive limit of a countable

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family of separable Fréchet spaces. More precisely, the results of Ref. 3 can be summarized in the following statements.

(i) $\mathcal{G}$ is an NLF–Lie group.

(ii) The set $\mathrm{Sec}_c\ P[\mathcal{g}]$ of the compact support sections of $P[\mathcal{g}]$ with pointwise defined operations is an NLF–Lie algebra, in fact the Lie algebra $L_{\mathcal{G}}$ of $\mathcal{G}$.

(iii) An exponential map $\mathrm{Exp}: \mathrm{Sec}_c\ P[\mathcal{g}] \to \mathrm{Sec}\ P[G]$ is defined by $(\mathrm{Exp}\,\sigma)\ (x): = \exp \sigma(x)\ \forall x \in M$, where exp: $P \underset{G}{\times} \mathcal{g} \to P \underset{G}{\times} G$ is the fiberwise defined exponential map, which is a local diffeomorphism at 0.

According to these results we more simply say that $\mathcal{G}$ is a Schwartz–Lie group and its Lie algebra a Schwartz–Lie algebra.

From the algebraic point of view, it is well known (see, for instance, Ref. 4) that the group $\mathcal{G}$ is isomorphic with the group $\mathcal{G}^{\#}$ of those diffeomorphisms f of the total space P of $P(M,G)$ such that

(a) $p \circ f = p$,

(b) $f(ua) = f(u)a, \quad \forall u \in P, \quad \forall a \in G.$

The group $\mathcal{G}^{\#}$, in turn, is isomorphic with the group $\hat{\mathcal{G}}$ of those maps $\hat{f}: P \to G$ such that

$$\hat{f}(ua) = a^{-1}\hat{f}(u)a, \quad \forall u \in P, \quad \forall a \in G.$$

The isomorphisms are

$$\iota: \mathcal{G} \to \mathcal{G}^{\#}, \quad \iota(s)(u) = ua,$$

where $a \in G$ is such that $(s \circ p)\ (u) = [(u,a)]_G$, and

$$\hat{}: \mathcal{G}^{\#} \to \hat{\mathcal{G}}, \quad f \mapsto \hat{f},$$

where $\hat{f}$ is defined by $f(u) = u\hat{f}(u)$.

Obviously, $\mathcal{G}^{\#}$ is a subgroup of the group Diff P of the diffeomorphisms of P. Now, as shown by Michor,[5] Diff P can be given the structure of NLF–Lie group with Lie algebra the NLF–Lie algebra $\mathcal{X}_c(P)$ of vector fields on P with compact support. It is easy to see that $\mathcal{G}^{\#}$ is closed in the FD-topology, which is the toplogy underlying the differential structure of Diff P. Under this topology the connected component of the identity contains only diffeomorphisms with compact support. If G is not compact, the only element of $\mathcal{G}^{\#}$ with compact support is the identity itself, owing to the equivariance property, therefore, in this case $\mathcal{G}^{\#}$ is a discrete subgroup of Diff P.

Analogously, $\hat{\mathcal{G}}$ is a closed subgroup of the Schwartz–Lie group $C^{\infty}(P,G)$ (see Ref. 3) and again, if G is not compact, $\hat{\mathcal{G}}$ is a discrete subgroup of $C^{\infty}(P,G)$.

From these remarks it clearly appears that to consider the gauge transformations as diffeomorphisms of P can be unsatisfactory. Indeed they are bundle automorphisms and only the group $\mathcal{G}$ fits completely this character, since, from the categorical point of view, bundle morphisms must be looked at as sections of a suitable bundle.

If the structure group G is compact, however, $\mathcal{G}^{\#}$ is a Lie subgroup of Diff P and $\hat{\mathcal{G}}$ a Lie subgroup of $C^{\infty}(P,G)$ as shown in the following theorems.

Theorem 2.1: If G is compact, $\mathcal{G}^{\#}$ is a splitting Lie subgroup of Diff P and its Lie algebra $\mathcal{X}_c^{\#}(P)$ is the splitting subalgebra of $\mathcal{X}_c(P)$ consisting of the vertical G-invariant vector fields on P with compact support.

Proof: First we note that the subspace $\mathcal{X}_c^V(P)$ of the vertical vector fields splits $\mathcal{X}_c(P)$. We introduce then the linear operator[6]

$$\int_G : \mathcal{X}_c^V(P) \to \mathcal{X}_c^V(P),$$

$$\left(\int_G X\right)(u) := \int_G (X \cdot a)(u)\, d\mu(a),$$

where $X \cdot a$ is the induced right action of G on vector fields of P and μ is the normalized Haar measure on the compact group G. It is immediate that $\int_G$ is a continuous projection onto $\mathcal{X}_c^{\#}(P)$, the subspace of $\mathcal{X}_c^V(P)$ consisting of the G-invariant elements. This shows that $\mathcal{X}_c^{\#}(P)$ is a splitting subspace of $\mathcal{X}_c(P)$; moreover, by standard arguments, $\mathcal{X}_c^{\#}(P)$ turns out to be a Lie subalgebra of $\mathcal{X}_c(P)$.

Now we recall that Diff P is a NLF–Lie group and that a chart at the identity e is given by $(U_{\mathrm{e}}^{\tau}, \chi, \mathcal{X}_c(P))$, where

(1) τ is a local addition on P,

(see, for definition, Ref. 3 or Ref. 5);

(2) $U_{\mathrm{e}}^{\tau} = \{f \in \mathrm{Diff}\ P \mid f \sim \mathrm{e},\ f(u) \in \tau_u(T_u P)\}$

[$f_1 \sim f_2$ means that the set $\{u \in P \mid f_1(u) \neq f_2(u)\}$ is relatively compact]; and

(3) $\chi: U_{\mathrm{e}}^{\tau} \to \mathcal{X}_c(P), \quad \chi(f) := X,$

$$\text{with } X(u) = \tau_u^{-1}(f(u)).$$

As we will show in the subsequent Lemma 2.2, there exists a local addition τ on P such that

(i) $\tau \circ TA^a = A^a \circ \tau$;

and (ii) the fibers of P are additively closed, i.e.,

$$\tau(\mathrm{Ver}_u P) \subset P_x, \quad x = p(u).$$

For such a local addition we have

$$\chi(U_{\mathrm{e}}^{\tau} \cap \mathcal{G}^{\#}) = \mathcal{X}_c^{\#}(P).$$

Actually, if $X = \chi(f)$ with $f \in U_{\mathrm{e}}^{\tau} \cap \mathcal{G}^{\#}$, then $X(u) \in \mathrm{Ver}_u P$ since $f(u) \in P_x$ and fibers are additively closed and X is G-invariant since τ is equivariant; vice versa, if $X \in \mathcal{X}_c^{\#}(P)$, the map $f = \tau \circ X$ is a diffeomorphism of P since χ is surjective and satisfies

$$f(ua) = (\tau \cdot X)(ua) = \tau[(TA^a \circ X)(u)]$$

$$= (\tau \circ X)(u)a = f(u)a,$$

$$(p \circ f)(u) = p(\tau(X(u))) = p(u),$$

hence $f \in \mathcal{G}^{\#}$. Thus $\mathcal{G}^{\#}$ is a splitting submanifold of Diff P, hence a Lie subgroup of Diff P and its Lie algebra is the splitting Lie subalgebra $\mathcal{X}_c^{\#}(P)$ of $\mathcal{X}_c(P)$. □

Lemma 2.2: Let $P(M,G)$ be a principal fiber bundle with principal action A. There exists a local addition τ on P satisfying conditions (i) and (ii) above.

Proof: Take a G-invariant partition of unity $\{f_\alpha\}$ of P subordinated to a local trivializing system $\{(U_\alpha, \varphi_\alpha)\}$. If ξ_G is the (right) invariant spray on G and ξ_α any spray on U_α, then

$$\xi = \sum_\alpha f_\alpha \xi_\alpha \oplus \xi_G$$

is a G-invariant spray on P. The corresponding exponential

map $\exp^{\xi}$ is equivariant and defined on an open G-invariant neighborhood V of the zero section of TP. Using a G-invariant metric on P, a contracting diffeomorphism h: $TP \to h(TP) \subset V$ with $h(0_u) = 0_u$, $\pi_P \circ h = \pi_P$, where π_P: $TP \to P$, can be constructed as in 10.2 of Michor[5], which, moreover, is equivariant. Therefore $\tau = \exp^{\xi} \circ h$ satisfies (i). As to (ii), it is enough to remark that the spray ξ, when restricted to the fiber P_x over x, gives a spray on P_x and the diffeomorphism h preserves Ver P.

Theorem 2.3: If G is compact, $\hat{\mathcal{G}}$ is a splitting Lie subgroup of $C^\infty(P,G)$ and its Lie algebra is the splitting subalgebra $C^\infty_{cG}(P,\mathcal{G})$ of the Lie algebra $C^\infty_c(P,\mathcal{G})$ of $C^\infty(P,G)$ consisting of those maps $\hat{\varphi}$: $P \to \mathcal{G}$ with compact support such that $\hat{\varphi}(ua) = \mathrm{Ad}_{a^{-1}}(\hat{\varphi}(u))$.

Proof: The linear operator

$$\int_G : C^\infty_c(P,\mathcal{G}) \to C^\infty_c(P,\mathcal{G}),$$

$$\left(\int_G \varphi\right)(u) := \int_G \mathrm{Ad}_a(\varphi(ua))\,d\mu(a)$$

is clearly a continuous projection onto $C^\infty_{cG}(P,\mathcal{G})$ and this shows that $C^\infty_{cG}(P,\mathcal{G})$ is a splitting subspace of $C^\infty_c(P,\mathcal{G})$; in fact $C^\infty_{cG}(P,\mathcal{G})$ is a Lie subalgebra of $C^\infty_c(P,\mathcal{G})$ since the Lie bracket is pointwise defined. A chart at the identity of the NLF–Lie group $C^\infty(P,G)$ is given by $(U_e, \chi, C^\infty_c(P,V) \subset C^\infty_c(P,\mathcal{G}))$, where, if $\exp_G : \mathcal{G} \to G$ is the exponential map of G, V is a zero neighborhood in $\mathcal{G}$ such that $\exp_G \restriction_V$: $V \to \exp_G(V) \equiv W \subset G$ is a diffeomorphism,

$$U_e = \{f \in C^\infty(P,G) \mid f \sim e,\ f(P) \subset W\}$$

and

$$\chi : U_e \to C^\infty_c(P,V)$$

is given by $\chi(f) = \log_G \circ f$, $\log_G = (\exp_G \restriction_V)^{-1}$: $W \to V$. We may assume that V is invariant under the adjoint action (e.g., an open ball with respect to a G-invariant metric on $\mathcal{G}$) so W is invariant under conjugation. Then

$$\hat{\mathcal{G}} \cap U_e = \hat{U}_e$$

$$:= \{f \in C^\infty(P,G) \mid f \sim e,\ f(P) \subset V,\ f(ua) = a^{-1} f(u) a,\ \forall a \in G\}.$$

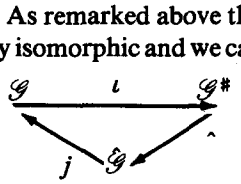
Clearly

$$\chi(\hat{U}_e) = \{\varphi \in C^\infty(P,\mathcal{G}) \mid \varphi \sim 0,\ \varphi(ua) = \mathrm{Ad}_{a^{-1}}\varphi(u),\ \varphi(U) \subset V\}$$

$$= \chi(U_e) \cap C^\infty_{cG}(P,\mathcal{G}).$$

Then $\hat{\mathcal{G}}$ is a splitting submanifold of $C^\infty(P,G)$, hence a Lie subgroup with Lie algebra the subalgebra $C^\infty_{cG}(P,\mathcal{G})$ of $C^\infty_c(P,\mathcal{G})$. □

As remarked above the groups $\mathcal{G}$, $\mathcal{G}^\#$, $\hat{\mathcal{G}}$ are algebraically isomorphic and we can consider the following diagram:



where the isomorphism j is given by

$$h(\hat{f})(x) := [(u, \hat{f}(u))]_G, \quad u \in p^{-1}(x).$$

Now we know that in the case of compact G the three groups are NLF–Lie groups. The following result is expected.

Theorem 2.4: If G is compact, the $\mathcal{G}$, $\mathcal{G}^\#$, and $\hat{\mathcal{G}}$ are isomorphic as NLF–Lie groups.

Proof: We must just prove that the maps in the above diagram are smooth.

(a) The map ι is smooth. Introduce the smooth map

$$r : (P \underset{G}{\times} G) \underset{M}{\times} P \to P, \quad r([(u,a)]_G, u)) := ua,$$

where $(P \underset{G}{\times} G) \underset{M}{\times} P$ is the total space of the fiber product of the bundles $P[G]$ and $P(M,G)$, and consider the following maps:

$$\iota_0 : \mathcal{G} \to C^\infty(M, P \underset{G}{\times} G), \text{ the canonical embedding,}$$

$$\iota_1 : C^\infty(M, P \underset{G}{\times} G) \to C^\infty(P, P \underset{G}{\times} G), \quad f \mapsto f \circ p,$$

$$\iota_2 : C^\infty(P, P \underset{G}{\times} G) \to C^\infty(P, (P \underset{G}{\times} G) \times P),$$

$$(\iota_2(f))(u) := (f(u), u),$$

$$\iota_3 : C^\infty(P, (P \underset{G}{\times} G) \underset{M}{\times} P) \to C^\infty(P,P), \quad \psi \times \eta \mapsto r \circ (\psi \circ \eta).$$

The maps ι_1 and ι_3 are smooth by Theorem 11.4 of Ref. 5; the map ι_2 is smooth by Proposition 10.5 of Refs. 5; finally, ι_0 is smooth by Proposition 10.10 of Ref. 5. Note that $\iota_2 \circ \iota_1 \circ \iota_0$ takes the values in the submanifold $C^\infty(P, (P \underset{G}{\times} G) \underset{M}{\times} P)$ of $C^\infty(P, (P \underset{G}{\times} G) \times P)$ and that $\iota = \iota_3 \circ \iota_2 \circ \iota_1 \circ \iota_0$.

(b) The map $\hat{}$ is smooth. Introduce the smooth map

$$\nu : P \underset{M}{\times} P \to G, \quad \nu(u,v) := a, \quad \text{where } ua = v,$$

and consider the following maps:

$$\kappa_0 : \mathcal{G}^\# \to C^\infty(P,P), \quad \text{the canonical embedding,}$$

$$\kappa_1 : C^\infty(P,P) \to C^\infty(P, P \times P), \quad (\kappa_1(f))(u) := (f(u), u),$$

$$\kappa_2 : C^\infty(P, P \underset{M}{\times} P) \to C^\infty(P,G), \quad \kappa_2(f) = \nu \circ f.$$

Note that $\hat{} = \kappa_2 \circ \kappa_1 \circ \kappa_0$; its smoothness follows by the same arguments as at the end of (a).

(c) The map j is smooth. As is shown in Ref. 3 we can use as charts at the identities of the groups $\hat{\mathcal{G}}$ and $\mathcal{G}$ the canonical charts using the exponential mappings

$$\mathrm{Exp} : L_{\mathcal{G}} \equiv \mathrm{Sec}_c\, P[\mathcal{G}] \to \mathcal{G}, \quad (\mathrm{Exp}\,\lambda)(x) = \exp_x(\lambda(x)),$$

where $\exp : P \underset{G}{\times} \mathcal{G} \to P \underset{G}{\times} G$ is the pointwise defined exponential map, and

$$\hat{\mathrm{Exp}} : L_{\hat{\mathcal{G}}} \equiv C^\infty_{cG}(P,\mathcal{G}) \to \hat{\mathcal{G}}, \quad (\hat{\mathrm{Exp}}\,\hat{\sigma})(x) = \exp_G(\hat{\sigma}(u)).$$

The two charts are clearly j-correlated and the local expression of j is the continuous linear operator

$$C^\infty_{cG}(P,\mathcal{G}) \ni \hat{\lambda} \mapsto \lambda \in \mathrm{Sec}_c\, P[\mathcal{G}]$$

with

$$\lambda(x) = [(u, \hat{\lambda}(u))]_G, \quad u \in p^{-1}(x).$$

Hence the isomorphism j is smooth. □

We remark that, taking into account the properties of the exponential map of $\mathcal{G}$,[3] Theorem 2.4 shows that the exponential map of the group Diff P restricted to $\mathcal{G}^{\#}$ is a local diffeomorphism in the case of compact G.

We conclude this section calling attention to two interesting properties of the Schwartz–Lie group $\mathcal{G}$.

(1) The group $\mathcal{G}$ has no small subgroups; this can be easily seen and essentially stems from the fact that the group G, as every ordinary Lie group, has the same property.[7]

(2) The group $\mathcal{G}$ is analytic and the Baker–Campbell–Hausdorff formula holds

$$\operatorname{Exp}\sigma \operatorname{Exp}\sigma' = \operatorname{Exp}\{(\sigma+\sigma') + \tfrac{1}{2}[\sigma,\sigma'] + \tfrac{1}{12}([\sigma,[\sigma,\sigma']] - [\sigma',[\sigma,\sigma']] + \cdots\},$$

for every σ,σ' in a suitable neighborhood of 0 in $L_{\mathcal{G}}$.

This can be seen rather easily using the canonical atlas defined by the exponential map and again remembering that the same property holds for the group G.

Obviously also the group $\mathcal{G}^{\#}$ and $\hat{\mathcal{G}}$ are these two properties in the case of compact G.

III. THE MANIFOLD OF PRINCIPAL CONNECTIONS

In gauge theories an important step is the study of the action of $\mathcal{G}$ on the space $\mathcal{C}$ of principal connections. Usually this action is introduced essentially as a pullback via the gauge transformations considered as diffeomorphisms of P.

As pointed out in Sec. II, the gauge transformations are in fact bundle automorphisms and this point of view is perhaps the only suitable way, in the general case, to treat smoothness properties of the group of gauge transformations.

Accordingly it might be convenient to look at connections too as sections of a suitable bundle over the base space M. This is just the aim of this section.

We need some preliminaries.

As is well known the tangent space TG of the Lie group G with multiplication $\mu: G\times G\to G$ can be given a Lie group structure with multiplication $T\mu$.

The group TG can be made to act on the Lie algebra of G by introducing the affine action

$$B: TG\times\mathcal{g}\to\mathcal{g},\quad B(\alpha_a,\delta):\mathrm{Ad}_a\delta-\alpha,$$

where $\alpha_a\in T_aG$, $\alpha\in\mathcal{g}$, and $\alpha_a = (T_eR_a)\alpha$.

Moreover the group TG can be considered as the structure group of the tangent principal bundle $TP(TM,TG)\equiv(TP,Tp,TM;TG)$. Actually if $(U_\alpha,\varphi_\alpha)$ is a trivializing system for $P(M,G)$ with transition functions $\varphi_{\alpha\beta}$, then $(TU_\alpha,T\varphi_\alpha)$ is a trivializing system for $TP(TM,TG)$ with transition functions $T\varphi_{\alpha\beta}$.

We recall that a connection one-form ω on the principal bundle $P(M,G)$ is a $\mathcal{g}$-valued one-form on P such that

(a) $\omega(\alpha_u^*)=\alpha,\quad \forall u\in P,$

for every fundamental vector field α^* on P, i.e.,

$$\alpha_u^* = (T_eA_u)\alpha,\quad \alpha\in\mathcal{g};$$

and

(b) $\omega\circ TA^a = \mathrm{Ad}_a - 1\circ\omega,\quad \forall a\in G.$

Looking at ω as a map from TP into $\mathcal{g}$ we can investigate its equivariant properties with respect to the actions of TG on TP and $\mathcal{g}$.

We have, with $\xi_u\in T_uP$, $\alpha_a\in T_aG$, and $\alpha\in\mathcal{g}$ such that $\alpha_a = (T_e,R_a)\alpha$,

$$\begin{aligned}\omega(T_{(u,a)}A(\xi_u,\alpha_a)) &= \omega((T_uA^a)(\xi_u) + (T_aA_u)(\alpha_a))\\ &= \mathrm{Ad}_{a^{-1}}\omega(\xi_u) + \omega((T_aA_u)((T_eR_a)\alpha))\\ &= \mathrm{Ad}_{a^{-1}}\omega(\xi_u) + \omega((T_uA^a\circ T_eA_u)\alpha)\\ &= \mathrm{Ad}_{a^{-1}}\omega(\xi_u) + \mathrm{Ad}_{a^{-1}}\omega((T_eA_u)\alpha)\\ &= \mathrm{Ad}_{a^{-1}}\omega(\xi_u) + \mathrm{Ad}_{a^{-1}}\alpha\\ &= B((\alpha_a)^{-1},\omega(\xi_u)).\end{aligned}$$

Thus connection one-forms can be considered as (particular) B-type $\mathcal{g}$-valued maps on TP. It is well known that the B-type $\mathcal{g}$-valued maps on TP correspond bijectively to the sections of the bundle $TP[\mathcal{g}]$ associated to the principal bundle $TP(TM,TG)$. To get a precise characterization of connection one-forms we must investigate this associated bundle.

First of all we remark that $TP[\mathcal{g}] = (TP\underset{TG}{\times}\mathcal{g},Tp_{\mathcal{g}},TM)$ is an affine bundle, that is, a bundle of affine spaces; actually the action B of TG on $\mathcal{g}$ is affine. The transition functions $\psi_{\alpha\beta}$ take values in the group of affine transformations of $\mathcal{g}$ and are given by

$$\begin{aligned}\psi_{\alpha\beta}(\xi_x)\delta &= B((T_x\varphi_{\alpha\beta})\xi_x,\delta)\\ &= \mathrm{Ad}\varphi_{\alpha\beta}(x)\delta - (d_x\varphi_{\alpha\beta})\xi_x,\quad \xi_x\in TU_{\alpha\beta},\end{aligned}$$

where $d_x\varphi_{\alpha\beta} = (T_eR\varphi_{\alpha\beta(x)})^{-1}\circ T_x\varphi_{\alpha\beta}$ is the (right) logarithmic derivative of the transition function $\varphi_{\alpha\beta}$ of the principal bundle $P(M,G)$.

We now introduce the fiber bundle $TP_M[\mathcal{g}]\equiv(TP\underset{TG}{\times}\mathcal{g},\pi_M\circ Tp,M)$, where $\pi_M: TM\to M$ is the projection of the tangent bundle of M.

By standard arguments it can be seen that $TP_M[\mathcal{g}]$ is a *vector* bundle for which the fiber over x is $T_xM\times\mathcal{g}$.

If $O_P: P\to TP$, $O_M: M\to TM$, and $O_G: G\to TG$ are the zero sections of the corresponding tangent bundles, the following diagram commutes:

$$\begin{array}{ccc} P & \xrightarrow{O_P} & TP\\ \downarrow & & \downarrow\\ M & \xrightarrow{O_M} & TM\end{array}.$$

The pair (O_P,O_G) is an injection of principal bundles over O_M, so it induces uniquely a map

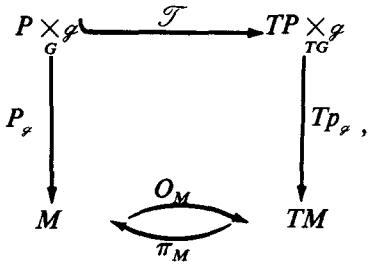
$$\mathcal{T}: P\underset{G}{\times}\mathcal{g}\to TP\underset{TG}{\times}\mathcal{g},$$

which is a bundle injection over O_M of the associated bundles $P[\mathcal{g}]$ and $TP[\mathcal{g}]$. Moreover $\mathcal{T}$ is a vector bundle injection of $P[\mathcal{g}]$ and $TP_M[\mathcal{g}]$ over id_M.

Now we can prove the following decomposition theorem, which will be very important later on.

Theorem 3.1: $TP_M[\mathcal{g}]\cong P[\mathcal{g}]\oplus TM$, that is, the vector bundle $TP_M[\mathcal{g}]$ is the Whitney sum of $P[\mathcal{g}]$ and the tangent bundle of M.

Proof: The image $\mathscr{T}(P[\mathscr{g}])$ of $P[\mathscr{g}]$ is a subbundle of $TP_M[\mathscr{g}]$. Hence there exists a Whitney complement of $\mathscr{T}(P[\mathscr{g}])$, i.e., a subbundle W of $TP_M[\mathscr{g}]$ such that $TP_M[\mathscr{g}] = \mathscr{T}(P[\mathscr{g}]) \oplus W$. Looking at the diagram

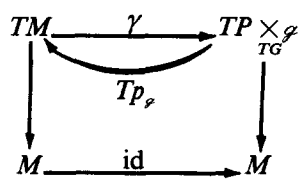


we get $Tp_{\mathscr{g}} \circ \mathscr{T} = O_M \circ p_{\mathscr{g}}$, so that $\operatorname{Im}\mathscr{T} \subset \operatorname{Ker} Tp_{\mathscr{g}}$, $Tp_{\mathscr{g}}$ being a vector bundle morphism over M. But $\dim \operatorname{Im}\mathscr{T} = \dim \mathscr{g} = \dim \operatorname{Ker} Tp_{\mathscr{g}}$, so $\operatorname{Im}\mathscr{T} = \operatorname{Ker} Tp_{\mathscr{g}}$. Hence $Tp_{\mathscr{g}}$ induces a vector bundle isomorphism of W and TM. □

Now we can give a precise characterization of the connections on $P(M,G)$ among the sections of $TP[\mathscr{g}]$. To every connection one-form ω there corresponds a section γ of $TP[\mathscr{g}]$ with

$$\gamma(\xi_x) = [(\xi_u, \omega(\xi_u))]_{TG},$$

where $Tp(\xi_u) = \xi_x$. Clearly the connections are exactly those sections γ of $TP[\mathscr{g}]$ that satisfy the following diagram:



and are linear on the fibers, that is on those sections of $TP[\mathscr{g}]$ which are also vector bundle morphisms over the identity of TM and $TP_M[\mathscr{g}]$.

Thus we have, denoting by $\mathscr{C}$ the set of the principal connections,

$$\mathscr{C} \equiv \{\gamma \in \operatorname{Sec} L(TM, TP_M[\mathscr{g}]),\quad Tp_{\mathscr{g}} \circ \gamma(x) = \mathbf{1}_x,\ \forall x \in M\},$$

where $L(TM,TP_M[\mathscr{g}])$ is the vector bundle over M whose fiber at x consists of the linear maps from T_xM into $(\pi_M \circ Tp_{\mathscr{g}})^{-1}(x)$ and $\mathbf{1}_x$ is the identity operator on T_xM.

On the basis of the above identification we can give $\mathscr{C}$ a suitable differentiable structure.

It is shown in Ref. 5, Proposition 10.10, that the vector space Sec E of the sections of an ordinary vector bundle (E,π,X) is a splitting submanifold of $C^\infty(X,E)$ modeled on the NLF-space $\operatorname{Sec}_c E$. For any $s \in \operatorname{Sec} E$, the set $s + \operatorname{Sec}_c E$ is an open neighborhood of s in FD-topology and an affine subspace, which is isomorphic to $\operatorname{Sec}_c E$; for this reason Sec E is called a local topological affine space. We now prove that $\mathscr{C}$ is an affine subspace and a splitting submanifold (shortly a local topological affine splitting subspace) of the local topological affine space Sec $L(TM,TP_M[\mathscr{g}])$.

Theorem 3.2: $\mathscr{C}$ is a topological affine splitting subspace of Sec $L(TM,TP_M[\mathscr{g}])$ isomorphic to Sec $L(TM,P[\mathscr{g}])$ as topological affine space.

Proof: Fix $\gamma_0 \in \mathscr{C}$; since $Tp_{\mathscr{g}} \circ (\gamma(x) - \gamma_0(x)) = 0_x$, $\forall x \in M$, implies $\gamma - \gamma_0 \in \operatorname{Ker} Tp_{\mathscr{g}} = \operatorname{Im}\mathscr{T}$, then $\gamma - \gamma_0 \in \operatorname{Sec} L(TM, \mathscr{T}(P[\mathscr{g}]))$. Conversely, let $\sigma \in \operatorname{Sec} L(TM, \mathscr{T}(P[\mathscr{g}]))$. One can easily prove that $\gamma_0 + \sigma \in \mathscr{C}$; moreover, by Theorem 3.1, $\operatorname{Sec} L(TM,TP_M[\mathscr{g}])) \cong \operatorname{Sec} L(TM,TM) \oplus \operatorname{Sec} L(TM,P[\mathscr{g}])$ as locally convex vector spaces, hence Sec $L(TM,P[\mathscr{g}])$ is a splitting submanifold of Sec $L(TM,TP_M[\mathscr{g}])$ modeled on Sec $L(TM,P[\mathscr{g}])$. □

Remark: There is another interesting way to look at connections of $P(M,G)$; they can be considered as reductions of the principal bundle $TP(TM,TG)$ to the subgroup G of the structure group TG. This follows from the fact that the bundles $TP[\mathscr{g}]$ and TP/G are isomorphic and by Proposition 5.6 (Chap. I of Ref. 8).

Here we will not exploit further this point of view on connections.

IV. SMOOTHNESS OF THE ACTION OF $\mathscr{G}$ ON $\mathscr{C}$

In order to prove the smoothness of the action of $\mathscr{G}$ on $\mathscr{C}$ we need some preliminary results of geometric nature.

Given the principal bundle $P(M,G)$, let $Z: G \times F \to F$ be the left action of G on a manifold F which defines the associated bundle $P[F]$; then $TZ: TG \times TF \to TF$ is again a left action and defines the associated bundle $TP[TF]$.

The following theorem can be proved by standard arguments.

Theorem 4.1: (a) The associated bundle $TP[TF]$ is isomorphic to the tangent bundle $(T(P \underset{G}{\times} F), Tp_F, TM)$ of the bundle $P[F]$.

(b) The triple $\Theta(P \underset{G}{\times} F) = (TP \underset{TG}{\times} TF, \vartheta_F, P \underset{G}{\times} F)$, where $\vartheta_F([(\xi_u,\xi_f)]_{TG}) = [(u,f)]_G$, is a vector bundle isomorphic to the tangent bundle of the manifold $P \underset{G}{\times} F$.

Given two vector bundles $\xi_1 = (E,\pi_1,X)$ and $\xi_2 = (F,\pi_2,Y)$, we recall that $L(\xi_1,\xi_2)$ stands for the vector bundle $(L(E,F),\alpha \times \omega, X \times Y)$, where $L(E,F)_{(x,y)}$ consists of the linear maps $L_{(x,y)}: E_x \to F_y$ and $(\alpha \times \omega)(L_{(x,y)}) = (x,y)$. We denote by $L_X(\xi_1,\xi_2)$ the bundle over X obtained by the composition of $\alpha \times \omega$ with the canonical projection on X.

Moreover, if X and Y are smooth manifolds, the one-jet map $j^1: C^\infty(X,Y) \to C^\infty(X,J^1(X,Y))$ is a smooth map by Proposition 11.1 of Ref. 5. Now, identifying $J^1(X,Y)$ with $L(TX,TY)$, we remark that the map j^1 takes values in the splitting submanifold Sec $L_X(TX,TY)$ of $C^\infty(X,L(TX,TY))$. Therefore the map

$$j^1: \mathscr{G} = \operatorname{Sec} P[G] \to \operatorname{Sec} L_M(TM, T(P \underset{G}{\times} G))$$

is a smooth map and by Theorem 4.1 we can consider it as a map

$$j^1: \mathscr{G} \to \operatorname{Sec} L_M(TM, \Theta(P \underset{G}{\times} G)).$$

Coming to the action of $\mathscr{G}$ on $\mathscr{C}$, first we recall that in the definition of $TP \underset{TG}{\times} TG$ we use the action of TG on itself by inner automorphisms $\alpha_a \rightsquigarrow \beta_b \alpha_a \beta_b^{-1}$ and in $TP \underset{TG}{\times} \mathscr{g}$ the

above defined action B: $TG \times \mathscr{g} \to \mathscr{g}$. One can easily check that

$$B(\beta_b \alpha_a \beta_b^{-1}, B(\beta_b, \delta)) = B(\beta_b, B(\alpha_a, \delta)).$$

Then the following "fibered action" is well defined:

$$\tilde{B}: (TP \underset{TG}{\times} TG) \underset{TM}{\times} (TP \underset{TG}{\times} \mathscr{g}) \to TP \underset{TG}{\times} \mathscr{g},$$

$$\tilde{B}([(\xi_u, \alpha_a)]_{TG}, [(\xi_u, \delta)]_{TG}) := [(\xi_u, \mathrm{Ad}_a \delta - \alpha)]_{TG},$$

where $\alpha_a = T_e R_a \cdot \alpha$.

Using $\tilde{B}$ we define the left action of $\mathscr{G}$ on $\mathscr{C}$

$$\tilde{A}: \mathscr{G} \times \mathscr{C} \to \mathscr{C}, \quad \tilde{A}(s, \gamma) = \tilde{\gamma},$$

where

$$\tilde{\gamma}(\xi_x) := \tilde{B}((j^1 s)(\xi_x), \gamma(\xi_x)), \quad \text{for } \xi_x \in T_x M.$$

Theorem 4.2: The action $\tilde{A}$ is smooth.

Proof: We can decompose $\tilde{A}$ as follows:

$$\mathscr{G} \times \mathscr{C} \overset{j^1 \times i}{\to} \mathrm{Sec}\, L_M(TM, \Theta(P \underset{G}{\times} G)) \times \mathrm{Sec}\, L(TM, TP_M[\mathscr{g}])$$

$$\overset{\mathrm{Comp}_{\tilde{B}}}{\to} \mathrm{Sec}\, L(TM, TP_M[\mathscr{g}]) \overset{i^{-1}}{\to} \mathscr{C},$$

where $i: \mathscr{C} \to \mathrm{Sec}\, L(TM, TP_M[\mathscr{g}])$ is the canonical inclusion and use of the fact that $\mathrm{Comp}_{\tilde{B}}(j^1 \times i)(\mathscr{G} \times \mathscr{C}) \subseteq \mathrm{Im}\, i$ is made. We have just recalled that j^1 is a smooth map; the inclusion i is an embedding by Theorem 3.2 and $\mathrm{Comp}_{\tilde{B}}$ is smooth by Proposition 11.4 of Ref. 5. □

Remark: We recall that, for every $\gamma \in \mathscr{C}$, $\gamma(\xi_x) = [(\xi_u, \omega(\xi_u))]_{TG}$, where $Tp(\xi_u) = \xi_x$ and ω is the connection one-form corresponding to γ. Analogously if $s \in \mathscr{G}$ there exists an $\hat{f} \in \hat{\mathscr{G}}$ such that $s(x) = [(u, \hat{f}(u))]_G$ with $u \in p^{-1}(x)$. Moreover

$$(j^1 s)(\xi_x) = (Ts)(\xi_x) = [(\xi_u, (T\hat{f})(\xi_u))]_{TG}$$

so that we have

$$\tilde{B}([(\xi_u, (T, \hat{f})(\xi_u))]_{TG}, [(\xi_u, \omega, \xi_u))]_{TG})$$
$$= [(\xi_u, \mathrm{Ad}_{\hat{f}(u)} \omega(\xi_u) - (d\hat{f})(\xi_u))]_{TG},$$

where $d\hat{f} = (T_e R_{\hat{f}(u)})^{-1} \circ T_u \hat{f}$ is the (right) logarithmic derivative of $\hat{f}$ at u.

If we change the left action into a right action

$$\bar{A}: \mathscr{C} \times \mathscr{G} \to \mathscr{C}, \quad \bar{A}(\gamma, s) = \bar{\gamma} := \tilde{A}(s^{-1}, \gamma),$$

we have

$$\bar{\gamma}(\xi_x) = [(\xi_u, \mathrm{Ad}_{(\hat{f}(u))^{-1}} \omega(\xi_u) - (d\hat{f})^{-1}(\xi_u))]_{TG}$$
$$= [(\xi_u, \mathrm{Ad}_{\hat{f}(u))^{-1}} \omega(\xi_u)$$
$$+ (T_{\hat{f}(u)} L_{(\hat{f}(u))^{-1}} \circ T_u \hat{f})(\xi_u)]_{TG},$$

since

$$(df)^{-1}(\xi_u) = ((T_e R_{(\hat{f}(u))^{-1}})^{-1} \circ T_u \hat{f}^{-1}(\xi_u)$$
$$= (T_{\hat{f}(u)^{-1}} R_{\hat{f}(u)} \circ T_u \hat{f}^{-1})(\xi_u)$$
$$= -(T_{\hat{f}(u)} L_{(\hat{f}(u))^{-1}} \circ T_u \hat{f})(\xi_u).$$

In the expression

$$\mathrm{Ad}_{(\hat{f}(u))^{-1}} \omega(\xi_u) + (T_{\hat{f}(u)} L_{(\hat{f}(u))^{-1}} \circ T_u \hat{f})(\xi_u),$$

one can easily recognize the usual transformation $f^* \omega$ of the one-form ω via pullback with the automorphism f defined by $f(u) = u\hat{f}(u)$ (i.e., the corresponding element of $\mathscr{G}^\#$).

Once the smoothness of the action $\tilde{A}$ has been proved, a natural development is the investigation of the properties of the orbits and the structure of the orbit space. In this context the main difficulties one is faced with arise from the lack of inverse map theorems for manifolds modeled on locally convex vector spaces more general than Banach spaces. Perhaps for this reason it is common in physical applications to retire to Banach manifolds or to chains of Banach manifolds. However, a workable version of the inverse map theorem (the Nash–Moser theorem) is now available for a significant subcategory of Fréchet manifolds called "tame Fréchet manifolds" by Hamilton.[9]

Now, if the base manifold M is assumed to be compact, the group $\mathscr{G}$ clearly becomes a nuclear Fréchet–Lie group and $\mathscr{C}$ a splitting affine subspace of a nuclear Fréchet space. Actually we can show that $\mathscr{G}$ is a tame Fréchet–Lie group, $\mathscr{G}$ a tame Fréchet manifold, and the action a tame smooth action.

To some extent, moreover, even the case of noncompact M can be handled: the connected component of the unit of $\mathscr{G}$ can be shown to be a strict inductive limit (in the category of topological groups) of tame Fréchet–Lie groups.

As a consequence of the tameness properties we can prove, in general, that every locally compact subgroup of $\mathscr{G}$ is a splitting Lie subgroup. This result appears as a generalization to $\mathscr{G}$ of a classical Cartan theorem and will be useful in the study of stability subgroups of the action $\mathscr{G}$ on $\mathscr{C}$.

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Approach to equilibrium for random walks on graphs and for stochastic infinite particle processes

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Associated with a finite connected graph g is a doubly stochastic (Laplacian) matrix $G(g)$. A lower bound on the "mass gap" for $G(g)$ is obtained, i.e., the first nonzero eigenvalue of $G(g)$. This estimate is then used to estimate the mass gap for some infinite particle stochastic generators with corresponding processes that are closely related to Monte Carlo methods employed in statistical mechanics calculations.

I. INTRODUCTION

Let g be a finite connected graph consisting of n vertices and (nondirected) bonds connecting various pairs of vertices. Then we can associate with g a Markov semigroup generator (doubly stochastic matrix) $G(g)$ with matrix elements

$$\begin{aligned} G(g)_{ii} &= n(i) \text{ with } n(i) \text{ the number of bonds emanating from vertex } i, \\ G(g)_{ij} &= -1 \text{ (or 0) according to whether there is a bond (no bond) between vertices } i \text{ and } j,\ i \neq j. \end{aligned} \tag{1.1}$$

The matrix $G(g)$ is just a (negative) Laplacian on g. Here, our first objective is to obtain a lower bound on the mass gap [i.e., the first nonzero eigenvalue of $G(g)$]. This mass gap, of course, controls the rate at which the semigroup generated by $G(g)$ approaches equilibrium.

Generalizing this problem, we let Ω be a perturbation of a countable direct sum of operators of the form $G(g)$. More precisely, let g be a fixed graph, $X(g)$ its vertices, $\mathbb{Z}^d$ the d-dimensional integer lattice, and r a site in $\mathbb{Z}^d$. Define the (compact) state space $X = \Pi_{r\in\mathbb{Z}^d} X(g)$ and let σ denote a point in X with $\sigma(r)$ its rth coordinate. Then we formally define Ω acting in $C(X)$, the space of continuous functions on X in the sup norm, by

$$\Omega = \sum_{r\in\mathbb{Z}^d} c(r,\cdot)(G(r,g) \otimes 1); \tag{1.2}$$

here, the $c(r,\sigma)$ are non-negative continuous functions on X and $G(r,g)$ is a copy of $G(g)$ corresponding to the site r. [Under suitable hypotheses on the $c(r,\sigma)$ including boundedness and decaying dependence on $\sigma(s)$ at sites s remote from r, functions of the form $f(\sigma) = g(\sigma(r_1),\ldots,\sigma(r_m))$ form a core for Ω (cf. Ref. 1, for the stochastic Ising case), and so the closure of Ω generates a unique semigroup.] Our second and main objective is to show that if the $c(r,\sigma)$ are nearly constant [so that the terms in Eq. (1.2) nearly commute], then the mass gap of Ω is approximately that of one of the terms; hence the need for a mass gap estimate on $G(g)$. We add that the semigroup generated by Ω is closely related to the (discrete) Monte Carlo methods employed by many authors to study the Gibbs states of statistical mechanical and field theoretical models, and so the mass gap of Ω is related to the rate at which the Monte Carlo method converges to equilibrium. Moreover, this exponential approach to equilibrium can be used to show that the correlation functions for the invariant state cluster exponentially (cf. Ref. 2 for the stochastic Ising model).

Section II provides the estimate on the mass gap for $G(g)$. The proof is split into two parts. The first part consists of an abstract version of the interlacing theorem for self-adjoint matrices and its principal submatrices; the second part applies this result to $G(g)$ in order to obtain the mass gap estimate roughly in terms of the number of vertices and the diameter of g. Our result should be contrasted with Cheeger[3] who considers the same problem for the Laplacian on compact manifolds. For additional results on the spectral properties of operators associated with graphs, see Ref. 4.

Finally, in Sec. III, we obtain an estimate on the mass gap for Ω defined in Eq. (1.2). Actually Ω need not be self-adjoint so that the mass gap estimate is phrased in terms of the rate at which the semigroup generated by Ω approaches equilibrium. This result is an adaptation of Liggett's argument for the stochastic Ising model.[1] The proof is adaptable to a broader class of operators (e.g., operators with drift terms), but for simplicity we have confined ourselves to operators Ω of the form Eq. (1.2). See also Faris[5] for an analogous result on the stochastic Heisenberg (rotator) model.

II. SPECTRAL PROPERTIES FOR THE GRAPH LAPLACIAN

We begin with a general result concerning the eigenvalues of an arbitrary self-adjoint matrix. The result is really just an abstract version of the interlacing theorem (cf. Ref. 6, p. 203) sometimes called Cauchy inequalities for eigenvalues.

Theorem 2.1: Let A be an $n\times n$ self-adjoint matrix, V: $\mathbb{R}^m \to \mathbb{R}^n$ a linear isometry, $m \leqslant n$, and define the $m\times m$ self-adjoint matrix A^c by

$$\langle x, A^c y\rangle_m = \langle Vx, AVy\rangle_n , \tag{2.1}$$

where $\langle\cdot,\cdot\rangle_p$ denotes the usual dot product in $\mathbb{R}^p$. Then

$$\lambda_k \leqslant \lambda_k^c \leqslant \lambda_{n-m+k}, \quad 1 \leqslant k \leqslant m , \tag{2.2}$$

where $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$ are the eigenvalues of A and

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$\lambda_1^c \leqslant \lambda_2^c \leqslant \cdots \leqslant \lambda_m^c$ are the eigenvalues of A^c.

Proof: For any k-dimensional subspace $\tilde{W} \subset R^n$, $\tilde{W}$ contains a normalized element $u \in \text{span}\{e_k,...,e_n\}$, where e_i is a normalized eigenvector of A corresponding to λ_i. Thus

$$\max_{\substack{u\in\tilde{W} \\ \|u\|=1}} \langle u,Au\rangle_n \geqslant \lambda_k .$$

On the other hand, if e_i^c is a normalized eigenvector corresponding to λ_i^c, $W = \text{span}\{e_1^c,...,e_k^c\}$ and $\tilde{W} = VW$, then

$$\lambda_k^c = \max_{\substack{x\in W \\ \|x\|=1}} \langle x, A^c x\rangle_m = \max_{\substack{u\in\tilde{W} \\ \|u\|=1}} \langle u, Au\rangle \geqslant \lambda_k$$

by Eq. (2.1). The other inequality of inequality (2.2) follows by replacing A by $-A$ and employing the above argument.

We actually only use this theorem here in the following manner.

Theorem 2.2 (Interlacing Theorem): Let A be a self-adjoint matrix A^c the principal submatrix obtained from A by suppressing the ith row and column, for any i, $1 \leqslant i \leqslant n$. Then

$$\lambda_k \leqslant \lambda_k^c \leqslant \lambda_{k+1}, \quad 1 \leqslant k \leqslant n , \tag{2.3}$$

where $\lambda_1 \leqslant \cdots \leqslant \lambda_n$ and $\lambda_1^c \leqslant \cdots \leqslant \lambda_{n-1}^c$ are the eigenvalues of A and A^c, respectively.

Proof: Let

$$V = (x_1,...,x_{n-1}) \in \mathbb{R}^{n-1} \to (x_1,...,x_{i-1},0,x_i,...,x_{n-1}) \in \mathbb{R}^n$$

and apply Theorem 2.1.

Remark: As another illustration of Theorem (2.1), however, we show the well-known fact that a self-adjoint rank 1 perturbation of a self-adjoint matrix A, $A+P$, has eigenvalues $\{\lambda_i'\}$ interlacing those of A. It is no restriction to assume P is positive so clearly $\lambda_i \leqslant \lambda_i'$, $i = 1,...,n$, with n the dimension of A. Let Q be projection onto the orthogonal complement of the range P. Then by Theorem (2.1) it is easy to see that $Q(A+P)Q = QAQ$, restricted to ran Q, has eigenvalues λ_i^Q interlacing those of A and $A+P$ so that in particular, $\lambda_i' \leqslant \lambda_i^Q \leqslant \lambda_{i+1}$, $i = 1,...,n-1$. Hence, $\lambda_i \leqslant \lambda_i' \leqslant \lambda_{i+1}$, $i = 1,...,n-1$.

As an application of this Theorem 2.2, we return to the problem of obtaining a lower bound on the first nonzero eigenvalue of $G(g)$ defined in the Introduction. The idea is to estimate this eigenvalue by the first nonzero eigenvalue of $G(g_\tau)$, where g_τ is any tree graph (a simply connected graph) linking all vertices in g and which is a subgraph of g. We call such a tree graph allowable. Given a tree graph g_τ, suppose vertex i is removed along with the bonds emanating from i. We let $b_i(j,g_\tau)$, $j = 1,...,j(i)$ denote the remaining disjoint connected branches, the index j just labeling the branch, $|b_i(j,g_\tau)|$ the number of vertices in $b_i(j,g_\tau)$, and $d_i(j,g_\tau)$ the length of the longest path in $b_i(j,g_\tau)$.

Theorem 2.3: Let λ_1 be the least nonzero eigenvalue of $G(g)$. Then for any allowable tree graph g_τ in g,

$$\lambda_1 \geqslant \sup_{i\in g_\tau} \inf_j (1 + d_i(j,g_\tau))^{-1} |b_i(j,g_\tau)|^{-1} . \tag{2.4}$$

Examples: Suppose g is a ring of n vertices and n bonds connecting adjacent vertices, $n \geqslant 2$. Removing a single bond, we obtain g_τ. Removing a vertex from the middle of g_τ or as close to the middle as possible, we obtain $\lambda_1 \geqslant 4/(n^2-1)$, n odd, $\lambda_1 \geqslant (4/n(n+2))$, n even, whereas

$$\lambda_1 = 2 - 2\cos(2\pi/n) \cong (4\pi^2/n^2) ,$$

n large.

As another example, we take g to be as above but with an additional vertex at the center of the ring and bonds (spokes) emanating from the center out to each ring vertex. (There are altogether $2n$ bonds.) For g_τ we take the graph consisting of all vertices and the spoke bonds only, and then remove the center vertex. We obtain $\lambda_1 \geqslant \frac{1}{2}$, whereas λ_1 can be calculated to be $\lambda_1 = 3 - 2\cos(2\pi/n)$. In both of these examples, the estimate exhibits the correct leading n dependence, up to a constant, $n \to \infty$.

To begin the proof of the theorem, we have the obvious lemma.

Lemma 2.4: Let g_1 and g_2 be graphs on $\{1,2,...,n\}$ with $g_1 \subset g_2$ so that g_1 is obtained from g_2 by removing some subset of bonds. Then

$$G(g_1) \leqslant G(g_2) . \tag{2.5}$$

In particular the k th eigenvalue of $G(g_1)$ is less than the k th eigenvalue of $G(g_2)$.

Proof: Note that

$$G(g_2) = G(g_1) + \sum_{\{i,j\}}{}' P(i,j) , \tag{2.6}$$

where Σ' extends over the removed bonds, and

$$P(i,j)_{kl} = \begin{cases} 1, & \text{if } k=l=i \text{ or } j, \\ -1, & \text{if } k=i,\ l=j \text{ or } k=j,\ l=i, \\ 0, & \text{otherwise.} \end{cases} \tag{2.7}$$

But as an $n \times n$ matrix $P(i,j) \geqslant 0$ so the lemma follows.

Thus this lemma enables us to give a lower bound on λ_1 of $G(g)$ by the first nonzero eigenvalue of $G(g_\tau)$ where g_τ is any tree that is a subset of g. By Theorem 2.2, we need to estimate the least eigenvalue of $G(i,g_\tau)$, the matrix obtained from $G(g_\tau)$ by suppressing the ith row and column. Since g_τ is a tree, however, removal of the ith vertex disconnects g_τ into the connected branches $b_i(j,g_\tau)$ and causes $G(i,g_\tau)$ to decompose into a direct sum

$$G(i,g_\tau) = \bigoplus_j G_i(j,g_\tau) ,$$

where $G_i(j,g_\tau)$ corresponds to the branch $b_i(j,g_\tau)$. The least eigenvalue of $G(i,g_\tau)$ is thus the least of those of $G_i(j,g_\tau)$. We have for a normalized vector x,

$$\langle x, G_i(j,g_\tau)x\rangle = {\sum}''(x_l - x_k)^2 + x_{i(j)}^2 , \tag{2.8}$$

where Σ'' extends over all bonds $\{l,k\}$ in $b_i(j,g_\tau)$ and $i(j)$ is the vertex in this branch that had a bond in g_τ connecting to vertex i.

Since x is normalized there is a vertex l such that $x_l^2 \geqslant |b_i(j,g_\tau)|^{-1}$ and a path $x_l = x_{l(1)}, x_{l(2)},...,x_{l(n)} = x_{i(j)}$ with $n \leqslant d_i(j,g_\tau)$ such that the expectation [Eq. (2.8)] exceeds

$$\sum_{k=2}^{n}(x_{l(k)}-x_{l(k-1)})^2+x_{i(j)}^2$$

$$\geqslant\frac{1}{n+1}x_i^2\geqslant(d_i(j,g_\tau)+1)^{-1}|b_i(j,g_\tau)|^{-1}. \qquad (2.9)$$

The first inequality is an application of Schwarz's inequality. Taking the infimum over all branches, we obtain the theorem.

Remark: An alternative approach to obtaining a lower bound on λ_1 for $G(g)$ is simply to note that if x is normalized and orthogonal to the ground state, then x must somewhere change sign so that

$$\langle x,G(g)x\rangle=\sum_{\{i,j\}\in g}(x_i-x_j)^2$$

$$\geqslant\sum_{\{i,j\}\in g}{}'(x_i-x_j)^2+\sum_{\{i,j\}\in g}{}''(x_i^2+x_j^2), \qquad (2.10)$$

where the first sum extends over all bonds with $x_ix_j\geqslant 0$ and the second sum extends over all bonds with $x_ix_j<0$. It then remains to estimate the right-hand side of the inequality, which amounts to estimating $\mathscr{D}G(g)$, i.e., the Laplacian on G with Dirichlet boundary conditions imposed on some (unknown) set of bonds. This estimate is analogous to that of Cheeger[3] who considers the Laplacian on a Riemannian manifold. Theorem 2.2 gives additional spectral information and, together with Theorem 2.3, gives a sharper estimate on λ_1.

III. INFINITE PARTICLE STOCHASTIC GENERATORS

In this section we consider the rate at which the semigroup generated by Ω, Eq. (1.2) of the Introduction, approaches equilibrium, in the case where the functions $c(r,\cdot)$ are nearly constant. (Henceforth g is fixed.) The basic idea is that if the $c(r,\cdot)\cong 1$, then the terms in the sum for Ω nearly commute and the approach to equilibrium is exponentially fast, behaving approximately as $e^{-\lambda_1 t}$, with λ_1 the first nonzero eigenvalue of $G(g)$.

To incorporate the assumption that $c(r,\cdot)\cong 1$, we set

$$c(r,\cdot)=1+c_1(r,\cdot), \qquad (3.1)$$

with $c_1(r,\cdot)\geqslant 0$ for convenience. Each $G(r)$ in the sum [Eq. (1.2)] is self-adjoint (we suppress the g and the $\otimes 1$ notation) and so we let $P_r(\alpha)(=P_r(\alpha)\otimes\mathbf{1})$ be the projection onto the αth eigenspace of $G(r)$ with λ_α the corresponding eigenvalue (the same for all sites r), observing the convention that $0=\lambda_0<\lambda_1\leqslant\lambda_2\leqslant\cdots\leqslant\lambda_{n-1}$ with n the dimension of each G. Finally, we set

$$\gamma(r,\alpha;s,\beta)=\|[P_r(\alpha),c_1(s,\cdot)]\|_\beta, \qquad (3.2)$$

where we use the operator norm in $C(X)$. We will think of γ as the kernel of an operator Γ on $\ell^1(Z^d\times X(g))$ [$X(g)$ is the set of vertices g]. Let $\|\Gamma\|$ denote the norm of this operator.

Given a function f on $C(X)$ we set

$$|||f|||=\sum_r\sum_\alpha\sup_\sigma|P_r(\alpha)f(\sigma)|. \qquad (3.3)$$

Theorem (3.1): Suppose $\lambda_1>\|\Gamma\|$. Then $\exp(-t\Omega)$ approaches equilibrium exponentially fast in the sense that

$$|||\exp(-t\Omega)g|||\leqslant\exp-t(\lambda_1-\|\Gamma\|)|||g|||. \qquad (3.4)$$

Thus the mass gap for Ω is at least $\lambda_1-\|\Gamma\|$.

Proof: Again, the proof is a straightforward adaptation of Liggett's argument for the stochastic Ising model.[1] Suppose that f is the solution to

$$(1+\epsilon\Omega)f=g. \qquad (3.5)$$

Operating on the left of this equation with $P_r(\alpha)$, we obtain

$$(1+\epsilon\Omega)P_r(\alpha)f$$

$$=P_r(\alpha)g-\epsilon\sum_{s,\beta}[P_r(\alpha),c_1(s)]\lambda_\beta P_s(\beta)f, \qquad (3.6)$$

where we have used the spectral representation of $G(r)$. At the point $\sigma_{\max}$, where $P_r(\alpha)f$ is maximum [recall $X=\Pi_{Z^d}X(g)$ is compact so this function attains its maximum], we have that

$$(1+\epsilon\lambda_\alpha)P_r(\alpha)f(\sigma_{\max})$$

$$\leqslant P_r(\alpha)g(\sigma_{\max})+\epsilon\sum_{s,\beta}\gamma(r,\alpha;s,\beta)|P_s(\beta)f(\sigma_{\max})| \qquad (3.7)$$

by a simple maximum principle argument applied to all the $r'\neq r$ terms of Ω and c_1 terms [e.g., $G(s)P_r(\alpha)f(\sigma_{\max})\geqslant 0$] and by Eq. (3.2). An analogous inequality holds at $\sigma_{\min}$. It follows that ($\|\cdot\|_\infty$ is the sup norm)

$$\|P_r(\alpha)f\|_\infty\leqslant\|((1+\epsilon(\lambda_1-\Gamma))^{-1}P)_r(\alpha)g\|_\infty \qquad (3.8)$$

and so

$$|||f|||\leqslant(1+\epsilon(\lambda_1-\|\Gamma\|))^{-1}|||g|||. \qquad (3.9)$$

Iterating this inequality, we obtain

$$|||\exp(-t\Omega)g|||=|||\lim_{n\to 0}(1+(t/n)\Omega)^{-n}g|||$$

$$\leqslant\lim_{n\to\infty}(1+(t/n)(\lambda_1-\|\Gamma\|))^{-n}|||g|||$$

$$=\exp(-(\lambda_1-\|\Gamma\|)t)|||g|||. \qquad (3.10)$$

This concludes the proof of the theorem.

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Sites and googly twistor spaces. I. Vacuum

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(Anti-) self-dual Yang–Mills fields may be described by twistors of the same or opposite handedness as the fields. These are called the leg-break and googly descriptions, respectively. The leg-break twistor space is a complex manifold; the Yang–Mills field is given by a vector bundle over this manifold, and massless fields minimally coupled to the Yang–Mills field are given by elements of certain sheaf cohomology groups on the manifold. In this paper, the structure of the googly twistor space when no Yang–Mills field is present is elucidated. It is shown that the googly twistor space is a *site*. Sites are generalizations of topological spaces, in which the primitive concept is that of an open set rather than that of a point. The massless fields on space-time are given by the elements of a sheaf cohomology group on the site. Also, this site is isomorphic to a leg-break site, consisting of a family of open sets in the leg-break manifold. This provides a strong link between the googly and the leg-break spaces. The following paper treats the case where a Yang–Mills field is present.

I. INTRODUCTION

The successes of gauge theories in recent years have led to an increased interest in solutions of the Yang–Mills field equations. The largest known class of these is given (implicitly) by a construction due to Ward.[1,2] He showed that, if the curvature is anti-self-dual, solutions of the field equations correspond exactly to certain bundles over twistor space $\mathbb{P}$. Thus, instead of trying to solve differential equations on Minkowski space, one can specify (essentially freely, locally) transition matrices over twistor space. Similarly, self-dual fields are described by bundles over dual twistor space $\mathbb{P}^*$.

This construction also allows a concise characterization of massless fields minimally coupled to the (anti-) self-dual Yang–Mills field.[1,3,4] (Such massless fields are important in instanton physics.[5]) They are given by elements of certain *sheaf cohomology groups* on twistor space. These elements are represented by certain equivalence classes of functions on $\mathbb{P}$. (This is called the *Čech* representation.)

It is hoped that twistor theory will be able to provide the *full*, non-self-dual, local solution to the Yang–Mills equations. As a first step, one wishes to develop a new description of self-dual fields on $\mathbb{P}$ (or anti-self-dual fields on $\mathbb{P}^*$). One would then combine this with the Ward construction, to arrive at the non-self-dual fields as some sort of nonlinear superpositions of the two. The description of self-dual fields on $\mathbb{P}$ is called the *googly*[6] (a cricketing term); by contrast, the Ward construction is called the *leg-break* (ditto).

Recently, a googly description of massless fields minimally coupled to a self-dual Yang–Mills background has been achieved.[7–9] The idea is this. One starts with the Čech leg-break representation of such fields on $\mathbb{P}^*$:

massless fields$\leftrightarrow$equivalence classes of functions on $\mathbb{P}^*$.

Then a new kind of *twistor transform* is introduced, which carries functions on $\mathbb{P}^*$ to certain second cohomology elements on $\mathbb{P}$. Then the leg-break description induces a googly one:

massless fields$\leftrightarrow$equivalence classes of second cohomology elements on $\mathbb{P}$.

From this, it has been possible to derive a number of explicit expressions for the massless fields. They are given by integral formulas with a remarkable contour (the "Pochhammer" contour[10]), and seem related to certain twistor-diagrammatic calculations of scattering amplitudes.[11–13]

This previous googly work focused on obtaining explicit expressions for the fields. In the present paper and a sequel, we elucidate the general theoretical framework into which the googly description fits. We show that googly twistor space has the structure of a site (sites are generalizations of topological spaces), that there are certain sheaves on the site, and massless fields are given by Čech cohomology elements of the site with coefficients in these sheaves. These parallel leg-break results. Furthermore, the Yang–Mills field is represented by a bundle over this site. In each case, the googly site may naturally be identified with a leg-break site.

These results are easy to establish, being mostly a matter of checking definitions. Their significance is that they systematize all the previous results, and allow one to bring the techniques of the theory of sites to bear on the googly problems. Additionally, these techniques will be useful in areas of twistor theory other than the study of googlies.[14]

This paper is divided into five sections. The next one reviews the twistor transform used in the googly construction. The third outlines the relevant elements of the theory of sites. Here, generality has been sacrificed for simplicity. (The sites we consider have underlying categories that are partially ordered sets which have greatest lower bounds of pairs of elements.) The reader will find more detailed accounts in Refs. 15–17. The fourth section establishes the site structures of googly and leg-break spaces when no Yang–Mills field is present, and their equivalence; the last section is devoted to discussion. In the sequel, we describe the site structures when Yang–Mills fields are present.

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We assume a knowledge of twistor theory[18,19] and an elementary acquaintance with sheaves.[20]

II. THE τ-TWISTOR TRANSFORM

The core of the googly construction is the following result.[8,9] Let V be an open set in $\mathbb{P}$. Then

$$U = \{W_\alpha \in \mathbb{P}^* | \text{the plane } W_\alpha \subset V\} \tag{1}$$

is Stein, and there is a group

$$\underline{H}^2(V, \mathscr{O}(-2-r)) \tag{2}$$

isomorphic to

$$H^0(U, \hat{\mathscr{O}}(-2+r)). \tag{3}$$

Here

$$\hat{\mathscr{O}}(n) = \mathscr{O}(n)/\text{polynomials},$$

U and V are called *corresponding* sets, and the isomorphism from (3) and (2) is called the (τ-) *twistor transform*, and denoted τ.

The definition of $\underline{H}^2$ is given in the Appendix; we shall not need it. The following properties will be used, however.[8,9] If $V' \subset V$, then there is a restriction homomorphism

$$\underline{H}^2(V, \mathscr{O}(-2-r)) \to \underline{H}^2(V', \mathscr{O}(-2-r))$$

and

$$\begin{array}{ccc} H^0(U, \hat{\mathscr{O}}(-2+r)) & \to & H^0(U', \hat{\mathscr{O}}(-2+r)) \\ \downarrow & & \downarrow \\ \underline{H}^2(V, \mathscr{O}(-2-r)) & \to & \underline{H}^2(V', \mathscr{O}(-2-r)) \end{array}$$

commutes, where U' corresponds to V', the horizontal maps are restrictions and the vertical ones twistor transforms.

Now set

$$\underline{H}^2(V, \mathscr{O}(n) \otimes S) = \underline{H}^2(V, \mathscr{O}(n)) \otimes S,$$

for any fixed vector space S. Then there are maps Z^α, $\partial/\partial Z^\alpha$ such that

$$\begin{array}{ccc} H^0(U, \hat{\mathscr{O}}(-2+r)) & \xrightarrow{\partial/\partial W_\alpha} & H^0(U, \hat{\mathscr{O}}^\alpha(-3+r)) \\ \tau \downarrow & & \tau \downarrow \\ \underline{H}^2(U, \mathscr{O}(-2-r)) & \xrightarrow{-Z^\alpha} & \underline{H}^2(V, \mathscr{O}^\alpha(-1-r)) \end{array}$$

and

$$\begin{array}{ccc} H^0(U, \hat{\mathscr{O}}(-2+r)) & \xrightarrow{W_\alpha} & H^0(U, \hat{\mathscr{O}}_\alpha(-1+r)) \\ \tau \downarrow & & \tau \downarrow \\ \underline{H}^2(V, \mathscr{O}(-2-r)) & \xrightarrow{\partial/\partial Z^\alpha} & \underline{H}^2(V, \mathscr{O}_\alpha(-3-r)) \end{array}$$

commute. The maps Z^α, $\partial/\partial Z^\alpha$ commute with restriction. These diagrams are the τ-twistor transform analogs of the more familiar helicity changing formulas.[21]

Lastly, we make some remarks about the corresponding sets. For every point omitted from $\mathbb{P}$ in forming V, a plane is omitted from $\mathbb{P}^*$ in forming U. Thus, the U's that arise from (1) are those gotten by omitting families of planes from $\mathbb{P}^*$. (So not every open set in $\mathbb{P}^*$ arises as the set corresponding to some $V \subset \mathbb{P}$.) In particular, note that there are arbitrarily small U's (take V to be a neighborhood of a plane in $\mathbb{P}$), and any open set in $\mathbb{P}^*$ can be covered by U's.

In general, more than one V corresponds to a single U. (For instance, any set in $\mathbb{P}$ that contains no plane corresponds to $\emptyset$ in $\mathbb{P}^*$.) However, the intersection $\tilde{V}$ of all the V's corresponding to U will correspond to U, since if any $W_\alpha \in U$, the plane W_α will be contained in every V. Then

$$\tilde{V} = \{Z^\alpha \in \mathbb{P} | Z^\alpha \text{ is on some plane in } V\}.$$

We call $\tilde{V}$ *the canonical set corresponding to* U.

III. SITES AND RELATED STRUCTURES

A. Sites

Sites are generalizations of topological spaces, in which the primitive concept is that of an open set, rather than that of a point. Thus the "open sets" in a site need not be sets of points, and they are called the *objects* of the site.

The structure of the site is described in two stages. First, there is a system of inclusions: we know what it means for one object to be contained in another. This is called *the underlying category* of the site. Then, there is a system of covers: we know what it means for a family of objects to cover another object. This is *the Grothendieck topology* of the site.

Recall that for a topological space, inclusion satisfies the following properties:

(i) $U \subset U$ for any open set U;

(ii) $U \subset V$, $V \subset W$ imply $U \subset W$.

A category[22] $\mathscr{C}$ is a set of objects (also denoted $\mathscr{C}$) together with a relation $\subset$ satisfying

(i) $U \subset U$ for any U,

(ii) $U \subset V$, $V \subset W$ imply $U \subset W$ for any U, V, $W \in \mathscr{C}$.

We shall also need a notion of intersection. For a topological space, $U \cap V$ is the largest set contained in both U and V. We shall require that the intersection of two arbitrary objects be defined. Thus we assume the following.

(iii) Let U, $V \in \mathscr{C}$. Then there is a unique largest $U \cap V \in \mathscr{C}$ with $U \cap V \subset U$, $U \cap V \subset V$; i.e., for any $X \in \mathscr{C}$ with $X \subset U$, $X \subset V$, then $X \subset U \cap V$.

Examples: (1) Let $\mathscr{C}$ be the collection of open sets of a topological space, and $\subset$ as usual.

(2) Let $\mathscr{C}$ be the integers, and define

$$m \subset n \quad \text{iff} \quad m \leqslant n.$$

Then $m \cap n = \min(m,n)$. This example does not arise as a special case of the first one: if it did, the object that is the whole topological space would include every other object, but there is no greatest integer.

(3) Let $\mathscr{C}$ be any order set, with $\subset$ and $\cap$ as in (2).

We now turn to the system of covers. Recall that a cover of a set U in a topological space is a set $\{U_i\}$ of subsets of U with $\cup_i U_i = U$. We have no notion of union, in general, in a category, so we cannot use this definition for a site. However, covers have three important properties:

(a) $\{U\}$ is a cover of U, for any U;

(b) if $\{V_i\}$ covers U, and $\{W_{ij}\}$ covers V_i for each i, then $\{W_{ij}\}$ covers U;

(c) if $\{V_i\}$ covers U and $W \subset U$, then $\{V_i \cap W\}$ covers W.

A *cover* of an object $U \in \mathscr{C}$ is a collection $\{U_i\}$ of objects included in U. A *Grothendieck topology*[23] on $\mathscr{C}$ is an assignment of a set of covers to each object in $\mathscr{C}$, satisfying (a)–(c) (with "cover" replaced by "cover from the assigned set"). A category with a Grothendieck topology is called a *site*. We

speak of "the site $\mathscr{C}$," when the Grothendieck topology is understood. Also, by a cover, we mean one in the Grothendieck topology unless otherwise noted.

Examples: (1) A topological space with the usual notion of cover.

(2) $\mathscr{C}$ = the integers, $m \subset n$ iff $m \leqslant n$. The covers are given by

$\{m_i\}$ covers n iff $n \in \{m_i\}$

(and $m_i \subset n$ for all m_i, of course).

(3) $\mathscr{C}$ = an ordered set, inclusion and covers as in (2).

In examples (2) and (3), the objects are not sets of points; the idea of a point appears nowhere in the definitions. Also note that no largest object (which would be the analog of the whole topological space) need exist; nor any smallest object (analog of $\varnothing$). As remarked before, unions need not exist either. [In example (2), finite unions—in the sense of smallest objects containing a given family of objects—exist, but not the infinite unions which would in a topological space.]

There is a further axiom on Grothendieck topologies that it will be convenient to impose:

(d) if $\mathscr{U}$ is a cover of U in the Grothendieck topology, and $\mathscr{U}'$ is *any* cover of U with $\mathscr{U}' \supset \mathscr{U}$, then $\mathscr{U}'$ is a cover of U in the Grothendieck topology.

This may be done without loss of generality, by adjoining to a Grothendieck topology those sets $\mathscr{U}'$ satisfying the above hypothesis. Henceforth we will assume sites have this property.

We now define subsites. These will be analogs of open subspaces of topological spaces.

Let $\mathscr{C}$ be a site, and $\mathscr{C}'$ a subset of the set of objects in $\mathscr{C}$ such that $U \in \mathscr{C}'$, $V \subset U$ implies $V \in \mathscr{C}'$. Then $\mathscr{C}'$ becomes a category with inclusions and intersections inherited from $\mathscr{C}$. Furthermore, $\mathscr{C}'$ becomes a site with covers inherited from $\mathscr{C}$. Thus $\mathscr{C}'$ is said to be a *subsite* of $\mathscr{C}$.

B. Sheaves

Recall that a presheaf $\mathscr{P}$ (of Abelian groups, say) over a topological space X is a mapping

open sets in $X \to$ Abelian groups,

$$U \mapsto \Gamma(U, \mathscr{P}),$$

together with restriction maps

$$\rho_{VU}\colon\ \Gamma(U,\mathscr{P}) \to \Gamma(V,\mathscr{P}) \quad \text{if } V \subset U,$$

satisfying (i) the restrictions are group homomorphisms; and

(ii) if $V \subset U$, $W \subset V$, $\rho_{WV}\rho_{VU} = \rho_{WU}$.

A presheaf $\mathscr{P}$ over a site $\mathscr{C}$ is a mapping

objects in $\mathscr{C} \to$ Abelian groups,

$$U \mapsto \Gamma(U, \mathscr{P}),$$

together with restrictions maps, as above, satisfying (i) and (ii). We shall often write $f_{|V}$ for $\rho_{VU} f$.

Recall that a presheaf $\mathscr{P}$ over a topological space X is a sheaf if (iii) for every cover $\{U_i\}$ of U and $f, g \in \Gamma(U, \mathscr{P})$, then $f_{|U_i} = g_{|U_i}$ for all i implies $f = g$; and (iv) for every cover $\{U_i\}$ of U, if $f_i \in \Gamma(U_i, \mathscr{P})$ and $f_{i|U_j} = f_{j|U_i}$ for all i, j, then there is $f \in \Gamma(U, \mathscr{P})$ with $f_i = f_{|U_i}$.

A sheaf over a site is a presheaf satisfying (iii) and (iv). As usual, we call the elements of $\Gamma(U, \mathscr{P})$ the *sections* of $\mathscr{P}$ over U.

C. Cohomology

We may define the Čech cohomology[24] of a site by analogy to that of a topological space. A subset $\mathscr{U}$ of the set of objects of a site $\mathscr{C}$ is called *a cover for* $\mathscr{C}$ if for every $U \in \mathscr{C}$, some cover of U is contained in $\mathscr{U}$. A second cover $\mathscr{U}'$ for $\mathscr{C}$ is said to be *finer* than $\mathscr{U}$ if $U \in \mathscr{U}'$ implies $U \subset V$ for some $V \in \mathscr{U}$. Note that $\mathscr{C}$ is always a cover for itself, so every site has covers.

A p-cochain with respect to $\mathscr{U}$, with coefficients in a sheaf $\mathscr{S}$, is a set of sections, one for every $(p+1)$-fold intersection of objects in $\mathscr{U}$,

$$\left\{ f_{i_0 \cdots i_p} \in \Gamma(U_{i_0} \cap \cdots \cap U_{i_p}, \mathscr{S}) \right\},$$

with $f_{i_0 \cdots i_p} = f_{[i_0 \cdots i_p]}$. The set of these p-cochains is denoted $C^p(\mathscr{U}, \mathscr{S})$. The coboundary operator is

$$\left\{ f_{i_0 \cdots i_p} \right\} \mapsto \left\{ \rho_{[i_0} f_{i_1 \cdots i_{p+1}]} \right\},$$

where ρ_{i_0} is restriction to U_{i_0}. The cocycles $Z^p(\mathscr{U}, \mathscr{S})$ and coboundaries $B^p(\mathscr{U}, \mathscr{S})$ are defined as usual, and

$$H^p(\mathscr{U}, \mathscr{S}) = Z^p(\mathscr{U}, \mathscr{S}) / B^p(\mathscr{U}, \mathscr{S})$$

is *the Čech cohomology of $\mathscr{S}$ with respect to $\mathscr{U}$*. One verifies that if $\mathscr{U}'$ is a finer cover than $\mathscr{U}$, there is a canonical homomorphism

$$H^p(\mathscr{U}, \mathscr{S}) \to H^p(\mathscr{U}', \mathscr{S})$$

and that such homomorphisms commute on passage to finer covers. Thus one can form

$$\check{H}^p(\mathscr{C}, \mathscr{S}) = \lim_{\mathscr{U}} H^p(\mathscr{U}, \mathscr{S}),$$

the Čech cohomology of $\mathscr{C}$ with coefficients in $\mathscr{S}$.

IV. SITE STRUCTURES OF TWISTOR SPACES

A. Googly twistor space

In this section, we define googly twistor space as a site. It is equipped with certain sheaves; later we shall show that the cohomology of these sheaves gives massless fields on space-time.

Denote by $\mathscr{G}$ the site whose objects are open sets in $\mathbb{P}$, whose inclusions are the usual ones, but whose covers are given by $\{V_i\}$ covers V iff every plane is V is in some V_i. (The verification that this is a Grothendieck topology is elementary and will be omitted.) We call $\mathscr{G}$ *googly twistor space*.

Let $\mathscr{A}(-2-r)$ denote the presheaf

$$V \mapsto \underline{H}^2(V, \mathscr{O}(-2-r))$$

on $\mathscr{G}$. We claim $\mathscr{A}(-2-r)$ is a sheaf, i.e., satisfies (iii) and (iv) of Sec. III B. Let $\{V_i\}$ cover V.

(iii) Suppose $f, g \in \underline{H}^2(V, \mathscr{O}(-2-r))$. Let V_i correspond to U_i and V to $\bar{U}$. Note that $\{U_i\}$ covers U (in the usual sense). Then $f_{|V_i} = g_{|V_i}$ implies $(\tau^{-1} f)_{|U_i} = (\tau^{-1} g)_{|U_i}$. Since $\hat{\mathscr{O}}(-2+r)$ is a sheaf on $\mathbb{P}^*$, we have then $\tau^{-1} f = \tau^{-1} g$, whence $f = g$, as was to be shown.

(iv) Let $f_i \in \underline{H}^2(V_i, \mathscr{O}(-2-r))$ be given, with

$f_{i|V_i\cap V_j}=f_{j|V_i\cap V_j}$. Then

$$(\tau^{-1}f_i)_{|U_i\cap U_j}=(\tau^{-1}f_j)_{|U_i\cap U_j},$$

so there is $g\in H^0(U,\hat{\mathcal{O}}(-2+r))$ with $g_{|U_i}=\tau^{-1}f_i$. Then $\tau g\in \underline{H}^2(V,\mathcal{O}(-2-r))$ with $(\tau g)_{|V_i}=f_i$, as was to be shown.

B. Low-helicity massless fields

We call a region in complexified conformally compactified Minkowski space *β-elementary*[25] if every β-plane that meets it does so in a connected and simply connected set. Let X be such a region. We shall give a googly description of the low-helicity massless fields on X.

Let $\mathcal{G}_X$ be the subsite of $\mathcal{G}$ whose objects are the open sets in $\mathbb{P}$ every β-plane of which meets X, and

$$\mathbb{P}^*_X=\{W_\alpha\in\mathbb{P}^*\,|\,W^\alpha \text{ meets } X\}.$$

We know that[4]

$$H^1(\mathbb{P}^*_X,\mathcal{O}(-2+2s))\simeq\mathcal{I}_s(X), \tag{4}$$

the space of helicity s massless fields on X. We will prove

$$\check{H}^1(\mathcal{G}_X,\mathcal{A}(-2-2s))\simeq\mathcal{I}_s(X),\quad s<1. \tag{5}$$

This formula (together with its counterpart for $s\geqslant 1$, below) is one of the main results of this paper. It is a concise characterization of massless fields, and comes close to giving us as good an understanding of the googly description as we have of the leg-break.

The proof of the isomorphism really follows from the definitions. Let $\mathcal{V}=\{V_i\}$ be a cover $\mathcal{G}_X$. Then $\mathcal{U}=\{U_i$ corresponding to $V_i\}$ is a (Stein) cover of $\mathbb{P}^*_X$. Since $U_i\cap U_j$ corresponds to $V_i\cap V_j$, there is a bijection of cochains

$$C^p(\mathcal{U},\hat{\mathcal{O}}(-2+2s))\simeq C^p(\mathcal{V},\mathcal{A}(-2-2s)),$$

whence

$$H^p(\mathcal{U},\hat{\mathcal{O}}(-2+2s))\simeq H^p(\mathcal{V},\mathcal{A}(-2-2s)).$$

However, if $s<1$,

$$\hat{\mathcal{O}}(-2+2s)\simeq\mathcal{O}(-2+2s)$$

and

$$H^p(\mathcal{U},\mathcal{O}(-2+2s))\simeq H^p(\mathcal{V},\mathcal{A}(-2-2s)).$$

The inductive limit in the definition of H is then trivial, and the isomorphism (5) results from (4).

C. High-helicity massless fields

The previous analysis must be modified for helicities $\geqslant 1$, because in that case

$$\hat{\mathcal{O}}(-2+2s)\not\simeq\mathcal{O}(-2+2s)$$

and, in general,

$$H^1(\mathcal{G}_X,\mathcal{A}(-2-2s))\simeq H^1(\mathbb{P}^*_X,\hat{\mathcal{O}}(-2+2s))\not\simeq\mathcal{I}_s(X).$$

There are several ways to do this; we give only one here. We shall define a new sheaf on $\mathcal{G}_X$ whose cohomology is $\mathcal{I}_s(X)$. For the moment, we take $s=1$, for simplicity.

First note

$$H^0(U,\mathcal{O})\simeq H^0(U,\mathcal{O}^\alpha(-1))/H^0(U,\mathcal{O}^{[\alpha\beta]}(-2)), \tag{6}$$

whenever U is Stein. This follows from the exact sequence of sheaves on $\mathbb{P}^*$:

$$\mathcal{O}^{[\alpha\beta]}(-2)\xrightarrow{W_\beta}\mathcal{O}^\alpha(-1)\xrightarrow{W_\alpha}\mathcal{O}\to 0.$$

We know how to twistor transform the groups on the right of (6): we define a presheaf $\mathcal{B}(-4)$ on $\mathcal{G}_X$ by

$$V\mapsto\underline{H}^2(V,\mathcal{O}^\alpha(-3))/\underline{H}^2(V,\mathcal{O}^{[\alpha\beta]}(-2)),$$

where the quotient is formed with respect to $\partial/\partial Z^\alpha$. As before, this is a sheaf, and an argument parallel to the previous one gives

$$\check{H}^1(\mathcal{G}_X,\mathcal{B}(-4))\simeq\mathcal{I}_1(X).$$

For higher helicities, one has

$$\check{H}^1(\mathcal{G}_X,\mathcal{B}(-2-2s))\simeq\mathcal{I}_s(X),$$

where $\mathcal{B}(-2-2s)$ is the sheaf

$$V\mapsto\underline{H}^2(V,\mathcal{O}^{(\alpha_1\cdots\alpha_{2s-1})}(-3))/(V,\mathcal{O}^{[\beta\alpha_1]\alpha_2\alpha_3\cdots\alpha_{2s-1}}(-2)).$$

D. Equivalence with leg-break space

The results of the previous three subsections were established by "twistor transforming" properties of $\mathbb{P}^*$ to $\mathbb{P}$. The reader has probably already noticed close correspondences between the sites $\mathbb{P}^*$ and $\mathcal{G}$ and the sheaves $\mathcal{O}(-2+2r)$ and $\mathcal{A}(-2-2r)$, $\mathcal{B}(-2-2r)$. In fact, they are very nearly identical, as we now show.

Let $\mathcal{P}^*$ be the site whose objects are those sets in $\mathbb{P}^*$ that correspond to open sets in $\mathbb{P}$, and whose inclusions and cover are as usual. Since intersections in $\mathbb{P}^*$ and $\mathcal{P}^*$ are the same and every cover in $\mathcal{P}^*$ is a cover in $\mathbb{P}^*$, $\mathcal{O}(-2+r)$ and $\hat{\mathcal{O}}(-2+r)$ are sheaves on $\mathcal{P}^*$.

Let $\tilde{\mathcal{G}}$ be the site whose objects are those objects $\tilde{V}\in\mathcal{G}$ that are canonical sets (i.e., every point in V is on a plane in V, cf. Sec. II), with inclusions and covers as usual. Note that intersections in $\tilde{\mathcal{G}}$ are not the same as in $\mathcal{G}$. This is because there may be points common to V_1 and V_2 that do not lie on common planes. Nevertheless, one has

$$\tilde{V}_1\underset{\tilde{\mathcal{G}}}{\cap}\tilde{V}_2=V_1\underset{\mathcal{G}}{\cap}\tilde{V}_2$$

(where the underscripts to $\cap$ indicate the category in which intersection is taken). Also note

$$\underline{H}^2(V,\mathcal{O}(-2-r))\simeq\underline{H}^2(\tilde{V},\mathcal{O}(-2-r)),$$

since both are isomorphic to $H^0(U,\hat{\mathcal{O}}(-2+r))$. For these observations and the fact that every cover $\tilde{\mathcal{G}}$ is a cover in $\mathcal{G}$, it follows that $\mathcal{A}(-2-r)$, $\mathcal{B}(-2-r)$ are sheaves on $\tilde{\mathcal{G}}$.

We know from Sec. II that the objects in $\mathcal{P}^*$ and $\tilde{\mathcal{G}}$ are in one-to-one correspondence, and that $U_1\subset U_2$ iff $V_1\subset V_2$, so the underlying categories of these sites may be identified. From the definition of covers in $\tilde{\mathcal{G}}$ (which is that of $\mathcal{G}$, cf. Sec. IV A), one sees that the covers may be identified as well. *Thus $\mathcal{P}^*$ and $\tilde{\mathcal{G}}$ are equivalent as sites.*

The sheaf $\hat{\mathcal{O}}(-2+r)$ over $\mathcal{P}^*$ may be identified with $\mathcal{A}(-2-r)$ over $\tilde{\mathcal{G}}$, and similarly $\mathcal{O}(-2+2s)$ over $\mathcal{P}^*$ with $\mathcal{B}(-2-2s)$, $s\geqslant 1$. This is immediate because τ identifies sections over identified objects.

Let X be a β-elementary region in complexified confor-

mally compactified Minkowski space, $\tilde{\mathcal{G}}_X$ the subsite of $\tilde{\mathcal{G}}$ whose objects are those in $\tilde{\mathcal{G}}$ every β-plane of which meets X, and $\mathcal{P}^*_X$ the subsite of $\mathcal{P}^*$ with objects

$$\{U \in \mathcal{P}^* | \text{every point in } U \text{ is a } \beta\text{-plane meeting } X\}.$$

Then, arguments parallel to those of the preceding subsections give

$$\begin{aligned}\mathcal{L}_s(X) &\simeq \check{H}^1(\mathcal{P}^*_X, \mathcal{O}(-2+2s)) \\ &\simeq \check{H}^1(\tilde{\mathcal{G}}_X, \mathcal{A}(-2-2s)), \quad s<1, \\ &\simeq \check{H}^1(\tilde{\mathcal{G}}_X, \mathcal{B}(-2-2s)), \quad s\geqslant 1.\end{aligned}$$

Thus, a description of massless fields can be recovered from either the leg-break site $\mathcal{P}^*$ or its googly equivalent $\tilde{\mathcal{G}}$.

The construction of $\tilde{\mathcal{G}}$ from $\mathcal{G}$ may seem *ad hoc*, but is in fact a special case of a very natural and general construction. Let us suppose we are given a site $\mathcal{C}$ and a sheaf $\mathcal{S}$ on $\mathcal{C}$, which we think of as being the *structure sheaf* on $\mathcal{C}$ (i.e., the "most important" class of functions on $\mathcal{C}$). Then if the restriction

$$\Gamma(U,\mathcal{S}) \to \Gamma(V,\mathcal{S}) \tag{7}$$

is an isomorphism for two objects $U,V \in \mathcal{C}$, then U and V are indistinguishable by sections over them in $\mathcal{S}$. It is then natural to define an equivalence relation on the set of objects in $\mathcal{C}$, generated by $U \sim V$ if (7) is an isomorphism.[26]

This is essentially how $(\tilde{\mathcal{G}}, \mathcal{A}(-2-2s))$ arises from $(\mathcal{G}, \mathcal{A}(-2-2s))$: one has $V_1 \sim V_2$ if $\tilde{V}_1 = \tilde{V}_2$. In general, the construction of the underlying category $\tilde{\mathcal{C}}$ and its covers is a little involved technically, and we shall not pursue it.

V. DISCUSSION

At the heart of the googly construction is the elementary observation that points in $\mathbb{P}^*$ correspond to planes in $\mathbb{P}$. The identity of the googly and leg-break sites is only an extension of this: sets of points in $\mathbb{P}^*$ correspond to sets of planes in $\mathbb{P}$. The set of points is an object in $\mathcal{P}^*$; the set of points on a family of planes is an object in $\tilde{\mathcal{G}}$. The virtue of the site-theoretic approach is that it systematizes previous results and provides a useful framework.

The identity of the sheaves over the sites is remarkable: after all, elements of $\underline{H}^2$ are quite different from ordinary functions (cf. the Appendix and Refs. 8 and 9). It is this difference that is responsible for the novelty of the googly integral formulas for massless fields.[7-9]

Another difference worth noting is that between $\mathcal{P}^*$ and $\mathbb{P}^*$: not all open sets in the latter are objects in the former (cf. Sec. II). Still, as we know, $\mathcal{P}^*$ has enough objects to satisfactorily describe massless fields, and indeed, every open set in $\mathbb{P}^*$ is covered by others that are objects in $\mathcal{P}^*$.

The prominence of planes, as opposed to points, in the googly construction is unusual but not surprising. Points would correspond to planes in the dual leg-break space. One knows that, if a self-dual Yang–Mills field is present, such planes will generically encounter singularities where the Ward bundle is not defined.[1] In the gravitational case, when a space-time with self-dual Weyl curvature is given by a curved dual leg-break twistor space, this space itself will not in any obvious way contain any planes.[27] Thus points in leg-break spaces are more natural than planes; so planes in googly spaces will be more natural than points.

We close by listing some of the work that remains to be done in the site-theoretic study of googlies.

The calculus of the sheaves on the googly sites and their cohomology groups must be more fully developed, in parallel to the extensive calculus that exists for sheaves over topological spaces. Much of the general theory has been worked out[15-17]: it remains to specialize it to twistor theory.

The relation of these techniques of the *googly map approach*[6,28] to the googly problem should be investigated. One of the reasons this approach has not had more success is its lack of a clear framework; perhaps sites will help.

The use of sites for gravitational googlies (i.e., googly twistor spaces describing space-times with self-dual Weyl curvatures) should be developed.

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APPENDIX: DEFINITION OF $\underline{H}^2$

Let Φ be a pseudo-Hermitian form of signature $+\ +\ +\ -$ on $\mathbb{P}^*$, and

$$U = \{W_\alpha \in \mathbb{P}^* | \Phi(W_\alpha) < 0\},$$
$$V = \{Z^\alpha \in \mathbb{P} | \Phi^{-1}(Z^\alpha) > 0\}.$$

Then U and V correspond in the sense of Sec. II. Here U is called a *regular ball*. It is known that

$$H^0(U, \hat{\mathcal{O}}(-2+r)) \simeq H^2(V, \mathcal{O}(-2-r))$$

and that the isomorphism commutes with restriction.[7-9,29]

Now let V be any open set in $\mathbb{P}$. Put

$$\mathcal{V} = \{V_\lambda \subset V | V_\lambda \text{ corresponds to a regular ball}\}.$$

A googly two-function with coefficients in $\mathcal{O}(-2-r)$ is a set

$$\{\varphi_\lambda \in H^2(V_\lambda, \mathcal{O}(-2-r)) | V_\lambda \in V\}$$

such that

$$\varphi_{\lambda | V_\mu} = \varphi_\mu \quad \text{if} \quad V_\mu \subset V_\lambda.$$

The set of all such googly two-functions is

$$\underline{H}^2(V, \mathcal{O}(-2-r)).$$

For more details, see Refs. 8 and 9.

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[23]What we call a Grothendieck topology is usually called a *pre-topology*. For our categories, the concepts are equivalent.
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Sites and googly twistor spaces. II. Yang–Mills fields

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(Anti-) self-dual Yang–Mills fields may be described by twistors of the same or opposite handedness as the fields. These are called the leg-break and googly descriptions, respectively. The leg-break twistor space is a complex manifold; the Yang–Mills field is given by a vector bundle over this manifold; and massless fields minimally coupled to the Yang–Mills field are given by elements of certain sheaf cohomology groups on the manifold. In the previous paper, we analyzed the structure of the googly twistor space when no Yang–Mills field is present, and showed that it was a *site*. (Sites are generalizations of topological spaces, in which the primitive concept is that of an open set rather than that of a point.) In this paper, we treat the case where a gauge field is present. We show that the field is represented by a vector bundle over the site, and that massless fields minimally coupled to the Yang–Mills field are given by the elements of a sheaf cohomology group on the site. Also, this vector bundle is isomorphic to one over a leg-break twistor site. This provides a strong link between the googly and the leg-break spaces.

I. INTRODUCTION

This is the second of two papers outlining the structure of *googly twistor spaces*. These spaces describe self-dual Yang–Mills fields with twistors of the opposite-to-usual handedness (purely right-handed fields with left-handed twistors or vice versa). It is hoped that a combination of googly techniques and the usual ones will lead to the general local solution of the source-free Yang–Mills equations as a nonlinear superposition of left- and right-handed pieces.

The previous paper[1] described the structure of googly twistor space when no Yang–Mills field was present. The space is a *site* (sites are generalizations of topological spaces) equipped with certain sheaves. The cohomology of these sheaves over appropriate subsites described massless fields on space-time. This parallels the usual ("leg-break") twistor description of massless fields as cohomology elements of sheaves on twistor space.

In this paper, we include the effects of the self-dual Yang–Mills field. We show that this field is given by a bundle over the googly site, and that massless fields minimally coupled to the Yang–Mills field are given by cohomology elements of sheaves "twisted" by the bundle. Again, these are parallel to the leg-break results. As in the previous paper, we are concerned with the structure of the googly space rather than with explicit computational techniques (see Refs. 2–4).

We assume the results and notation of the previous paper, and an acquaintance with the Ward construction[5,6] (the usual twistor description of self-dual fields).

II. THE GOOGLY CONVOLUTION

We describe here the googly operation corresponding to the multiplication of holomorphic functions on the leg-break space. Over any open set $U\subset\mathbb{P}^*$, there is a multiplication

$$\Gamma(U,\mathscr{O})\times\Gamma(U,\mathscr{O})\to\Gamma(U,\mathscr{O}),$$
$$(f,g)\mapsto fg,$$

which, of course, commutes with restrictions to subsets. We define the googly counterpart of this as

$$\Gamma(V,\mathscr{B}(-4))\times\Gamma(V,\mathscr{B}(-4))\to\Gamma(V,\mathscr{B}(-4)),$$
$$(\alpha,\beta)\mapsto\alpha*\beta=\tau((\tau^{-1}\alpha)(\tau^{-1}\beta)),$$

and call it *the googly convolution*. An explicit formula is given for it in Ref. 2. We will not need this here.

III. SOME MORE SITE THEORY

In this section, we introduce some more site-theoretic analogs of familiar topological ideas. Our aim is to keep the technicalities to a minimum.

We first discuss the sheaves of sections of vector bundles over sites. We do this rather than dealing directly with vector bundles over sites because it is much less involved to formulate the local triviality condition for the sheaves of sections. For a vector bundle over a topological space, the vector-space structure of the fibers is reflected in the fact that the sheaf of continuous sections of the vector bundle is a *module* over the sheaf of continuous functions. This is how such sheaves are defined on sites, as sheaves of modules over distinguished sheaves.

The second main idea we introduce is that of a *continuous functor of sites*, which is the counterpart of the concept of a continuous map of topological spaces.

A. Sheaves of rings and modules

Recall that a ring is a set R with two binary operations $+,\cdot$ such that (i) $+$ and $\cdot$ are associative, $+$ is commutative, and $\cdot$ distributes over $+$; and (ii) there is an additive identity element $0\in R$, and every $a\in R$ has an additive inverse $-a\in R$. We will generally omit the dot for multiplication. If multiplication is commutative, the ring is *commutative*; if there is a multiplicative identity $1\in R$, the ring is said to *possess a unity*. All our rings will be commutative rings with

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unity, and we will just call them rings, for short.

Examples: The real numbers, the complex numbers, the integers, and the ring of continuous real-valued functions on an open set in a topological space. Note that, in the last two cases, multiplicative inverses of nonzero elements do not exist. This is what distinguishes rings from *fields*. (The reals and the complex numbers are fields.)

A homomorphism from a ring R to a ring S is a map that preserves the ring structure, i.e., products, sums, identities, and inverses.

A sheaf of rings[7] is a sheaf $\mathscr{R}$ such that, for all U, $\Gamma(U,\mathscr{R})$ is a ring and, if $V\subset U$, then the restriction

$$\Gamma(U,\mathscr{R})\to\Gamma(V,\mathscr{R})$$

is a ring homomorphism.

Examples: (1) The sheaf $\mathscr{C}^0$ of continuous real-valued functions on a topological space, the sheaf $\mathscr{C}^\infty$ of smooth real-valued functions on a smooth manifold, and the sheaf $\mathscr{O}$ of holomorphic functions on a complex manifold.

(2) The sheaf $\mathscr{B}(-4)$ on $\mathscr{G}$ or $\bar{\mathscr{G}}$, with multiplication $*$.

Let R be a ring. *A module over R* is a set M together with two operations,

$$+ : M\times M\to M \quad \text{(addition)},$$

$$\cdot : R\times M\to M \quad \text{(scalar multiplication)},$$

such that (again, sometimes omitting the dot for multiplication) (i) addition is commutative and associative, there is an additive identity $0\in M$, and every $\mu\in M$ has an additive inverse $-\mu\in M$; (ii) scalar multiplication distributes over addition;

(iii) $r(s\mu)=(rs)\mu$, for all $r,s\in R$, $\mu\in M$;

and

(iv) $1\cdot\mu=\mu$, $0\cdot\mu=0$, for all $\mu\in M$.

Observe that a module is to a ring as a vector space is to a field.

A module homomorphism is a map of modules preserving module structure, and *a sheaf of modules*[7] *$\mathscr{M}$ over a sheaf of rings $\mathscr{R}$* has

$$\Gamma(U,\mathscr{M}) \text{ a } \Gamma(U,\mathscr{R})\text{-module},$$

for all U, and restrictions are module homomorphisms.

Example: Let E be a vector bundle over a topological space. Then the sheaf $\mathscr{E}$ of continuous sections of E is a module over $\mathscr{C}^0$. Similarly, one can work with smooth manifolds, vector bundles, and sections, or complex manifolds and holomorphic vector bundles and sections.

If M is a module over R, and there are $\mu_1,\dots,\mu_n\in M$ such that any $\mu\in M$ can be expressed as

$$\mu=r_1\mu_1+\cdots+r_n\mu_n,$$

for some $r_1,\dots,r_n\in R$, $\{\mu_1,\dots,\mu_n\}$ is said to *generate* M. The smallest n such that this is true is called the *rank* of M. These concepts are the module analogs of span and dimension for vector spaces.

Examples: (1) Let M be the module of *global* sections of a vector bundle E over a topological space X. (R is the ring of globally defined continuous real functions on X.) In general, the rank of M is greater than the dimension of the fiber of E, because sections of E will necessarily have zeros. At a zero, the section will not help to span the fiber.

(2) Another important example of an R-module is R^n. In particular, $\mathscr{R}^n$ is a sheaf of modules over $\mathscr{R}$.

We close this subsection with some remarks about matrices over R. First, R^{n^2} is the set of all $n\times n$ matrices with entries in R. Matrix multiplication is defined in the usual way. It is associative. There is an identity element, 1 on the diagonal and zero elsewhere. The determinant may be defined in the usual way; it is an element of R. A matrix is *nonsingular* if its determinant has a multiplicative inverse in R. Nonsingular matrices have unique inverses. One may, of course, consider sheaves of matrices.

Examples: Let $\mathscr{R}$ be a sheaf of rings. Then $\mathscr{R}^{n^2}$ is the sheaf of $n\times n$ $\mathscr{R}$-valued matrices. One can also consider the sheaf of such matrices with determinant unity.

B. Vector bundles

Let E be a vector bundle over a topological space X. The local triviality of E is reflected in the following property of the $\mathscr{C}^0$-module $\mathscr{E}$.

(i) There is a cover $\mathscr{U}=\{U_i\}$ of X such that $\Gamma(U_i,\mathscr{E})$ has finite rank for all i. For fine enough covers, a generating set on U_i restricts to one on any $U\subset U_i$; also, the rank is independent of i and of $\mathscr{U}$: it is called the *rank* of the bundle.

It is easy to show that this condition of an *arbitrary* $\mathscr{C}^0$-module $\mathscr{E}$ *implies* $\mathscr{E}$ arises as the sheaf of sections of a vector bundle (unique up to isomorphism). Choose a sufficiently fine cover $\{U_i\}$, and let $\mu_{i\alpha}$, $\alpha=1,\dots,n$, be the generating set on U_i. The patching relation over $U_i\cap U_j$ is given by (the v_i^α are fiber coordinates over U_i)

$$v_i^\alpha\,\mu_{i\alpha}|_{U_j}=v_j^\alpha\,\mu_{j\alpha}|_{U_i}$$

(summation convention on α but not i,j).

The analogous results for smooth vector bundles over smooth manifolds and holomorphic vector bundles over complex manifolds also hold. In these cases, the sheaves of rings are $\mathscr{C}^\infty$ and $\mathscr{O}$. The sheaves $\mathscr{C}^0$, $\mathscr{C}^\infty$, and $\mathscr{O}$ play such fundamental roles—can indeed be regarded as defining their spaces—that they are called *structure sheaves*. Thus a module $\mathscr{E}$ over the structure sheaf is the sheaf of sections of a vector bundle iff it satisfies (i).

Now let $\mathscr{C}$ be a site, and $\mathscr{R}$ be a distinguished sheaf of rings over $\mathscr{C}$; we shall call $\mathscr{R}$ the structure sheaf. *By the sheaf of sections of a vector bundle over the site $\mathscr{C}$ with structure sheaf $\mathscr{R}$, we mean an $\mathscr{R}$-module $\mathscr{E}$ satisfying (i)* (with X replaced by $\mathscr{C}$).

$\mathscr{E}$ is called *trivial* if it is isomorphic to $\mathscr{R}^n$ for some n (necessarily the rank of $\mathscr{E}$). For $\mathscr{E}$ arising as a sheaf of sections of a vector bundle E, this is the same thing as saying that E is trivial. (We omit the verification of this, which is easy.)

We now show how to explicitly construct sheaves of bundles over sites from "transition functions," and vice versa.

Let $\mathscr{U}=\{U_i\}$ be a cover of $\mathscr{C}$, and suppose we are given a set of nonsingular $\mathscr{R}$-valued matrices

$$f=\{f_{ij}\in\Gamma(U_i\cap U_j,\mathscr{R}^{n^2})\},$$

satisfying

$$f_{ij} = f_{ji}^{-1}, \quad f_{ij} f_{jk} = f_{ik} \text{ on } U_i \cap U_j \cap U_k.$$

These will be the *transition matrices* defining a sheaf $\mathscr{E}_f$:

$$\Gamma(U,\mathscr{E}_f) = \ker \bigoplus_i \Gamma(U\cap U_i,\mathscr{R}^n) \xrightarrow{\varphi} \bigoplus_{i,j} \Gamma(U\cap U_i\cap U_j,\mathscr{R}^n),$$

where

$$\{\mu_i\} \xrightarrow{\varphi} \{\mu_i - f_{ij}\mu_j\}.$$

More abstractly, let $\mathscr{R}_i^n$ be the restriction of $\mathscr{R}^n$ to U_i, $\mathscr{R}_{ij}^n$ its restriction to $U_i\cap U_j$. Then $\mathscr{E}_f$ may be defined by the exact sequence

$$0 \to \mathscr{E}_f \to \bigoplus_i \mathscr{R}_i^n \xrightarrow{\varphi} \bigoplus_{i,j} \mathscr{R}_{ij}^n.$$

It is easy to see that $\mathscr{E}_f$ satisfies (i) with respect to $\mathscr{U}$.

Contrariwise, if a bundle $\mathscr{E}$ is given satisfying (i), choose a cover $\mathscr{U}$ of $\mathscr{E}$ so that $\Gamma(U_i,\mathscr{E})$ has finite rank n for every $U_i\in\mathscr{U}$. Let $\mu_{i\alpha}$ be a generating set for $\Gamma(U_i,\mathscr{E})$ as before. Then, on $U_i\cap U_j$,

$$\mu_{i\alpha} = f_{ij\alpha}{}^{\beta}\mu_{j\beta}$$

for some matrix f_{ij}. It is easy to see that $\{f_{ij}\}$ satisfies the conditions above.

In parallel with the usual result for vector bundles over topological spaces, one can easily derive the condition that two sets of transition matrices $f = \{f_{ij}\}, g = \{g_{i'j'}\}$ (with respect to two covers) give isomorphic sheaves of sections, $\mathscr{E}_f \simeq \mathscr{E}_g$. The result is that on a sufficiently fine cover $\mathscr{U} = \{U_i\}$ there should be nonsingular matrices

$$\{t_i \in \Gamma(U_i,\mathscr{R}^{n^2})\}$$

such that

$$f_{ij} = t_i^{-1} g_{ij} t_j$$

(no summation implied).

C. Tensor products

We will now define tensor products of sheaves of modules on a site. First, we need a technical definition.

Let $\mathscr{P}$ be a presheaf on a site $\mathscr{C}$. *The sheaf associated to* $\mathscr{P}$ is

$$U \mapsto \lim_{\mathscr{U}} \check{H}^0(\mathscr{U},\mathscr{P}),$$

where $\mathscr{U}$ ranges over the covers of U. It is not hard to see that this is indeed a sheaf.

Now let $\mathscr{R}$ be a sheaf of rings over $\mathscr{C}$, and let $\mathscr{L}$, $\mathscr{M}$ be $\mathscr{R}$-modules. *The tensor product* $\mathscr{L} \underset{\mathscr{R}}{\otimes} \mathscr{M}$ is the sheaf associated to the presheaf

$$U \mapsto \Gamma(U,\mathscr{L}) \underset{\Gamma(U,\mathscr{R})}{\otimes} \Gamma(U,\mathscr{M}),$$

where the tensor product of modules is defined analogously to that of vector spaces.

D. Continuous functors

Recall that a map of topological spaces

$$f: X \to Y$$

is continuous iff the *inverse* image of every open set in Y is open in X. (In general, the image of an open set in X need not be open in Y.) A continuous map of sites will thus be described by an analog of f^{-1}. Note that f^{-1} preserves inclusions, intersections, and covers:

(i) $U\subset V$ implies $f^{-1}(U)\subset f^{-1}(V)$;
(ii) $\{U_i\}$ covers U implies $\{f^{-1}(U_i)\}$ covers $f^{-1}(U)$;
(iii) $f^{-1}(U\cap V) = f^{-1}(U)\cap f^{-1}(V)$.

For topological spaces, (i)–(iii) hold because f^{-1} arises from a mapping of points in X to points in Y. For sites, they will be extra hypotheses.

A continuous functor of sites, denoted

$$f: \mathscr{C} \to \mathscr{D}$$

is by definition a map, denoted f^{-1}, *from the set of objects of* $\mathscr{D}$ *to those of* $\mathscr{C}$, *satisfying* (i)–(iii).[8]

Examples: (1) A continuous map of topological spaces gives rise to a continuous functor between their sites.

(2) Let $\mathscr{C}$ be the site arising from the topological space of real numbers, and $\mathscr{D}$ be the non-negative integers as in example (3) of Sec. II A of the previous paper.[1] Define

$$f^{-1}(n) = (-n,n).$$

It is easy (and left to the reader) to verify (i)–(iii).

If $f: X\to Y$ is a continuous map of topological spaces, and $s: Y\to Z$ is another, *the pullback of* s *to* X *via* f, f^*s, is the composition $sf: X\to Z$. The idea extends readily (if a little technically) to sheaves over sites.[8]

Let $f: \mathscr{C}\to\mathscr{D}$ be a continuous functor of sites, and $\mathscr{S}$ a sheaf over $\mathscr{D}$. Define a presheaf $f_!\mathscr{S}$ over $\mathscr{C}$ by

$$U \mapsto \lim_{\substack{V\in\mathscr{D} \\ U\subset f^{-1}(V)}} \Gamma(V,\mathscr{S}).$$

The sheaf associated to this presheaf (see Sec. III C, above) is *the pullback of* $\mathscr{S}$ *to* $\mathscr{C}$ *via* f, denoted $f^*\mathscr{S}$.

Examples: (1) Pullbacks of sheaves over topological spaces via continuous maps.

(2) Let $\mathscr{C}$ be the usual site associated to the topological space of real numbers, $\mathscr{D}$ the site of non-negative integers, and $f: \mathscr{C}\to\mathscr{D}$ as above. Define a sheaf $\mathscr{S}$ on $\mathscr{D}$ by

$$\Gamma(n,\mathscr{S}) = \mathbb{R}^n$$

(where we understand $\mathbb{R}^0 = \{0\}$) with restriction from $\mathbb{R}^n$ to $\mathbb{R}^m$ by

$$(x^1,\ldots,x^n) \mapsto (x^1,\ldots,x^m), \quad \text{if } 0<m\leqslant n,$$
$$\mapsto 0, \quad \text{if } m = 0.$$

The pullback of $\mathscr{S}$ to $\mathscr{C}$ is given as follows. If O is open in $\mathbb{R}$, then $f_!\mathscr{S}$ is

$$O \mapsto \lim_{\substack{n\in\mathscr{D} \\ O\subset(-n,n)}} \mathbb{R}^n.$$

This limit is $\mathbb{R}^n$, where n is the least integer such that $|x|<n$ for all $x\in O$. It is easy to verify that this is a sheaf, so $f^*\mathscr{S} = f_!\mathscr{S}$.

IV. THE GOOGLY BUNDLE AND MASSLESS FIELDS

In the leg-break picture, a self-dual Yang–Mills field is represented by a vector bundle over a region of $\mathbb{P}^*$ (see Refs.

5 and 6). The vector bundle is required to be trivializable over those lines in $\mathbb{P}^*$ representing points in space-time where the field is to be defined. The set of such points, of course, depends on the problem under consideration. (It may be Minkowski space, or Euclideanized space-time, or some other region.) We call this *the Ward triviality condition*.

Massless fields minimally coupled to the Yang–Mills background (i.e., test fields, which do not produce a back reaction on the gauge field) are described by cohomology elements:

$$H^1(\mathbb{P}^*_X, E \otimes \mathcal{O}(-2+2s))$$

is the space of fields of helicity s on the region X in space-time.[6] Here E is the Ward bundle. Of course, this group is the same as

$$H^1(\mathbb{P}^*_X, \mathscr{E} \otimes \mathcal{O}(-2+2s)),$$

where $\mathscr{E}$ is the sheaf of holomorphic sections of E.

In this section, we present the googly counterparts of these results. Throughout, we regard $\mathscr{B}(-4)$ on $\mathscr{G}_X$ or $\tilde{\mathscr{G}}_X$ as a ring with multiplication given by $\star$. Also, for convenience, we let

$$\mathscr{B}(-2-2s) = \mathscr{A}(-2-2s), \quad s<1,$$

so $\mathscr{B}(-2-2s)$ is the "twistor transform" of $\mathcal{O}(-2+2s)$ for all s.

A. The googly bundle

Let $\mathscr{G}_X$, $\tilde{\mathscr{G}}_X$, $\mathbb{P}^*_X$, and $\mathbb{P}^*_X$ be as in the preceding article. Our goal is to show that the sheaves of sections of the Ward bundles over $\mathbb{P}^*_X$ may be identified naturally with sheaves of sections of various bundles over the other sites. We begin by ignoring the Ward triviality condition.

Lemma: There is a natural one-to-one correspondence between isomorphism classes of $\mathscr{B}(-4)$-modules satisfying the local triviality condition [Sec. III B (i)] on $\mathscr{G}_X$ and $\tilde{\mathscr{G}}_X$.

Proof: This follows from the fact that

$$\underline{H}^2(V_i, \mathscr{B}(-4)) \simeq \underline{H}^2(\tilde{V}_i, \mathscr{B}(-4)) \simeq \underline{H}^2(V_j, \mathscr{B}(-4))$$

if $\tilde{V}_i = \tilde{V}_j$. The argument is straightforward and the details will be omitted.

Proposition: Between any two of the following sets of isomorphism classes of modules over sites satisfying the local triviality condition [Sec. III B (i)], there is a natural one-to-one correspondence:

(a) $\mathscr{B}(-4)$-modules on $\mathscr{G}_X$,

(b) $\mathscr{B}(-4)$-modules on $\tilde{\mathscr{G}}_X$,

(c) $\mathcal{O}$-modules on $\mathscr{P}^*_X$,

(d) $\mathcal{O}$-modules on $\mathbb{P}^*_X$.

Proof: We have the bijection between (a) and (b) by the previous lemma; since $(\mathscr{P}^*_X, \mathcal{O})$ may naturally be identified with $(\tilde{\mathscr{G}}_X, \mathscr{B}(-4))$, there is a bijection between (b) and (c). The one between (c) and (d) follows from the fact that the sets in $\mathbb{P}^*_X$ that are objects in $\mathscr{P}^*_X$ suffice for the trivialization of any holomorphic vector bundle.

Since we know that (d) is equivalent to the set of isomorphism classes of holomorphic sections of holomorphic vector bundles on $\mathbb{P}^*_X$, this proposition identifies the sheaves of sections of such vector bundles with googly structures.

We will, in what follows, denote the leg-break sheaf of modules $\mathscr{E}$, and its corresponding googly sheaf $\mathscr{F}$.

B. The triviality condition

For the leg-break space $\mathbb{P}^*_X$, the triviality condition is that, for certain points $x \in X$, the vector bundle E (or equivalently its sheaf of sections $\mathscr{E}$) should be trivializable over L_x. Restriction to L_x is the same thing as pulling back via the inclusion map

$$\xi\colon L_x \to \mathbb{P}^*_X,$$

so we may express the triviality condition as

$$H^0(L_x, \xi^*\mathscr{E}) \simeq H^0(L_x, \xi^*\mathcal{O}^n), \tag{1}$$

where n is the rank of $\mathscr{E}$. We now translate this to a statement about googlies.

Let $\mathscr{L}_x$ denote the site associated to the topological space of planes in $\mathbb{P}$ containing the line corresponding to x. Since planes in $\mathbb{P}$ containing x are naturally identified with points in $L_x \subset \mathbb{P}^*$, $\mathscr{L}_x = L_x$. We use $\mathscr{L}_x$ to indicate we are thinking of a structure in googly rather than leg-break space.

There is a continuous functor

$$\zeta\colon \mathscr{L}_x \to \mathscr{G}_X,$$

given by $\zeta^{-1}(V) = \{\text{planes in } V \text{ containing } x\}$. (We omit the proof, which is elementary, that this is indeed a continuous functor.) *Then the Ward triviality condition at x is*

$$\check{H}^0(\mathscr{L}_x, \zeta^*\mathscr{F}) \simeq \check{H}^0(\mathscr{L}_x, \zeta^*(\mathscr{B}(-4))^n) \simeq \mathbb{C}^n, \tag{2}$$

where n is the rank of $\mathscr{F}$.

We sketch the proof, the details of which are not hard to supply. One may work equally well with the continuous functor

$$\tilde{\zeta}\colon \mathscr{L}_x \to \tilde{\mathscr{G}}_X$$

defined analogously. Similarly, let

$$\tilde{\xi}\colon L_x \to \mathscr{P}^*_X$$

be the analog of ξ, above. Then

$$\begin{array}{ccc} \mathscr{L}_x & \xrightarrow{\tilde{\zeta}} & \tilde{\mathscr{G}}_X \\ \updownarrow & & \updownarrow \\ L_x & \xrightarrow{\tilde{\xi}} & \mathscr{P}^*_X \end{array}$$

commutes, where the vertical arrows represent the natural identifications of the sites. Since this also naturally identifies (the isomorphism classes of) $\mathscr{E}$ and $\mathscr{F}$, (2) follows from (1). Also, $\zeta^*\mathscr{B}(-4)$ is isomorphic to the sheaf of holomorphic functions on L_x.

C. Massless fields

From the leg-break results and our previous machinery, we have the following. *Massless fields of helicity s on X, minimally coupled to the self-dual Yang–Mills background, are given by the elements of*

$$\check{H}^1(\mathcal{G}_{\nu},\mathcal{F}\otimes\mathcal{B}(-2-2s))$$

or similarly for $\tilde{\mathcal{G}}_{x}$. Of course, these are fields in the representation defined by the Ward bundle. Fields in other representations can be obtained, as in the leg-break case, by replacing $\mathcal{F}$ with the sheaf of sections of another representation (e.g., tensor products of $\mathcal{F}$).

V. DISCUSSION

This paper and the preceding one provide a coherent framework for the study of googly twistor spaces. These papers have been concerned with the general structures of such spaces; another (Ref. 3) gave many explicit calculational techniques.

Within this framework, it may be possible to develop aspects of googly Yang–Mills theory that have been in need of such a structure. Perhaps most important would be to understand the *googly maps* that are supposed to characterize the points in the space-time bundle on which the gauge group acts.[2] This would, one hopes, connect with *gravitational* googlies (twistor spaces describing gravitational fields with self-dual curvatures). In this case, the googly maps are supposed to give the space-time points from a knowledge of the twistor space.[9,10] Indeed, many of the techniques of the present paper generalize to gravitational googlies, as will be discussed in a future publication.

The googly was intended to complement, rather than compete with, the leg-break. Despite this, it is reasonable to compare their usefulness. It seems that, as an abstract tool for classifying Yang–Mills solutions (instantons, etc.), the googly will not be as useful. This is because, for leg-breaks, one has a body of classical results about holomorphic vector bundles over complex manifolds to draw on; whereas, for googlies, there are (at present) fewer site-theoretic tools. On the other hand, it seems possible that googly techniques for computing fields will be as useful as leg-break ones.[2,3]

Lastly, it is possible that sites will be useful in uniting the leg-break and googly to describe non-self-dual fields. This is the next major problem in the twistor description of Yang–Mills theory.

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Comment on a paper by Espindola, Teixeira, and Espindola [J. Math. Phys. 27, 151 (1986)]

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It is shown that the criterium to decide whether two Hamiltonians are equivalent given by Espindola *et al.* [O. Espindola, N. L. Teixeira, and M. L. Espindola, J. Math. Phys. **27**, 151 (1986)] is incorrect.

I. INTRODUCTION

Recently, Espindola *et al.* devised a procedure to generate equivalent Hamiltonians in two dimensions starting from the Hamilton–Jacobi equation.[1] The purpose of this comment is to show that such a procedure does not, in general, yield correct results.

In what follows Ref. 1 is briefly summarized.

(a) Definition: Two Hamiltonians

$$H(q_1,q_2,p_1,p_2) \quad \text{and} \quad \overline{H}(q_1,q_2,p_1,p_2)$$

are equivalent if the Hamilton–Jacobi equations generated by them yield the same solutions for the generating function S.

(b) Statement: $\overline{H}$ is equivalent to H iff $\overline{H}$ is any (time-independent) constant of the motion generated by H and

$$J \equiv \frac{\partial(H,\overline{H})}{\partial(p_1,p_2)} \neq 0.$$

I will show that (b) yields, in general, incorrect results.

II. COUNTEREXAMPLE

Consider a particle moving in a two-dimensional central potential

$$H = \tfrac{1}{2}(p_1^2 + p_2^2) + V(q_1^2 + q_2^2).$$

One of its time-independent constants of motion is

$$L_z = q_1 p_2 - q_2 p_1.$$

Define $\overline{H} = L_z = q_1 p_2 - q_2 p_1$, which is equivalent to H according to the statement (b) given in Ref. 1. It is straightforward to see that the Hamilton–Jacobi equations generated by H and $\overline{H}$ do *not* have the same solutions. Moreover, it is easy to understand why H and $\overline{H}$ are *not* equivalent.

(i) H is regular $[\det(\partial^2 H/\partial p_i \partial p_j) \neq 0]$ while $\overline{H}$ is singular $[\det(\partial^2 \overline{H}/\partial p_i \partial p_j) = 0]$.

(ii) $\overline{H}$ is a constant of motion for *any* central potential, while H has detailed information about what potential V we are dealing with, namely $V = V(q_1^2 + q_2^2)$.

Moreover, if statement (b) would indeed define an equivalence relation, all the Hamiltonians for different central potentials would be equivalent, due to the transitive property of equivalence relations.

With this counterexample I have proved that the criterium (b) given in Ref. 1, to decide whether two Hamiltonians H and $\overline{H}$ are equivalent, is incorrect.

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Canonical transformations and the equivalence problem

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Several equivalence relations for Hamiltonian systems are studied. The relationship to the theory of canonical transformations is analyzed. In the hyperregular case, the results are transformed into the Lagrangian formulation. The gauge group of Lagrangian mechanics is obtained by looking at the generating functions for canonical fiber invariant transformations. An intrinsic proof of a theorem of Henneaux [M. Henneaux, Ann. Phys. (NY) **140**, 45 (1982)] is given.

I. INTRODUCTION

Consider a dynamical system X on the cotangent bundle T^*Q over the configuration space Q. We assume that X describes the dynamics of a mechanical system. Then the classically observable trajectories in Q are the projections of the solution curves of X in T^*Q. Any diffeomorphism φ: $T^*Q \to T^*Q$ will transform any vector field X on T^*Q into a vector field $\varphi_* X$ on T^*Q ($\varphi_* X$ is the push-forward of X by φ). Clearly X and $\varphi_* X$ are differentiably conjugate, that is, they have "similar" phase portraits: φ is a one-to-one mapping carrying oriented orbits of X to oriented orbits of $\varphi_* X$. The mappings considered in this paper are fiber-invariant diffeomorphisms, connecting systems (phase flows) which are called *equivalent*. It is verified easily that the solution curves for equivalent dynamical systems coincide when projected to configuration space.

Suppose now that $X = X_H$ is a Hamiltonian vector field on T^*Q. Then the above consideration leads to the well-known fact that the classically observable trajectories of some mechanical systems do not uniquely describe their Hamiltonian; this may result in inequivalent quantum and statistical theories. We observe that this type of ambiguity ("gauge invariance") occurs in several physical theories. We refer, e.g., to classical Maxwell fields on manifolds, and to gauge theories on principal fiber bundles.[1] In the case of classical electrodynamics, the origin of gauge invariance lies in the fact that the potentials $\mathbf{A}$ and ϕ are not unique for given physical fields $\mathbf{E}$ and $\mathbf{B}$. The transformations which $\mathbf{A}$ and ϕ may undergo while preserving $\mathbf{E}$ and $\mathbf{B}$ (and hence the Maxwell equations) unchanged are called gauge transformations, and the group of all gauge transformations is called the gauge group.

In the present paper we examine the connection between the theory of canonical transformations and the problem of gauge invariance (equivalence problem) for conservative mechanical systems. For the nonconservative case, we refer, e.g., to Ref. 2. Because of the role that the cotangent bundle (with its canonical symplectic structure) plays in the theory of canonical transformations, it is convenient to start with the Hamiltonian point of view (differential geometrically, the Hamiltonian involves the cotangent bundle, the Lagrangian the tangent bundle). Let $\mathcal{F}(T^*Q)$ denote the space of all smooth real-valued functions on T^*Q. The equivalence relation for dynamical systems on T^*Q induces an equivalence relation on $\mathcal{F}(T^*Q)$, called q-equivalence. Of particular interest are two stronger equivalence relations on $\mathcal{F}(T^*Q)$: c-equivalence and s-equivalence. Proposition 2 tells us that c-equivalence classes and s-equivalence classes are orbits of certain group actions on $\mathcal{F}(T^*Q)$. The group classifying c-equivalent Hamiltonians is essentially $\mathrm{Can}_i(T^*Q)$, the group of canonical fiber-invariant transformations on T^*Q; the corresponding group for s-equivalence is the subgroup $\mathrm{Sp}_i(T^*Q) \subset \mathrm{Can}_i(T^*Q)$ of symplectic fiber-invariant transformations. A similar result in the Lagrangian formulation is given by Proposition 7. The corresponding group is the additive group $\Omega_c^1 Q$ of closed one-forms on Q. Here $\Omega_c^1 Q$ is called *gauge group* of Lagrangian mechanics (see Ref. 3, p. 216) and acts via gauge transformations on $\mathcal{F}_r(TQ)$. By Proposition A2, $\Omega_c^1 Q$ is isomorphic to $\mathrm{Sp}_i(T^*Q)$. This is most useful when applied to the hyperregular situation. Indeed, the natural one-to-one correspondence χ: $\mathcal{F}_{hr}(TQ) \to \mathcal{F}_{hr}(T^*Q)$ between hyperregular Lagrangian and Hamiltonian functions turns out to be equivariant with respect to (extended) gauge transformations and canonical transformations (Theorem 2).

II. HAMILTONIAN MECHANICS

Let Q be a differentiable manifold (configuration space) and T^*Q its cotangent bundle (the associated phase space). Denote by $\mathrm{Diff}(T^*Q)$ the group of all diffeomorphisms on T^*Q, and let $\mathrm{Diff}_i(T^*Q)$ denote the subgroup of all fiber-invariant diffeomorphisms φ on T^*Q (i.e., $\tau_Q^* \circ \varphi = \tau_Q^*$). Any $\varphi \in \mathrm{Diff}(T^*Q)$ will transform any vector field X on T^*Q into a vector field $\varphi_* X$ on T^*Q ($\varphi_* X$ is the push-forward of X by φ). If H is any Hamiltonian, i.e., any function on T^*Q, then X_H denotes the associated Hamiltonian vector field on T^*Q. Now consider a Hamiltonian $H \in \mathcal{F}(T^*Q)$. Then $\varphi \in \mathrm{Diff}(T^*Q)$ is called *H-canonoid* if $\varphi_* X_H$ is a Hamiltonian vector field, i.e., if there is a $H' \in \mathcal{F}(T^*Q)$ such that $\varphi_* X_H = X_{H'}$. Any H-canonoid fiber-invariant φ is called an *H-fouling transformation*.[4]

Definition 1: Two Hamiltonians H, H' are called q-equivalent if there exists a $\varphi \in \mathrm{Diff}_i(T^*Q)$ such that $\varphi_* X_H = X_{H'}$.

This clearly defines an equivalence relation $\overset{q}{\sim}$ on $\mathcal{F}(T^*Q)$. Since φ is fiber-invariant, the (classically observable) base integral curves of X_H and $X_{H'}$ on Q coincide:

$$\tau_Q^* \circ \phi_t^{X_H}(\alpha_q) = \tau_Q^* \circ \varphi \circ \phi_t^{X_H}(\alpha_q) = \tau_Q^* \circ \phi_t^{X_{H'}}(\varphi(\alpha_q)) .$$

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Clearly φ is an H-fouling transformation, and φ^{-1} is an H'-fouling transformation.

$\omega_0 = -d\theta_0$ denotes the canonical symplectic structure on T^*Q. Here $\varphi \in \mathrm{Diff}(T^*Q)$ is called a *canonical transformation* if there is a $\lambda_\varphi \in \mathbb{R} - \{0\}$ such that $g^*\omega_0 = \lambda_\varphi \omega_0$, if $\lambda_\varphi = 1, \varphi$, is a *symplectic transformation*. We observe that $\varphi \in \mathrm{Diff}(T^*Q)$ is a canonical transformation if and only if φ is H-canonoid for any $H \in \mathcal{F}(T^*Q)$, i.e., iff φ preserves the canonical formalism for any Hamiltonian.[5] Denote by $\mathrm{Can}(T^*Q)$ the group of all canonical transformations, with subgroup $\mathrm{Sp}(T^*Q) \subset \mathrm{Can}(T^*Q)$ of all symplectic transformations. Finally, consider

$$\mathrm{Can}_i(T^*Q) = \mathrm{Can}(T^*Q) \cap \mathrm{Diff}_i(T^*Q)$$

and its subgroup

$$\mathrm{Sp}_i(T^*Q) = \mathrm{Sp}(T^*Q) \cap \mathrm{Diff}_i(T^*Q).$$

Definition 2: Two Hamiltonians H, H' are called c-equivalent if there exists a $\varphi \in \mathrm{Can}_i(T^*Q)$ such that $\varphi_* X_H = X_{H'}$; if $\varphi \in \mathrm{Sp}_i(T^*Q)$, H and H' are called s-equivalent.

The corresponding equivalence relations are denoted by $\overset{c}{\sim}$ and $\overset{s}{\sim}$, respectively. Note that s-equivalence implies c-equivalence, while c-equivalence implies q-equivalence. By Jacobi's theorem, a diffeomorphism $\varphi \in \mathrm{Diff}(T^*Q)$ is a canonical transformation if and only if $\varphi_* X_H = X_{\lambda_\varphi H \circ \varphi^{-1}}$, for any $H \in \mathcal{F}(T^*Q)$. Thus we obtain the following.

Proposition 1: Let H, H' be two Hamiltonians. Then (i) H and H' are c-equivalent if and only if there exist a $\varphi \in \mathrm{Can}_i(T^*Q)$ and a $c \in R$ such that $H' = \lambda_\varphi H \circ \varphi^{-1} - c$; and (ii) H and H' are s-equivalent if and only if there exist a $\varphi \in \mathrm{Sp}_i(T^*Q)$ and a $c \in R$ such that $H' = H \circ \varphi^{-1} - c$.

We now turn to the study of group actions. First consider the semidirect product $\mathrm{Can}_i(T^*Q) \times_\lambda R$, where λ: $\mathrm{Can}_i(T^*Q) \to \mathrm{Aut}(R)$ is the group homomorphism given by $(\lambda(\varphi))(c) = \lambda_\varphi c$. The group structure in $\mathrm{Can}_i(T^*Q) \times_\lambda R$ is the semidirect product structure given by

$$(\varphi, c)(\varphi', c') = (\varphi \circ \varphi',\ c + \lambda_\varphi c').$$

Then $\mathrm{Can}_i(T^*Q) \times_\lambda R$ acts on $\mathcal{F}(T^*Q)$, the group action

$$\rho_c\colon (\mathrm{Can}_i(T^*Q) \times_\lambda R) \times \mathcal{F}(T^*Q) \to \mathcal{F}(T^*Q)$$

given by

$$\rho_c((\varphi, c), H) = \lambda_\varphi H \circ \varphi^{-1} - c.$$

Here $\mathrm{Sp}_i(T^*Q) \times_\lambda R$ is a subgroup of $\mathrm{Can}_i(T^*Q) \times_\lambda R$; by restriction, we obtain the group action

$$\rho_s\colon (\mathrm{Sp}_i(T^*Q) \times_\lambda R) \times \mathcal{F}(T^*Q) \to \mathcal{F}(T^*Q),$$

$\rho_s((\varphi, c), H) = H \circ \varphi^{-1} - c$. Using these terms, we can make the following observation.

Proposition 2: The orbits of ρ_c are the c-equivalence classes, and the orbits of ρ_s are the s-equivalence classes.

To any $H \in \mathcal{F}(T^*Q)$ we associate a map FH: $T^*Q \to T^{**}Q$ by $FH(\alpha_q)\beta_q = dH(\beta_q)^v_{\alpha_q}$; here

$$(\beta_q)^v_{\alpha_q} := \left.\frac{d}{dt}\right|_{t=0} (\alpha_q + t\beta_q) \in T_{\alpha_q} T^*Q$$

denotes the vertical lift of $\beta_q \in T^*_q Q$ with respect to $\alpha_q \in T^*_q Q$.

Define $\overline{FH}$: $T^*Q \to TQ$ by $\overline{FH} = \phi^{-1} \circ FH$, where ϕ denotes the natural bijection $TQ \cong T^{**}Q$. We shall need the following result.

Proposition 3: $\overline{FH} = T\tau^*_Q \circ X_H$.

Proof: We must show $FH = \phi \circ \tau^*_Q \circ X_H$, i.e.,

$$FH(\alpha_q)\beta_q = \beta_q(T\tau^*_Q \circ X_H(\alpha_q)), \quad \text{for all } \alpha_q, \beta_q \in T^*_q Q.$$

Now

$$FH(\alpha_q)\beta_q = dH(\beta_q)^v_{\alpha_q} = (i_{X_H}\omega_0)(\beta_q)^v_{\alpha_q}$$
$$= -d\theta_0(X_H(\alpha_q), (\beta_q)^v_{\alpha_q}).$$

Choose two (local) vector fields η and X on T^*Q such that

(i) η is vertical and $\eta(\alpha_q) = (\beta_q)^v_{\alpha_q}$;

(ii) $[X, \eta] = 0$ and $X(\alpha_q) = X_H(\alpha_q)$.

Then (see Ref. 3, p. 117)

$$-d\theta_0(X_H(\alpha_q), (\beta_q)^v_{\alpha_q})$$
$$= \eta(\alpha_q)\theta_0(X) - X(\alpha_q)\theta_0(\eta) + \theta_0(\alpha_q)[X, \eta]$$
$$= \eta(\alpha_q)\theta_0(X) = \left.\frac{d}{dt}\right|_{t=0} \theta_0(X(\phi^\eta_t(\alpha_q)))$$
$$= \left.\frac{d}{dt}\right|_{t=0} \phi^\eta_t(\alpha_q)(T\tau^*_Q X(\phi^\eta_t(\alpha_q))).$$

Observe that $T\tau^*_Q \cdot X(\phi^\eta_t(\alpha_q)) \in T_q Q$ since $\phi^\eta_t(\alpha_q)$ is a vertical flow. We obtain

$$FH(\alpha_q)\beta_q = \left.\frac{d}{dt}\right|_{t=0} \phi^\eta_t(\alpha_q)(T\tau^*_Q X(\alpha_q)) + \left.\frac{d}{dt}\right|_{t=0} \alpha_q(T\tau^*_Q X(\phi^\eta_t(\alpha_q)))$$
$$= \beta_q(T\tau^*_Q X(\alpha_q)).$$

This proves the assertion.

We shall now specialize to the important case when H is hyperregular. Here $H \in \mathcal{F}(T^*Q)$ is called hyperregular if FH is a diffeomorphism, and $\mathcal{F}_{hr}(T^*Q) \subset \mathcal{F}(T^*Q)$ denotes the set of all hyperregular Hamiltonians.

Proposition 4: Let $H \in \mathcal{F}_{hr}(T^*Q)$, $H' \in \mathcal{F}(T^*Q)$, and suppose that H and H' are q-equivalent. Then $H' \in \mathcal{F}_{hr}(T^*Q)$, and $\varphi := (FH')^{-1} \circ FH$ is the unique fiber-invariant diffeomorphism such that $\varphi_* X_H = X_{H'}$.

Proof: By definition, $\varphi_* X_H = X_{H'}$ for a $\varphi \in \mathrm{Diff}_i(T^*Q)$. By Proposition 3, $\overline{FH} = T\tau^*_Q \circ X_H$ and $\overline{FH'} = T\tau^*_Q \circ X_{H'}$. Consequently,

$$\overline{FH'} = T\tau^*_Q \circ \varphi_* \circ X_H = T\tau^*_Q \circ T\varphi \circ X_H \circ \varphi^{-1}$$
$$= T\tau^*_Q \circ X_H \circ \varphi^{-1} = \overline{FH} \circ \varphi^{-1}.$$

Since H is hyperregular, hyperregularity of H' and $\varphi = (FH')^{-1} \circ FH$ result.

This last result tells us that the group actions ρ_c and ρ_s leave $\mathcal{F}_{hr}(T^*Q) \subset \mathcal{F}(T^*Q)$ invariant, thus inducing group actions

$$\rho^{hr}_c\colon (\mathrm{Can}_i(T^*Q) \times_\lambda R) \times \mathcal{F}_{hr}(T^*Q) \to \mathcal{F}_{hr}(T^*Q)$$

and

$$\rho^{hr}_s\colon (\mathrm{Sp}_i(T^*Q) \times_\lambda R) \times \mathcal{F}_{hr}(T^*Q) \to \mathcal{F}_{hr}(T^*Q),$$

$$\rho^{hr}_c((\varphi, c), H) = \lambda_\varphi H \circ \varphi^{-1} - c,$$

$$\rho_s^{hr}((\varphi,c),H) = H\circ\varphi^{-1} - c\,.$$

We say that a group action ρ: $G\times M\to M$ is effective (resp. free) if $\rho(g,m) = m$ for all $m\in M$ (resp. for some $m\in M$) implies that $g = e$.

Proposition 5: (i) The group actions ρ_c and ρ_s are effective, but not free.

(ii) ρ_c^{hr} and ρ_s^{hr} act freely on $\mathscr{F}_{hr}(T^*Q)$.

Proof: It is verified easily that (a) if ρ_c^{hr} is free, then ρ_s^{hr} is free and ρ_c, ρ_s are effective; and (b) if ρ_s is not free, then ρ_c is not free.

We first prove that ρ_c^{hr} is free. Suppose that $\rho_c^{hr}((\varphi,c),H) = H$ for a $H\in\mathscr{F}_{hr}(T^*Q)$. Then $\lambda_\varphi H\circ\varphi^{-1} - c = H$ and hence $X_{\lambda_\varphi H\circ\varphi^{-1}} = X_H$. By Jacobi's theorem, $\varphi_* X_H = X_H$. Since H is hyperregular, Proposition 4 yields $\varphi = \mathrm{id}_{T^*Q}$. Consequently $(\varphi,c) = (\mathrm{id}_{T^*Q},0)$, i.e., the identity in $\mathrm{Can}_i(T^*Q)\times_\lambda R$. Thus ρ_c^{hr} is free. Finally, ρ_s is not free since $\rho_s((\varphi,c),H) = H$ for $H = 0$, $c = 0$, and φ any element in $\mathrm{Sp}_i(T^*Q)$.

Corollary 1: Assume that H: $T^*Q\to R$ is hyperregular. Then Hamiltonians c-equivalent to H are in one-to-one correspondence with elements of $\mathrm{Can}_i(T^*Q)\times_\lambda R$, and Hamiltonians s-equivalent to H are in one-to-one correspondence with elements of $\mathrm{Sp}_i(T^*Q)\times_\lambda R$.

It is natural to ask whether one can give a (infinite-dimensional) manifold structure to $\mathscr{F}_{hr}(T^*Q)$ such that the free group actions ρ_c^{hr} and ρ_s^{hr} induce principal fiber bundles with total space $\mathscr{F}_{hr}(T^*Q)$ and structure groups $\mathrm{Can}_i(T^*Q)\times_\lambda R$ and $\mathrm{Sp}_i(T^*Q)\times_\lambda R$, respectively. Although there are many formal analogies between our work and the theory of principal fiber bundles, we are not prepared at this time to go into these considerations.

III. LAGRANGIAN MECHANICS

$\mathscr{F}(TQ)$ denotes the space of real-valued functions on the tangent bundle over Q. Take a Lagrangian L, i.e., any $L\in\mathscr{F}(TQ)$. The analog of FH in the Lagrangian approach is the Legendre transformation FL: $TQ\to T^*Q$, $FL(v_q)w_q = dL(w_q)^v_{v_q}$, $v_q, w_q\in T_qQ$. Here $L\in\mathscr{F}(TQ)$ is called regular if FL is a local diffeomorphism; if FL is a diffeomorphism, we say that L is hyperregular. In the following, $\mathscr{F}_{hr}(TQ)\subset\mathscr{F}_r(TQ)\subset\mathscr{F}(TQ)$ denote the subsets of hyperregular Lagrangians and regular Lagrangians, respectively. For $L\in\mathscr{F}_r(TQ)$, ω_L denotes the symplectic structure $(FL)^*\omega_0$ on TQ. Observe that $\omega_L = -d\theta_L$, with $\theta_L = (FL)^*\theta_0$. Finally, Λ_L denotes the Lagrangian vector field (for regular L) on TQ given by $i_{\Lambda_L}\omega_L = dE_L$, where $E_L\in\mathscr{F}(TQ)$ is the energy given by $E_L(v_q) = FL(v_q)v_q - L(v_q)$. Λ_L is a second-order equation on TQ. Therefore the (observable) base integral curves on Q determine Λ_L uniquely. However, the Lagrangian vector field does not determine the Lagrangian uniquely. Recall that the situation for Hamiltonian systems is as follows: there are different Hamiltonians yielding the same base integral curves, and two Hamiltonians lead to the same Hamiltonian vector field if and only if they differ by a constant. These are some of the main differences between the Hamiltonian and Lagrangian formulations.

The equivalence problem appears in the Lagrangian formulation as follows.

Definition 3: Two regular Lagrangians L, L' are called q-equivalent if $\Lambda_L = \Lambda_{L'}$; if, furthermore, $\omega_{L'} = \lambda\omega_L$ for a $\lambda\in R - \{0\}$, they are called e-equivalent; if $\lambda = 1$, they are called g-equivalent.

The corresponding equivalence relations on $\mathscr{F}_r(TQ)$ are denoted by $\overset{q}{\sim}$, $\overset{e}{\sim}$ (extended gauge equivalence), and $\overset{g}{\sim}$ (gauge equivalence). Clearly, the g-equivalence relation is finer than the e-equivalence relation, and the e-equivalence relation is finer than the q-equivalence relation. In the following, Ω^1Q denotes the space of one-forms on Q, and $\Omega^1_cQ\subset\Omega^1Q$ is the subspace of all closed one-forms on Q. Given $\alpha\in\Omega^1Q$, define $\tilde\alpha\in\mathscr{F}(TQ)$ by $\tilde\alpha(v_q) = \alpha_q(v_q)$. Let $\dot R = R - \{0\}$.

Proposition 6: Suppose $L\in\mathscr{F}(TQ)$, $\lambda\in\dot R$, $\alpha\in\Omega^1Q$, $c\in R$. Then

(i) $F(\lambda L + \tilde\alpha + c) = \lambda FL + \alpha\circ\tau_Q$;
(ii) $\theta_{\lambda L+\tilde\alpha+c} = \lambda\theta_L + (\tau_Q)^*\alpha$;
(iii) $E_{\lambda L+\tilde\alpha+c} = \lambda E_L - c$.

Proof: We have

$$\begin{aligned}F(\lambda L + \tilde\alpha + c)(v_q)w_q &= d(\lambda L + \tilde\alpha + c)(w_q)^v_{v_q} = \lambda dL(w_q)^v_{v_q} + d\tilde\alpha(w_q)^v_{v_q}\\ &= \lambda FL(v_q)w_q + \alpha_q(w_q) = (\lambda FL + \alpha\circ\tau_Q)(v_q)w_q\,;\end{aligned}$$

thus, (i) follows. Now $\theta_{\lambda L+\tilde\alpha+c} = F(\lambda L + \tilde\alpha + c)^*\theta_0$. By (i), we obtain

$$\theta_{\lambda L+\tilde\alpha+c} = \lambda(FL)^*\theta_0 + (\tau_Q)^*\alpha^*\theta_0.$$

Since $\alpha^*\theta_0 = \alpha$ (see Ref. 3, p. 179), the assertion (ii) follows. Finally,

$$\begin{aligned}E_{\lambda L+\tilde\alpha+c}(v_q) &= F(\lambda L + \tilde\alpha + c)\ (v_q)v_q\\ &\quad - \lambda L(v_q) - \alpha_q(v_q) - c\,;\end{aligned}$$

(i) yields $E_{\lambda L+\tilde\alpha+c}(v_q) = \lambda E_L(v_q) - c$, as required.

As a consequence of Proposition 6, we get the following two results.

Corollary 2: Suppose $L\in\mathscr{F}(TQ)$, $\lambda\in\dot R$, $\alpha\in\Omega^1_cQ$, $c\in R$. Then $\omega_{\lambda L+\tilde\alpha+c} = \lambda\omega_L$.

Corollary 3: Suppose $\lambda\in\dot R$, $\alpha\in\Omega^1Q$, $c\in R$. Then

(i) for $L\in\mathscr{F}_r(TQ)$, $\lambda L + \tilde\alpha + c\in\mathscr{F}_r(TQ)$;
(ii) for $L\in\mathscr{F}_{hr}(TQ)$, $\lambda L + \tilde\alpha + c\in\mathscr{F}_{hr}(TQ)$.

We observe that the second part of Corollary 3 corresponds to the first part of Proposition 4. The dual to Proposition 1 is the following theorem.

Theorem 1: Let $L, L'\in\mathscr{F}_r(TQ)$. Then we have the following.

(i) L and L' are e-equivalent if and only if there exist $\lambda\in\dot R$, $\alpha\in\Omega^1_cQ$, $c\in R$ such that $L' = \lambda L + \tilde\alpha + c$.

(ii) L and L' are g-equivalent if and only if there exist $\alpha\in\Omega^1_cQ$, $c\in R$ such that $L' = L + \tilde\alpha + c$.

Proof: It suffices to prove (i). Suppose that $L' = \lambda L + \tilde\alpha + c$ for a $(\lambda,\alpha,c)\in\dot R\times\Omega^1_cQ\times R$. By Proposition 6, $E_{L'} = \lambda E_L - c$. By Corollary 2, $\omega_{L'} = \lambda\omega_L$. It follows that $\Lambda_{L'} = \Lambda_L$. This proves $L\overset{e}{\sim}L'$. Conversely, suppose that $\Lambda_{L'} = \Lambda_L$ and $\omega_{L'} = \lambda\omega_L$ for a $\lambda\in\dot R$. Then $i_{\Lambda_{L'}}\omega_{L'} = dE_{L'}$, i.e., $\lambda i_{\Lambda_L}\omega_L = dE_{L'}$. Consequently,

$\lambda\, dE_L = dE_{L'}$, i.e., $\lambda E_L = E_{L'} + c$, for a $c \in R$. Moreover, $d\theta_{L'} = \lambda\, d\theta_L$, i.e., $\theta_{L'} - \lambda\theta_L \in \Omega_c^1(TQ)$. Since $\lambda\theta_L - \theta_{L'}$ is a semibasic one-form on TQ, Proposition A1 tells us that there is a unique $\alpha \in \Omega_c^1 Q$ such that $\theta_{L'} - \lambda\theta_L = (\tau_Q)^*\alpha$. Because τ_Q: $TQ \to Q$ is a submersion, we obtain $FL'(v_q) - \lambda FL(v_q) = \alpha_q$, for any $v_q \in T_qQ$. Thus

$$L'(v_q) - \lambda L(v_q) = FL'(v_q)v_q - \lambda FL(v_q)v_q - E_{L'}(v_q) + \lambda E_L(v_q) = \alpha_q(v_q) + c\,,$$

i.e., $L' = \lambda L + \tilde{\alpha} + c$.

We note that if L and L' are g-equivalent Lagrangians, then locally (ii) corresponds to the usual gauge variance $L' = L + f$ (up to a constant). A discussion of the nonautonomous case can be found in Ref. 7.

We shall now discuss our results in terms of group actions. Consider the group homomorphism σ: $\dot{R} \to \mathrm{Aut}(\Omega_c^1 Q \times R)$ given by $\sigma(\lambda)(\alpha, c) = (\lambda\alpha, \lambda c)$. The group structure in $\dot{R} \times_\sigma (\Omega_c^1 Q \times R)$ is the semidirect product structure given by $(\lambda, \alpha, c)\ (\lambda', \alpha', c') = (\lambda\lambda', \alpha + \lambda\alpha', c + \lambda c')$. Define the group action

$$\delta_e^r\colon\ (\dot{R} \times_\sigma (\Omega_c^1 Q \times R)) \times \mathscr{F}_r(TQ) \to \mathscr{F}_r(TQ)$$

by $\delta_e^r((\lambda, \alpha, c), L) = \lambda L + \tilde{\alpha} + c$. Now consider the subset $\mathscr{F}_{hr}(TQ) \subset \mathscr{F}_r(TQ)$. By Corollary 3, δ_e^r leaves $\mathscr{F}_{hr}(TQ)$ invariant. Arguing as in the Hamiltonian case, we obtain group actions

$$\delta_g^r\colon\ (\Omega_c^1 Q \times R) \times \mathscr{F}_r(TQ) \to \mathscr{F}_r(TQ)\,,$$

$$\delta_g^r((\alpha, c), L) = L + \tilde{\alpha} + c\,,$$

and

$$\delta_e^{hr}\colon\ (\dot{R} \times_\sigma (\Omega_c^1 Q \times R)) \times \mathscr{F}_{hr}(TQ) \to \mathscr{F}_{hr}(TQ)\,,$$

$$\delta_g^{hr}\colon\ (\Omega_c^1 Q \times R) \times \mathscr{F}_{hr}(TQ) \to \mathscr{F}_{hr}(TQ)\,.$$

The analog of Proposition 2 is the following result.

Proposition 7: (i) The orbits of δ_e^r are the e-equivalence classes in $\mathscr{F}_r(TQ)$.

(ii) The orbits of δ_g^r are the g-equivalence classes in $\mathscr{F}_r(TQ)$.

The proof of Proposition 7 is a direct consequence of Theorem 1. Next we prove a result similar to Proposition 5.

Proposition 8: The group actions δ_e^r, δ_g^r, δ_e^{hr}, and δ_g^{hr} are free.

Proof: It suffices to show that δ_e^r acts freely on $\mathscr{F}_r(TQ)$. Suppose that $\delta_e^r((\lambda, \alpha, c), L) = L$, for a $L \in \mathscr{F}_r(TQ)$. Then $(1 - \lambda)L = \tilde{\alpha} + c$. It is verified easily that $F(\tilde{\alpha} + c)(v_q) = \alpha_q$, for $v_q \in T_qQ$. Consequently, $(1 - \lambda)L$ is not regular, but then $\lambda = 1$ since L is regular. It follows that $\alpha = 0, \tilde{c} = 0$, i.e., $(\lambda, \alpha, c) = (1,0,0)$ is the identity in $\dot{R} \times_\sigma (\Omega_c^1 Q \times R)$.

Corollary 4: Assume that L: $TQ \to R$ is regular. Then $(\lambda, \alpha, c) \to \lambda L + \tilde{\alpha} + c$ is a one-to-one correspondence between $\dot{R} \times \Omega_c^1 Q \times R$ and the e-equivalence class containing L; similarly, $(\alpha, c) \to L + \tilde{\alpha} + c$ is a bijection between $\Omega_c^1 Q \times R$ and the g-equivalence class containing L.

IV. THE HYPERREGULAR CASE

We shall now discuss the relationship between the results obtained in Sec. II and Sec. III. Consider the bijection χ: $\mathscr{F}_{hr}(TQ) \to \mathscr{F}_{hr}(T^*Q)$ given by $\chi(L) = E_L \circ (FL)^{-1}$. One knows[3] that for $H = \chi(L)$, $(FL)^{-1} = \bar{F}H$. Moreover, $(FL)_* \Lambda_L = X_H$, and, conversely, $(\bar{F}H)_* X_H = \Lambda_L$. The next result shows that χ is compatible with the equivalence relations introduced on $\mathscr{F}_{hr}(TQ)$ and $\mathscr{F}_{hr}(T^*Q)$.

Proposition 9: Let $L, L' \in \mathscr{F}_{hr}(TQ)$, and write $\chi(L) = H, \chi(L') = H'$. Then

(i) $L \overset{q}{\sim} L'$ if and only if $H \overset{q}{\sim} H'$;

(ii) $L \overset{e}{\sim} L'$ if and only if $H \overset{c}{\sim} H'$;

and

(iii) $L \overset{g}{\sim} L'$ if and only if $H \overset{s}{\sim} H'$.

Proof: By Proposition 4, $H \overset{q}{\sim} H'$ iff $\varphi_* X_H = X_{H'}$, for $\varphi = (FH')^{-1} \circ FH$. Thus $H \overset{q}{\sim} H'$ iff $(\bar{F}H)_* X_H = (\bar{F}H')_* X_{H'}$, i.e., $\Lambda_L = \Lambda_{L'}$. This proves (i). But since $(\bar{F}H^{-1})^* \omega_0 = \omega_L$ we also get (ii) and (iii).

There is a natural group isomorphism ϕ: $\Omega_c^1 Q \to \mathrm{Sp}_i(T^*Q)$ given by $(\phi(\alpha))\ (\beta_q) := \beta_q + \alpha_q$, for $\alpha \in \Omega_c^1 Q$, $\beta_q \in T_q^* Q$ (Proposition A2). We also write $\phi(\alpha) = \varphi_\alpha$. For $\lambda \in \dot{R}$, define T_λ: $T^*Q \to T^*Q$ by $T_\lambda(\beta_q) := \lambda\beta_q$ (scaling transformation). A straightforward calculation shows that

$$\eta_e\colon\ \dot{R} \times_\sigma (\Omega_c^1 Q \times R) \to \mathrm{Can}_i(T^*Q) \times_\lambda R$$

given by $\eta_e(\lambda, \alpha, c) := (\varphi_\alpha \circ T_\lambda, c)$ is a group isomorphism with inverse $\eta_e^{-1}(\varphi, c) = (\lambda_\varphi, \phi^{-1}(\varphi \circ T_{\lambda_\varphi^{-1}}), c)$.

Theorem 2: The diagram

$$\begin{array}{ccc} (\dot{R} \times_\sigma (\Omega_c^1 Q \times R)) \times \mathscr{F}_{hr}(TQ) & \xrightarrow{\delta_e^{hr}} & \mathscr{F}_{hr}(TQ) \\ \downarrow \eta_e \times \chi & & \downarrow \chi \\ (\mathrm{Can}_i(T^*Q) \times_\lambda R) \times \mathscr{F}_{hr}(T^*Q) & \xrightarrow[\rho_c^{hr}]{} & \mathscr{F}_{hr}(T^*Q) \end{array}$$

commutes.

Proof: By Proposition 6,

$$\chi(\lambda L + \tilde{\alpha} + c) = (\lambda E_L - c) \circ (\lambda FL + \alpha \circ \tau_Q)^{-1} = \lambda E_L \circ (\varphi_\alpha \circ T_\lambda \circ FL)^{-1} - c = \lambda\chi(L) \circ T_\lambda^{-1} \circ \varphi_\alpha^{-1} - c\,.$$

Since $\lambda_{\varphi_\alpha \circ T_\lambda} = \lambda$, we obtain $\chi \circ \delta_e^{hr} = \rho_c^{hr} \circ (\eta_e \times \chi)$. This proves the assertion.

Thus the results obtained in Sec. II and Sec. III are equivalent in the hyperregular case, and are transformed one into the other by the Legendre transformation.

V. CLOSING REMARKS

In this paper we discussed the ambiguities in the choice of the Hamiltonian (or Lagrangian) of a conservative mechanical system. Apart from the rather obvious applications in classical and quantum mechanics our results may be of interest to mathematicians in the area of "differentiable dynamics" in connection with the so-called "equivalence problem" (see e.g., Ref. 6, p. 141).

There are well-known examples of q-equivalent Hamil-

tonians which are not c-equivalent (e.g., $H = p_1 p_2$ for the two-dimensional free particle). This motivates the introduction of weaker concepts of equivalence (including the aspect of symmetry). By an interesting result of Henneaux,[7] however, such examples are "exceptional," i.e., "in general" H is unique up to c-equivalence.

We finally observe that the above treatment can be extended in various directions, such as, e.g., nonautonomous systems and systems with generalized forces.

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APPENDIX: A CHARACTERIZATION OF FIBER-INVARIANT SYMPLECTIC TRANSFORMATIONS

$\theta \in \Omega^1(TQ)$ is called semibasic if $\theta(\xi_{v_q}) = 0$, for any $\xi_{v_q} \in T_{v_q} TQ$ with $T\tau_Q \xi_{v_q} = 0$.

Proposition A1: For any closed semibasic one-form β on TQ there exists a unique closed one-form α on Q such that $\beta = (\tau_Q)^* \alpha$. Moreover, if β is exact, then α is exact, too.

Proof: First suppose that β is exact, i.e., $\beta = dF$ for a $F \in \mathcal{F}(TQ)$. Since β is semibasic, F is constant on the fibers. Hence $F = g \circ \tau_Q$ for a $g \in \mathcal{F} Q$. It follows that $\beta = (\tau_Q)^* \alpha$ for $\alpha = dg$. Since τ_Q is a submersion, α is unique. Now suppose that β is closed. Let $\{U_\lambda\}_{\lambda \in \Lambda}$ be a covering of Q by open contractible sets such that $TU_\lambda \cong U_\lambda \times R^n$. By Poincaré's lemma, $\beta \mid TU_\lambda$ is exact for any $\lambda \in \Lambda$. It follows that there is a unique $\alpha_\lambda \in \Omega_c^1 U_\lambda$ such that $(\tau_Q)^* \alpha_\lambda = \beta \mid TU_\lambda$. Define $\alpha \in \Omega_c^1 Q$ by $\alpha \mid U_\lambda = \alpha_\lambda$. Clearly $\beta = (\tau_Q)^* \alpha$, which proves the assertion.

Observe that the analog of Proposition A1 on the cotangent bundle is true and can be proven in the same way. Given $\alpha \in \Omega_c^1 Q$, define φ_α: $T^*Q \to T^*Q$ by $\varphi_\alpha(\beta_q) = \beta_q + \alpha_q$ (fiberwise translation by α). It is well known (see Ref. 3, p. 186) that φ_α is a symplectic transformation. Thus we have an injective group homomorphism ϕ: $\Omega_c^1 Q \to \mathrm{Sp}_i(T^*Q)$, $\phi(\alpha) = \varphi_\alpha$.

Proposition A2: ϕ is surjective.

Proof: For $\varphi \in \mathrm{Sp}_i(T^*Q)$, consider $\varphi^* \theta_0 - \theta_0 \in \Omega^1(T^*Q)$. It is verified easily that $\varphi^* \theta_0 - \theta_0$ is closed and semibasic. According to Proposition A1, there exists a unique $\alpha \in \Omega_c^1 Q$ such that $\varphi^* \theta_0 - \theta_0 = (\tau_Q)^* \alpha$. Consequently, $(\varphi^* \theta_0)\ (\xi_{\beta_q}) = \theta_0(\xi_{\beta_q}) + ((\tau_Q)^* \alpha)(\xi_{\beta_q})$ for any $\xi_{\beta_q} \in T^*TQ$. Since φ is fiber invariant, we obtain $\varphi(\beta_q) = \beta_q + \alpha_q$, i.e., $\phi(\alpha) = \varphi$.

We observe that locally, when $\alpha = df$, then

$$\varphi_\alpha^* \theta_0 - \theta_0 = d(f \circ \tau_Q);$$

thus f is a *generating function* for the canonical transformation φ_α.

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Dirac's theory of constraints in field theory and the canonical form of Hamiltonian differential operators

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A simple algorithm for constructing the canonical form of Hamiltonian systems of evolution equations with constant coefficient Hamiltonian differential operators is given. The result of the construction is equivalent to the canonical system derived using Dirac's theory of constraints from the corresponding degenerate Lagrangian.

I. INTRODUCTION

In the classical theory of Hamiltonian systems, great emphasis is placed on the introduction of canonical coordinates—the positions and conjugate momenta of classical mechanics.[1] Canonical coordinates serve to simplify many of the equations and transformations required in the study of finite-dimensional Hamiltonian systems. Most quantization procedures require that the Hamiltonian system be in canonical form before proceeding. Hamiltonian perturbation theories are much easier to develop in canonical coordinates.[2,3] However, in recent years there has been a renewed interest in Hamiltonian systems in noncanonical coordinates. The principle motivation has been the development of an infinite-dimensional theory of Hamiltonian systems of evolution equations in which the role of the skew-symmetric symplectic matrix J is played by a skew-adjoint Hamiltonian differential operator, and the Hamiltonian function is replaced by a Hamiltonian functional.[4,5] Applications to stability questions in fluid mechanics and plasma physics[6] and also to completely integrable (soliton) equations[7,8] have been just a few of the important consequences of this general theory. A significant open problem in this theory is the *Darboux problem* of whether one can always determine suitable canonical coordinates for such a Hamiltonian system. In this paper, a general result of this type for constant coefficient Hamiltonian differential operators is proved, along with some extensions of the result to more general field-dependent Hamiltonian operators.

In the case of finite-dimensional Hamiltonian systems, Darboux' theorem guarantees that canonical coordinates can always be found, provided that the Poisson bracket has constant rank.[9] For maximal rank (symplectic) Poisson brackets, the proof of Weinstein[10] is especially appealing in that it readily extends to certain infinite-dimensional situations. There are two main steps in Weinstein's proof: first the Hamiltonian operator is reduced to a constant operator by a clever change of variables; second, one shows that any constant-coefficient skew-adjoint operator can be placed into canonical form. In this light, the present paper can be viewed as an implementation of the second part of Weinstein's proof in the case of constant-coefficient skew-adjoint differential operators. The first part of the proof is far more difficult, and, unfortunately, the infinite-dimensional version of Darboux' theorem due to Weinstein does not appear to be applicable to the Hamiltonian differential operators of interest. The problem is that Weinstein requires some form of Banach manifold structure to effect his proof, but for differential operators that depend on the dependent variables it is not at all obvious how to impose such a structure. Even if one could mimic Weinstein's proof, the resulting changes of variable would be horribly nonlocal, and therefore be of limited use. Thus the question of whether Darboux' theorem is valid for Hamiltonian differential operators remains an important open problem. Only in special cases, including first- and third-order scalar operators, and some first-order matrix operators is the answer known.[11,26] (Results of Dubrovin and Novikov[12] indicate that Darboux' theorem may not hold for matrix operators involving more than one independent variable, but they only consider a limited class of changes of variable, so the general Darboux problem remains unanswered.)

The underlying motivation of this paper can be found in the recent applications of Dirac's theory of constraints by Nutku to produce canonical forms of a number of Hamiltonian systems of evolution equations of physical interest, including the equations of shallow water waves and gas dynamics[13] and the Korteweg–de Vries equation.[14] In the finite-dimensional theory of the calculus of variations, for nondegenerate Lagrangians the passage from the Euler–Lagrange equations to the corresponding canonical form of Hamilton's equations is classical.[1] Dirac's theory of constraints was designed to handle degenerate Lagrangians and produce canonical Hamiltonian systems, which, when subjected to the appropriate constraints, reduce to the original Euler–Lagrange equations.[15] In Nutku's applications of this theory, one begins with a Hamiltonian system of evolution equations, whose Poisson bracket is not in canonical form. The next step is to replace the original Hamiltonian system of evolution equations by an equivalent system of Euler–Lagrange equations; this appears to require that the Hamiltonian operator be constant coefficient. The resulting Lagrangian function is inevitably degenerate, so to construct a corresponding canonical Hamiltonian system one is required to invoke the Dirac machinery. The details of the construction can be found in Refs. 13 and 14.

However, given the fact that one begins with a (noncanonical) Hamiltonian system, the entire procedure seems to be a bit roundabout, and it would be useful to have a direct method of constructing canonical Hamiltonian systems from more general Hamiltonian evolution equations. In this paper a simple constructive procedure for effecting this

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transformation to canonical coordinates is presented. The only restriction is that the original Hamiltonian differential operator does not depend on the field variables or their derivatives; typically the operator will be a constant-coefficient, skew-adjoint differential operator, but explicit dependence on the spatial variables is also allowed. The method is illustrated with a number of examples, including elementary derivations of Nutku's Hamiltonians for gas dynamics and the Korteweg–de Vries equation. More general Hamiltonian operators are less easy to deal with directly. At present, the only recourse is to first determine a transformation that will place the operator in constant-coefficient form, and then apply the method described here.

II. HAMILTONIAN OPERATORS

For the basic theory of Hamiltonian systems of evolution equations, we refer the reader to the works of Gel'fand and Dorfman,[4] and the author.[5,16] We let $x = (x^1,...,x^p)$ denote the spatial variables, and $u = (u^1,...,u^q)$ the field variables (dependent variables), so each u^α is a function of $x^1,...,x^p$ and the time t. We will be concerned with autonomous systems of evolution equations

$$u_t = K[u],$$

in which $K[u] = (K_1[u],...,K_q[u])$ is a q-tuple of *differential functions*, where the square brackets indicate that each K_α is a function of x, u, and finitely many partial derivatives of each u^α with respect to $x^1,...,x^p$. A system of evolution equations is said to be *Hamiltonian* if it can be written in the form

$$u_t = \mathscr{D}\cdot E_u(H). \tag{1}$$

Here $\mathscr{H}[u] = \int H[u]\,dx$ is the Hamiltonian functional, and the Hamiltonian function $H[u]$ depends on x, u, and the derivatives of the u's with respect to the x's; $E_u = (E_1,...,E_q)$ denotes the Euler operator or variational derivative with respect to u. The Hamiltonian operator $\mathscr{D}$ is a $q\times q$ matrix differential operator, which may depend on both x, u, and derivatives of u (but not on t), and is required to be (formally) skew-adjoint relative to the L^2-inner product $\langle f,g\rangle = \int f\cdot g\,dx = \int \Sigma f^\alpha\cdot g^\alpha\,dx$, so

$$\mathscr{D}^* = -\mathscr{D},$$

where * denotes the formal L^2 adjoint of a differential operator.[16] In addition, $\mathscr{D}$ must satisfy a nonlinear "Jacobi condition" that the corresponding Poisson bracket

$$\{\mathscr{P},\mathscr{Q}\} = \int E_u(P)\cdot\mathscr{D}E_u(Q)\,dx,$$

$$\mathscr{P} = \int P[u]\,dx, \quad \mathscr{Q} = \int Q[u]\,dx,$$

satisfies the Jacobi identity.[4,5,16] In the special case that $\mathscr{D}$ is a field-independent skew-adjoint differential operator, meaning that the coefficients of $\mathscr{D}$ do not depend on u or its derivatives (but may depend on x), the Jacobi conditions are automatically satisfied; for more general field-dependent operators, there is a nontrivial computation to be effected to determine whether or not it is genuinely Hamiltonian.

Since we will be using changes of variables, it is essential that we determine how they affect objects like Euler operators and Hamiltonian operators. The changes of variables to be considered here are of the form $u = Q[v]$, where $Q[v] = (Q_1[v],...,Q_q[v])$ is a q-tuple of differential functions, depending on the variables x, $v = (v^1,...,v^q)$ and derivatives of v with respect to x. Let D_Q denote the *Fréchet derivative* of Q with repect to v, which is the $q\times q$ matrix differential operator defined by the formula

$$D_Q(w) = \frac{d}{d\epsilon}\bigg|_{\epsilon=0} Q[v+\epsilon w], \quad w = (w^1,...,w^q).$$

Alternatively, note that if $u = Q[v]$, then

$$u_t = D_Q[v_t]. \tag{2}$$

Let D_Q^* denote the (formal) L^2 adjoint of D_Q.

Proposition 1: Let $u = Q[v]$ be a change of variables. Then the variational derivatives with respect to u and v are related by the formula

$$E_v = D_Q^*\cdot E_u. \tag{3}$$

Proposition 2: Let $u_t = \mathscr{D}\cdot E_u(H)$ be a Hamiltonian system with Hamiltonian operator $\mathscr{D}$. Let $u = Q[v]$ be a change of variables. Then the corresponding Hamiltonian operator $\tilde{\mathscr{D}}$ in the v variables is related to that in the u variables by the formula

$$D_Q\cdot\tilde{\mathscr{D}}\cdot D_Q^* = \mathscr{D}. \tag{4}$$

The corresponding Hamiltonian system in the v variables is

$$v_t = \tilde{\mathscr{D}}\cdot E_v(H),$$

in which we take the variational derivative of H with respect to v.

These results are special cases of an even more general theorem on how Euler operators and Hamiltonian operators behave under changes in both the independent and dependent variables.[11,17] Note that (4) follows easily from (2) and (3).

Example 3: Suppose $u(x,t)$ is scalar valued, $x\in\mathbb{R}$, and let $\varphi(x,t)$ be a potential function for u, so the change of variables is

$$u = Q[\varphi] = \varphi_x.$$

The corresponding Fréchet derivative is easily seen to be $D_Q = D_x$, with adjoint $D_Q^* = -D_x$. Therefore, by (3),

$$E_\varphi(H) = -D_x E_u(H), \tag{5}$$

for any differential function H.

Similarly, if $\mathscr{D}$ is any Hamiltonian operator in the u variables, then the corresponding Hamiltonian operator in the v variables $\tilde{\mathscr{D}}$ is related by the formula

$$D_x\cdot\tilde{\mathscr{D}}\cdot(-D_x) = \mathscr{D}.$$

For example, consider the Harry Dym equation[7]

$$u_t = D_x^3(u^{-1/2}), \tag{6}$$

which is in Hamiltonian form (1) with Hamiltonian operator

$$\mathscr{D} = D_x^3,$$

and Hamiltonian function

$$H = 2\sqrt{u}.$$

If we introduce a potential function $\varphi_x = u$, then the corresponding potential form of (6) is the equation

$$\varphi_t = D_x^2(\varphi_x^{-1/2}) . \tag{7}$$

(Here, and elsewhere, we set the integration constants to 0 when introducing a potential function.) The Hamiltonian for (7) is just

$$\tilde{H} = H = 2\sqrt{\varphi_x} ,$$

and the Hamiltonian operator is $\tilde{\mathscr{D}} = -D_x$, since $D_x^3 = D_x\cdot(-D_x)\cdot(-D_x)$. Indeed, (7) is the same as the evolution equation

$$\varphi_t = \tilde{\mathscr{D}}\cdot E_\varphi(\tilde{H}) ,$$

as the reader can check.

III. THE GARDNER HAMILTONIAN OPERATOR

In order to simply illustrate the main ideas of the paper, we begin by discussing the elementary Hamiltonian operator $\mathscr{D} = D_x$, originally found by Gardner in connection with the Korteweg–de Vries equation.[18] Thus we are looking at a single evolution equation of the form

$$u_t = D_x\cdot E_u(H) , \tag{8}$$

in which $\mathscr{H} = \int H[u]\,dx$ is the corresponding Hamiltonian functional. We first show that any such Hamiltonian system can always be derived from a Lagrangian variational problem.[19]

Proposition 4: Let $u_t = D_x\cdot E_u(H)$ be a Hamiltonian evolution equation relative to the Hamiltonian operator D_x. Let $\varphi(x,t)$ be the potential of $u(x,t)$, so $\varphi_x = u$. Then the Hamiltonian evolution equation is equivalent to the Euler–Lagrange equation for the variational problem $\mathscr{L} = \int L[\varphi]\,dx$ with Lagrangian

$$L[\varphi] = \varphi_x\varphi_t - 2H[\varphi_x] . \tag{9}$$

Proof: Formula (5) immediately implies that the Euler–Lagrange equation for $\mathscr{L}$ is

$$E_\varphi(L) = -2\varphi_{xt} - 2E_\varphi(H) = -2\{u_t - D_xE_u(H)\} = 0 ,$$

which coincides with a multiple of the original Hamiltonian system (8).

We now apply Dirac's theory of constraints to the Lagrangian (9) as explained in Nutku.[13,14] The Lagrangian is degenerate, and the first constraint should be determined by

$$c_1 = \pi - \frac{\partial L}{\partial \varphi_t} = \pi - \varphi_x = \pi - u = 0 ,$$

in which π will be the canonical momentum dual to φ. As shown by Nutku, this constraint is second class in the terminology of Dirac, and so to derive the further constraints we need to investigate the canonical Poisson brackets of the constraint with the Hamiltonian.

In the version of the Dirac theory used by Nutku, the Lagrangian is required to only depend on first-order derivatives of the potential φ. This is equivalent to the fact that the Hamiltonian $H = H(x,u)$ depends only on x and u, and not any derivatives of u, so that the Hamiltonian system (8) is a simple nonlinear wave equation

$$u_t = [H_u(x,u)]_x = H_{xu}(x,u) + H_{uu}(x,u)\cdot u_x .$$

The corresponding potential form is the equation

$$\varphi_t = H_u(x,\varphi_x) .$$

The Lagrangian (9) for this equation is

$$L = \varphi_x\varphi_t - 2H(x,\varphi_x) .$$

Therefore, provided there are no further constraints coming from the Poisson brackets of the constraint with the Hamiltonian, the total Hamiltonian has the form

$$H^* = 2H(x,\varphi_x) + \lambda(\pi - \varphi_x) ,$$

where the multiplier λ remains to be determined. [In the notation of Ref. 13, the free part of the Hamiltonian has been determined as

$$H_0 = \varphi_t\pi - L = \varphi_t\pi - \varphi_x\varphi_t + 2H(x,\varphi_x) = 2H(x,\varphi_x) .]$$

Using the canonical Poisson bracket relations[14]

$$\{\varphi(x),\pi(x')\} = \delta(x-x') ,$$

δ being the Dirac delta function, we find

$$\{c_1(x),c_1(x')\} = -2\delta'(x-x') .$$

Therefore

$$\{c_1(x),H^*(x')\} = 2[H_u(x',\varphi_x(x')) - \lambda]\cdot\delta'(x-x') ,$$

from which we see that $\lambda = H_u(x,\varphi_x)$ is required in order to make the Poisson bracket vanish. Thus the total Hamiltonian is

$$H^*[\varphi,\pi] = \pi\cdot H_u(x,\varphi_x) + 2H(x,\varphi_x) - H_u(x,\varphi_x)\cdot\varphi_x . \tag{10}$$

The canonical equations corresponding to H^*, which are

$$\varphi_t = E_\pi[H^*] = H_u(x,\varphi_x) ,$$
$$\pi_t = -E_\varphi[H^*] = D_x\{(\pi-\varphi_x)H_{uu}(x,\varphi_x) + H_u(x,\varphi_x)\} ,$$

are easily seen to reduce to the original wave equation when subjected to the constraint $\pi = u$.

The goal now is to generalize this construction to Hamiltonian functions which depend on higher-order derivatives of the field variable u. Rather than try to follow through the complete derivation using the Dirac theory, as in Ref. 14, we proceed directly to the general result. In order to state it, we need to introduce the multiplication operator

$$N = u\frac{\partial}{\partial u} + u_x\frac{\partial}{\partial u_x} + u_{xx}\frac{\partial}{\partial u_{xx}} + \cdots ,$$

whose action on differential functions is to multiply each term by its algebraic degree in u and its derivatives. For example,

$$N(u_{xx} + xu^2u_x + u^5) = u_{xx} + 3xu^2u_x + 5u^5 .$$

Theorem 5: Let $u_t = D_x\cdot E_u(H)$ be a Hamiltonian system with Hamiltonian operator D_x. Then the corresponding canonical Hamiltonian system has total Hamiltonian

$$H^*[\pi,\varphi] = \pi\cdot E_u(H) + (2-N)H , \tag{11}$$

in which φ is the potential for u, π the corresponding momentum, and u is to be replaced by φ_x on the right-hand side of (11). The corresponding canonical Hamiltonian system for H^* takes the form

$$\varphi_t = E_\pi(H^*), \quad \pi_t = -E_\varphi(H^*) , \tag{12}$$

and, when subjected to the constraint $\pi = u = \varphi_x$, is equivalent to the original Hamiltonian system.

For example, in the case that $H = H(x,u)$ just depends on u, then (11) reduces to the formula (10) derived using the Dirac theory.

Proof: It suffices to check that when $\pi = u$, the pair of evolution equations in (12) reduce to the original evolution equation (8). The first one is easy, since $E_\pi(H^*) = E_u(H)$, and so we just derive the potential form $\varphi_t = E_u(H)$ of the original equation. For the second, we require a lemma of Olver and Shakiban.[20]

Lemma 6: Let $u(x)$ be real valued, and let $L[u]$ be any differential function. Then

$$E_u(u\cdot E_u(L)) = (N+1)E_u(L)\,. \tag{13}$$

[Indeed, if P is a differential polynomial, then the condition $E_u(u\cdot P) = (N+1)P$ is both necessary and sufficient that $P = E_u(L)$ be the Euler–Lagrange expression for some Lagrangian L.]

Corollary 7: Let $u(x)$ and $\pi(x)$ be real-valued functions, and $L[u]$ any differential function depending only on u and its derivatives. Then

$$E_u(\pi\cdot E_u(L))|_{\pi=u} = N[E_u(L)] = E_u((N-1)L)\,. \tag{14}$$

Proof: The second equality is clear since the Euler operator E_u reduces the algebraic degree of a differential function by 1. To prove the first, we use the well-known formula for the Euler operator

$$E_u = \sum_{n=0}^{\infty} (-D_x)^n \cdot \frac{\partial}{\partial u_n}\,,$$

where $u_n = \partial^n u/\partial x^n$. Therefore

$$E_u(u\cdot E_u(L)) = E_u(L) + \sum_n (-D_x)^n \left\{ u\cdot \frac{\partial E_u(L)}{\partial u_n} \right\}.$$

On the other hand, since the restriction to $\pi = u$ commutes with the operation of total differentiation D_x (but not with the partial derivatives $\partial/\partial u_n$), the left-hand side of (14) equals

$$\sum_n (-D_x)^n \left\{ \pi\cdot \frac{\partial E_u(L)}{\partial u_n} \right\}\Bigg|_{\pi=u} = \sum_n (-D_x)^n \left\{ u\cdot \frac{\partial E_u(L)}{\partial u_n} \right\}.$$

The equivalence of (14) and (13) is now clear.

Returning to the proof of the theorem, we only need compute

$$E_\varphi(H^*) = E_\varphi\{\pi\cdot E_u(H) + (2-N)H\} = -D_x\cdot E_u\{\pi\cdot E_u(H) + (2-N)H\}\,,$$

cf. (5), and restrict to $\pi = u$. According to (14), this equals

$$E_\varphi(H^*)|_{\pi=u} = -D_x\cdot E_u\{(N-1)H + (2-N)H\} = -D_x\cdot E_u(H)\,,$$

which explains the factor $(2-N)$ in the formula (11) for the total Hamiltonian. Therefore, when restricted to the constraint $\pi = u$, the second evolution equation in (12) becomes

$$u_t = -E_\varphi(H^*)|_{\pi=u} = D_x\cdot E_u(H)\,,$$

which is the same as the original Hamiltonian system! This completes the proof.

Example 8: Consider the evolution equation

$$u_t = u_x + u_{xxx} + uu_x + u^2u_x\,, \tag{15}$$

which is a combination of the Korteweg–de Vries and modified Korteweg–de Vries equations. This is in Hamiltonian form (8), with Hamiltonian

$$H = \tfrac{1}{2}u^2 - \tfrac{1}{2}u_x^2 + \tfrac{1}{6}u^3 + \tfrac{1}{12}u^4\,.$$

Note that

$$E_u(H) = u + u_{xx} + \tfrac{1}{2}u^2 + \tfrac{1}{3}u^3\,,$$

while

$$(N-2)H = \tfrac{1}{6}u^3 + \tfrac{1}{6}u^4\,.$$

Therefore the total Hamiltonian (11) is

$$H^* = \pi(u + u_{xx} + \tfrac{1}{2}u^2 + \tfrac{1}{3}u^3) - \tfrac{1}{6}u^3 - \tfrac{1}{6}u^4 = \pi(\varphi_x + \varphi_{xxx} + \tfrac{1}{2}\varphi_x^2 + \tfrac{1}{3}\varphi_x^3) - \tfrac{1}{6}\varphi_x^3 - \tfrac{1}{6}\varphi_x^4\,.$$

The corresponding canonical Hamiltonian system is

$$\begin{aligned} \varphi_t &= E_\pi(H^*) = \varphi_x + \varphi_{xxx} + \tfrac{1}{2}\varphi_x^2 + \tfrac{1}{3}\varphi_x^3\,,\\ \pi_t &= -E_\varphi(H^*) = \pi_x + \pi_{xxx} + \pi_x\varphi_x + \pi\varphi_{xx}\\ &\quad + \pi_x\varphi_x^2 + 2\pi\varphi_x\varphi_{xx} - \varphi_x\varphi_{xx} - 2\varphi_x^2\varphi_{xx}\,. \end{aligned} \tag{16}$$

The first is just the potential form of the original equation (15); restricting to $\pi = \varphi_x = u$, the second reduces to (15) identically. Thus we are justified in labeling (16) as the canonical form of the modified Korteweg–de Vries equation (15). If the last term in (15) does not appear, we are back to the Korteweg–de Vries equation as treated by Nutku.[14]

IV. CANONICAL FORMS AND FACTORIZATIONS OF HAMILTONIAN OPERATORS

Theorem 5 readily generalizes to systems of evolution equations which are in field-independent Hamiltonian form

$$u_t = \mathscr{D}\cdot E(H)\,, \tag{17}$$

in which the Hamiltonian H depends on $x = (x^1,\ldots,x^p)$, $u = (u^1,\ldots,u^q)$, and the derivatives of the u's with respect to the x's. The corresponding Lagrangian form of such a system is written in terms of the "potential" $\psi = (\psi^1,\ldots,\psi^q)$, satisfying $\mathscr{D}\psi = u$. The Lagrangian function is

$$L[\psi] = (\mathscr{D}\psi)\cdot\psi_t - 2H\,,$$

in which $\mathscr{D}\psi$ is to be substituted for u in H. Using the change of variables formula (3), which is

$$E_\psi(H) = \mathscr{D}^*\cdot E_u(H) = -\mathscr{D}\cdot E_u(H)$$

(the second equality following from the skew-adjointness of $\mathscr{D}$), we easily check that the Euler–Lagrange equations $E_\psi(L) = 0$ for L are the same as the Hamiltonian system (17).

As it turns out, for each possible *factorization*,

$$\mathscr{D} = \mathscr{D}_1\cdot\mathscr{D}_2\,, \tag{18}$$

of the differential operator $\mathscr{D}$ into the product of two differential operators $\mathscr{D}_1$ and $\mathscr{D}_2$, there is a corresponding canonical Hamiltonian system that reduces to (17). Either $\mathscr{D}_1$ or $\mathscr{D}_2$ can be the identity operator, in which case the other

one coincides with $\mathscr{D}$, but this is not the only possible choice in (18). Once a factorization has been chosen, we define canonically conjugate "positions" $\varphi = (\varphi^1,...,\varphi^q)$ and momenta $\pi = (\pi^1,...,\pi^q)$ by the equations

$$\mathscr{D}_1\varphi = u, \quad \mathscr{D}_2^*\pi = u,$$

where $\mathscr{D}_2^*$ is the adjoint of $\mathscr{D}_2$. Thus, the choice of $\mathscr{D}_1$ and $\mathscr{D}_2$ might be determined on physical grounds as to which variables might reasonably be labeled "position" or "momentum"; however, from a mathematical point of view, any choice of $\mathscr{D}_1$ and $\mathscr{D}_2$ satisfying (18) is allowable.

We also need the general multiplication operator

$$N = \sum u_J^\alpha \frac{\partial}{\partial u_J^\alpha}, \quad u_J^\alpha = \frac{\partial^n u^\alpha}{\partial x^{j_1} \cdots \partial x^{j_n}},$$

the sum being over all $\alpha = 1,...,q$ and all multi-indices $J = (j_1,...,j_n)$, $n \geqslant 0$, $1 \leqslant j_\nu \leqslant p$, corresponding to all possible derivatives of the u's. The effect of N is, as before, to multiply a monomial by its algebraic degree in the u's and their derivatives. With this definition, Lemma 6 has an immediate generalization due to Shakiban.[21] In this case, formula (13) still holds, with $u \cdot E_u(H) \equiv \Sigma u^\alpha \cdot E_\alpha(H)$.

Theorem 9: Consider a Hamiltonian system of evolution equations $u_t = \mathscr{D} \cdot E(H)$, in which the Hamiltonian operator $\mathscr{D}$ is a skew-adjoint $q \times q$ matrix differential operator, whose coefficients do not depend on u or their derivatives. Let $\mathscr{D} = \mathscr{D}_1 \cdot \mathscr{D}_2$ be any factorization of $\mathscr{D}$ as a product of two differential operators. Define canonically conjugate variables φ and π by the equations $\mathscr{D}_1\varphi = u$, $\mathscr{D}_2^*\pi = u$. Define the total Hamiltonian

$$H^*[\varphi,\pi] = (\mathscr{D}_2^*\pi) \cdot E_u(H) + (2 - N)H, \tag{19}$$

in which one substitutes $\mathscr{D}_1\varphi$ for u wherever it occurs on the right-hand side of (19). Then the original Hamiltonian system is equivalent to the canonical Hamiltonian system

$$\varphi_t = E_\pi(H^*), \quad \pi_t = -E_\varphi(H^*), \tag{20}$$

when subjected to the constraints

$$\mathscr{D}_1\varphi = u = \mathscr{D}_2^*\pi. \tag{21}$$

Proof: The first canonical equation is easy; we find it has the form

$$\varphi_t = E_\pi(H^*) = \mathscr{D}_2 E_u(H),$$

evaluated at $u = \mathscr{D}_1\varphi$. Applying the operator $\mathscr{D}_1$ to both sides of this equation, we recover the original Hamiltonian system since $\mathscr{D} = \mathscr{D}_1 \cdot \mathscr{D}_2$. For the second canonical system, we require the identity

$$E_u\{(\mathscr{D}_2^*\pi) \cdot E_u(H)\}\big|_{u = \mathscr{D}_2^*\pi} = E_u[(N-1)H],$$

which follows from formula (13) (in the general case) just as (14) did before. Therefore, evaluating the canonical equation

$$\pi_t = -E_\varphi(H^*) = -E_\varphi\{(\mathscr{D}_2^*\pi) \cdot E_u(H) + (2 - N)H\}$$

on the constraint $u = \mathscr{D}_2^*\pi$, we find, using (3),

$$\begin{aligned}\pi_t &= -\mathscr{D}_1^* \cdot E_u[(N-1)H + (2-N)H] \\ &= -\mathscr{D}_1^* \cdot E_u(H).\end{aligned}$$

Finally applying $\mathscr{D}_2^*$ to this system, we recover

$$u_t = \mathscr{D}_2^* \cdot \mathscr{D}_1^* \cdot E_u(H) = -\mathscr{D}^* \cdot E_u(H) = \mathscr{D} \cdot E_u(H),$$

since $\mathscr{D}$ is skew-adjoint. Thus the second canonical equation, when evaluated on the constraints, is equivalent to the original Hamiltonian system, and Theorem 9 is proven.

Example 10: Consider the equations of gas dynamics for a polytropic gas

$$\begin{aligned}&u_t + uu_x + v^{\gamma-2}v_x = 0, \\ &v_t + uv_x + vu_x = 0,\end{aligned}$$

the case $\gamma = 2$ also covering the equations of shallow water wave motion.[13] These are in Hamiltonian form

$$\begin{aligned}\begin{pmatrix} u \\ v \end{pmatrix}_t &= \mathscr{D} \begin{pmatrix} E_u(H) \\ E_v(H) \end{pmatrix} \\ &= \begin{pmatrix} 0 & D_x \\ D_x & 0 \end{pmatrix} \begin{pmatrix} -uv \\ -\frac{1}{2}u^2 - (\gamma-1)^{-1}v^{\gamma-1} \end{pmatrix},\end{aligned}$$

with Hamiltonian function

$$H[u,v] = -\tfrac{1}{2}u^2 v - \{\gamma(\gamma-1)\}^{-1}v^\gamma.$$

Let $\varphi_x = u$, $\psi_x = v$ be the corresponding potentials, with $\pi = v$, $\rho = u$, the canonically conjugate momenta. The reader can see that this corresponds to the factorization (18) in which $\mathscr{D}_1 = D_x$, and $\mathscr{D}_2 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$. Note that

$$(2 - N)H = \frac{1}{2}u^2 v + \frac{\gamma - 2}{\gamma(\gamma-1)}v^\gamma.$$

Therefore, according to (19), the corresponding canonical total Hamiltonian is

$$\begin{aligned}H^*[\varphi,\psi,\pi,\rho] &= -\left\{\frac{1}{2}u^2 + \frac{1}{(\gamma-1)}v^{\gamma-1}\right\}\pi - uv\rho \\ &\quad + \frac{1}{2}u^2 v + \frac{\gamma-2}{\gamma(\gamma-1)}v^\gamma \\ &= -\left\{\frac{1}{2}\varphi_x^2 + \frac{1}{(\gamma-1)}\psi_x^{\gamma-1}\right\}\pi - \varphi_x\psi_x\rho \\ &\quad + \frac{1}{2}\varphi_x^2\psi_x + \frac{\gamma-2}{\gamma(\gamma-1)}\psi_x^\gamma.\end{aligned}$$

This is the same as that derived by Nutku,[13] but the derivation here is far more straightforward. The Hamiltonian system

$$\begin{aligned}&u_t = E_\pi(H^*), \quad v_t = E_\rho(H^*), \\ &\pi_t = -E_u(H^*), \quad \rho_t = -E_v(H^*),\end{aligned}$$

when subjected to the constraints

$$\varphi_x = \rho = u, \quad \psi_x = \pi = v,$$

is easily seen to be equivalent to the original system.

There are, of course, other possible factorizations of the Hamiltonian operator $\mathscr{D}$, and these lead to different canonical total Hamiltonians. For example, if we choose $\mathscr{D}_1$ to be the identity operator, while $\mathscr{D}_2 = \mathscr{D}$, then the velocities u,v are the canonical "positions," while the conjugate momenta π,ρ are related by $\pi_x = -v$, $\rho_x = -u$. In this case formula (19) gives the total Hamiltonian as

$$\begin{aligned}H^*[\varphi,\psi,\pi,\rho] &= -uv\pi - \left\{\frac{1}{2}u^2 + \frac{1}{(\gamma-1)}v^{\gamma-1}\right\}\rho \\ &\quad + \frac{1}{2}u^2 v + \frac{\gamma-2}{\gamma(\gamma-1)}v^\gamma,\end{aligned}$$

and the gas dynamic equations are equivalent to the canonical system

$$u_t = E_\pi(H^*), \quad v_t = E_\rho(H^*),$$
$$\pi_t = -E_u(H^*), \quad \rho_t = -E_v(H^*),$$

when subject to the constraints $\pi_x = -v$, $\rho_x = -u$, as can be easily checked.

This last remark indicates that there are other possible canonical formulations of the Korteweg–de Vries example (15) above. The procedure of example 8 amounts to choosing the factorization (18) with $\mathscr{D}_2$ the identity operator. If, on the other hand, we were to choose $\mathscr{D}_1$ to be the identity, then we would have canonically conjugate variables u and π, with $\pi_x = -u$, and total Hamiltonian

$$H^* = \pi(u + u_{xx} + \tfrac{1}{2}u^2 + \tfrac{1}{3}u^3) - \tfrac{1}{6}u^3 - \tfrac{1}{6}u^4.$$

While simpler than the Hamiltonian found above, this is not the version prescribed by the Dirac theory. It is, however, related to the Dirac Hamiltonian by a canonical transformation.

Example 11: For a higher-order example, consider the Harry Dym equation

$$u_t = D_x^3(u^{-1/2}), \tag{22}$$

which is in Hamiltonian form (17) with

$$\mathscr{D} = D_x^3, \quad H = 2\sqrt{u}.$$

If we choose $\mathscr{D}_1 = D_x^2$, $\mathscr{D}_2 = D_x$, so that $\varphi_{xx} = u$, $\pi_x = -u$ are conjugate variables, then the total Hamiltonian is

$$H^* = -\pi_x \varphi_{xx}^{-1/2} + 3\varphi_{xx}^{1/2},$$

with the canonical system (20) equivalent to the Harry Dym equation when subjected to the constraints $\varphi_{xx} = u$, $\pi_x = -u$.

Alternatively, we can choose $\mathscr{D}_1$ to be the identity, so u and π are conjugate, where $\pi_{xxx} = -u$, in which case

$$H^* = -\pi_{xxx} \cdot u^{-1/2} + 3u^{1/2}$$

is the total Hamiltonian. Other factorizations are also possible.

V. FIELD-DEPENDENT HAMILTONIAN OPERATORS

If the Hamiltonian operator depends explicitly on the dependent variables u, or their derivatives, then the above theory does not appear to be directly applicable. Indeed, a significant outstanding problem in the subject is whether some version of Darboux' theorem is true for all Hamiltonian differential operators, i.e., given a Hamiltonian differential operator, is it always possible to find canonical coordinates? The only case that has been completely answered to date is the case of first-order scalar differential operators in one independent variable.[11] In this case, provided one admits differential substitutions,[22] which change both the independent and dependent variables in the problem, one can always reduce such an operator to constant coefficient form, and hence, using the methods of this paper, to canonical form. The proof, however, is constructive, and does not appear to easily generalize to either higher-order or matrix operators, so the general "Darboux problem" for differential operators remains open. See, also, Ref. 26.

If one *can* reduce a Hamiltonian operator to constant coefficient form using some change of variables, then the methods discussed above are applicable, and canonical coordinates can always be found. In the case of bi-Hamiltonian systems,[4,7] or even multi-Hamiltonian systems,[23,24] this opens up the possibility of several different systems of canonical variables, which are *not* related to each other by canonical transformations. The implications of this phenomenon for quantization theory or perturbation theory remain to be developed. Here we just present a few examples to illustrate the main ideas.

Example 12: The Harry Dym equation (22) has a second Hamiltonian structure,[7] with first-order Hamiltonian operator

$$\tilde{\mathscr{D}} = 2uD_x + u_x,$$

and Hamiltonian function

$$\tilde{H} = \tfrac{1}{8}u^{-5/2} \cdot u_x^2.$$

Using the results in Ref. 11, or by direct inspection, we see that the transformation

$$u = \tfrac{1}{2}v^2$$

transforms $\tilde{\mathscr{D}}$ into the constant-coefficient operator D_x; indeed

$$D_Q \cdot D_x \cdot D_Q^* = v \cdot D_x \cdot v = v^2 D_x + v v_x = 2uD_x + u_x = \tilde{\mathscr{D}}.$$

In terms of v,

$$\tilde{H} = 2^{-1/2} v^{-3} v_x^2,$$

and

$$E_v(\tilde{H}) = \sqrt{2}(-v^{-3}v_{xx} + \tfrac{3}{2}v^{-4}v_x^2).$$

Therefore, using Theorem 9, the canonical total Hamiltonian is

$$\tilde{H}^*[\varphi,\pi] = \sqrt{2}\{\pi(-\varphi_x^{-3}\varphi_{xxx} + \tfrac{3}{2}\varphi_x^{-4}\varphi_{xx}^2) + \tfrac{3}{2}\varphi_x^{-3}\varphi_{xx}^2\},$$

where $\varphi_x = v$, $\pi = v$ are the canonically conjugate variables. The reader can check that the canonical Hamiltonian system (20) for $\tilde{H}^*$, when subjected to the constraints $u = \frac{1}{2}\varphi_x^2 = \frac{1}{2}\pi^2$, coincides with the Harry Dym equation (22). Thus we have constructed a second, inequivalent, canonical form for this equation.

Example 13: As a final example, consider the Korteweg–de Vries equation

$$u_t = u_{xxx} + uu_x.$$

The first Hamiltonian structure was considered in example 8. There is also a second Hamiltonian structure,[7] with Hamiltonian operator

$$\tilde{\mathscr{D}} = D_x^3 + \tfrac{2}{3}uD_x + \tfrac{1}{3}u_x,$$

and Hamiltonian function

$$\tilde{H} = \tfrac{1}{2}u^2.$$

According to Kupershmidt and Wilson,[8] the second Hamiltonian operator for the Korteweg–de Vries equation can be

put into constant-coefficient form D_x by the Miura transformation[25]

$$u = v_x - \tfrac{1}{6} v^2 ,$$

which has the effect of transforming the Korteweg–de Vries equation into the modified Korteweg–de Vries equation

$$v_t = v_{xxx} - \tfrac{1}{6} v^2 v_x .$$

Indeed,

$$\begin{aligned} D_Q \cdot D_x \cdot D_Q^* &= (D_x - \tfrac{1}{3} v) \cdot D_x \cdot (-D_x - \tfrac{1}{3} v) \\ &= -D_x^3 - (\tfrac{2}{3} v_x - \tfrac{1}{9} v^2) D_x - (\tfrac{2}{3} v_{xx} - \tfrac{1}{9} v v_x) \\ &= -D_x^3 - \tfrac{2}{3} u D_x - \tfrac{1}{3} u_x = -\mathscr{D} . \end{aligned}$$

Thus, using (19), we obtain the canonical total Hamiltonian

$$\tilde{H}^*[\varphi,\pi] = \pi(\varphi_{xxx} - \tfrac{1}{18} \varphi_x^3) + \tfrac{1}{36} \varphi_x^4 ,$$

where $\varphi_x = \pi = v$. In this case, we obtain a second canonical representation of the Korteweg–de Vries equation corresponding to the canonical Hamiltonian system for $\tilde{H}^*$ subject to the constraints[26]

$$u = \varphi_{xx} - \tfrac{1}{6} \varphi_x^2 = \pi_x - \tfrac{1}{6} \pi^2 .$$

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A Dyson-like expansion for solutions to the quantum Liouville equation

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Given a Hamiltonian of the form $H = h + \lambda v$, the convergence of a Dyson-like expansion (in λ) is constructed and shown for the Wigner distribution function that solves the quantum Liouville equation that corresponds to H. Here, h is a quadratic polynomial in $\mathbf{p}$, $\mathbf{q}$; its coefficients may depend continuously on time. The potential v is a function of $\mathbf{p}$ and t as well as $\mathbf{q}$; roughly speaking, it is the Fourier transform of a time-dependent measure.

I. INTRODUCTION

For a system with n degrees of freedom, a state in the Wigner–Weyl phase-space formulation of quantum mechanics is a function ρ (the Wigner distribution function) that is defined and continuous on $\mathbb{R}^{2n}$, and that satisfies certain positivity conditions.[1,2,3] If the system is subject to forces arising from a Hamiltonian function $H(\mathbf{q},\mathbf{p},t)$, then its state changes according to the quantum Liouville equation[3,4]

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar}[\rho, H] \equiv \frac{i}{\hbar}(\rho \circ H - H \circ \rho), \tag{1.1}$$

where the product $\rho \circ H$ is the phase-space function that corresponds to the operator product $\hat{\rho} \times \hat{H}$. [If $a(\mathbf{q},\mathbf{p})$ and $b(\mathbf{q},\mathbf{p})$ are two functions on phase space, and if one adopts the conventions for the Weyl correspondence used by Voros (cf. Ref. 5, Sec. III), then

$$\begin{aligned}(a \circ b)(\mathbf{q},\mathbf{p}) = \frac{1}{(\pi\hbar)^{2n}} \int d^n P_1\, d^n Q_1\, d^n P_2\, d^n Q_2 \\ \times \{a(\mathbf{q}+\mathbf{Q}_1, \mathbf{p}+\mathbf{P}_1) b(\mathbf{q}+\mathbf{Q}_2, \mathbf{p}+\mathbf{P}_2) \\ \times \exp[(2i/\hbar)(\mathbf{Q}_1 \cdot \mathbf{P}_2 - \mathbf{Q}_2 \cdot \mathbf{P}_1)]\}.\end{aligned} \tag{1.2}$$

The integration is to be understood in a (Schwartz) distributional sense.]

In this paper, I will construct and show the convergence of "Dyson" expansions for solutions to the quantum Liouville equation, given that the Hamiltonian H has the form

$$H(\mathbf{q},\mathbf{p},t) = h(\mathbf{q},\mathbf{p},t) + \lambda v(\mathbf{q},\mathbf{p},t). \tag{1.3}$$

Here, h is a real-valued, time-dependent quadratic function of $\mathbf{q}$, $\mathbf{p}$; specifically,

$$\begin{aligned}h(\mathbf{q},\mathbf{p},t) = \frac{1}{2}\Big\{\sum_{j,k=1}^{n} [a_{jk}(t) q_j q_k \\ + b_{jk}(t)(q_j p_k + q_k p_j) + c_{jk}(t) p_j p_k]\Big\},\end{aligned} \tag{1.4}$$

where the various coefficients are real-valued, continuous functions of t only, and the matrices a_{jk}, b_{jk}, and c_{jk} are symmetric. (I do *not*, however, need to assume that they are nonnegative matrices.)

The perturbing potential v, which depends on momentum and time as well as position, is real valued, and it is assumed to have the form

$$v(\mathbf{q},\mathbf{p},t) = \frac{\hbar}{2}\int f(\mathbf{q}',\mathbf{p}',t)\exp\left(\frac{2i}{\hbar}(\mathbf{p}\mathbf{q}' - \mathbf{q}\cdot\mathbf{p}')\right) d\mu(\mathbf{q}',\mathbf{q}'), \tag{1.5}$$

where $d\mu$ is a positive, finite measure on $\mathbb{R}^{2n}$, and f is in $L^{\infty}(\mathbb{R}^{2n+1}, d\mu \times dt)$. In addition, the condition that v be real valued forces f and $d\mu$ to obey a reflection condition,[6]

$$\overline{f(\mathbf{q}',\mathbf{p}',t)}\, d\mu(\mathbf{q}',\mathbf{p}') = f(-\mathbf{q}', -\mathbf{p}', t)\, d\mu(-\mathbf{q}', -\mathbf{p}'). \tag{1.6}$$

Finally, that v is of the form (1.5) implies that, for all $\mathbf{p},\mathbf{q},t$,

$$|v(\mathbf{p},\mathbf{q},t)| \leqslant (\hbar/2)\|f\|_{\infty}\mu(\mathbb{R}^{2n}) \tag{1.7}$$

and that, when t is fixed, v is continuous in $\mathbf{q}$ and $\mathbf{p}$.[7]

I have chosen to work with the class of potentials described above because it is the natural one for the mathematical techniques that I will use, and because it contains a number of physically interesting examples. For instance, every periodic, one-dimensional potential of the form

$$v(q,t) = \sum_{n=-\infty}^{\infty} a_n(t) b_n \exp\left\{\frac{2\pi i q}{G} n\right\},$$

where G is the period, $|a_n(t)| \leqslant C$ for all n, and where $\Sigma |b_n| < \infty$, is in the class. (Higher-dimensional periodic potentials satisfying similar conditions also belong to it.)

One novel feature of this class is that the potentials in it can be functions of momentum, time, and position. In the usual configuration space approach to quantum mechanics, such potentials would be nonlocal and troublesome to handle, but in the phase-space approach they can be handled in the same way as potentials that depend only on position.

Several workers have dealt with potentials belonging to classes that are similar to the one worked with here. In particular, Osborn and Fujiwara,[6] Albeverio and Høegh-Krohn,[8] Ito,[9] and Combe *et al.*[1] all employ them.

Indeed, Combe *et al.*[1] solve the quantum Liouville equation for a class of time-independent Hamiltonians that are perturbations of a harmonic-oscillator Hamiltonian by a potential that is of the form (1.5), except that it does not depend on time. The results they get and the methods they use involve dealing with stochastic processes in a "Fourier transformed" phase space.

The paper is organized this way. In Sec. II, I introduce notation, review the theory of Wigner–Weyl transforms, and

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determine the distribution that corresponds to the commutator in (1.1). In Sec. III, after reviewing the definition of "state" in the phase-space formulation of quantum mechanics, I put the quantum Liouville equation into a form, an integral form, suitable for solving via the method of successive approximations. In Sec. IV, I obtain a Dyson-like expansion that solves the quantum Liouville equation when its initial conditions are taken to be in a Banach space X that has certain "nice" properties. I then show that one may take X to be any of a wide variety of spaces, among which is included the space of functions that are Wigner transforms of trace-class operators, T. In Sec. V, I show that the solution to the quantum Liouville equation not only preserves the cone of states, but it also preserves the set of pure (extremal) states. In Sec. VI, I discuss possible applications, and I show how to treat Hamiltonians that are of the form (1.3), but that have additional linear terms. Finally, I make a few concluding remarks.

II. THE WIGNER AND WEYL TRANSFORMS

I want to introduce and establish notation, review briefly the Wigner and Weyl transforms, and prove a few results that will enable me to determine the tempered distribution that corresponds to the commutator that appears in the quantum Liouville equation (1.1).

There are two pieces of notation that will simplify many of the formulas used in the rest of the paper. First, let

$$z=(\mathbf{p},\mathbf{q})=(q_1,\ldots,q_n;p_1,\ldots,p_n), \qquad dz=dq_1\cdots dq_n\,dp_1\cdots dp_n, \tag{2.1}$$

and, second, define the symplectic form σ via

$$\sigma(z,z')\equiv(2/\hbar)(\mathbf{p}\cdot\mathbf{q}'-\mathbf{q}\cdot\mathbf{p}'). \tag{2.2}$$

Using (2.1) and (2.2), one may rewrite (1.2) as

$$(a\circ b)(z)=\frac{1}{(\pi\hbar)^{2n}}\int dz_1\,dz_2\,a(z+z_1)b(z+z_2)e^{-i\sigma(z_1,z_2)}, \tag{2.3}$$

and (1.5) as

$$v(z,t)=\frac{\hbar}{2}\int f(z',t)e^{i\sigma(z,z')}\,d\mu(z'). \tag{2.4}$$

This notation also simplifies the formulas for the "symplectic" Fourier transform. If $g(z)$ is a phase-space function that is in, say, $L^1(\mathbb{R}^{2n})$, then its symplectic Fourier transform is

$$\tilde{g}(z)\equiv\frac{1}{(\pi\hbar)^n}\int g(z')e^{i\sigma(z,z')}\,dz'. \tag{2.5}$$

The formula giving the inverse of the transform is identical to (2.5), except that $\tilde{g}$ and g are interchanged:

$$g(z)=\frac{1}{(\pi\hbar)^n}\int\tilde{g}(z')e^{i\sigma(z,z')}\,dz'. \tag{2.6}$$

Symplectic Fourier transforms play an important role in the Wigner–Weyl phase-space formalism. Both the Weyl transform, which takes phase-space functions into operators on a quantum mechanical system's Hilbert space, and the Wigner transform, which inverts the Weyl transform, are closely related to such Fourier transforms.

The Weyl transform[1,3,4,5] works this way: Let $\mathscr{H}$ be the Hilbert space $L^2(\mathbb{R}^n,d^n\xi)$, and let $\hat{q}_j,\hat{p}_j$ $(j=1,\ldots,n)$, and $\hat{z}$ be defined by

$$\hat{q}_jf(\xi)=\xi_jf(\xi),\quad(\hat{p}_jf)(\xi)=-ih\frac{\partial f}{\partial\xi_j}(\xi), \qquad \hat{z}=(\hat{q}_1,\ldots,\hat{q}_n;\hat{p}_1,\ldots,\hat{p}_n). \tag{2.7}$$

The operator on $\mathscr{H}$ associated with the phase-space function $g(z)$ is

$$\hat{g}=\frac{1}{(\pi\hbar)^n}\int\tilde{g}(z')e^{i\sigma(\hat{z},z')}\,dz', \tag{2.8}$$

where the Weyl operators $e^{i\sigma(\hat{z},z')}$ satisfy the Weyl relations[1,3,4,10,11]

$$e^{i\sigma(\hat{z},z_1)}e^{i\sigma(\hat{z},z_2)}=e^{i\sigma(z_1,z_2)}\cdot e^{i\sigma(\hat{z},z_1+z_2)}. \tag{2.9}$$

[The action of $e^{i\sigma(\hat{z},z)}$ on a function in $\mathscr{H}$ is[1]

$$(\exp[i\sigma(\hat{z},z)]f)(\xi)=\exp[-(2i/h)\mathbf{p}\cdot(\mathbf{q}+\xi)]f(\xi+2\mathbf{q}).] \tag{2.10}$$

In addition to being able to map functions into operators, one can extend the Weyl transform in a way that allows mapping finite measures to operators,[2] or even distributions to operators.[11–15] For example, the operator

$$\hat{v}=\frac{\hbar}{2}\int f(z',t)e^{i\sigma(\hat{z},z')}\,d\mu(z') \tag{2.11}$$

is the one associated with the measure used in (2.4) to define v.

Remarkably, it is also possible to directly write $\hat{v}$ in terms of v. Grossmann[10] has shown that if one is given a function $g(z)$ defined on phase space, and if one defines the parity operator Π by

$$\Pi f(\xi)=f(-\xi), \tag{2.12}$$

then one obtains for $\hat{g}$

$$\hat{g}=\frac{1}{(\pi\hbar)^n}\left(\int g(z)\Pi e^{i\sigma(\hat{z},z)}\,dz\right). \tag{2.13}$$

Replacing g by v in (2.13) gives $\hat{v}$ in terms of v.

One inverts the Weyl transform by means of the Wigner transform. If $\hat{g}$ is a trace-class operator that corresponds to g, then[1]

$$\tilde{g}(z)=2^n\,\mathrm{trace}(\hat{g}e^{i\sigma(z,\hat{z})}). \tag{2.14}$$

Since, by (2.13), $\Pi\hat{g}=\hat{\tilde{g}}$, and since $\tilde{\tilde{g}}=g$, one has[10,11]

$$g(z)=2^n\,\mathrm{trace}(\Pi\,\hat{g}e^{i\sigma(z,\hat{z})}). \tag{2.15}$$

Using this form for g, one can easily prove this proposition, which contains well-known results (Ref. 13, Theorem 3.5.4).

Proposition 2.1: If $\hat{g}$ is trace class, and if g is the Wigner transform of $\hat{g}$, then $g(z)$ is continuous in z, vanishes at infinity, and is in $L^2(\mathbb{R}^{2n})$. In addition, one can choose an orthonormal basis in $\mathscr{H}=L^2(\mathbb{R}^n)$ for which $\mathrm{trace}(\Pi\hat{g}e^{i\sigma(z,\hat{z})})$ will be, when expanded in terms of this basis, an absolutely and uniformly convergent series.

Proof: The only statement that requires comment is the existence of the basis mentioned in the proof. Using rather standard results from operator theory (Ref. 16, Secs. 2.2 and

2.3), we can easily show that the orthonormal basis $\{\psi_j\}_{j=1}^{\infty}$ gotten from diagonalizing the non-negative operator $\Pi\,\hat{g}\hat{g}^*\Pi$ will work.

Later on I will need $g\circ v - v\circ g$, where $g(z)$ is the Wigner transform of a trace-class operator and v is defined by (2.4). While I could use (2.3) to do this, I will not. It is easier to obtain the formula directly from (2.15).

Corollary 2.1: Let $\hat{g}$ be a trace-class operator defined on the Hilbert space $\mathscr{H}\equiv L^2(\mathbb{R}^n, d^n\xi)$, and let $g(z)$ be its Wigner transform. If v is given by (2.4), then

$$(g\circ v - v\circ g)(z) = -i\hbar\int g(z+z')\mathrm{Im}\{f(z',t)e^{i\sigma(z,z')}\}\,d\mu(z'). \quad (2.16)$$

Proof: The operator $\hat{v}$ defined by (2.11) is bounded, and so both $\hat{g}\hat{v}$ and $\hat{v}\hat{g}$ are trace-class operators.[16] Thus (2.15) applies:

$$g\circ v = 2^n\,\mathrm{trace}(\Pi\,\hat{g}\hat{v}e^{i\sigma(z,\hat{z})}). \quad (2.17)$$

One may put this into the form of an integral this way. First, in (2.17) replace $\hat{v}$ by its integral form (2.11), then interchange trace and integral; this may be justified by expanding the trace in the orthonormal basis described in the proof of Proposition 2.1. Second, use the Weyl relations (2.9) to simplify the integrand. Third, employing (2.15), (1.6), and an obvious change of variables in the integral, one gets

$$g\circ v(z) = \frac{\hbar}{2}\cdot\int g(z+z')e^{-i\sigma(z,z')}\,\overline{f(z',t)}\,d\mu(z'). \quad (2.18)$$

A similar computation gives

$$v\circ g(z) = \frac{\hbar}{2}\cdot\int g(z+z')e^{i\sigma(z,z')}f(z',t)\,d\mu(z'). \quad (2.19)$$

Subtract (2.19) from (2.18) and use $-2i\,\mathrm{Im}(c) = \bar{c} - c$ to get (2.16). This ends the proof.

There is a second commutator that I want to compute, $g\circ h - h\circ g$, where h is defined by (1.4) and g is the Wigner transform of a trace-class operator $\hat{g}$. Since $\hat{h}$, the operator that corresponds to h, is unbounded, the products $\hat{g}\hat{h}$ and $\hat{h}\hat{g}$ may also be unbounded; even worse, $\hat{h}\hat{g}$ may not be densely defined. Even so, it is possible to interpret both $g\circ h$ and $h\circ g$ as tempered distributions.[5,11,12,13]

To get this interpretation, first note that the mappings $\phi\to\phi\circ h$ and $\phi\to h\circ\phi$ are well-defined, continuous mappings from Schwartz space into itself. (See Ref. 5, Theorem 2.4.1; $\phi\in S_{-\infty}$ and $h\in S_2$ in Voros's notation.) In addition, the mapping $\psi\to(2\pi h)^n\,\mathrm{trace}(\hat{g}\hat{\psi})$ defines a continuous linear functional in Schwartz space, and so both $\phi\to(2\pi h)^n\,\mathrm{trace}\,(\hat{g}(\phi\circ h))$ and $\phi\to(2\pi h)^n\,\mathrm{trace}(\hat{g}h\circ\phi)$ define such functionals. Finally, define $g\circ h$ and $h\circ g$ to be the tempered distributions given by these continuous linear functionals:

$$\phi\to\int(g\circ h)(z)\phi(z)dz\equiv(2\pi\hbar)^n\,\mathrm{trace}(\hat{g}h\circ\phi), \quad (2.20)$$

$$\phi\to\int(h\circ g)(z)\phi(z)dz\equiv(2\pi\hbar)^n\,\mathrm{trace}(\hat{g}\phi\circ h),$$

where ϕ is a Schwartz function.

Having defined $h\circ g$ and $g\circ h$ by (2.20), I can now compute the comutator $g\circ h - h\circ g$.

Proposition 2.2: If $g(z)$ is the Wigner transform of a trace-class operator $\hat{g}$, and if $h(z)$ is given by (1.4), then $g\circ h - h\circ g$ is the tempered distribution

$$g\circ h - h\circ g = -(\hbar/i)\{g,h\}, \quad (2.21)$$

where $\{\ ,\ \}$ is the usual Poisson bracket

$$\{g,h\}\equiv\sum_{j=1}^{n}\left(\frac{\partial g}{\partial q_j}\frac{\partial h}{\partial p_j} - \frac{\partial g}{\partial p_j}\frac{\partial h}{\partial q_j}\right), \quad (2.22)$$

and where the derivatives are taken in a distributional sense.[17]

Proof: Let $\phi(z)$ be a Schwartz function. From (2.20) and the formula $(2\pi h)^n\,\mathrm{trace}(\hat{a}\hat{b}) = \int a(z)b(z)dz$,[11,18] one has

$$\int(g\circ h(z) - h\circ g(z))\phi(z) = (2\pi h)^n\,\mathrm{trace}[\hat{g}(h\circ\phi - \phi\circ h)] = \int g(z)(h\circ\phi(z) - \phi\circ h(z))dz. \quad (2.23)$$

Using a formula found in Ref. 5 [Theorem 2.4.1, part (iii)], one can compute $h\circ\phi - \phi\circ h$ when ϕ is a Schwartz function; the result is

$$h\circ\phi - \phi\circ h = -(\hbar/i)\{h,\phi\}. \quad (2.24)$$

Inserting (2.24) into (2.23) and integrating by parts in a distributional sense yield (2.21). This completes the proof.

I want to make a few remarks about what I have just discussed. First of all, one can define $g\circ h$ or $h\circ g$ whenever h belongs to one of Voros's[5] classes S_m. Functions in these classes are infinitely differentiable and, at infinity, behave like polynomials. Indeed, even when h is a polynomial of degree more than two, one can get a formula for $g\circ h - h\circ g$ that is similar to (2.21).

The second remark is that one can define operator products like $\hat{h}\hat{g}$ and $\hat{g}\hat{h}$ in a purely operator-theoretic setting. This in fact has been done by Hagedorn, Loss, and Slawny.[19]

Finally, an approach that in some sense comes halfway between what I have talked about above and what Hagedorn *et al.*[19] use is taken by Combe *et al.*[1] They define certain commutator products via a combination of Fourier transforms of Wigner distribution functions and weak-operator products similar to the ones used in Ref. 19.

III. AN INTEGRAL FORM FOR THE QUANTUM LIOUVILLE EQUATION

States in the Schrödinger formulation of quantum mechanics are the density matrices. (Recall that a density matrix is a non-negative, trace-class operator whose trace is unity.) In the Wigner–Weyl phase-space formulation of quantum mechanics, the states are Wigner distribution functions, which are related to density matrices this way: If $\hat{r}$ is a density matrix whose Wigner transform is $r(z)$, then the Wigner distribution that corresponds to $\hat{r}$ is[3]

$$\rho(z) = (2\pi\hbar)^{-n}r(z) = (\pi\hbar)^{-n}\,\mathrm{trace}(\Pi\hat{r}e^{i\sigma(z,\hat{z})}). \quad (3.1)$$

[I have used (2.15) to get the far right term in (3.1).]

For the system described in the Introduction, states in

the Wigner–Weyl formulation evolve according to the quantum Liouville equation

$$\frac{\partial \rho}{\partial t} = \frac{i}{\hbar}(\rho \circ H - H \circ \rho), \tag{3.2}$$

where H is given by (1.3). Since ρ is the Wigner transform of a trace-class operator, one may evaluate the commutator that appears in (3.2) by means of Corollary 2.1 and Proposition 2.2. Doing the evaluation results in

$$\frac{\partial \rho}{\partial t} = -\{\rho,h\} + \lambda \int \rho(z+z',t) \times \mathrm{Im}\{f(z',t)e^{i\sigma(z,z')}\}d\mu(z'), \tag{3.3}$$

where the derivatives are taken in a distributional sense; also, the initial condition is $\rho(z,0) = \rho_{\mathrm{in}}(z)$.

The form of the quantum Liouville equation given in (3.3) is not the best one for my purpose, which is to expand ρ in a power series in λ. To get a more suitable form, first let $\Phi(\tau)$ be the unique $(2n)\times(2n)$ fundamental solution that is associated with the linear, homogeneous, τ-dependent Hamiltonian system

$$\frac{dp_j}{d\tau} = -\frac{\partial h}{\partial q_j}, \quad \frac{dq_j}{d\tau} = \frac{\partial h}{\partial p_j}, \quad j = 1,\ldots,n, \tag{3.4}$$

and that is subject to the initial condition $\Phi(0) = I$. Next, set

$$\Lambda(\tau,t) \equiv \Phi(\tau)\Phi(t)^{-1}. \tag{3.5}$$

Finally, a straightforward calculation shows that (3.3) is equivalent to

$$\rho(z,t) - \rho_{\mathrm{in}}(\Lambda(0,t)z) = \lambda \int_0^t d\tau \int d\mu(z')\rho(z' + \Lambda(\tau,t)z,\tau)\mathrm{Im}\{f(z',\tau) \times \exp[i\sigma(\Lambda(\tau,t)z,z')]\}, \tag{3.6}$$

which is the form of (3.3) that I want.

There are several things that ought to be said now. First, the linear transformation $z \to \Phi(\tau)z$ is, for each τ, a canonical one, for it is generated by the time evolution of a Hamiltonian system.[20] This means that the matrix $\Phi(\tau)$ is symplectic[20]; that is,

$$\sigma(\Phi z_1, \Phi z_2) = \sigma(z_1,z_2). \tag{3.7}$$

Clearly, the mapping $z \to \Lambda(\tau,t)z$ is also a linear canonical transformation, and so the operation $\rho(z) \to \rho(\Lambda(\tau,t)z)$ preserves both the cone of classical states and the cone quantum mechanical states (the Wigner distribution functions).[1,19,21] Second, if one sets $\lambda = 0$ in (3.6), one gets that $\rho(z,t) = \rho_{\mathrm{in}}(\Lambda(0,t)z)$. This is interesting because it very clearly shows that for the system with Hamiltonian h, the difference between quantum and classical behavior is due entirely to the state chosen initially.[19,21]

Last, the work of Hagedorn *et al.*[19] contains a very nice discussion of topics related to time-dependent, quadratic Hamiltonians. In particular, this paper makes use of the connection between the quantum and classical time evolution for such Hamiltonians.

IV. A SERIES SOLUTION TO THE QUANTUM LIOUVILLE EQUATION

Having put the quantum Liouville equation into its integral form (3.6), one can easily generate a formal power series (in λ) that "solves" the equation. To do this and to simplify many of the expressions involved, first define the integral operator K by

$$(K\rho)(z,t) = \int_0^t dt \int d\mu(z')[\rho(\Lambda(\tau,t)z + z',\tau) \times \mathrm{Im}\{f(z',\tau)\exp[i\sigma(\Lambda(\tau,t)z,z')]\}], \tag{4.1}$$

and note that with this bit of notation (3.6) becomes

$$\rho(z,t) = \rho_0(z,t) + \lambda(K\rho)(z,t), \qquad \rho_0(z,t) = \rho_{\mathrm{in}}(\Lambda(0,t)z). \tag{4.2}$$

Applying the method of successive approximations,[22] one gets the Neumann series

$$\rho(z,t;\lambda) = \sum_{j=0}^{\infty} \lambda^j (K^j \rho_0)(z,t) \tag{4.3}$$

as a formal solution to (4.2). (This series is, in fact, gotten in the same way as the Dyson expansion that solves the operator version of Schrödinger's equation.[8,23])

What I want to do in this section is to show that when $\rho_{\mathrm{in}}(z)$ belongs to one of several function spaces, the series (4.3) converges and defines an entire function of λ. Before I can show this, I need to introduce some notation. Throughout the rest of the section, let α be a fixed, positive number and let J be the closed interval $J = [0,\alpha]$. Also, take X to be a Banach space having the norm $\|\cdot\|_X$, and take $C[J,X]$ to be the Banach space of functions that continuously map J into X; the norm in $C[J,X]$ is $\|x(t)\|_C = \sup_{t\in J}\|x(t)\|_X$.

I should mention that I will specify what spaces can be taken for X later on. Also, the only significance of J is that it provides a compact time interval, which is easier to deal with than $[0,\infty)$. Finally, one has for K

$$K\rho(z,t) = \frac{1}{2i} D_{\Phi(t)} \left\{ \int_0^t d\tau \int d\mu(z') \times \left[f(z',\tau)(D_{\Phi(\tau)^{-1}} S_{z'}^{+} \rho)(z,\tau) - \overline{f(z',\tau)}(D_{\Phi(\tau)^{-1}} S_{z'}^{-} \rho)(z,\tau) \right] \right\}, \tag{4.4}$$

where the operators D_M and $S_{z'}^{\pm}$ are defined by

$$(S_{z'}^{\pm} g)(z) \equiv g(z+z')e^{\pm i\sigma(z,z')}, \qquad (D_M g)(z) \equiv g(M^{-1}z), \tag{4.5}$$

for all $g \in X$, $z' \in \mathbb{R}^{2n}$, and every symplectic matrix M.

The set of $2n \times 2n$ symplectic matrices is a topological group, the symplectic group $\mathrm{Sp}(2n)$.[20] My reason for working with such matrices stems from a fact that I discussed at the end of Sec. III: $\Phi(s)$ is symplectic for every value of s.

In order to make the method of successive approximations work, I need to make these assumptions about X, D_M, and the $S_{z'}^{\pm}$.

(i) There exist constants c_1 and c_2 such that, for all $g \in X$, $M \in \mathrm{Sp}(2n)$, and $z' \in \mathbb{R}^{2n}$, one has $\|D_M g\|_X \leqslant c_1\|g\|_X$ and

$\|S_{z'}^{\pm} g\|_X \leqslant c_2 \|g\|_X$.

(ii) For each fixed $g \in X$, the mappings $M \to D_M g$ and $z' \to S_{z'}^{\pm} g$ are strongly continuous mappings from $\mathrm{Sp}(2n)$ and $\mathbb{R}^{2n}$ (respectively) into X.

A function space X will be called *admissible* if it is a separable Banach space that satisfies (i) and (ii). For such spaces, one has the following technical lemmas.

Lemma 4.1: Let X be admissible. If $\rho \in C[J,X]$, then $D_{\Phi(\tau)^{-1}} S_{z'}^{\pm} \rho(\cdot,\tau)$ are strongly continuous X-valued functions of (z',τ), for all $(z',\tau) \in \mathbb{R}^{2n} \times J$. Moreover,

$$\|D_{\Phi(\tau)^{-1}} S_{z'}^{\pm} \rho(\cdot,\tau)\|_X \leqslant c_1 c_2 \|\rho(\cdot,\tau)\|_X \leqslant c_1 c_2 \|\rho\|_C. \tag{4.6}$$

Proof: It is easy to show that $D_M S_{z'}^{\pm} \rho(\cdot,\tau)$ is jointly and strongly continuous in M, z', τ. Since $\tau \to \Phi(\tau)$ is a continuous map from $\mathbb{R}$ to $\mathrm{Sp}(2n)$, and since taking inverses is a continuous transformation on a topological group, the mapping $\tau \to \Phi(\tau)^{-1}$ is continuous, and

$$(\tau,z') \to D_{\Phi(\tau)^{-1}} S_{z'}^{\pm} \rho(\cdot,\tau)$$

are thus jointly and strongly continuous maps from $J \times \mathbb{R}^{2n}$ into X.

The norm estimate is a direct consequence of (i), which holds because X is admissible. This finishes the proof.

Lemma 4.2: Let X be admissible. If $\rho \in C[J,X]$, then the X-valued functions

$$\rho_+(\cdot,z',\tau) \equiv f(z',\tau)\,(D_{\Phi(\tau)^{-1}} S_{z'}^{+} \rho)(\cdot,\tau),$$
$$\rho_-(\cdot,z',\tau) \equiv \overline{f(z',\tau)}\,(D_{\Phi(\tau)^{-1}} S_{z'}^{-} \rho(\cdot,\tau) \tag{4.7}$$

are Bochner-integrable (cf. Ref. 24, Sec. 3.7) with respect to the measure $d\tau \times d\mu(z')$. Moreover,

$$F(\cdot,t) \equiv \frac{1}{2i} \int_{[0,t] \times \mathbb{R}^{2n}} d\tau\, d\mu(z')\,[\,\rho^+(\cdot,z',\tau) - \rho^-(\cdot,z',\tau)\,] \tag{4.8}$$

is in $C[J,X]$, can be computed via

$$F(\cdot,t) \equiv \frac{1}{2i} \int_0^t d\tau \int d\mu(z')\,[\,\rho^+(\cdot,z',\tau) - \rho^-(\cdot,z',\tau)\,], \tag{4.9}$$

and satisfies the inequality

$$\|F(\cdot,t)\|_X \leqslant c_1 c_2 \|f\|_\infty\, \mu(\mathbb{R}^{2n}) \int_0^t \|\rho(\cdot,\tau)\|_X\, d\tau. \tag{4.10}$$

Proof: By Lemma 4.1, the X-valued functions $(D_{\Phi(\tau)^{-1}} S_{z'}^{\pm} \rho)(\cdot,\tau)$ are strongly continuous in (z',τ). Thus for every continuous linear functional $g^* \in X^*$, the scalar-valued functions $g^*[\,(D_{\Phi(\tau)^{-1}} S_{z'}^{\pm} \rho)(\cdot,\tau)\,]$ are continuous in (z',τ), and are therefore measurable with respect to $d\tau\, d\mu(z')$. This means that $(D_{\Phi(\tau)^{-1}} S_{z'}^{\pm} \rho)(\cdot,\tau)$ are, by definition (Ref. 24, Definition 3.5.4), weakly measurable with respect to $d\tau\, d\mu(z')$, and, because X is separable they are in fact strongly measurable with respect to $d\tau\, d\mu(z')$ (cf. Ref. 24, Corollary 2, p. 73). Finally, since the product of measurable scalar-valued functions and strongly measurable vector-valued functions is itself a strongly measurable vector-valued function (cf. Ref. 24, Theorem 3.5.4), and since $f(z',\tau)$, $\overline{f(z',\tau)}$ are both bounded, measurable functions, the two functions ρ^+ and ρ^- are strongly measurable.

To see that the functions $\rho^{\pm}$ are Bochner-integrable with respect to $d\tau \times d\mu(z')$, note that from (4.6), (4.7), and the fact that $f \in L^\infty$, one has

$$\|\rho^{\pm}(\cdot,z',\tau)\|_X \leqslant \|f\|_\infty\, c_1 c_2 \|\rho\|_{C[J,X]}, \tag{4.11}$$

and so

$$\int_{J \times \mathbb{R}^{2n}} d\tau\, d\mu(z') \|\rho^{\pm}(\cdot,z',\tau)\|_X \leqslant \alpha c_1 c_2\, \mu(\mathbb{R}^{2n}) \|f\|_\infty \|\rho\|_{C[J,X]}. \tag{4.12}$$

From (4.12) and the strong measurability of $\rho^{\pm}$, it follows that $\rho^{\pm}$ are Bochner-integrable with respect to $d\tau\, d\mu(z')$ (cf. Ref. 24, Theorem 3.7.4).

Seeing that $F(\cdot,t)$ is in $C[J,X]$ is not hard. From (4.11) and Theorem 3.7.6 of Ref. 24, one has the inequality

$$\|F(\cdot,t_2) - F(\cdot,t_1)\|_X \leqslant \text{const} \times |t_2 - t_1|, \tag{4.13}$$

which implies the continuity of $F(\cdot,t)$ in t on J.

Equation (4.9) follows from (4.8) and the Bochner-integral analog of Fubini's theorem (Ref. 24, Theorem 3.7.13). The inequality (4.10) results from applying Theorem 3.7.6 of Ref. 24 to (4.8) and then using the inequality in (4.6). The proof is ended.

Lemma 4.2 is important because it shows how to make sense out of the integral used to define $K\rho(z,t)$ in (4.4). Indeed, using (4.4) and the function $F(\cdot,t)$ defined in (4.8), one has

$$K\rho(z,t) = D_{\Phi(t)} F(z,t). \tag{4.14}$$

Assuming that the hypotheses of Lemma 4.2 hold, one can show that $(K\rho)(z,t)$ is in $C[J,X]$, and one can get bounds for the norm of K^j. To see that $K\rho \in C[J,X]$, first note that $F \in C[J,X]$, and that $t \to \Phi(t)$ is a continuous mapping of J into $\mathrm{Sp}(2n)$. Using an argument similar to the one employed in the proof of Lemma 4.1, one then gets that $K\rho \in C[J,X]$.

One gets the norm estimates this way. First, since X is admissible and $\Phi(t) \in \mathrm{Sp}(2n)$, assumption (i) from the definition of admissibility implies that

$$\|K\rho(\cdot,t)\|_X \leqslant c_1 \|F(\cdot,t)\|_X. \tag{4.15}$$

Combining (4.10) and (4.15) yields

$$\|K\rho(\cdot,t)\|_X \leqslant c \int_0^t \|\rho(\cdot,\tau)\|_X\, d\tau,$$
$$c \equiv c_1^2 c_2 \|f\|_\infty\, \mu(\mathbb{R}^{2n}). \tag{4.16}$$

"Bootstrapping" (4.16), using $\|\rho(\cdot,t)\|_X \leqslant \|\rho\|_{C[J,X]}$, and doing a standard multiple integral result in

$$\|K^j \rho(\cdot,t)\|_X \leqslant [\,(ct)^j/j!\,] \|\rho\|_{C[J,X]}. \tag{4.17}$$

Finally, taking the supremum in (4.17) gives

$$\|K^j \rho\|_{C[J,X]} \leqslant [\,(c\alpha)^j/j!\,] \|\rho\|_{C[J,X]}. \tag{4.18}$$

The norm estimates in (4.18) are sufficient to guarantee the convergence of (4.3), provided $\rho_0(z,t) \in C[J,X]$. For if $\rho_0 \in C[J,X]$, then the series in (4.3) is majorized by the power series for $\exp(c\alpha|\lambda|)$, and so it converges for all values of λ to a $C[J,X]$-valued entire function of λ, $\rho(z,t;\lambda)$.

By plugging the series of $\rho(z,t;\lambda)$ into the integral equation in (4.2), one can see that, apart from the special form of ρ_0 used there, ρ satisfies the equation for every $\rho_0 \in C[J,X]$. Also, a standard argument shows that the solution is unique.

Thus, the only question left is whether the function

$$\rho_0(z,t) \equiv D_{\Phi(t)}\,\rho_{\rm in}(z) \tag{4.19}$$

belongs to $C[J,X]$. [Note: $\Lambda(0,t) = \Phi(t)^{-1}$ because $\Phi(0) = I$.] The answer is yes, provided only that $\rho_{\rm in}(z) \in X$. The argument is much the same as that used in Lemma 4.1 or the one used to show that K: $C[J,X] \to C[J,X]$, and so I will omit it.

The next theorem is a summary of the results gotten in the discussion given above.

Theorem 4.1: Let X be admissible and let $\rho_0(z,t)$ be in $C[J,X]$. If in (4.4) the integrals are taken in the sense of Bochner, then K maps $C[J,X]$ into itself, and satisfies the bounds (4.16) and (4.17). In addition, the Neumann series (4.3) converges to a $C[J,X]$-valued entire function $\rho(z,t;\lambda)$ that uniquely solves the integral equation in (4.2). Finally, if $\rho_{\rm in}(z) \in X$, then $\rho_0(z,t) \equiv \rho_{\rm in}(\Lambda(0,t)z)$ belongs to $C[J,X]$, and the corresponding function $\rho(z,t;\lambda)$ defined by (4.3) uniquely solves the problem posed in (4.2).

The main hypothesis of Theorem 4.1, whose conclusions regarding the convergence of (4.3) and the solution of (4.2) are what I have been working towards, is the admissibility of X. In the lemma below, I give a list of spaces that are admissible.

Theorem 4.2: The following spaces are admissible: $C_0(\mathbb{R}^{2n})$, the space of functions continuous on $\mathbb{R}^{2n}$ and vanishing at ∞; $L^p(\mathbb{R}^{2n})$, with $1 \leqslant p < \infty$; T, the space of functions that are Wigner transforms of trace-class operators (the norm for $g \in T$ is $\|g\|_T \equiv \|\hat{g}\|_{\rm trace}$); and $X_1 \cap X_2$, whenever X_1 and X_2 are admissible. (The norm in $X_1 \cap X_2$ is $\|\cdot\|_{X_1 \cap X_2} = \max\{\|\cdot\|_{X_1}, \|\cdot\|_{X_2}\}$.)

Proof: The L^p spaces ($1 \leqslant p < \infty$) and $C_0(\mathbb{R}^{2n})$ are all well known to be separable spaces. T is also separable because it is isometrically isomorphic to $C_1(\mathscr{H})$, the Banach space of trace-class operators on $\mathscr{H} = L^2(\mathbb{R}^{2n})$; $C_1(\mathscr{H})$ is the trace-norm closure of the span of finite rank operators,[16] and so it is separable. Finally, because the intersection of separable Banach spaces is separable, and because X_1 and X_2, being admissible, are separable, the intersection $X_1 \cap X_2$ is separable. [It is very easy to check that $X_1 \cap X_2$ satisfies assumptions (i) and (ii), and so there is no need to discuss $X_1 \cap X_2$ in the rest of the proof.]

Fix $M \in {\rm Sp}(2n)$, the set of $2n \times 2n$ real symplectic matrices, and consider the operator D_M defined in (4.5). Because[20] $\det M = \det(M^{-1}) = 1$, the measure $dz = dq_1 \cdots dq_n\, dp_1 \cdots dp_n$ is invariant under the transformation $z \to M^{-1}z$, so the operator D_M is actually an isometry for the L^p spaces. Also, because $D_M g(z) = g \circ M^{-1}(z)$, D_M will not affect $\sup|g|$, the behavior of g at ∞, or the continuity properties of g; hence D_M is an isometry for $C_0(\mathbb{R}^{2n})$.

D_M is an isometry for T, too. If $g \in T$, then (2.15) gives

$$D_M g(z) = 2^n\,{\rm trace}(\Pi\,\hat{g} e^{i\sigma(M^{-1}z,\hat{z})}) \tag{4.20}$$

Using the fact that M^{-1} leaves σ invariant [see Eq. (3.7)] and (2.9), one finds that the operators

$$W_M(z) = e^{i\sigma(\hat{z},M^{-1}z)} \tag{4.21}$$

satisfy the Weyl relations,

$$W_M(z_1)\,W_M(z_2) = e^{i\sigma(z_1,z_2)}\,W_M(z_1+z_2). \tag{4.22}$$

Since, in addition, for M fixed, they form an irreducible, unitary family, von Neumann's theorem[25] implies the existence of a unitary operator U_M such that for every $z \in \mathbb{R}^{2n}$

$$W_M(z) \equiv e^{i\sigma(\hat{z},M^{-1}z)} = U_M^* e^{i\sigma(\hat{z},z)} U_M. \tag{4.23}$$

From this, (4.20), and (2.15), one gets that

$$D_M g = \Pi U_M \Pi \hat{g} U_M^*. \tag{4.24}$$

Moreover, neither pre- nor postmultiplying by unitary operators changes the trace-norm, so

$$\|D_M g\|_T = \widehat{\|D_M g\|}_{\rm trace} = \|\hat{g}\|_{\rm trace} = \|g\|_T; \tag{4.25}$$

hence D_M is an isometry for T.

Even the $S_{z'}^{\pm}$ are isometries for $C_0(\mathbb{R}^{2n})$, the L^p, and T. Except for T, this is obvious. To deal with T, let $g \in T$. Note that, from (2.15) and the Weyl relations (2.9), one has

$$\begin{aligned} S_{z'}^{-} g &= \hat{g} e^{i\sigma(z',\hat{z})} \\ S_{z'}^{+} g &= \Pi e^{i\sigma(z',\hat{z})} \Pi\,\hat{g}. \end{aligned} \tag{4.26}$$

Again, because pre- or postmultiplying by a unitary operator leaves the trace-norm unchanged, one gets

$$\|S_{z'}^{\pm} g\|_T = \widehat{\|S_{z'}^{\pm} g\|}_{\rm trace} = \|\hat{g}\|_{\rm trace} = \|g\|_T, \tag{4.27}$$

and so that $S_{z'}^{\pm}$ are isometries for T.

Having verified that the spaces listed satisfy assumption (i), I now want to turn to showing that the D_M and $S_{z'}^{\pm}$ are strongly continuous in M and z', respectively. I will do the D_M first.

Using the definition of D_M, one can easily show that the mapping $M \to D_M$ is a faithful representation of ${\rm Sp}(2n)$, and so, in the usual way, one sees that D_M being continuous at given M_0 is equivalent to D_M being continuous at $M = I$, the identity matrix. This reduction and standard analytical arguments are enough to show that D_M is continuous on $C_0(\mathbb{R}^{2n})$ and on the L^p-spaces ($1 \leqslant p < \infty$).

Once again, T's case takes some work. First of all, if $g \in T$, then $\hat{g} \in C_1(\mathscr{H})$, and it looks like[16]

$$\hat{g} = \hat{g}_1 \hat{g}_2, \tag{4.28}$$

where $\hat{g}_1$ and $\hat{g}_2$ are in $C_2(\mathscr{H})$, the set of Hilbert–Schmidt operators. The space $C_2(\mathscr{H})$ is, under the Wigner–Weyl transform, isometrically isomorphic to $L^2(\mathbb{R}^{2n})$ (see Ref. 18), and the function g equivalent to $\hat{g}$ in (4.28) has the form

$$g(z) = g_1 \circ g_2(z), \tag{4.29}$$

where "$\circ$" is the same as in (2.3), and where g_1 and g_2 are in $L^2(\mathbb{R}^{2n})$. By making the changes of variables $z_1 \to M^{-1}z_1$ and $z_2 \to M^{-1}z_2$ in (2.3), and by noting that $\sigma(M^{-1}z_1, M^{-1}z_2) = \sigma(z_1,z_2)$ and that $\det(M) = 1$, one sees that

$$(D_M g)(z) = (D_M g_1) \circ (D_M g_2)(z), \tag{4.30}$$

and that

$$D_m g - g = D_M g_1 \circ (D_M g_2 - g_2) + (D_M g_1 - g_1) \circ g_2, \tag{4.31}$$

and, finally, that

$$\widehat{D_M g - g} = \widehat{D_M g_1}\,\widehat{(D_M g_2 - g_2)} + \widehat{(D_M g_1 - g_1)}\,\hat{g}_2. \tag{4.32}$$

Second, take the trace-norm of both sides, and use $\|AB\|_{\rm trace} \leqslant \|A\|_{C_2} \|B\|_{C_2}$ (see Ref. 16) to get the inequality

$$\begin{aligned} &\|\widehat{D_M g - g}\|_{\rm trace} \\ &\leqslant \|\widehat{D_M g_1}\|_{C_2} \|\widehat{D_M g_2 - g_2}\|_{C_2} + \|\widehat{D_M g_1 - g_1}\|_{C_2} \|\hat{g}_2\|_{C_2}. \end{aligned} \tag{4.33}$$

Since C_2 is isometrically isomorphic to $L^2(\mathbb{R}^{2n})$, the Wigner-transformed version of (4.33) is

$$\|D_M g - g\|_T \leqslant \|g_1\|_{L^2}\|D_M g_2 - g_2\|_{L^2} + \|g_2\|_{L^2}\|D_M g_1 - g_1\|_{L^2}; \tag{4.34}$$

here, I have also used the fact that the D_M are isometries on $L^2(\mathbb{R}^{2n})$. Using the continuity of D_M on $L^2(\mathbb{R}^{2n})$ and the inequality (4.34) gives $\lim_{M\to I}\|D_M g - g\|_T = 0$, so the D_M are continuous at the identity when they act on T. By the remarks made earlier, this means that D_M is strongly continuous on T.

Similar arguments are sufficient to get the continuity of $S_{z'}^{\pm}$ in z' for the spaces $C_0(\mathbb{R}^{2n})$, $L^P(\mathbb{R}^{2n})$, and T. As in the case of the D_M, one may reduce the problem of showing continuity on T to one of showing continuity on L^2 via

$$\begin{aligned} S_{z'}^{+}(g_1 \circ g_2)(z) &= [(S_{z'}^{+} g_1)\circ g_2](z), \\ S_{z'}^{-}(g_1 \circ g_2)(z) &= [g_1 \circ (S_{z'}^{-} g_2)](z). \end{aligned} \tag{4.35}$$

This completes the proof.

Of course, one immediately has this corollary.

Corollary 4.1: The conclusions of Theorem 4.1 hold when X is $C_0(\mathbb{R}^{2n})$, any $L^P(\mathbb{R}^{2n})$ with $1 \leqslant p < \infty$, T, or any finite intersection of the preceding spaces. Moreover, for these spaces, one may take $c_1 = 1$ and $c_2 = 1$ in (4.16)–(4.18).

Proof: Only the last statement requires comment. In proving Theorem 4.2, I actually showed that D_M and $S_{z'}^{\pm}$ were isometries on $C_0(\mathbb{R}^{2n})$, the L^P and T. Hence, for these spaces one has $c_1 = c_2 = 1$. Indeed, examining the definition of the intersection of two Banach spaces shows that the operators are isometries for intersections too; hence, $c_1 = c_2 = 1$ for these as well. The proof is done.

I remark that $L^\infty(\mathbb{R}^{2n})$ is conspicuously absent from the list of spaces in Corollary 4.1. This is because L^∞ is not admissible, for it is not separable and it fails to satisfy assumption (ii).

Of course, from the point of view of quantum mechanics, T is the most important of the spaces listed in Corollary 4.1. Unfortunately, it is also the most difficult to work with. The other spaces, though of less physical importance, are, from a mathematical point of view, more tractable.

Among the spaces listed, the best substitute for T is perhaps $C_0(\mathbb{R}^{2n}) \cap L^2(\mathbb{R}^{2n})$. To the best of my knowledge, this space encompasses all of the known "generic" properties of T, and, indeed, it contains T. (See Ref. 13, Theorem 3.5.4.)

The reverse inclusion does not hold, however. The function g defined by

$$g(q,p) = \frac{\hbar}{\pi qp}\sin\left(\frac{2qp_0'}{\hbar}\right)\sin\left(\frac{2pq_0'}{\hbar}\right) \tag{4.36}$$

is the symplectic Fourier transform of $\tilde{g}$, the characteristic function for the rectangle $[-q_0', q_0'] \times [-p_0', p_0']$. Clearly, g is continuous, falls to 0 at ∞, and is in L^2. On the other hand, $\tilde{g}$ is *not* continuous and therefore cannot be in T. Since taking symplectic transforms preserves T, and since $\tilde{\tilde{g}} = g$, g cannot be in T either.

V. TIME EVOLUTION OF THE CONE OF STATES

There is one point that I have not touched upon, but that I ought to say something about. In Sec. IV, I showed that (4.2) is uniquely solved by (4.3) for a variety of spaces, including T, the space of functions that are Wigner transforms of trace-class operators. Now, T contains the cone of Wigner distribution functions (the phase-space functions that correspond to the usual quantum mechanical states, the density matrices), and the solution (4.3) should preserve this cone as well as T itself. I want to show that this is indeed the case.

The first step in showing that the cone is preserved is to rewrite (4.2) with K in terms of a commutator instead of an integral over $d\mu(z')$. One can do this by combining (2.16), (4.2), (4.4), and (4.19). The result is

$$\rho(z,t) = D_{\Phi(t)}\left\{\rho_{\text{in}}(z) + \frac{i}{\hbar}\int_0^t d\tau\, D_{\Phi(\tau)^{-1}}[\rho(\cdot,\tau), v(\cdot,\tau)](z)\right\}, \tag{5.1}$$

where $[a,b] = a\circ b - b\circ a$.

Two things follow from (5.1). The first is that

$$\int \rho(z,t)dz = \int \rho_{\text{in}}(z)dz, \tag{5.2}$$

because, for every $M \in \mathrm{Sp}(2n)$, $\int (D_M g)(z)dz = \int g(z)dz$ and because $\int [a,b](z)dz = 0$; the second is that

$$\frac{\partial}{\partial t}[(D_{\Phi(t)^{-1}}\rho)(z,t)] = (i/\hbar)D_{\Phi(t)^{-1}}[\rho(\cdot,t), v(\cdot,t)](z), \tag{5.3}$$

which holds for almost every t. Using (4.30), one may rewrite (5.3) as

$$\frac{\partial}{\partial t}[(D_{\Phi(t)^{-1}}\rho)(z,t)] = (i/\hbar)[D_{\Phi(t)^{-1}}\rho, D_{\Phi(t)^{-1}}v](z). \tag{5.4}$$

If ρ_1 and ρ_2 are two arbitrary T-valued solutions to (5.1), with $\rho_1(z,0) = \rho_{\text{in}}^{(1)}(z)$ and $\rho_2(z,0) = \rho_{\text{in}}^{(2)}(z)$, then a straightforward computation, using (5.4), (4.30), and elementary properties of commutators, yields

$$\frac{\partial}{\partial t}[D_{\Phi(t)^{-1}}(\rho_1\circ\rho_2)(z,t)] = (i/\hbar)D_{\Phi(t)^{-1}}[\rho_1\circ\rho_2, v](z). \tag{5.5}$$

Integrating (5.5) then implies that $\rho_1\circ\rho_2$ satisfies (5.1) with $\rho_{\text{in}} = \rho_{\text{in}}^{(1)}(z)\circ\rho_{\text{in}}^{(2)}$. The uniqueness of solutions to (5.1) then gives the following theorem.

Theorem 5.1: If $\rho(z,t)$ solves (5.1) with $\rho(z,0) = \rho_{\text{in}}^{(1)}\circ\rho_{\text{in}}^{(2)}(z)$, where both $\rho_{\text{in}}^{(1)}$ and $\rho_{\text{in}}^{(2)}$ are in T, then

$$\rho(z,t) = (\rho_1\circ\rho_2)(z,t), \tag{5.6}$$

where ρ_1 and ρ_2 solve (5.5) with the initial conditions $\rho_1(z,0) = \rho_{\text{in}}^{(1)}(z)$, $\rho_2(z,0) = \rho_{\text{in}}^{(2)}(z)$.

As corollaries to this theorem, I will now show that the solution to (5.1) not only preserves the cone of states, but that it also preserves the pure (extremal) states of that cone.

Corollary 5.1: If $\rho_{\text{in}}(z)$ is a Wigner distribution function

that corresponds to a pure state (rank-one orthogonal projection), then the solution $\rho(z,t)$ to (5.1) does too.

Proof: The function $\rho_{\text{in}}(z)$ corresponds to a pure state if and only if $\int \rho_{\text{in}}(z)dz = 1$ and $\rho_{\text{in}} \circ \rho_{\text{in}}(z) = (2\pi\hbar)^n \rho_{\text{in}}(z)$. Now, let $\rho(z,t)$ be the solution to (5.1) that has $\rho_{\text{in}}(z)$ as its initial value. By Theorem 5.1, $\rho \circ \rho(z,t)$ is the solution to (5.1) that has initial value $\rho_{\text{in}}(z) \circ \rho_{\text{in}}(z) = (2\pi\hbar)^n \rho_{\text{in}}(z)$. By the uniqueness of solutions to (5.1), one then gets that $\rho \circ \rho(z,t) = (2\pi\hbar)^n \rho(z,t)$. Since $\int \rho_{\text{in}}(z)dz = 1$, (5.2) implies that $\int \rho(z,t)dz = 1$. Hence, for each fixed t, $\rho(z,t)$ is a Wigner distribution function that corresponds to a pure state.

Corollary 5.2: If $\rho_{\text{in}}(z)$ is a Wigner distribution function (WDF) that corresponds to a state (density matrix), then the solution $\rho(z,t)$ to (5.1) does too.

Proof: Using the spectral resolution of the density matrix, one may write $\rho_{\text{in}}(z)$ as this convex combination of WDF's coming from pure states:

$$\rho_{\text{in}}(z) = \sum_{j=1}^{\infty} \beta_j \rho_{\text{in}}^{(j)}(z), \tag{5.7}$$

where $\beta_j \geqslant 0$ and $\Sigma_{j=1}^{\infty} \beta_j = 1$. By the principle of superposition,

$$\rho(z,t) = \sum_{j=1}^{\infty} \beta_j \rho_j(z,t), \tag{5.8}$$

where the $\rho_j(z,t)$ are the solutions to (5.1) that correspond to the initial values of $\rho_{\text{in}}^{(j)}(z)$. By Corollary 5.1, the $\rho_j(z,t)$'s correspond to pure states; thus $\rho(z,t)$ is a convex combination of WDF's corresponding to pure states, and so it itself is a WDF corresponding to a mixed state. This ends the proof.

These two corollaries show that mixed states evolve into mixed states, and pure states into pure states. No crossing of one type into the other ever occurs.

VI. CONCLUDING REMARKS

I want to begin by indicating where one might apply the results I have gotten. One place is in approximating the time evolution of the WDF for a system subject to forces arising from a uniform electromagnetic field plus some small perturbing potential. (The perturbation need not be electromagnetic in origin.)

As an example of such a system, consider a spinless, charged particle bathed in an electromagnetic field described by the vector and scalar potentials:

$$\mathbf{A}(\mathbf{r}) = \tfrac{1}{2}\mathbf{B}_0 \times \mathbf{r}, \quad \Phi(\mathbf{r},t) = -\mathbf{E}_0 \mathbf{r} + \lambda\phi(\mathbf{r},t). \tag{6.1}$$

The vectors $\mathbf{E}_0$ and $\mathbf{B}_0$ are constant; $\phi(\mathbf{r},t)$ is the perturbation. If the particle has a positive charge of Ne, then the classical nonrelativistic Hamiltonian corresponding to this system is[23]

$$H(\mathbf{r},\mathbf{p},t) = (1/2m)(\mathbf{p} - \text{Ne}\,\mathbf{A})^2 - \text{Ne}\,\mathbf{E}_0 \mathbf{r} + \lambda v(\mathbf{r},t), \tag{6.2}$$

where $v = \text{Ne}\,\phi$. (The speed of light is taken to be 1.)

When $\mathbf{E}_0 = 0$, this system is a crude model of a positively charged particle in a cyclotron. Let $\rho(\mathbf{r},\mathbf{p},t,\lambda)$ be the WDF that represents the state of this system as it evolves from some initial state $\rho_{\text{in}}(\mathbf{r},\mathbf{p})$. Assuming that v has the form (1.5), one sees that the Hamiltonian for this system has the form (1.3), with

$$h(\mathbf{r},\mathbf{p},t) = (1/2m)(\mathbf{p} - \text{Ne}\,\mathbf{A})^2. \tag{6.3}$$

Thus Theorem 4.1 applies, and one sees that $\rho(\mathbf{r},\mathbf{p},t,\lambda)$ is entire in λ. In addition, if $\rho_0(\mathbf{r},\mathbf{p},t)$ is the state classically evolved out of $\rho_{\text{in}}(\mathbf{r},\mathbf{p})$ via the Hamiltonian h in (6.3), one gets the inequality

$$\|\rho(\mathbf{r},\mathbf{p},t,\lambda) - \rho_0(\mathbf{r},\mathbf{p},t)\|_T \leqslant (\exp(ct|\lambda|) - 1)\|\rho_{\text{in}}\|_T \tag{6.4}$$

from the bounds (4.16)–(4.18). [Here, c is given by (4.16); it is *not* the speed of light, which is 1 in the units I have chosen.]

The point is that, for $ct|\lambda| \ll 1$, the exact quantal state ρ is well approximated by the classically evolved state ρ_0. This observation clears up one of those little mysteries that come up when one first learns quantum mechanics. Particles in a cyclotron are treated quite successfully with *classical* dynamics, even though the particles are certainly subject to quantum dynamics. (Curiously, this explanation does not involve the one tool one would expect it to, semiclassical analysis.) It would be interesting to see this kind of treatment applied to a more realistic model of the system, and, for that model, to have quantum corrections to the dynamics calculated.

When $\mathbf{E}_0 \neq 0$, the Hamiltonian in (6.2) contains linear terms, and thus it is not, strictly speaking, in the form (1.3). Such terms are, however, easy to handle, for they can be removed via a time-dependent translation of the system.

Suppose that a system has the Hamiltonian

$$H'(\mathbf{q},\mathbf{p},t) = h'(\mathbf{q},\mathbf{p},t) + v'(\mathbf{q},\mathbf{p},t), \tag{6.5}$$

where v' is of the form (1.5) and

$$h'(\mathbf{q},\mathbf{p},t) = h(\mathbf{q},\mathbf{p},t) + \sum_{j=1}^{n} (d_j(t)q_j + e_j(t)p_j); \tag{6.6}$$

the function h is given by (1.4). In addition, suppose that at any time t, the system is in a state represented by $\rho'(\mathbf{q},\mathbf{p},t)$. Let $(\boldsymbol{\beta}(t),\boldsymbol{\alpha}(t))$ be the unique solution to the linear system

$$\frac{d\beta_j}{dt} = \frac{\partial h'}{\partial \alpha_j}(\boldsymbol{\beta},\boldsymbol{\alpha},t), \quad \frac{d\alpha_j}{dt} = -\frac{\partial h'}{\partial \beta_j}(\boldsymbol{\beta},\boldsymbol{\alpha},t), \tag{6.7}$$
$$\alpha_j(0) = \beta_j(0) = 0, \quad j = 1,\ldots,n.$$

A straightforward calculation shows that the translated WDF

$$\rho(\mathbf{q},\mathbf{p},t) \equiv \rho'(\mathbf{q} + \boldsymbol{\beta}(t), \mathbf{p} + \boldsymbol{\alpha}(t), t) \tag{6.8}$$

evolves via the Hamiltonian (1.3), with v given by

$$v(\mathbf{q},\mathbf{p},t) \equiv v'(\mathbf{q} + \boldsymbol{\beta}(t), \mathbf{p} + \boldsymbol{\alpha}(t), t). \tag{6.9}$$

It is easy to check that v satisfies (1.5) if and only if v' does, and so the translations (6.8) and (6.9) remove the linear terms. One can thus get expansions for ρ' using those for ρ.

Although I have not looked at Hamiltonians with spin-dependent terms, I believe that all the results that I have gotten will hold for them too, provided they satisfy conditions like the ones I have imposed upon spin-independent Hamiltonians. About the only difference is that the notation will become more complicated.

There are, however, Hamiltonians for which the techniques I have used break down. For example, any $v(\mathbf{q},\mathbf{p})$ that is discontinuous is problematical. (Such potentials include, unfortunately, both the Coulomb potential and the square

well.) It is likely that if the potential is not too badly singular, the results still hold. On the other hand, if the potential is too singular, they will probably not. My opinion is that they will hold for potentials like the square well, but they will *not* hold for Coulomb potentials.

In Sec. 4, I developed the various theorems about the convergence of (4.3) for admissible spaces. I did this because the space T is, from a mathematical point of view, less tractable than some of the others. Are there admissible spaces other than the ones I have listed in Theorem 4.2? In particular, are the Wigner transforms of the von Neumann–Schatten p-classes admissible? (See Ref. 13, Sec. 3.5 for a discussion of these spaces.) Also, are there better substitutes for T than $C_0 \cap L^2$?

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Conformal collineations and anisotropic fluids in general relativity

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Recently, Herrera *et al.* [L. Herrera, J. Jimenez, L. Leal, J. Ponce de Leon, M. Esculpi, and V. Galino, J. Math. Phys. **25**, 3274 (1984)] studied the consequences of the existence of a one-parameter group of conformal motions for anisotropic matter. They concluded that for special conformal motions, the stiff equation of state ($p=\mu$) is singled out in a unique way, provided the generating conformal vector field is orthogonal to the four-velocity. In this paper, the same problem is studied by using conformal collineations (which include conformal motions as subgroups). It is shown that, for a special conformal collineation, the stiff equation of state is not singled out. Non-Einstein Ricci-recurrent spaces are considered as physical models for the fluid matter.

I. INTRODUCTION

A space-time (V_4, g) admits a one-parameter group of conformal motions (Conf M) generated by a vector field ξ if

$$L_\xi g_{ab} = 2\sigma g_{ab} \quad (a,b = 0,...,3), \tag{1}$$

where L is the Lie operator and σ is an arbitrary function of the coordinates. Every (Conf M) must satisfy

$$L_\xi \{{}^a_{bc}\} = \delta^a_b \sigma_{;c} + \delta^a_c \sigma_{;b} - g_{bc} g^{ad} \sigma_{;d}. \tag{2}$$

Definition 1: A space-time V_4 is said to admit a conformal collineation (Conf C) (see Ref. 1) if there exists a vector field ξ for which (2) holds.

It follows that every (Conf M) is a (Conf C) but the converse is not necessarily true.[2] However, it is known[3] that condition (2) is equivalent to

$$L_\xi g_{ab} = 2\sigma g_{ab} + h_{ab}, \tag{3}$$

where h_{ab} is a (0,2) covariant constant (symmetric) tensor.

Definition 2: A vector field ξ is called *affine conformal*[2] if (2) or equivalently (3) holds.

Thus, (Conf C) is equivalent to the existence of an affine conformal vector which is conformal iff $h_{bc} = A g_{bc}$; $A = \text{const}$. For the existence of an affine conformal vector it is necessary that there exists a covariant constant symmetric tensor other than the metric tensor. In 1923, Eisenhart[4] proved that a Riemannian space with positive definite metric is reducible iff there exists a covariant constant (symmetric) tensor other than the metric tensor. Patterson[5] generalized this result, in 1951, for the spaces of indefinite metrics under some conditions. In general, the problem of characterizing h_{bc} still remains open. However, we state a few recent results satisfying (3) (for which h_{bc} is not necessarily a covariant constant), which have been obtained with reference to a symmetry property called "curvature collineation" (CC) defined by a vector ξ satisfying

$$L_\xi R^a{}_{bcd} = 0, \tag{4}$$

where $R^a{}_{bcd}$ is the Riemannian curvature tensor.

(1) Collinson[6] has shown that a necessary condition for ξ to generate (CC) in an empty space-time of Petrov type N is that (3) holds with $h_{bc} = \alpha \ell_b \ell_c$, α a real scalar and ℓ^b the unique (in direction) principal vector of the Weyl tensor.

(2) Katzin *et al.* [7]: A nonflat conformally flat space admits a (Conf C) such that $h_{bc} = \alpha R_{bc}$ (c.f. also Refs. 8–10).

(3) As a counterexample, Levine *et al.*[11] have shown that a space of nonzero constant curvature admits only one $h_{bc} = g_{bc}$. Thus, for this case a proper (Conf C) cannot exist.

Definition 3: A Conf C (Conf M) with a (CC) is called a special conformal collineation (motion) denoted by S Conf C (S Conf M).

The purpose of this paper is to study the consequences of the existence of a (S Conf C) *in a class of space-times having anisotropic and isotropic matter.*

As the paper progresses, we will indicate some advantages of the use of a (S Conf C) over a (S Conf M), in particular reference to a recent study of Herrera *et al.*[12] on conformal motions.

II. CONFORMAL COLLINEATIONS AND THE HYDRODYNAMICAL VARIABLES

Let the Einstein field equations, in appropriate units, be

$$R_{ab} - \tfrac{1}{2} g_{ab} R = T_{ab}, \tag{5}$$

where the energy-momentum tensor is prescribed by

$$\begin{aligned} T_{ab} &= (\mu + \bar{p}) U_a U_b + \bar{p} g_{ab} + (p - \bar{p}) S_a S_b, \\ R &= -T = -T^b{}_b = \mu - p - 2\bar{p}, \end{aligned} \tag{6}$$

where U^b is the four-velocity, S^b is a unit spacelike vector orthogonal to U^b, μ is the energy density, p is the pressure in the direction of S^b, and $\bar{p}$ is the pressure on the two-space orthogonal to S^b.

We consider a class of space-times, satisfying Eqs. (5) and (6), that admit a (S Conf C). It is well known[7] that a (Conf C) is a (S Conf C) iff $\sigma_{;bc} = 0$. The following results are immediate.

Proposition 1: If a V_4 admits a (S Conf C), then

(1) ξ generates a "Ricci collineation" $L_\xi R_{bc} = 0$,

(2) $L_\xi R^b{}_c = -2\sigma R^b{}_c - h^d{}_c R^b{}_d$,

(3) $L_\xi R = -2\sigma R - h^b{}_c R^c{}_b$.

To study the consequences of our hypothesis, we calculate the Lie derivative of the Einstein equations (5) and (6). This provides

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$$L_\xi(R_{ab}-\tfrac{1}{2}g_{ab}R)=h^{c}{}_{d}R^{d}{}_{c}g_{ab}-\tfrac{1}{2}(\mu-p-2\bar{p})h_{ab}, \quad (7)$$

where we have used Proposition 1 and (3). Furthermore,

$$h^{c}{}_{b}R^{b}{}_{c}=[(\mu-p)/2]h^{b}{}_{b}+(\mu+\bar{p})h_{bc}U^{b}U^{c}+(p-\bar{p})h_{bc}S^{b}S^{c}. \quad (8)$$

The four-velocity vector U^b can be represented by dx^b/ds, for the world line $x^b=x^b(s)$ of the fluid. Using the well-known[2] result $L_\xi dx^b=0$ and $ds^2=-g_{bc}\,dx^b dx^c$, we get

$$L_\xi U_b=(\sigma+\tfrac{1}{2}h_{cd}U^cU^d)U_b+h_{bc}U^c. \quad (9)$$

In a similar way, we can obtain the following:

$$L_\xi S_b=(\sigma-\tfrac{1}{2}h_{cd}S^cS^d)S_b+h_{bc}S^c. \quad (10)$$

Thus, the Lie derivative of the energy-momentum tensor is

$$\begin{aligned}L_\xi T_{ab}=&[L_\xi\mu+L_\xi\bar{p}+(\mu+\bar{p})(2\sigma+h_{cd}U^cU^d)]U_aU_b\\&+(L_\xi p+2\sigma\bar{p})g_{ab}\\&+[L_\xi p-L_\xi\bar{p}+(p-\bar{p})(2\sigma-h_{cd}S^cS^d)]S_aS_b\\&+\bar{p}h_{ab}+(\mu+\bar{p})[h_{ac}U^cU_b+U_ah_{bc}U^c]\\&+(p-\bar{p})[h_{ac}S^cS_b+S_ah_{bc}S^c]. \quad (11)\end{aligned}$$

Now equating (7) with (11) and then taking projections, we get

$$L_\xi\mu+2\sigma\mu=\tfrac{1}{2}[(p+\bar{p})h_{bc}U^bU^c-(p-\bar{p})h_{bc}S^bS^c]-[(\mu-p)/4]h^{b}{}_{b}, \quad (12)$$

$$L_\xi p+2\sigma p=\tfrac{1}{2}[(\mu+\bar{p})h_{bc}U^bU^c-(\mu-\bar{p})h_{bc}S^bS^c]+[(\mu-p)/4]h^{b}{}_{b}, \quad (13)$$

$$L_\xi\bar{p}+2\sigma\bar{p}=[(\mu+\bar{p})h_{bc}U^bU^c+(p-\bar{p})h_{bc}S^bS^c-(\mu-\mathrm{p})h_{bc}W^bW^c]+[(\mu-p)/4]h^{b}{}_{b}, \quad (14)$$

$$(\mu-p+4\bar{p})h_{bc}U^bS^c=0, \quad (15)$$

$$(\mu+p+2\bar{p})h_{bc}U^bW^c=0, \quad (16)$$

$$(\mu+p+2\bar{p})h_{bc}S^bW^c=0, \quad (17)$$

where W^b is a unit spacelike vector orthogonal to S^b and U^b. Equations (12)–(14) express the infinitesimal variations in the hydrodynamical variables under the (S Conf C) generated by ξ. We observe the following from Eqs. (15)–(17).

(i) If one of the components $h_{bc}U^bS^c$, $h_{bc}U^bW^c$, and $h_{bc}S^bW^c$ survives, then either $\mu=p-4\bar{p}$ or $\mu+p+2\bar{p}=0$ (whose isotropic counterpart is $\mu+3p=0$, called "curvature fluid").[13]

(ii) If $h_{bc}U^bS^c$ and either of $h_{bc}U^bW^c$ and $h_{bc}S^bW^c$ survives, then the anisotropy disappears ($p=\bar{p}$) and again we have $\mu+3p=0$. A general geometric/physical interpretation of Eqs. (12)–(14) is difficult to obtain. Therefore, in this paper, we concentrate on a few special cases in the following section.

III. ξ SPACELIKE

We consider two specific directions, namely, (A) ξ is collinear with S, and (B) ξ is orthogonal to U and S. These cases are specially discussed to compare our results with that of Herrera *et al.*[12]

(A) $\xi=\alpha S$, where α is a scalar. Then, $T^{b}{}_{c}\xi^{c}=p\xi^{b}$. Taking the divergence of this equation, using the conservation law equation $T^{b}{}_{c;b}=0$, Eqs. (13) and (14) and (3), we obtain

$$(\mu+p-2\bar{p})(4\sigma+h-2h_{bc}S^bS^c)=0, \quad \text{where } h\equiv h^{b}{}_{b}. \quad (18)$$

This leads to the following two nontrivial possibilities:

$$\text{(i) } \mu+p-2\bar{p}=0 \quad \text{or} \quad \text{(ii) } 4\sigma+h-2h_{bc}S^bS^c=0. \quad (19)$$

For perfect fluids, Eq. (19) (i) reduces to the stiff state ($\mu=p$). To prove that the stiff equation of state is not singled out, we must show that other solutions are possible from Eq. (19)(ii). For this purpose, we consider the following special case.

As mentioned in the Sec. II, for a non-Einstein conformally flat space $h_{bc}=\gamma R_{bc}$, but the converse need not be true. We study the converse problem by prescribing

$$h_{bc}=\gamma R_{bc}, \quad \gamma\neq 0. \quad (20)$$

For a (Conf C), h_{bc} has to be a covariant constant. Thus, our space-time must be Ricci recurrent (see Hall[14]). Using the field equations (5) and (6) and (20), we get

$$\begin{aligned}&\text{(i) } 2h_{bc}U^bU^c=\gamma(2\mu-R),\\&\text{(ii) } 2h_{bc}S^bS^c=\gamma(2p+R),\\&\text{(iii) } \gamma R=h^{b}{}_{b}=h, \quad \text{where } R=\mu-p-2\bar{p}.\end{aligned} \quad (21)$$

For $R\neq 0$, using Eqs. (21) (ii) and (21)(iii) in (19) (ii), we obtain

$$2\sigma(\mu-p-2\bar{p})=ph, \quad \sigma\neq 0. \quad (22)$$

As h_{bc} is parallel$\Rightarrow h^{b}{}_{b}=h$ is const. Thus, Eq. (22) can provide different classes of solutions for different suitable choices of the function σ. Therefore, the stiff equation of state is not singled out when ξ is orthogonal to U.

(B) ξ is orthogonal to U and S. Proceeding exactly as in (A), we obtain the following two nontrivial possibilities:

$$\text{(i) } \mu=p \quad \text{or} \quad \text{(ii) } 4\sigma=h+h_{bc}U^bU^c-h_{bc}S^bS^c. \quad (23)$$

For Ricci-recurrent spaces satisfying (20), Eq. (23) (ii) reduces to

$$2\sigma(\mu-p-2\bar{p})=h\bar{p}, \quad \sigma\neq 0. \quad (24)$$

Thus, for this case, either $\mu=p$ with no constraints on $\bar{p}$ or there are other possible solutions generated from Eq. (24) for suitable values of σ. The dominant energy condition for (A) and (B) is satisfied if $4\sigma+h\geqslant 0$.

Conclusions: (1) The stiff equation of state is not singled out when ξ is orthogonal to U.

(2) Equations (22) and (24) provide perfect fluid solutions iff

$$\sigma=ph/(2\mu-6p), \quad R\neq 0, \quad \sigma\neq 0. \quad (25)$$

(3) For any choice of nonzero σ other than (25) (satisfying energy condition) different anisotropic solutions are possible.

Remark 1: Herrera *et al.*[12] have recently discussed this topic with respect to conformal motion. Some of their conclusions are the following.

(a) Under their assumptions, the existence of a one-

parameter group of conformal motions introduces specific restrictions on the hydrodynamical variables.

(b) Furthermore, for a (S Conf M), the stiff equation of state is singled out in a unique way, provided ξ is orthogonal to U.

Comparing their conclusion (b) with the present work, it is clear from Eqs. (19)–(25) that the use of an affine conformal vector field has certain advantages. For example, the stiff equation of state is not singled out when ξ is orthogonal to U.

IV. ξ TIMELIKE

In this section, we assume that $\xi = \alpha U$, α being a scalar. Then, proceeding exactly as in Sec. III (A), we can obtain the following two nontrivial possibilities of solutions:

$$\text{(i) } \mu + p + 2\bar{p} = 0 \quad \text{or} \quad \text{(ii) } 4\sigma + h + 2h_{bc}U^bU^c = 0. \tag{26}$$

For perfect fluids, (26) (i) reduces to $\mu + 3p = 0$. This equation of state has been used earlier in several exact solutions (see, for example, conformally flat solutions, Sec. 32.5.3, pp. 370 and 371 of Ref. 15) (cf., also, McIntosh).[16,17] To investigate the case (26) (ii), we take the Lie derivative of $\xi^b = \alpha U^b$. This provides

$$L_\xi U_b = [2\sigma - L_U\alpha]U_b + h_{bc}U^c. \tag{27}$$

Making use of Eq. (9) in above equation, we get

$$L_U\alpha = \sigma - \tfrac{1}{2}h_{bc}U^bU^c. \tag{28}$$

Now taking the divergence of $\xi^b = \alpha U^b$ and using (27), we obtain

$$L_U\alpha = 4\sigma - \alpha\theta + h, \tag{29}$$

where $\theta = U^b{}_{;b}$ is the volume expansion of the fluid. Finally eliminating $L_U\alpha$ from Eqs. (28) and (29) and using (26) (ii), we obtain

$$8\sigma = 4\alpha\theta - h. \tag{30}$$

Thus, σ is const iff $\alpha\theta = \text{const} \Leftrightarrow \xi$ is an affine collineation.[7]

To show that solutions (other than curvature fluid $\mu + 3p = 0$) are possible from the Eq. (26) (ii), we use the Ricci-recurrent spaces satisfying Eqs. (20) and (21). This provides

$$2\sigma(\mu - p - 2\bar{p}) + h\mu = 0, \quad R \neq 0 \text{ and } \sigma \neq 0. \tag{31}$$

Thus, it is possible to generate solutions (other than the curvature fluid) for the case (26) (ii) by assigning in Eq. (31) suitable values of the function σ. The dominant energy condition is satisfied for $4\sigma - h \geqslant 0$.

Conclusions: (1) The curvature fluid solution is not singled out when ξ is collinear with U.

(2) Equation (31) provides perfect fluid solutions iff

$$\sigma = h\mu/(6p - 2\mu), \quad R \neq 0, \quad \sigma \neq 0. \tag{32}$$

(3) For any choice of nonzero σ other than (32) and satisfying the energy condition, different anisotropic solutions are possible.

(4) For $\sigma = \text{const}$ a (S Conf C) in a non-Einstein conformally flat space reduces to a (AC).[7] In particular, the volume expansion $\theta = 0 \Rightarrow \sigma = -h/8$. Observe that for this case, the energy condition is satisfied if h is negative. An example of such a space is the Einstein cosmological model.[7]

Remark 2: Following Sec. III. of Herrera *et al.*,[12] we have found that for static spherically symmetric spaces, either we get the stiff equation of state or the curvature fluid for all the cases discussed in this paper.

V. CONCLUDING REMARK

Although we also do not know for sure the precise reasons for the link between the stiff equation of state (as observed in Ref. 12) and the group of special conformal motions, nevertheless, we have shown that this possibility can be avoided by the use of a more general group of special conformal collineations [see Eqs. (22) and (24)].

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Collision-free gases in static space-times

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Collision-free gases in static space-times are analyzed by developing previous work in static spherically symmetric space-times and extending the analysis to include the cases of planar and hyperbolic symmetry. By assuming that the distribution function of the gas inherits the space-time symmetries, distribution solutions to the Einstein–Liouville equations, which are without expansion, rotation, shear, and heat flow, but which have an anisotropic stress are found. The conditions for the gas to behave like a perfect fluid are considered and the relation between equations of state and the distribution function are investigated. In particular, distribution functions that generate the γ-law equation of state are found. The solutions are extended to find invariant Einstein–Maxwell–Liouville solutions for a charged gas, subject to a consistency condition on the invariant electromagnetic potential. Finally, the general solution of Liouville's equation in the static space-times is obtained and a particular nonstatic solution is considered, which can be shown to lead to a self-gravitating gas with expansion, shear, and heat flow.

I. INTRODUCTION

Static spherically symmetric space-times have been considered in the context of general relativistic kinetic theory by Fackerell[1] and Ray.[2] In this paper we seek to extend aspects of their work. We include static space-times with planar and hyperbolic symmetry because they are naturally related to the spherical geometry, and our analysis allows for a unified treatment. (Compare the unified treatment by Collins[3] for perfect fluids.) However, only the spherical case has a clear physical interpretation, for example in astrophysics and cosmology.

The purpose of this paper is to obtain physically acceptable distribution functions f, in order to study the gas behavior. Following the method of a previous paper,[4] we assume f is invariant under the space-time group of motions. This allows us to construct solutions of Liouville's equation. Invariant Liouville solutions are found in Sec. II, applying the techniques of Ref. 4. We show the redundancy of the assumption that f be a function of Killing vector constants of the motion. The kinematics and dynamics of the gas are considered in Sec. III, and we show that the invariant Liouville solutions satisfy the Einstein field equations. These Einstein–Liouville solutions are nonexpanding, nonrotating, and shear-free, as in the perfect fluid case, but they have an anisotropic stress. For the case of perfect fluid behavior, we investigate the relation between f and the energy density and pressure, using Fackerell's techniques[1]; in particular, we find an f that generates the γ-law equation of state. In Sec. IV we find an invariant distribution solution to the Einstein–Maxwell–Liouville equations for a gas of charged particles, extending the results of Ray.[2] In Sec. V, we find the complete general solution of the Liouville equation in static space-time. Nonstatic distributions with spherical (planar, hyperbolic) symmetry are shown to be related to rank 2 Killing tensors in special space-times. These nonstatic Liouville solutions are expanding and shearing, and can be shown[5] to satisfy Einstein's equations under reasonable conditions.

Since this paper is based on the methods of our previous paper[4] [which considered the same problems in locally rotationally symmetric (LRS) Bianchi space-times], we do not repeat the review in Ref. 4 of kinetic theory and symmetries, but refer directly to Ref. 4 where necessary, using a "P" to identify equations from Ref. 4 [e.g., P(3.1)].

II. INVARIANT DISTRIBUTION FUNCTIONS

The static space-times are given in standard coordinates $x^i = (t,r,\theta,\phi) = (t,x^\alpha)$ by[6]

$$ds^2 = -e^{\nu(r)}\,dt^2 + e^{\lambda(r)}\,dr^2 + r^2(d\theta^2 + \Sigma^2\,d\phi^2), \tag{2.1}$$

where $\Sigma = (\theta,\sin\theta,\sinh\theta)$, for $k = (0,1,-1)$, giving (planar, spherical, hyperbolic) symmetry. The Killing vectors X_I of (2.1) are

$$\begin{aligned} X_1 &= \cos\phi\partial_\theta - \sin\phi(\Sigma'/\Sigma)\partial_\phi, \\ X_2 &= \sin\phi\,\partial_\theta + \cos\phi(\Sigma'/\Sigma)\partial_\phi, \\ X_3 &= \partial_\phi, \quad X_4 = \partial_t, \end{aligned} \tag{2.2}$$

giving the nonzero structure constants

$$\begin{aligned} &C^1{}_{23} = -C^1{}_{32} = C^2{}_{31} = -C^2{}_{13} = k^2 + k - 1, \\ &C^3{}_{12} = -C^3{}_{21} = k^2. \end{aligned} \tag{2.3}$$

In the orthonormal one-form basis

$$\omega^a = \{e^{\nu/2}\,dt, e^{\lambda/2}\,dr, r\,d\theta, r\Sigma\,d\phi\}, \tag{2.4}$$

the Einstein tensor is

$$\begin{aligned} G^{00} &= kr^{-2} - e^{-\lambda}(r^{-2} - r^{-1}\lambda'), \\ G^{11} &= -kr^{-2} + e^{-\lambda}(r^{-2} + r^{-1}\nu'), \\ G^{22} &= G^{33} = e^{-\lambda}[2\nu'' + (\nu' - \lambda')(\nu' + 2r^{-1})]/4, \\ G^{ab} &= 0 \quad \text{for} \quad a \neq b. \end{aligned} \tag{2.5}$$

A collision-free gas of particles (mass m, four-momentum p) has distribution function $f(x^i, p^\alpha)$ with $g_{ij}\,p^i p^j = -m^2$, satisfying Liouville's equation

$$Lf \equiv p^i\left(\frac{\partial}{\partial x^i} - \Gamma^\alpha{}_{ij}\,p^j\frac{\partial}{\partial p^\alpha}\right)f = 0. \tag{2.6}$$

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We begin by looking for physically realistic solutions to the Ehlers equation P(2.19). So we are assuming that (a) f is invariant under the G_4 of motions, and (b) f is a function only of Killing vector constants of the motion, $y_I = X_I^i p_i$. Using (2.3) we find the general solution of P(2.19),

$$f(x^i, p^\alpha) = F(y_4, y_1^2 + y_2^2 + k y_3^2),$$

which becomes, using (2.1), (2.2), and (2.4),

$$\begin{aligned} f &= F[e^{\nu} p^t, r^4((p^\theta)^2 + \Sigma^2 (p^\phi)^2)] \\ &= F[e^{\nu/2} p^0, r^2((p^2)^2 + (p^3)^2)], \end{aligned} \tag{2.7}$$

in agreement with Fackerell[1] and Ray[2] for static spherical symmetry ($k = 1$).

Note how the static Killing vector leads to dependence of f on the constant $e^{\nu/2} p^0$, which is isotropic in momentum space, while the G_3 invariance of f leads to dependence on $r^2((p^2)^2 + (p^3)^2)$, which is axially symmetric in momentum space, corresponding to the local rotational symmetry at each point in space-time about the ∂_r direction. (This feature is similar to that found in locally rotationally symmetric, spatially homogeneous space-times.[4])

We now drop the assumption that f be a function of the constants y_I, and insist only that P(2.15) holds. That is, the only restriction placed on f is that it inherits the space-time symmetries. Using (2.2) we obtain the general solution of P(2.15),

$$f = F[r, p^r, (p^\theta)^2 + \Sigma^2 (p^\phi)^2], \tag{2.8}$$

which is also axially symmetric in momentum space. The most general invariant distribution function (2.8) has been obtained purely from geometric considerations; the collision-free behavior has not been used. Therefore we must impose the Liouville equation on the invariant distribution function F to obtain a physical solution. The Liouville equation (2.6) for f given by (2.8) has the general solution (2.7). Hence we have shown the redundancy of the assumption that f be a function of the Killing vector constants. This result is also true in spatially homogeneous locally rotationally symmetric space-times.[4]

Without solving (2.6) for (2.8) to obtain (2.7), we can show geometrically that the invariant Liouville solution must be based on Killing vector constants. Since $[L, \tilde{X}_I] = 0$ [$\tilde{X}_I$ is given by P(2.15)], the G_4 acts on the six-dimensional manifold P of phase trajectories of fixed mass m. A function f obeying $Lf = 0$ and $\tilde{X}_I f = 0$ is constant on the orbits of that G_4 action. Since these orbits are four dimensional, f depends only on any two phase functions that label these orbits. One such pair is given by $e^{\nu/2} p^0$ and $r^2((p^2)^2 + (p^3)^2)$, by (2.7), which is a known invariant Liouville solution. Hence every invariant Liouville solution is of the form (2.7).

Theorem 2.1: In the static space-times (2.1), containing a neutral one-component collision-free gas, if the distribution function is invariant under the G_4 of motions and satisfies Liouville's equation, then it is a function of the Killing vector constants of the motion, and is given by (2.7).

Thus if f depends on any constants of the motion not generated by Killing vectors, then f cannot be G_4 invariant. This will be the case, for example, if f depends on quadratic first integrals generated by irreducible rank 2 Killing tensors such as those found in certain static spherically symmetric space-times by Hauser and Malhiot[7] and Kimura.[8] (See Sec. V for further discussion.)

III. KINEMATICS AND DYNAMICS OF THE GAS

A. Kinematics

The invariance of the distribution function f implies invariance of the four-current density n by P(2.16). Hence the number density N and the kinematic average four-velocity u are G_4 invariant. Thus u must be of the form

$$u = e^{-\nu/2} \cosh\psi\, \partial_t + e^{-\lambda/2} \sinh\psi\, \partial_r, \tag{3.1}$$

where $\psi(r)$ is the hyperbolic angle of tilt relative to ∂_t. In the orthonormal tetrad (2.4), the four-current density P(2.5) for the distribution (2.7) is

$$n^a = \int p^a \left(\frac{1}{p^0}\right) F[e^{\nu/2} p^0, r^2((p^2)^2 + (p^3)^2)]\, dp^{123}, \tag{3.2}$$

where the integration is over all of $\mathbb{R}^3$. The integrands of n^1, n^2, n^3 in (3.2) are odd functions of p^1, p^2, and p^3, respectively. Hence $n^1 = n^2 = n^3 = 0$, and $\psi = 0$ in (3.1):

$$u = e^{-\nu/2} \partial_t. \tag{3.3}$$

Thus u must be orthogonal to the surfaces $t = \text{const}$ for collision-free gases with invariant distribution functions. The most general invariant distribution (2.8) is an even function of p^2 and p^3, but not of p^1 in general. For this distribution, only n^2 and n^3 are forced to be zero so that u may be tilted. It is precisely the collision-free behavior of the gas that forces u to be orthogonal. Then the kinematic quantities [given by P(2.9)] take the same form as for a perfect fluid[6]:

$$\dot{u} = \nu' e^{-\lambda}/2 \partial_r, \quad \theta = \sigma = \omega = 0. \tag{3.4}$$

B. Dynamics: The self-gravitating gas

In the orthonormal tetrad (2.4), the energy–momentum tensor P(2.6) for the gas distribution (2.7) is

$$T^{ab} = \int p^a p^b \left(\frac{1}{p^0}\right) F[e^{\nu/2} p^0, r^2((p^2)^2 + (p^3)^2)]\, dp^{123}, \tag{3.5}$$

and since F in (3.5) is even in p^1, p^2, and p^3, and symmetric in p^2 and p^3, it follows that

$$T^{ab} = T^{ab}(r) = \text{diag}(T^{00}, T^{11}, T^{22}, T^{23}), \quad \text{with } T^{22} = T^{33}. \tag{3.6}$$

The form (3.6) of the energy–momentum tensor is the same as that of the Einstein tensor (2.5), and is thus consistent with the Einstein field equations $G^{ab} = T^{ab}$, which therefore impose no additional restrictions on the functional form of F in (3.5). In fact the three field equations given by (2.5) and (3.6) contain only two independent equations by virtue of the conservation equations $T^{ab}{}_{;b} = 0$, which hold identically as a consequence of Liouville's equation.[4] Thus any choice of F in (2.7) and (3.5), which already satisfies Liouville's theorem (Theorem 2.1), gives a solution of the field equations. Explicitly, given a choice of F of the form (2.7), the components T^{ab} are determined as functions of r and ν via

(3.5). Choosing $G^{00} = T^{00}$ and $G^{11} = T^{11}$ as the independent field equations, we therefore obtain a coupled first-order system for ν and λ, which may in principle be solved to determine the metric (2.1). Clearly, for a physical solution, the choice of F must be non-negative, suitably smooth, and suitably bounded on the mass shell.

Theorem 3.1: The invariant distribution function (2.7) is a solution of the Einstein–Liouville equations in the static space-times (2.1), where F is any physical function.

The invariance of the distribution function implies invariance of u, and of the energy–momentum tensor T by P(2.16). Thus the dynamic quantities of the gas, given by P(2.10), are invariant. Furthermore, u is orthogonal, so that the heat flow is zero, by (3.6). Thus

$$\mu = \mu(r), \quad p = p(r), \quad q^i = 0, \quad \pi^{ij} = \sqrt{3}S(r)(c^i c^j - h^{ij}/3), \tag{3.7}$$

where $c = e^{-\nu/2}\partial_r$ and S is the magnitude of the stress ($2S^2 = \pi_{ij}\pi^{ij}$). (Note that it is the collision-free behavior of the gas that forces the heat flow to vanish.) The invariant distribution functions are Einstein–Liouville solutions without expansion, shear, rotation, or heat flow. However, there is an anisotropic stress: the pressure in the radial direction differs in general from the pressure in the orthogonal two-plane. This possibility, which is ruled out in the usual perfect fluid models, is of importance in astrophysics. For example, in the study of neutron stars, energy–momentum tensors of the form given by (3.7) have been constructed by mixing two perfect fluids or introducing external fields.[9]

In terms of the components of T^{ab}: $\mu = T^{00}$, $p = (T^{11} + 2T^{22})/3$, $S = (T^{11} - T^{22})/\sqrt{3}$. We can simplify the triple integrals involved by introducing new coordinates on the mass shell. Following Fackerell[1] and Ray,[2] we define

$$E = e^{\nu/2}p^0, \quad J^2 = r^2((p^2)^2 + (p^3)^2), \quad e^{i\Phi} = rJ^{-1}(p^2 + ip^3), \tag{3.8}$$

where E represents the energy ($E \geqslant me^{\nu/2}$) and J the angular momentum of the particles ($J \geqslant 0$), so that the Einstein–Liouville solution becomes $f = F(E,J)$. Then the mass shell volume element $\pi_m = dp^{123}/p^0$ becomes

$$\pi_m = r^{-2}e^{-\nu}EJ(e^{-\nu}E^2 - r^{-2}J^2 - m^2)^{-1/2}\, dE \wedge dJ \wedge d\Phi,$$

and we obtain, from (3.5),

$$\mu = 2\pi r^{-2}e^{-3\nu/2}\iint E^2 J(e^{-\nu}E^2 - r^{-2}J^2 - m^2)^{-1/2} \times F(E,J)\,dE\,dJ, \tag{3.9}$$

$$p = \frac{2}{3}\pi r^{-2}e^{-\nu/2}\iint J(e^{-\nu}E^2 - m^2) \times (e^{-\nu}E^2 - r^{-2}J^2 - m^2)^{-1/2}F(E,J)\,dE\,dJ, \tag{3.10}$$

$$S = \frac{1}{\sqrt{3}}\pi r^{-2}e^{-\nu/2}\iint J(2e^{-\nu}E^2 - 3r^{-2}J^2 - 2m^2) \times (e^{-\nu}E^2 - r^{-2}J^2 - m^2)^{-1/2}F(E,J)\,dE\,dJ. \tag{3.11}$$

C. Perfect fluid

The Einstein–Liouville solution provides a kinetic theory basis for perfect fluid models in static space-times. Since the heat flow vanishes by the orthogonality of u, to obtain perfect fluid behavior[4] the stress (3.11) must vanish:

$$\iint J(2e^{-\nu}E^2 - 3r^{-2}J^2 - 2m^2) \times (e^{-\nu}E^2 - r^{-2}J^2 - m^2)^{-1/2}F(E,J)\,dE\,dJ = 0. \tag{3.12}$$

If F is independent of $J = r[(p^2)^2 + (p^3)^2]^{1/2}$ and is only a function of $E = e^{\nu/2}[(p^1)^2 + (p^2)^2 + (p^3)^2 + m^2]^{1/2}$, then f is still a function of p^1, p^2, and p^3, and will be physical if it vanishes sufficiently rapidly at infinity on the mass shell. This property follows essentially from invariance of f under the static Killing vector. (In spatially homogeneous, locally rotationally symmetric space-times without static symmetry, if F is independent of J, then f depends only on p^1, and therefore necessarily has unbounded moments.[4]) Now $f = F(E)$ implies that f is isotropic in p^1, p^2, and p^3, so that $T^{11} = T^{22} = T^{33} = p \Leftrightarrow S = 0$. Hence (3.12) is identically satisfied for all r, and the gas behaves like a perfect fluid. (Note that isotropy of the distribution function in momentum space always leads to perfect fluid behavior, even if there are collisions.[10])

This result was proved in the case of spherical symmetry by Ray[2] and, in fact, Fackerell[1] had earlier established essentially the same result (if f is independent of angular momentum, then the "pressure matrix" is isotropic). It is not clear whether the converse is true: Does (3.12) imply that f is isotropic ($\partial F/\partial J = 0$)? This seems unlikely, but we have been unable to find a nonisotropic f satisfying (3.12). Treciokas and Ellis[10] give an example of nonisotropic f generating perfect fluid behavior in Robertson–Walker space-time. The existence of such an f in our case would be consistent with the conjecture of Treciokas and Ellis[10,11] that perfect fluid behavior is possible only if the shear σ vanishes and there exists an acceleration potential R (in our case $R = e^{-\nu/2}$).

In order to study μ and p in the perfect fluid case, we assume $\partial F/\partial J = 0$. Then (3.9) and (3.10) become (since $F \to 0$ as $J \to \infty$)

$$\mu = 2\pi e^{-2\nu}\int E^2(E^2 - m^2e^{\nu})^{1/2}F(E)\,dE, \tag{3.13}$$

$$p = \frac{2}{3}\pi e^{-2\nu}\int (E^2 - m^2e^{\nu})^{3/2}F(E)\,dE. \tag{3.14}$$

These expressions agree in the case of spherical symmetry with those given by Fackerell[1] [Eqs. (47) and (48)]. Note that (3.13) and (3.14) imply $0 \leqslant p \leqslant \mu/3$ and $p = \mu/3 \Leftrightarrow m = 0$, which hold in general in kinetic theory.

By Theorem 3.1, any choice of the functional form $f = F(E,J)$, and in particular any isotropic choice $f = F(E)$ (leading to perfect fluid behavior), gives a solution of the Einstein–Liouville system, in the sense that μ and p are obtained as functions of ν from (3.13) and (3.14), and then substituted into the field equations $G^{ab} = T^{ab}$, leading to two independent equations in λ and ν. The isotropic Bel distribution

$$F = 4F_0 \exp(-E^2), \quad F_0 > 0, \tag{3.15}$$

has been used in Robertson–Walker space-time by Bel[12] and Ray and Zimmerman.[13] With (3.15) we can integrate (3.13) and (3.14) (see Ref. 14) for $m > 0$ in terms of the Kummer function U:

$$\mu = 2\pi^{3/2} m^4 F_0 \exp(-m^2 e^{\nu}) U(\tfrac{3}{2}, 3, m^2 e^{\nu}), \tag{3.16}$$

$$p = \pi^{3/2} e^{-2\nu} F_0 \exp(-m^2 e^{\nu}) U(\tfrac{1}{2}, -1, m^2 e^{\nu}). \tag{3.17}$$

It is then possible to construct graphs showing the behavior of μ, p, and p/μ as functions of e^{ν} (compare Ref. 13). What would be more useful is to obtain $\nu(r)$ and $\lambda(r)$ by substituting (3.16) and (3.17) into the field equations using (2.5). However, the resulting differential equations are extremely complex. What we can find is the behavior of μ and p for limiting values of the metric function e^{ν}, using the asymptotic forms[14] of U:

$$e^{\nu} \to 0 \Rightarrow p \to \mu/3; \quad e^{\nu} \to \infty \Rightarrow p \to 0, \quad \mu \to 0, \quad p/\mu \to 0.$$

Hence for the Bel distribution with $m > 0$, the ultrarelativistic equation of state $p = \mu/3$ and the dust equation of state $p = 0, \mu > 0$, are obtained as limiting equations of state.

Instead of assuming a functional form $f = F(E)$ and then determining μ and p as functions of e^{ν}, we can impose conditions on μ and p and then seek to determine $F(E)$. This approach was developed by Fackerell,[1] and allows one to investigate the kinetic theory (collision-free) basis for standard perfect fluid equations of state, or for special behavior of $\mu(r)$ (e.g., $\mu = \text{const.}$). Explicitly, we can either (a) assume an equation of state $p = p(\mu)$, or (b) assume a form for $\mu(r)$. Then the momentum conservation equation

$$(\mu + p)\nu' + 2p' = 0 \tag{3.18}$$

may be integrated, giving $\mu = M(\nu)$ in case (a), and $p = P(r,\nu)$ in case (b). Thus in both cases, μ and p are determined as functions of r and ν, which may be substituted in the field equations to determine $\nu(r)$ and $\lambda(r)$. However the resulting solution may be nonphysical (from a collision-free kinetic theory standpoint) if the distribution function is forced to be nonphysical by the conditions imposed on μ and p. These conditions reduce, by (3.13), (3.14), and (3.18), to an integral equation in $F(E)$. This equation will not in general have a unique physical solution $F(E)$. If μ and p are determined, then the average dynamical behavior of the gas is determined, but there may be no isotropic physical distribution that generates this behavior, or there may be many different isotropic physical distributions that generate the same average behavior. In the spherically symmetric case, Fackerell[1] shows that the Schwarzschild interior solution ($\mu = \mu_0 > 0$ for $r < r_0, \mu = 0$ for $r > r_0$) cannot be generated by a physical $F(E)$, while the polytropic equation of state ($p = K\mu^{(n+1)/n}$ for $r < r_0, p = 0 = \mu$ for $r > r_0$) can be generated by a physical $F(E)$, which he is able to determine.

The γ-law equation of state

$$p = (\gamma - 1)\mu, \quad \text{for all } r, \tag{3.19}$$

is usually assumed in the standard perfect fluid models, and is used by Collins[3] in his analysis of the static space-time (2.1). Kinetic theory imposes the restriction $1 \leqslant \gamma \leqslant \frac{4}{3}$ in (3.19). However $\gamma = 1$ is ruled out by (3.4) if F is a smooth isotropic non-negative function (and in any case, the field equations show that $p = 0 \Rightarrow \mu = 0$). For $\gamma = \frac{4}{3}$, we have a perfect fluid photon gas, and then (3.18), (3.14) imply

$$\int_0^{\infty} E^3 F(E) dE = c, \quad 3p = \mu = 2\pi c e^{-2\nu}, \tag{3.20}$$

where c is a positive constant. The integral equation for $F(E)$ in (3.20) has many different physical solutions for a given c; for example,

$$F(E;a) = 4ac(E^4 + a)^{-2}, \quad a > 0, \tag{3.21}$$

is an infinite family of isotropic physical distributions generating the same dynamical behavior. For $1 < \gamma < \frac{4}{3}$, (3.18) and (3.19) imply

$$p = \tfrac{1}{3}\pi m^{\delta} c e^{(\delta - 2)\nu}, \quad c > 0, \quad \delta = (3\gamma - 4)/2(\gamma - 1) < 0, \tag{3.22a}$$

and then (3.14) gives the integral equation

$$\int_z^{\infty} w^{-1/2}(w - z)^{3/2} F(w) dw = c z^{\delta}, \tag{3.22b}$$

where $w = E^2, z = m^2 e^{\nu}$. By inspection (3.22b) has a solution of form $F \sim w^b$, and we obtain[14]

$$F(E) = \tfrac{4}{3}\pi^{-1/2} c \Gamma[(2\gamma - 1)/2(\gamma - 1)] E^{2\gamma/(1-\gamma)} \times \Gamma[(4 - 3\gamma)/2(\gamma - 1)]^{-1}. \tag{3.23}$$

Since $\gamma/(1 - \gamma) < -4$ and $E \geqslant m e^{\nu/2} > 0$, (3.23) gives a physical distribution for each γ, which generates the γ-law equation of state. [Solutions $\nu(r), \lambda(r)$ of the field equations are given by Collins.[3]]

Theorem 3.2: The distribution functions (3.21) and (3.23) are physical Einstein–Liouville solutions in the static space-times (2.1) that generate a perfect fluid with $p = (\gamma - 1)\mu$, $1 < \gamma \leqslant \frac{4}{3}$.

IV. CHARGED PARTICLES

We now consider whether the static space-times can admit a self-gravitating gas of particles with charge ϵ, which themselves generate the electromagnetic field. Ray[2] shows that

$$\bar{y}_I = X_I{}^i(p_i + \epsilon A_i) \tag{4.1}$$

are "charged" constants of the motion for the charged Liouville equation

$$\bar{L}f \equiv \left(L + \epsilon p^i F^{\alpha}{}_i \frac{\partial}{\partial p^{\alpha}}\right) f = 0, \tag{4.2}$$

provided the four-potential $A (F = -2\,dA)$ is G_4 invariant $\Rightarrow A$ must be of the form $A = \alpha(r)\partial_t + \beta(r)\partial_r$, leading to the charged constants of motion

$$\bar{y}_I = y_I, \quad \text{for } I = 1,2,3, \quad \bar{y}_4 = -e^{\nu}(p^t + \epsilon\alpha), \tag{4.3}$$

and the electromagnetic field tensor

$$F = 2(\alpha e^{\nu})'\, dt \wedge dr, \tag{4.4}$$

which has zero magnetic field and radial electric field. The most general G_4-invariant distribution for a charged gas is still (2.8), and for this f the general solution of (4.2) is

$$f = \bar{F}[e^{\nu}(p^t + \epsilon\alpha), r^4((p^{\theta})^2 + \Sigma^2(p^{\phi})^2)] = \bar{F}[e^{\nu/2}(p^0 + \epsilon e^{\nu/2}\alpha), r^2((p^2)^2 + (p^3)^2)], \tag{4.5}$$

which by (4.3) is precisely the solution of the charged Ehlers equation. [Assuming that $f=\overline{F}(\bar{y}_I)$ and $\overline{X}_I f=0$, for all I, and using the charged Liouville operator $\overline{L}$, we obtain the Ehlers equation P(2.19) with y_I replaced by $\bar{y}_I$.] Thus the assumption[2] that f be based on the charged Killing vector constants of motion is redundant, as in the uncharged case (Theorem 2.1).

We must still show that (4.5) is consistent with Maxwell's equations $F^{ij}{}_{;j}=j^i$. [The remaining Maxwell equations $dF=0$ are satisfied by construction: $F=-2dA$.] Now the charged Liouville solution (4.5) has the same symmetries in momentum space as the uncharged (2.7). Thus the arguments of Sec. III A remain valid, and the kinetic average four-velocity remains orthogonal, so that the current $j^i=\epsilon n^i=\epsilon N u^i$ is orthogonal:

$$j=\epsilon N e^{-\nu/2}\partial_t. \tag{4.6}$$

Maxwell's equations $j^i=F^{ij}{}_{;j}$, using (4.4), give

$$j=-r^{-2}e^{-(\nu+\lambda)/2}[r^2(\alpha e^{\nu})'e^{-(\nu+\lambda)/2}]'\partial_t. \tag{4.7}$$

Comparing (4.6) and (4.7) we see that ϵ may indeed be nonzero; the static space-times (2.1) can admit an invariant Maxwell–Liouville solution. [This is not the case in locally rotationally symmetric spatially homogeneous space-times, except those of Bianchi type V (see Ref. 4).]

Ray[2] established this result in the case of spherical symmetry, although he did not give the consistency condition for the existence of the solutions that is contained in (4.6) and (4.7):

$$\int \overline{F}\,[e^{\nu/2}(p^0+\alpha\epsilon e^{\nu/2}),r^2[(p^2)^2+(p^3)^2)]dp^{123}$$
$$=-\epsilon^{-1}(r^{-2}e^{-\lambda/2})[r^2(\alpha\epsilon^{\nu})'e^{-(\nu+\lambda)/2}]', \tag{4.8}$$

where we have used (3.2) ($N=n^0$). Thus (4.4) and (4.5) are a Maxwell–Liouville solution provided $\alpha(r)$ satisfies (4.8). We show that this solution also satisfies the Einstein field equations. By (4.4) the tetrad components of the electromagnetic energy–momentum tensor

$$\overline{T}^{ab}=F^{ac}F^{b}{}_{c}-g^{ab}F_{cd}F^{cd}/4,$$

are diagonal, with $\overline{T}^{22}=\overline{T}^{33}$, and $\overline{T}^{ab}=\overline{T}^{ab}(r)$, which shows that the field equations $G^{ab}=T^{ab}+\overline{T}^{ab}$ impose no restrictions on the form of the electromagnetic field (4.4). The conservation equations $(T^{ij}+\overline{T}^{ij})_{;j}=0$, which ensure consistency of the Einstein–Maxwell–Liouville system, follow from the Liouville equation $\overline{L}f=0$ and the identity $\overline{T}^{ij}{}_{;j}=F^{ki}j_k$. Hence, by an argument similar to that for Theorem 3.1, any distribution function of the form (4.5) is a solution to the Einstein–Maxwell–Liouville system, provided $\alpha(r)$ satisfies (4.8).

Theorem 4.1: The invariant distribution function (4.5) is a solution of the Einstein–Maxwell–Liouville equations in the static space-times (2.1), where $\overline{F}$ is an arbitrary physical function, and α satisfies (4.8).

V. NONSTATIC DISTRIBUTION FUNCTIONS

We have seen how the distribution function invariant under the full G_4 of motions (2.2) and satisfying Liouville's equation leads to an orthogonal kinematic average four-velocity. Consequently the kinematic quantities of the gas have the same form as for the standard perfect fluid model, and the heat flow vanishes. If we drop the assumption of G_4 invariance, we will obtain a tilted u, and hence in general a nonzero expansion, shear, rotation, and heat flow. However, without G_4 invariance it is difficult to find a physical Liouville solution [besides the obvious Killing vector solution: $f=F(y_I)$, $\partial F/\partial y_4\neq 0$], and even more difficult to find noninvariant Einstein–Liouville solutions. We tackle the first problem in this section; the second problem is taken up elsewhere.[5]

In fact, we can find the general Liouville solution as follows. By (2.6), the general solution will be a function of six functionally independent constants of the motion (characteristics). The four Killing vectors (2.2) provide four independent (static) characteristics: $E=-y_4$, $J^2=y_1^2+y_2^2+ky_3^2$, $J_z=y_3$, and $J_x=y_2$ (or $J_y=y_1$). The remaining characteristic equations can be taken as $dt/p^t=dr/p^r=d\theta/p^\theta$, and since $p^t=e^{-\nu}E$, these can be integrated if we can express p^r as $P(r,y_I)$ and p^θ as $Q(r,\theta,y_I)$. By (2.1), (2.4), and (3.8), $p^r=\pm e^{-\lambda/2}[e^{-\nu}E^2-r^{-2}J^2-m^2]^{1/2}$, and $p^\theta=\pm r^{-2}[J^2-J_z^2/\Sigma^2(\theta)]^{1/2}$, since $p_\phi=J_z$. Thus $dt/p^t=dr/p^r$ can be integrated along the phase flow (E,J const) to give the time-dependent characteristic

$$C=t-\mathrm{sgn}(p^r)E\int e^{(\lambda-2\nu)/2}$$
$$\times[e^{-\nu}E^2-r^{-2}J^2-m^2]^{-1/2}\,dr, \tag{5.1}$$

while $dr/p^r=d\theta/p^\theta$ can be integrated[14] to give the static characteristic

$$D=\mathrm{sgn}(p^\theta)J^{-1}h(\theta)-\mathrm{sgn}(p^r)\int r^{-2}e^{\lambda/2}$$
$$\times[e^{-\nu}E^2-r^{-2}J^2-m^2]^{-1/2}\,dr, \tag{5.2a}$$

where

$$h(\theta)=\{[\theta^2-J_z^2/J^2]^{1/2},$$
$$-\arcsin[(1-J_z^2/J^2)^{-1/2}\cos\theta\,],$$
$$\mathrm{arcosh}[(1+J_z^2/J^2)^{-1/2}\cosh\theta\,]\},$$
$$\text{for } k=(0,1,-1). \tag{5.2b}$$

Clearly (5.1) and (5.2) are independent of the Killing vector characteristics. Hence we have found the general solution of (2.6):

$$f(x^i,p^\alpha)=F(E,J_x,J_y,J_z,C,D). \tag{5.3}$$

Theorem 5.1: The general solution of the Liouville equation in the static space-times (2.1) is (5.3), where F is an arbitrary physical function.

The non-Killing vector characteristics (5.1) and (5.2) depend on terms quadratic in the momentum components, and can be related to rank 2 Killing tensors[6] in special geometries. For example, in Minkowski space-time, (5.1) gives

$$C=(E^2-m^2)^{-1}K_{ij}p^ip^j,\quad K^{ij}=\sum_\alpha s_\alpha{}^{(i}l_\alpha{}^{j)},$$

where s_α are the spatial translations and l_α the Lorentz boosts, so that C is generated by a reducible Killing tensor.

(D has a similar interpretation.) In the Kimura space-time of case IIc (Theorem 6.18 of Ref. 8), $k=1$, $e^{\nu}=a^{-1}r^2$, $e^{\lambda}=(ar)^{-2}$, where $a>0$, and (5.1) gives

$$C=(aE^2-J^2)^{-1}K_{ij}\,p^ip^j,$$
$$K_{ij}=\mathrm{tr}^4\mathrm{diag}(a^{-1},0,-1,-\Sigma^2)+a^{-2}r\,\delta^t{}_{(i}\delta^r{}_{j)}, \tag{5.4}$$

with $\Sigma=\sin\theta$. Thus C is generated by one of the two irreducible Killing tensors found by Kimura. [Note the incorrect factor $\frac{1}{2}$ in K_{tr} as given by Kimura's equation (6.34).] The static characteristic D must be related to the static irreducible Killing tensors found by Hauser and Malhiot[7] in certain $k=1$ static space-times. In principle, C and D can be used to find irreducible Killing tensors, if they exist, for static space-times.

It is clear from P(2.5), (2.2), and (5.1) and (5.2), that the general Liouville solution (5.3) has a kinematic average four-velocity u, which at each point may tilt in any spatial direction, with a hyperbolic tilt angle that may be time dependent and anisotropic:

$$u=e^{-\nu/2}\cosh\psi(x^i)\partial_t+\sinh\psi(x^i)\tilde{c},\quad \tilde{c}\cdot\partial_t=0,\quad \tilde{c}\cdot\tilde{c}=1, \tag{5.5}$$

where ψ and $\tilde{c}$ are determined by integrating (5.3) over the mass shell. [Note that the Killing vector solution $f=F(E,J_x,J_y,J_z)$ has $\partial\psi/\partial t=0$.] From (5.5) it follows that the general Liouville solution represents a test gas in static space-time with nonstatic and anisotropic expansion, shear, rotation, and acceleration. This solution could be applicable, for example, in the study of noninteracting radiation in astrophysics, since (5.3) (with $k=1$) describes the most general possible collision-free behavior in static spherically symmetric space-time.

By (2.6), it follows that the completely general Liouville solution (5.3) may have a nondiagonal, nonstatic, and anisotropic energy–momentum tensor T^{ab}. Thus it is extremely unlikely that any nondegenerate choice of F in (5.3) could be found to bring T^{ab} into the form (3.6) and hence to satisfy Einstein's field equations. [Even the general Killing vector solution $f=F(E,J_x,J_y,J_z)$ ($\Rightarrow\partial T^{ab}/\partial t=0$) is extremely unlikely to provide a noninvariant Einstein solution.] However, we can find nonstatic solutions with G_3 invariance (i.e., with spherical, planar, or hyperbolic symmetry) that lead to physical distribution solutions of the Einstein–Liouville equations. (This is analogous to the anisotropic but spatially homogeneous solutions found by Ellis *et al.*[15] in Robertson–Walker space-time.) By (5.1), $C=C(t,r,p^1,(p^2)^2+(p^3)^2)$ is the (physical) nonstatic G_3-invariant characteristic, leading to radially tilted u with isotropic tilt angle in (5.5):

$$f=F(C)\Rightarrow u=e^{-\nu/2}\cosh\psi(t,r)\partial_t+e^{-\lambda/2}\sinh\psi(t,r)\partial_r. \tag{5.6}$$

Hence this distribution has time-dependent, isotropic kinematic, and dynamic behavior:

$$\theta=\theta(t,r),\quad \dot{u}^i=a(t,r)c^i,$$
$$\sigma_{ij}=\sqrt{3}\sigma(t,r)(c_ic_j-h_{ij}/3),\quad \omega_{ij}=0, \tag{5.7}$$
$$\mu=\mu(t,r),\quad p=p(t,r),\quad q^i=Q(t,r)c^i,$$
$$\pi_{ij}=\sqrt{3}S(t,r)(c_ic_j-h_{ij}/3). \tag{5.8}$$

It can be shown[5] that, under reasonable restrictions on the function $F(C)$, the dynamic quantities (5.8) [measured by the tilted observer (5.6)] lead to orthonormal components T^{ab} (measured by an orthogonal observer) of the form (3.6). Thus $f=F(C)$ gives a nonstatic Einstein–Liouville solution in static space-time. Note how we require the general solution of Liouville's equation in order to find a nonstatic Einstein–Liouville solution: the Killing vector Liouville solution is always static.

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Classical and quantum scattering theory for linear scalar fields on the Schwarzschild metric. II[a)]

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An alternate treatment of the results of paper I is given. As in that paper, the Unruh boundary condition is formulated, the Unruh vacuum is defined as a state satisfying this boundary condition, and the thermal character of the state is exhibited. The present work differs in that it uses the double-wedge region of the Kruskal manifold and defines and uses a precise notion of distinguished modes.

I. INTRODUCTION

In a recent paper Dimock and Kay[1] have given a treatment of the scattering theory for a scalar quantum field propagating on an external black-hole background. Using these results it was possible to define and characterize some of the standard states for the theory. These are (1) the Boulware vacuum or ground state, (2) the Hartle–Hawking vacuum or thermal state with $T = 1/8\pi M$, and (3) the Unruh vacuum, which represents the radiation of a black body at $T = 1/8\pi M$.

The Hawking effect can be formulated as the hypothesis that the Unruh vacuum is the natural state on the eternal black hole to mock-up the in-vacuum state for the collapsing black hole. The argument for this has two parts. In the first part, only heuristic at present, one argues that to mock-up the collapse situation one should select a state that satisfies a certain boundary condition on the past horizon and at past infinity—the Unruh boundary condition. In the second step, treated in Ref. 1 on the Schwarzschild manifold, one defines a state satisfying this boundary condition, and shows that it is the Unruh vacuum.

In the present paper we give an alternate treatment of the second step, which uses more of the Kruskal manifold, precisely the exterior region and its reflection through the origin—the double wedge. We also introduce and use a precise concept of "distinguished modes" in the formulation of our results. The treatment is close to that of Unruh's original paper.[2] (See also Israel.[3])

This paper can be read independently of Ref. 1. However, the latter contains more details about the formulation and interpretation of the problem, and also has a much more complete list of references. There are some differences in notation between the two papers.

II. CLASSICAL RESULTS

A. Notation

We consider a massless scalar field on the Schwarzschild manifold. (With modifications as in Ref. 1 the massive case could also be treated.) The manifold is $\mathbb{R}\times\mathscr{M}$, where $\mathscr{M} = \mathbb{R}\times S^2$, and the metric is such that the wave equation has the form

$$\frac{d^2f}{dt^2} + B^2 f = 0,$$

$$B^2 = \frac{-\partial^2}{\partial r_*^2} + \left(1 - \frac{2M}{r}\right)\left(\frac{2M}{r^3} - \frac{\Delta_\xi}{r^2}\right).$$

Here $r = r(r_*)$ is defined by $r_* = r + 2M\log(r/2M - 1)$ and Δ_ξ is the Laplacian on S^2. Introducing $p = df/dt$ this can also be written as a first-order system for $F = (f,p)$:

$$\frac{dF}{dt} = -HF, \quad H = \begin{pmatrix} 0 & -1 \\ B^2 & 0 \end{pmatrix}.$$

One can show that B^2 is positive and essentially self-adjoint on $C_0^\infty(\mathscr{M}) \subset L_2(\mathscr{M}, dr_*\, d\omega_\xi)$ ($d\omega_\xi$ = volume element on S^2). Then H is a skew-adjoint operator on the Hilbert space

$$\mathscr{H} = [D(B)] + L_2(\mathscr{M})$$

with

$$D(H) = ([D(B^2)] \cap [D(B)]) \oplus D(B).$$

Here $[D(B)]$ is the completion of $D(B) \subset L_2(\mathscr{M})$ in the norm $\|Bf\|$. (If B is realized as multiplication by a function $\beta(q)$ on some $L_2(Q,dq)$ by the spectral theorem, then $[D(B)]$ is all measurable functions ψ on Q so $\int|\beta(q)|^2 \times|\psi(q)|^2\, dq < \infty$. We have $D(B) = L_2 \cap [D(B)]$.) We now define the unitary e^{-Ht} and $F_t = e^{-Ht}F_0$ is the solution of the wave equation with data F_0.

For future reference we note that

$$H^{-1} = \begin{pmatrix} 0 & B^{-2} \\ -1 & 0 \end{pmatrix} \quad \text{on } D(B) \oplus D(B^{-1}),$$

$$H^{-2} = \begin{pmatrix} -B^2 & 0 \\ 0 & -B^{-2} \end{pmatrix}$$

$$\text{on } D(B) \cap D(B^{-1}) \oplus D(B^{-2}).$$

Since $D(H^{-1}) \subset L_2(\mathscr{M}) \oplus L_2(\mathscr{M})$ we may also define on $D(H^{-1}) \times D(H^{-1})$ the symplectic form

$$\sigma(F_1,F_2) = \int (f_1 p_2 - p_1 f_2)\, dr_*\, d\omega_\xi,$$

which is invariant under time evolution.

[a)] This paper appeared as a preprint under the title "Scattering for scalar quantum fields on black hole metrics. II."

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There are also asymptotic operators. For the Minkowskian region ($r_* \to \infty$) we have

$$B_0^2 = \frac{-\partial^2}{\partial r_*^2} - \frac{\Delta_\xi}{r_*^2}, \quad H_0 = \begin{pmatrix} 0 & -1 \\ B_0^2 & 0 \end{pmatrix}.$$

Then B_0^2 is positive self-adjoint on $L_2(\mathscr{M}^+)$, $\mathscr{M}^+ = \mathbb{R}^+ \times S$, and H_0 is skew-adjoint on

$$\mathscr{A}_0 = [D(B_0)] \oplus L_2$$

(with suitable domains). For the horizon ($r_* \to -\infty$) we have

$$B_1^2 = \frac{-\partial^2}{\partial r_*^2}, \quad H_1 = \begin{pmatrix} 0 & -1 \\ B_1^2 & 0 \end{pmatrix}.$$

Then B_1^2 is positive self-adjoint on $L_2(\mathscr{M})$ and H_1 is skew-adjoint on

$$\mathscr{A}_1 = [D(B_1)] \oplus L_2$$

(with suitable domains).

The space $L_2(\mathscr{M}) = L_2(\mathbb{R} \times S^2, dr_* \, d\omega_\xi)$ can be identified with $L_2(\mathbb{R}, L_2(S^2))$, where $L_2(S^2) = L_2(S^2, d\omega_\xi)$. On this space or on $\mathscr{S}'(\mathbb{R}, L_2(S^2))$ one can define a Fourier transform

$$\tilde{f}(k) = (2\pi)^{-1/2} \int \exp(-ikr_*) f(r_*) dr_*.$$

Then $B_1 = (-\partial^2/\partial r_*^2)^{1/2}$ is multiplication by $|k|$ and $[D(B_1)] = \{f \in \mathscr{S}' : |k| \tilde{f} \in L_2\}$.

The Hilbert space $\mathscr{A}_1$ splits to $\mathscr{A}_1 \equiv \mathscr{A}_L \oplus \mathscr{A}_R$, where

$$\mathscr{A}_{L/R} = \left\{ (f,p) \in \mathscr{A}_1 : p = \pm \frac{\partial f}{\partial r_*} \right\}$$

($\partial/\partial r_* : [D(B_1)] \to L_2(\mathscr{M})$ since it is multiplication by ik under the Fourier transform). These are data for left and right moving solutions under $e^{-H_1 t}$.

The scattering theory for $dF/dt = -HF$ was developed jointly by the authors and appears in Refs. 1, 4, and 5. The fundamental result is that there exist wave operators $\Omega_0^\pm : \mathscr{A}_0 \to \mathscr{A}$ and $\Omega_1^\pm : \mathscr{A}_1 \to \mathscr{A}$ defined on dense domains $\mathscr{D}_0 \times \mathscr{D}_0 \subset \mathscr{A}_0$ and $\mathscr{D}_1 \times \mathscr{D}_1 \subset \mathscr{A}_1$, by

$$\Omega_0^\pm F = \lim_{t \to \pm\infty} e^{Ht} J_0 e^{-H_0 t} F,$$

$$\Omega_1^\pm F = \lim_{t \to \pm\infty} e^{Ht} J_1 e^{-H_1 t} F,$$

where $J_0 : \mathscr{A}_0 \to \mathscr{A}$ and $J_1 : \mathscr{A}_1 \to \mathscr{A}$ are certain identification operators between these Hilbert spaces. Then $\Omega_0^\pm$ is an isometry and $\Omega_1^\pm$ is a partial isometry with initial subspace $\mathscr{A}_{L/R}$. Elements of $\mathscr{A}^{0,\pm} \equiv \mathrm{Ran}\, \Omega_0^\pm$ are data for solutions which are free as $t \to \pm\infty$ while elements of $\mathscr{A}^{1,\pm} \equiv \mathrm{Ran}\, \Omega_1^\pm$ are data for solutions which go to the horizon as $t \to \pm\infty$. We also have asymptotic completeness:

$$\mathscr{A}^{0,\pm} \oplus \mathscr{A}^{1,\pm} = \mathscr{A}.$$

Theorem II.1: Let $F_1 \in D(H_1^{-1}) \cap \mathscr{A}_{L/R}$ and $F = \Omega_1^\pm F_1 \in D(H^{-1}) \cap \mathscr{A}^{1,\pm}$. Then the first components of $e^{-Ht}F$ and $e^{-H_1 t}F_1$ determine continuous functions $f(t,r_*)$, $f_1(t,r_*)$ from $\mathbb{R}^2$ to $L_2(S^2)$ which satisfy

$$\lim_{t \to \pm\infty} \left\{ \sup_{r_*} |f(t,r_*) - f_1(t,r_*)| \right\},$$

where $|\cdot|$ is the norm in $L_2(S^2)$.

The limit holds in a mean sense just by the definition of the wave operators. The theorem asserts that the limit is uniform in r_*. The proof is given in Appendix A.

B. The Kruskal manifold

The Schwarzschild manifold extends to the Kruskal manifold. The Kruskal manifold is $\{(T,X) \in \mathbb{R}^2 : T^2 - X^2 < 1\} \times S^2$ together with a metric such that the wave equation takes the form

$$\left(\frac{\partial^2}{\partial T^2} - \frac{\partial^2}{\partial X^2} + 32M^3 r^{-1} e^{-r/2M} \left(\frac{2M}{r^3} - \frac{\Delta_\xi}{r^2} \right) \right) \phi = 0, \tag{1}$$

where r is defined by $T^2 - X^2 = e^{r/2M}(1 - r/2M)$. We divide the manifold into four regions:

region I: $X > |T|$,
region II: $T > |X|$,
region III: $-X > |T|$,
region IV: $-T > |X|$.

Then region I is isometric with the Schwarzschild manifold under the change of variables

$$T = e^{r_*/4M} \sinh(t/4M), \quad X = e^{r_*/4M} \cosh(t/4M),$$

and is identified with the exterior of the black hole. Region III is also isometric, but now we choose

$$T = -e^{r_*/4M} \sinh(t/4M),$$

$$X = -e^{r_*/4M} \cosh(t/4M),$$

so that t is negative timelike in this region if T is positive timelike.

Although one can solve the Kruskal wave equation globally, for our purposes it is convenient to only consider regions I and III where there is a timelike symmetry. Then it suffices to double up the constructions for the Schwarzschild manifold.

Thus we define

$$\underline{\mathscr{A}} = \mathscr{A}_{\mathrm{I}} \oplus \mathscr{A}_{\mathrm{III}},$$

where $\mathscr{A}_{\mathrm{I}}$, $\mathscr{A}_{\mathrm{III}}$ are copies of $\mathscr{A}$ and

$$\underline{H} = H \oplus H.$$

Then $e^{-\underline{H}t}$ generates solutions of the wave equation in I and III. It is a twist which goes forward in I and backward in III. Similarly we double $\mathscr{A}_1$, H_1, etc. to obtain $\underline{\mathscr{A}}_1$, $\underline{H}_1$, etc. An invariant symplectic form which respects the time orientation is

$$\underline{\sigma} = \sigma \oplus (-\sigma).$$

Now define

$$U = (T - X)/2, \quad V = (T + X)/2.$$

The past horizon is the $V = 0$ axis and the future horizon is the $U = 0$ axis. In spite of our restriction to regions I and III, the horizons are accessible as boundary values for our solutions. The following result for region I is typical. There is a similar result for region III.

Theorem II.2: Let $F_1 \in D(H_1^{-1}) \cap \mathscr{A}_R$ and $F = \Omega_1^- F_1$

$\in D(H^{-1})\cap\mathscr{A}^{1,-}$. Then the first components of $e^{-Ht}F$ and $e^{-H_1 t}F_1$, determine continuous functions $\phi(U,V)$, $\phi_1(U,V)$ from $V>0$, $U<0$ (region I) to $L_2(S^2)$ such that

$$\lim_{V\searrow 0}|\phi(U,V)-\phi_1(U,V)|=0.$$

Proof: The coordinates U,V are related to r_*,t by

$$t(U,V)=2M(\log V-\log(-U)),$$

$$r_*(U,V)=2M(\log V+\log(-U)).$$

Let f,f_1 be as in Theorem II.1. Then

$$|\phi(U,V)-\phi_1(U,V)|$$

$$\equiv|f(t(U,V),r_*(U,V))-f_1(t(U,V),r_*(U,V))|$$

$$\leqslant\sup_{r_*}|f(t(U,V),r_*)-f_1(t(U,V),r_*)|\to 0 \quad \text{as } V\searrow 0.$$

The last step follows by Theorem II.1 since $t(U,V)\to-\infty$ as $V\searrow 0$.

C. Complex solutions

Let $\mathscr{A}^{\mathbb{C}}$ be the complexification of $\mathscr{A}$. We define subspaces

$$\mathscr{A}_{t\text{-pos}/t\text{-neg}}\equiv\{F=(f,p)\in\mathscr{A}^{\mathbb{C}}:\ p=\mp iBf\}.$$

[Note that B is unitary from $[D(B)]$ to $L_2(\mathscr{M})$.] These subspaces are orthogonal and they span $\mathscr{A}^{\mathbb{C}}$ since we may write

$$(f,p)=\tfrac{1}{2}(f+iB^{-1}p,-iBf+p)+\tfrac{1}{2}(f-iB^{-1}p,iBf+p).$$

Thus we have

$$\mathscr{A}^{\mathbb{C}}=\mathscr{A}_{t\text{-pos}}\oplus\mathscr{A}_{t\text{-neg}}. \tag{2}$$

Now $(-iH)$ is a self-adjoint operator on $D(H)$, and we have $-iH=B\oplus B$ in $\mathscr{A}_{t\text{-pos}}$ and $-iH=-(B\oplus B)$ in $\mathscr{A}_{t\text{-neg}}$. Thus $\mathscr{A}_{t\text{-pos}}$ and $\mathscr{A}_{t\text{-neg}}$ are the positive and negative spectral subspaces for $-iH$. Note also that on $D(H)$,

$$|H|=|-iH|=B\oplus B. \tag{3}$$

By the spectral theorem we also have the characterization that $\mathscr{A}_{t\text{-pos}}$ is the subspace of all F such that

$$\exp(-tH)F=\exp[-i(-iH)t]F$$

is bounded and analytic in the lower half-plane in t. One uses to terminology "t-positive frequency."

We may similarly split $\mathscr{A}_1^{\mathbb{C}}=\mathscr{A}_{1,t\text{-pos}}\oplus\mathscr{A}_{1,t\text{-neg}}$ into the positive and negative subspaces for $-iH_1$.

Lemma II.3: (a) $\Omega_1^{\pm}:\mathscr{A}_{1,t\text{-pos}}\to\mathscr{A}_{t\text{-pos}}$ (also for t-neg).

(b) For any measurable function f, $\Omega_1^{\pm}$ maps $D(f(-iH_1))$ to $D(f(-iH))$ and on $D(f(-iH_1))$

$$f(-iH)\Omega_1^{\pm}=\Omega_1^{\pm}f(-iH_1).$$

Proof: (a) Use the intertwining relation $e^{-Ht}\Omega_1^{\pm}=\Omega_1^{\pm}e^{-H_1 t}$ on $\mathscr{A}^{\mathbb{C}}$. If $F\in\mathscr{A}_{1,t\text{-pos}}$, then $e^{-Ht}\Omega_1^{\pm}F$ is bounded and analytic in the lower half-plane and so $\Omega_1^{\pm}F\in\mathscr{A}_{t\text{-pos}}$ which gives (a).

(b) $\Omega_1^{\pm}$ is unitary from $(\mathscr{A}_{L/R})^{\mathbb{C}}$ to $(\mathscr{A}^{1,\pm})^{\mathbb{C}}$ so $e^{-H_1 t}$ on the former domain is unitarily equivalent to e^{-Ht} on the latter. These unitary groups have self-adjoint generators $-iH_1$, $-iH$ and so the statement of (b) in $(\mathscr{A}_{L/R})^{\mathbb{C}}$ follows. But the statement is trivial on the complement $(\mathscr{A}_{R/L})^{\mathbb{C}}$ and so holds generally. Q.E.D.

For the Kruskal manifold we split $\mathscr{A}^{\mathbb{C}}=\mathscr{A}_{\mathrm{I}}^{\mathbb{C}}\oplus\mathscr{A}_{\mathrm{III}}^{\mathbb{C}}$ into positive and negative spectral subspaces for $-i\underline{H}^{+}\equiv(-iH)\oplus iH$, which generates forward time evolution. We have

$$\mathscr{A}^{\mathbb{C}}=\mathscr{A}_{t\text{-pos}}\oplus\mathscr{A}_{t\text{-neg}},$$

where

$$\mathscr{A}_{t\text{-pos}}=\mathscr{A}_{\mathrm{I},t\text{-pos}}\oplus\mathscr{A}_{\mathrm{III},t\text{-neg}},$$

$$\mathscr{A}_{t\text{-neg}}=\mathscr{A}_{\mathrm{I},t\text{-neg}}\oplus\mathscr{A}_{\mathrm{III},t\text{-pos}}.$$

Now let $G\in D(\underline{H}^{-1})\subset\mathscr{A}^{\mathbb{C}}$ and let $\phi(U,V)$ be the solution $\exp(-t\underline{H})G$ expressed in Kruskal U,V coordinates for $U<0$, $V>0$ and for $U>0$, $V<0$ (regions I and III). We define a subspace $\mathscr{A}_{U\text{-pos}}$ of $\mathscr{A}^{\mathbb{C}}$ (not necessarily closed) as those G such that $\phi(U,V)$ has a boundary value $\phi(U,0)$ on $V=0$ [in the sense of $L_2(S^2)$ convergence] which is positive frequency in U. Thus

$$\mathscr{A}_{U\text{-pos}}=\{G\in D(\underline{H}^{-1})\subset\mathscr{A}^{\mathbb{C}}:\ \phi(U,0)\text{ is bounded and analytic in Im } U<0\}.$$

We similarly define a subspace $\mathscr{A}_{1,U\text{-pos}}$ of $D(\underline{H}_1^{-1})\subset\mathscr{A}_1^{\mathbb{C}}$ using the dynamics $\exp(-t\underline{H}_1)G$ instead of $\exp(-t\underline{H})G$.

The two notions of positive frequency (t-pos, U-pos) will be connected by a densely defined operator $\mathscr{L}$ on $\mathscr{A}=\mathscr{A}_{\mathrm{I}}\oplus\mathscr{A}_{\mathrm{III}}$ given by

$$\mathscr{L}=\begin{pmatrix}\cosh\phi(|H|) & \sinh\phi(|H|)\\ \sinh\phi(|H|) & \cosh\phi(|H|)\end{pmatrix}, \tag{4}$$

where

$$\cosh\phi(k)=(1-e^{-8\pi Mk})^{-1/2},$$

$$\sinh\phi(k)=e^{-4\pi Mk}(1-e^{-8\pi Mk})^{-1/2}.$$

To keep track of domains for $\mathscr{L}$ we consider $|H|^{-3/2}=B^{-3/2}\oplus B^{-3/2}$ with domain

$$D(|H|^{-3/2})=D(B)\cap D(B^{-1/2})\oplus D(B^{-3/2}).$$

We have $D(H^{-2})\subset D(|H|^{-3/2})\subset D(H^{-1})$.

Lemma II.4: (a) $\mathscr{L}$ maps $D(\underline{H}^{-2})\to D(|\underline{H}|^{-3/2})$ and $D(|\underline{H}|^{-3/2})\to D(\underline{H}^{-1})$.

(b) $\mathscr{L}$ is symplectic, i.e., $\mathscr{L}$ preserves $\underline{\sigma}$.

Proof: Both $\cosh\phi(k)$ and $\sinh\phi(k)$ are bounded as $k\to-\infty$ and are $\mathcal{O}(k^{-1/2})$ as $k\searrow 0$. Hence $\cosh\phi(|H|)$ and $\sinh\phi(|H|)$ map $D(H^{-2})$ to $D(|H|^{-3/2})$ and $D(|H|^{-3/2})$ to $D(H^{-1})$. Part (a) follows and part (b) is immediate from $\cosh^2\phi-\sinh^2\phi=1$. Q.E.D.

We similarly define $\mathscr{L}_1$ in $\mathscr{A}_1=\mathscr{A}_{1,\mathrm{I}}\oplus\mathscr{A}_{1,\mathrm{III}}$ with $|H_1|$ and domains $D(\underline{H}_1^{-2}),D(|\underline{H}_1|^{-3/2})$. We define $\underline{\Omega}_1^{\pm}:\underline{\mathscr{A}}_1\to\underline{\mathscr{A}}$ by

$$\underline{\Omega}_1^{\pm}=\Omega_1^{\pm}\oplus\Omega_1^{\pm}.$$

By Lemma II.3(b) we have on $D(|H_1|^{-3/2})$

$$\mathscr{L}\underline{\Omega}_1^{\pm}=\underline{\Omega}_1^{\pm}\mathscr{L}_1. \tag{5}$$

Thus $\mathscr{L}$ preserves $\mathscr{A}^{1,\pm}\equiv\mathrm{Ran}\,\underline{\Omega}_1^{\pm}$. We extend $\mathscr{L}$ to be complex linear on $\mathscr{A}^{\mathbb{C}}$.

Theorem II.5: Let $G\in D(|\underline{H}|^{-3/2})\cap(\mathscr{A}^{1,-})^{\mathbb{C}}$ so that $\mathscr{L}G\in D(\underline{H}^{-1})\cap(\mathscr{A}^{1,-})^{\mathbb{C}}$. Then $G\in\mathscr{A}_{t\text{-pos}}$ implies $\mathscr{L}G\in\mathscr{A}_{U\text{-pos}}$.

Proof: We have $G=\underline{\Omega}_1^- G_1$ with $G_1\in D(|H_1|^{-3/2})\cap(\mathscr{A}_R)^C$. Then $\mathscr{L}G=\underline{\Omega}_1^-\mathscr{L}_1 G_1$ by (5). Since $\exp(-\underline{H}t)\mathscr{L}G$ has the same boundary values as $\exp(-\underline{H}_1 t)\mathscr{L}_1 G_1$ by Theorem II.2 it is sufficient to prove the following theorem.

Theorem II.5′: Let $G\in D(|\underline{H}_1|^{-3/2})\cap(\mathscr{A}_R)^C$ so that $\mathscr{L}_1 G\in D(\underline{H}_1^{-1})\cap(\mathscr{A}_R)^C$. Then $G\in\mathscr{A}_{1,t\text{-pos}}$ implies $\mathscr{L}_1 G\in\mathscr{A}_{1,U\text{-pos}}$.

First consider $G=(F,0)$ with $F\in D(|H_1|^{-3/2})\cap\mathscr{A}_R^C\cap\mathscr{A}_{1,t\text{-pos}}$. We then have $F=(f,-\partial f/\partial r_*)=(f,-iB_1 f)$ with $f\in D(B_1)\cap D(B_1^{-1/2})$. Let $\tilde{f}$ be the $L_2(S^2)$ valued Fourier transform of f. Since $\partial/\partial r_*\leftrightarrow ik$ and $iB_1\leftrightarrow i|k|$ we must have $\tilde{f}(k)=0$, for $k<0$. The domain condition becomes

$$\int_0^\infty (1+k^2+k^{-1})|\tilde{f}(k)|^2\,dk<\infty. \tag{6}$$

Now $\mathscr{L}_1 G=(\cosh\phi(|H_1|)F,\ \sinh\phi(|H_1|)F)$, and $\cosh\phi(|H_1|)(f,p)=(\cosh\phi(B_1)f,\cosh\phi(B_1)p)$. Also $\cosh\phi(B_1)f$ has Fourier transform $\cosh\phi(|k|)\tilde{f}(k)$. We have

$$\exp(-\underline{H}_1 t)\mathscr{L}_1 G = (e^{-H_1 t}\cosh\phi(|H_1|)F, e^{-H_1 t}\sinh\phi(|H_1|)F)$$

and $e^{-H_1 t}$ is a translation by t on $(\mathscr{A}_R)^C$. Thus we have the $L_2(S^2)$ valued solutions:

$$\begin{aligned}&(2\pi)^{-1/2}\int_0^\infty e^{ik(r_*-t)}\cosh\phi(k)\tilde{f}(k)dk, \quad \text{region I},\\ &(2\pi)^{-1/2}\int_0^\infty e^{ik(r_*-t)}\sinh\phi(k)\tilde{f}(k)dk, \quad \text{region III}.\end{aligned} \tag{7}$$

[The integrands are L_1 by (6) and $\cosh\phi(k)=\mathcal{O}(k^{-1/2})$ as $k\to 0$.] In U,V coordinates we have

$$\begin{aligned}&(2\pi)^{-1/2}\int_0^\infty \exp(i4Mk\log(-U))\cosh\phi(k)\tilde{f}(k)dk, \quad U<0,\\ &(2\pi)^{-1/2}\int_0^\infty \exp(i4Mk\log U)\sinh\phi(k)\tilde{f}(k)dk, \quad U>0,\end{aligned} \tag{8}$$

which trivially has the same boundary value as $V\to 0$.

Now define $\log U$ in the lower half-plane with $-\pi\leqslant\arg U\leqslant 0$. We then have for U negative

$$\exp(i4Mk\log(-U))=e^{-4Mk\pi}\exp(i4Mk\log U).$$

Since also

$$e^{-4Mk\pi}\cosh\phi(k)=\sinh\phi(k),$$

we see that (8) is the boundary value as $\operatorname{Im} U\nearrow 0$ of the single analytic function in the lower half-plane

$$(2\pi)^{-1/2}\int_0^\infty \exp(i4Mk\log U)\sinh\phi(k)\tilde{f}(k)dk. \tag{9}$$

This is well defined and bounded in the lower half-plane since

$$|\exp(i4Mk\log U)|\leqslant\exp(4Mk\pi)$$

and

$$|\exp(4Mk\pi)\sinh\phi(k)|=|\cosh\phi(k)|$$

and $|\cosh\phi(k)\tilde{f}(k)|$ is in L_1. Thus we have that $\mathscr{L}_1 G\in\mathscr{A}_{1,U\text{-pos}}$ as required.

Now suppose $G=(0,F)$ with $F\in\mathscr{A}_{1,t\text{-neg}}$. Then $F=(f,-\partial f/\partial r_*)=(f,iB_1 f)$ and so $\tilde{f}(k)=0$, for $k>0$. Proceeding as before we obtain from $\exp(-H_1 t)\mathscr{L}_1 G$:

$$\begin{aligned}&(2\pi)^{-1/2}\int_0^\infty \exp(-i4Mk\log(-U))\sinh\phi(k)\tilde{f}(-k)dk, \quad U<0,\\ &(2\pi)^{-1/2}\int_0^\infty \exp(-i4Mk\log U)\cosh\phi(k)\tilde{f}(-k)dk, \quad U>0.\end{aligned} \tag{10}$$

This is the boundary value as $\operatorname{Im} U\nearrow 0$ of the function

$$(2\pi)^{-1/2}\int_0^\infty \exp(-i4Mk\log U)\cosh\phi(k)\tilde{f}(-k)dk, \tag{11}$$

which is bounded and analytic in the lower half-plane. Thus $\mathscr{L}_1 G\in\mathscr{A}_{1,U\text{-pos}}$ in this case as well. Q.E.D.

III. QUANTUM RESULTS

For the time-zero quantum field on the Schwarzschild manifold we take a representation of the CCR over $(D(H^{-2}),\sigma)$. This consists of operators $W(F)$ indexed by $F\in D(H^{-2})\subset\mathscr{A}$ which satisfy

$$W(F_1)W(F_2)=\exp(-i\sigma(F_1,F_2)/2)W(F_1+F_2).$$

The time-evolved field operator is then

$$W_t(F)=W(e^{Ht}F).$$

States for the system are states on the C^*-algebra generated by $W(F)$. The ground state is defined by

$$\omega(W(F))=\exp(-\tfrac{1}{2}\|KF\|^2),$$

where $K: D(H^{-1})\to\mathscr{H}\equiv L_2(\mathscr{M},\mathbb{C})$ is defined by

$$K(f,p)=2^{-1/2}(B^{1/2}f+iB^{-1/2}p)$$

and is symplectic from $(D(H^{-1}),\sigma)$ to $(\mathscr{H},2\operatorname{Im}(\cdot,\cdot))$.

Such a state can be characterized by its *distinguished modes* defined as those $F\in D(H^{-2})$ in the complexification $\mathscr{A}^C$ of $\mathscr{A}$ such that $K^C\bar{F}=0$, where K^C is the complex linear extension of K. The interpretation of this is that the state lacks field excitations of this type. For this particular K the distinguished modes satisfy $p=-iBf$ and so are elements of $\mathscr{A}_{t\text{-pos}}$. For more about distinguished modes see Appendix B.

For the Kruskal manifold (regions I and III) we take a representation of the CCR over $(D(\underline{H}^{-2}),\underline{\sigma})$. Thus we have operators $\underline{W}(G)$ indexed by $G\in D(\underline{H}^{-2})\subset\underline{\mathscr{A}}$ such that

$$\underline{W}(G_1)\underline{W}(G_2)=\exp(-i\underline{\sigma}(G_1,G_2)/2)\underline{W}(G_1+G_2).$$

The time-evolved field operator is

$$\underline{W}_t(G)=\underline{W}(e^{\underline{H}t}G).$$

Note that if we restrict to region I, $W_t(F)\equiv\underline{W}_t(F,0)$ is a field operator for the Schwarzschild manifold. A ground state on the C^*-algebra generated by $\underline{W}(G)$ is defined by

$$\underline{\omega}(\underline{W}(G))=\exp(-\tfrac{1}{2}\|\underline{K}G\|^2),$$

where $\underline{K}: D(\underline{H}^{-1})\to\mathscr{H}\oplus\mathscr{H}$ is defined by

$$\underline{K}=K\oplus CK.$$

Here C is complex conjugation and is necessary to make $\underline{K}$ symplectic from $(D(\underline{H}^{-1}),\underline{\sigma})$ to $(\mathscr{H}\oplus\mathscr{H},2\,\mathrm{Im}(\,\cdot\,,\cdot\,))$. The distinguished modes satisfy $\underline{K}^{\mathbb{C}}(\bar{G})=0$, where $\underline{K}^{\mathbb{C}}=K\oplus CKC$ and they are elements of $\mathscr{A}_{t\text{-pos}}$.

The Unruh vacuum will be defined on the same algebra, but with different distinguished modes. The choice of distinguished modes depends on the following considerations relating the collapsing star to the eternal black hole.

The exterior of a collapsing star can be represented as a portion of regions I and II of the Kruskal manifold that lies above a certain forward timelike curve $T(\lambda)$, $X(\lambda)$ going from I to II and representing the surface of the star. In the idealization in which the collapse occurs in the distant past this line approaches the $V=0$ axis and the exterior corresponds to all of regions I and II.

For the collapsing star we are interested in the state which has no particles in the distant past, the in-vacuum. This is the state for which the distinguished modes are t-positive frequency in the distant past. Now Unruh[2] argues that in the idealization mentioned above the t-positive frequency modes will have U-positive frequency when they emerge from the surface of the star, i.e., at $V=0$. (This statement is susceptible to proof if one takes a model for collapse.) The upshot is that we want to define a state which has distinguished modes which are U-positive frequency on the past horizon $V=0$, but still t-positive frequency at past infinity. This is the Unruh boundary condition.

With these remarks as motivation we define the Unruh vacuum by

$$\omega_U(\underline{W}(G))=\exp(-\tfrac{1}{2}\|K_U\underline{G}\|^2),$$

where $K_U: D(\underline{H}^{-2})\to\mathscr{H}\oplus\mathscr{H}$ is defined by

$$K_UG=\begin{cases}\underline{K}G, & G\in\mathscr{A}^{0,-},\\ \underline{K}\mathscr{L}^{-1}G, & G\in\mathscr{A}^{1,-}.\end{cases}$$

Note that K_U is symplectic since both $\underline{K}$ and $\mathscr{L}^{-1}$ are symplectic, since $\mathscr{A}^{0,-},\mathscr{A}^{1,-}$ are symplectic orthogonal, and since $\mathscr{L}^{-1}$ preserves $\mathscr{A}^{1,-}$.

The distinguished modes are those $G\in D(\underline{H}^{-2})\subset\mathscr{A}^{\mathbb{C}}$ such that $K_U^{\mathbb{C}}(\bar{G})=0$. The distinguished modes in $\mathscr{A}^{0,-}$ are elements of $\mathscr{A}_{t\text{-pos}}$. The distinguished modes in $\mathscr{A}^{1,-}$ are those G such that $\mathscr{L}^{-1}G\in D(|\underline{H}|)^{-3/2})$ is in $\mathscr{A}_{t\text{-pos}}$. For such G we have $G=\mathscr{L}(\mathscr{L}^{-1}G)$ in $\mathscr{A}_{U\text{-pos}}$ by Theorem II.5. Thus the Unruh boundary condition is satisfied.

Now we look at the Unruh vacuum on the exterior field $W(F)=\underline{W}(F,0)$, $F\in D(H^{-2})$.

Proposition III.1:

$$\omega_U(W(F))=\begin{cases}\exp(-\tfrac{1}{2}\|KF\|^2), & F\in\mathscr{A}^{0,-},\\ \exp(-\tfrac{1}{2}(KF,\coth(4\pi MB)KF)), & F\in\mathscr{A}^{1,-}.\end{cases}$$

Proof: For $F\in\mathscr{A}^{0,-}$ this is trivial, while for $F\in\mathscr{A}^{1,-}$ we make the calculation

$$\begin{aligned}&\|K\mathscr{L}^{-1}(F,0)\|^2\\ &\quad=(KF,(\cosh^2\phi(B)+\sinh^2\phi(B))KF)\\ &\quad=(KF,\coth(4\pi MB)KF).\end{aligned}$$

[Note that $KF\in D(B^{-1})$ and $\cosh\phi(B)$, $\sinh\phi(B)$, and $\coth(4\pi MB)$ are defined on this domain.] Q.E.D.

Now the state on the subalgebra generated by $\{W(F): F\in\mathscr{A}^{1,-}\}$ may be identified as the KMS state for $T=1/8\pi M$, for our dynamics. The state is thus thermal on modes coming from the star in the past and a ground state for modes coming from infinity in the past. In this sense it represents the radiation of a hot body ($T=1/8\pi M$) in a cold universe ($T=0$). The characterization of the state in the distant future is more complicated, see Ref. 1.

APPENDIX A: ESTIMATES

We give the proof of Theorem II.1. Using the Fourier transform on $L_2(\mathscr{M})=L_2(\mathbb{R},L_2(S^2))$ one can show that if $f\in D(B_1)$, then f is continuous from $\mathbb{R}$ to $L_2(S^2)$ and satisfies the Sobolev inequality

$$|f(r_*)|\leqslant C(\|B_1f\|+\|f\|), \tag{A1}$$

where $|\cdot|$ is the norm in $L_2(S^2)$. Since $B_1^2\leqslant B^2$ on the core $C_0^\infty(\mathscr{M})$ we may deduce that $D(B)\subset D(B_1)$ and that for $f\in D(B)$, $\|B_1f\|\leqslant\|Bf\|$. Thus for $f\in D(B)$, we also have $f\in C(\mathbb{R},L_2(S^2))$ and

$$|f(r_*)|\leqslant C[\|Bf\|+\|f\|]. \tag{A2}$$

If $F=(f,p)\in D(H^{-1})$, then $f\in D(B)$, $p\in D(B^{-1})$ and

$$\|H^{-1}F\|^2+\|F\|^2=\|f\|^2+\|B^{-1}p\|^2+\|Bf\|^2+\|p\|^2. \tag{A3}$$

A similar result holds for H_1^{-1}.

Combining the above we have the following lemma.

Lemma A1: Let $F=(f,p)\in D(H^{-1})$, then $f\in C(\mathbb{R},L_2(S^2))$ and

$$|f(r_*)|\leqslant C(\|H^{-1}F\|+\|F\|).$$

A similar result holds for $F\in D(H_1^{-1})$.

Now define $\mathscr{D}_1\subset L_2(\mathscr{M})$ by

$$\mathscr{D}_1=\left\{f=\sum_i f_i\,g_i:\ \tilde{f}_i\in C_0^\infty(\mathbb{R}\setminus\{0\}),\ g_i\in C^\infty(S^2)\right\}.$$

Then $\mathscr{D}_1\times\mathscr{D}_1$ is dense in $\mathscr{A}_1$ and the wave operator $\Omega_1^\pm$ exists as a limit on this domain.

Lemma A2: $(\mathscr{D}_1\times\mathscr{D}_1)\cap\mathscr{A}_{L/R}$ is a core for H_1^{-1} on $D(H_1^{-1})\cap\mathscr{A}_{L/R}$.

Proof: In $D(H_1^{-1})\cap\mathscr{A}_{L/R}$ we have

$$F=\begin{pmatrix}f,\ \pm\dfrac{\partial f}{\partial r_*}\end{pmatrix},\quad f\in D(B_1).$$

Then (A3) for H_1 becomes

$$\|H_1^{-1}F\|_1^2+\|F\|_1^2=2(\|B_1f\|^2+\|f\|^2).$$

The result now follows since $\mathscr{D}_1$ is a core for B_1. Q.E.D.

Now let $F_1\in D(H_1^{-1})\cap\mathscr{A}_{L/R}$ and $F=\Omega_1^\pm F_1\in D(H^{-1})\cap\mathscr{A}^{1,\pm}$. We define

$$e^{-Ht}F=(f_t,p_t),\quad e^{-H_1t}F_1=(f_{1,t},p_{1,t}).$$

By Lemma A1 $f_t, f_{1,t}$ determine functions $f(t,r_*)$, $f_1(t,r_*)$ from $\mathbb{R}^2$ to $L_2(S^2)$. Also by Lemma A1 these functions are continuous in t uniformly in r_* and hence they are continuous on $\mathbb{R}^2$.

Lemma A3 (Theorem II.1):

$$\lim_{t\to\pm\infty}\left\{\sup_{r_*}|f(t,r_*)-f_1(t,r_*)|\right\}=0.$$

Proof: We have the estimates from Lemma A1

$$|f_1(t,r_*)| \leqslant C\|H_1^{-1}F_1\|_1 + \|F_1\|_1$$
$$|f(t,r_*)| \leqslant C(\|H^{-1}\Omega_1^{\pm}F_1\| + \|\Omega_1^{\pm}F_1\|)$$
$$= C(\|H_1^{-1}F_1\|_1 + \|F_1\|_1).$$

Here we use $H^{-1}\Omega_1^{\pm} = \Omega_1^{\pm}H_1^{-1}$. By Lemma A2 we may pick $F_{1,j} \in (\mathscr{D}_1 \times \mathscr{D}_1) \cap \mathscr{A}_{L/R}$ so that $\|F_{1,j} - F_1\|_1$ and $\|H_1^{-1}(F_{1,j} - F_1)\|_1$ go to zero as $j \to \infty$. Then with $F_j = \Omega_1^{\pm}F_{1,j}$, we have, by the above estimates,

$$\lim_{j\to\infty}\left\{\sup_{r_*}|f_1(t,r_*) - f_{1,j}(t,r_*)|\right\} = 0,$$
$$\lim_{j\to\infty}\left\{\sup_{r_*}|f(t,r_*) - f_j(t,r_*)|\right\} = 0,$$

and the limits are uniform in t. Thus it suffices to prove fixed j that $\sup|f_j(t,r_*) - f_{1,j}(t,r_*)| \to 0$ as $t \to \pm\infty$, i.e., that the theorem holds for $F_1 \in (\mathscr{D}_1 \times \mathscr{D}_1) \cap \mathscr{A}_{L/R}$.

Now assuming $F_1 \in (\mathscr{D}_1 \times \mathscr{D}_1) \cap \mathscr{A}_{L/R}$ we have that $e^{-H_1 t}F_1$ is in $\mathscr{A}$ and

$$\|B(f_t - f_{1,t})\| \leqslant \|e^{-Ht}\Omega_1^{\pm}F_1 - e^{-H_1 t}F_1\|,$$

which goes to zero as $t \to \pm\infty$ [with the restriction to $(\mathscr{D}_1 \times \mathscr{D}_1) \cap \mathscr{A}_{L/R}$ the identification operator J_1 is unnecessary].

We also have that $H_1^{-1}F_1 \in (\mathscr{D}_1 \times \mathscr{D}_1) \cap \mathscr{A}_{L/R}$ and that $e^{-tH_1}(H_1^{-1}F)$ is in $\mathscr{A}$ and so

$$\|f_t - f_{1,t}\| \leqslant \|H^{-1}e^{-Ht}\Omega_1^{\pm}F_1 - H_1^{-1}e^{-H_1 t}F_1\|$$
$$= \|(e^{-Ht}\Omega_1^{\pm} - e^{-H_1 t})H_1^{-1}F_1\|,$$

which goes to zero as above. The result $\sup|f(t,r_*) - f_1(t,r_*)| \to 0$ now follows by the inequality (A2).

APPENDIX B: DISTINGUISHED MODES

Let $\mathscr{D}$ be a real pre-Hilbert space supplied with a symplectic form σ. Let $W(F)$ be a representation of the CCR over $(\mathscr{D},\sigma)$ consisting of operators $W(F)$ on some complex Hilbert space, indexed by $F \in \mathscr{D}$, and satisfying

$$W(F_1)W(F_2) = \exp(-i\sigma(F_1,F_2)/2)W(F_1 + F_2).$$

A state on the C^*-algebra generated by $W(F)$ may be defined by a pair $(\mathscr{H},K)$ consisting of a complex Hilbert space $\mathscr{H}$ regarded as a real symplectic space with symplectic form $2\,\mathrm{Im}(\cdot,\cdot)$, and a symplectic operator $K: \mathscr{D} \to \mathscr{H}$, which we assume has dense complex-linear range. The state is defined by

$$\omega(W(F)) = \exp(-\tfrac{1}{2}\|KF\|^2).$$

The state ω can be realized on Fock space as follows. Let $\mathscr{F}$ be the Fock space over $\mathscr{H}$ with vacuum state Ω. For $\psi \in \mathscr{H}$, let $a(\psi)$, $a(\psi)^*$ be creation and annihilation operators on $\mathscr{F}$ (a antilinear in ψ) and let

$$\sigma(\Phi,F) = a(KF) + a(KF)^*.$$

Then $\sigma(\Phi,F)$ is naturally self-adjoint on $\mathscr{F}$ and $W(F) = \exp(i\sigma(\Phi,F))$ gives a representation of the CCR. The state ω is realized as $\omega = (\Omega,[\,\cdot\,]\Omega)$.

Let $\mathscr{D}^{\mathbf{C}}$ be the complexification of $\mathscr{D}$. The definition of the field operator can be extended to $\mathscr{D}^{\mathbf{C}}$ by linearity and is still denoted $\sigma(\Phi,F)$. We also extend K to $\mathscr{D}^{\mathbf{C}}$ and denote it $K^{\mathbf{C}}$. Then we have

$$\sigma(\Phi,F) = a(K^{\mathbf{C}}\overline{F}) + a(K^{\mathbf{C}}F)^*.$$

Definition: $F \in \mathscr{D}^{\mathbf{C}}$ is a *distinguished mode* if

$$K^{\mathbf{C}}\overline{F} = 0.$$

Thus if F is a distinguished mode $\sigma(\Phi,F)$ is a pure creation operator and $\sigma(\Phi,\overline{F})$ is a pure annihilation operator. The identity $\sigma(\Phi,\overline{F})\Omega = 0$, expresses that Ω has no field excitations of this type. In some cases $\sigma(\Phi,F)$ can be interpreted as an operator creating a particle, but this needs some assumptions on time evolution which we do not make.

The following result (which we do not use) shows that there is a sense in which the distinguished modes determine K up to unitary equivalence, and hence ω.

Proposition B.1: Let $K_1: \mathscr{D} \to \mathscr{H}_1$ and $K_2: \mathscr{D} \to \mathscr{H}_2$ each be symplectic with dense complex-linear range and suppose $K_1^{\mathbf{C}}, K_2^{\mathbf{C}}$ have the same null space. Then there is a unitary U: $\mathscr{H}_1 \to \mathscr{H}_2$ so $UK_1 = K_2$.

Proof: Let $J_1 = K_1^{-1}iK_1$ and $J_2 = K_2^{-1}iK_2$ be the associated complex structures in the sense of Segal. Then $J_1 = J_2$ since $F = J_1G$ implies $K_1^{\mathbf{C}}(F - iG) = 0$, hence $K_2^{\mathbf{C}}(F - iG) = 0$, and hence $F = J_2G$. Now define $U = K_2K_1^{-1}$ from Ran K_1 to Ran K_2. Then U is symplectic and it is also complex linear since

$$K_2K_1^{-1}i = K_2J_1K_1^{-1} = K_2J_2K_1^{-1} = iK_2K_1^{-1}.$$

It follows that U is norm preserving since

$$\|U\psi\|^2 = \mathrm{Im}(U\psi,iU\psi) = \mathrm{Im}(\psi,i\psi) = \|\psi\|^2.$$

Since U has dense domain and dense range it extends to a unitary operator.

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Although the papers in this series represent the joint work of the authors, we would like to note that the presentation and point of view of paper I is more due to B.K., while the presentation and point of view of paper II is more due to J.D.

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Linear transport theory in a random medium

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The time-independent linear transport problem in a purely absorbing (no scattering) random medium is considered. A formally exact equation for the ensemble averaged distribution function $\langle\Psi\rangle$ is derived. Under the assumption of a two-fluid statistical mixture, with the transition from one fluid to the other assumed to be determined by a Markov process, an exact solution to this equation for $\langle\Psi\rangle$ is obtained. In the source-free case, this solution is shown to agree with the result obtained by ensemble averaging simple exponential attenuation. Several approximations to the exact equation for $\langle\Psi\rangle$ are considered, and numerical results given to assess the accuracy of these approximations.

I. INTRODUCTION

In this paper we consider the problem of describing particle transport in a statistical (random) medium. Specifically, we consider time-independent transport in a medium in which the only particle–medium interaction is annihilation (absorption). Allowing for an external source of particles in the medium, we then have the generic linear kinetic (transport) equation along a direction s given by

$$\frac{d\Psi(s)}{ds} + \sigma(s)\Psi(s) = S(s). \tag{1}$$

Here s is the spatial variable; $\Psi(s)$ is a distribution function defined such that the number of particles of speed v between s and $s + ds$ is given by $v^{-1}\Psi(s)ds$; $\sigma(s)$ is the annihilation (absorption) cross section, defined such that $\sigma(s)ds$ is the probability of absorption for a particle traversing a distance ds; and $S(s)$ is the external source strength, defined such that $S(s)ds$ is the number of particles introduced into the medium per unit time between s and $s + ds$. If Eq. (1) is assumed to hold for $s \geqslant 0$, we then have the boundary condition

$$\Psi(0) = \Psi_0, \tag{2}$$

where Ψ_0 is the prescribed incident distribution at $s = 0$. We assume that σ and S in Eq. (1) are known only in some statistical or probabilistic sense. That is, at each space point s there is some time-independent probability that each of these two quantities will assume certain values. Accordingly, we consider σ and S, as well as the distribution function Ψ, to be random variables. Assuming we know the complete statistical description of σ and S, we seek the solution for $\langle\Psi\rangle$, the ensemble averaged (expected value) of the distribution function Ψ. We emphasize that Eq. (1) is a transport equation for particle propagation along a particular direction s in a three-dimensional setting. That is, our analysis and results are applicable to a random, three-dimensional medium.

There are conceptually two distinct ways to proceed. In the first approach, one can immediately write the solution to Eqs. (1) and (2) as

$$\Psi(s) = \Psi_0 \exp\left[-\int_0^s ds'\,\sigma(s')\right] + \int_0^s ds'\,S(s')\exp\left[-\int_{s'}^s ds''\,\sigma(s'')\right], \tag{3}$$

and then ensemble average the right-hand side (rhs) of Eq. (3) to obtain $\langle\Psi(s)\rangle$. Alternately, as a second approach one could develop, from Eqs. (1) and (2), a transportlike equation for $\langle\Psi(s)\rangle$, and then solve this equation to obtain the ensemble averaged solution. In this paper, we primarily focus on the second approach, but we also consider the first approach in the source-free ($S = 0$) case.

Specifically, in Sec. II we develop the details of the second approach by using a projection operator technique, the method of smoothing as described by Keller[1,2,3] and Frisch,[4] to derive a formally exact equation for $\langle\Psi(s)\rangle$. This equation contains an infinite series, with the nth term in this series involving an n-fold integral arising from n applications of the inverse transport operator. This multiple integral acts on various spatial correlation functions describing the statistical nature of the medium. For small statistical fluctuations, this infinite series can be truncated to a single term to obtain the lowest-order (in the smallness parameter describing the fluctuations) statistical correction. The integral operator in this lowest-order approximation can be localized by invoking a standard Fokker–Planck approximation.

These formal results are specialized, in Sec. III, to a statistical mixture of two immiscible fluids, with σ and S at any space point each taking one of the two values that are associated with each fluid. We show that the assumption of a Markov (Poisson) process for the transition from one fluid to the other allows an explicit calculation of all of the required spatial correlations. In addition, under this Markovian model, one can also obtain an analytic expression for the probability density distribution function corresponding to the optical depth random variable τ, defined as

$$\tau(s) = \int_0^s ds'\,\sigma(s'). \tag{4}$$

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This distribution function can be used to ensemble average the right-hand side (rhs) of Eq. (3) in the source-free ($S=0$) case, since in this case Eq. (3) simply becomes $\Psi(s)=\Psi_0\exp(-\tau)$.

In Sec. IV we show that the transportlike equation for $\langle\Psi(s)\rangle$ derived in Sec. II can be solved exactly for the two-fluid Markovian medium, in the special case of a homogeneous (spatially independent statistics for σ and S) medium. We numerically compare this exact solution with the result predicted by the small fluctuation equation (that which truncates the infinite series to a single term), as well as to the Fokker–Planck approximation to this small fluctuation equation. We also use the probability density distribution function for the optical depth τ obtained in Sec. III to carry out the details of ensemble averaging Eq. (3) in the source-free ($S=0$) case. The results of these two approaches to obtain $\langle\Psi(s)\rangle$ in a source-free medium are shown to be identical. The final section of the paper is devoted to a few concluding remarks.

As is clear from the above outline, the emphasis in this paper is on particle transport in a random medium composed of two immiscible turbulently mixed materials. This work was motivated by the need for an accurate transport description in the calculation of the performance of laser- or beam-driven fusion pellets. At an interface between two materials, these pellets are susceptible to Rayleigh–Taylor instabilities which can lead to a two-fluid turbulent mixture around the interface. A review of Rayleigh–Taylor instabilities within the context of inertially confined fusion has recently been given by Jacobs.[5] We intend to implement our formalism in the laser fusion code LASNEX used at the Lawrence Livermore National Laboratory. Other areas of application also come to mind. In a boiling-water nuclear reactor, the water, which acts as both coolant and moderator, is in a two-fluid random state (liquid and vapor). A proper treatment of the neutron transport must take the statistical nature of the mixture into account. In shielding calculations through concrete, the random nature of the materials (e.g., gravel) in the concrete implies a need for a statistical transport treatment to obtain an accurate measure of the shield effectiveness. Still another area of application is the calculation of light transport through a two-component random medium, such as sooty air or murky water. In general, there seem to be numerous areas of application for a transport theory for random media.

Finally, we note that the equation of radiative transfer with certain stochastic coefficients has been studied rather extensively with the astrophysical community.[6,7] However, the emphasis in this work has been on line transport with random Doppler shifts of the absorption coefficient due to small random velocity fields. The problem we treat, that of two turbulently mixed materials, is quite different from this astrophysical problem, even though both involve a stochastic linear transport equation.

II. THE EQUATION FOR $\langle\Psi(s)\rangle$

We rewrite Eq. (1) as

$$L\Psi+M\Psi=\langle S\rangle+q, \tag{5}$$

where $\langle S\rangle$ is the ensemble averaged source, L is the ensemble averaged transport operator given by

$$L=\frac{d}{ds}+\langle\sigma\rangle, \tag{6}$$

and q and M are the corresponding fluctuating quantities, i.e.,

$$q=S-\langle S\rangle,\quad M=\sigma-\langle\sigma\rangle. \tag{7}$$

We now introduce $\phi(s)$ as the fluctuating portion of $\Psi(s)$, i.e.,

$$\Psi=\langle\Psi\rangle+\phi. \tag{8}$$

We note that q, M, and ϕ all have a zero expected value, i.e.,

$$\langle q\rangle=\langle M\rangle=\langle\phi\rangle=0. \tag{9}$$

Following Keller[1,2,3] and Frisch,[4] we use Eq. (8) in Eq. (5) and ensemble average to obtain

$$L\langle\Psi\rangle+\langle M\phi\rangle=\langle S\rangle. \tag{10}$$

The term $\langle M\phi\rangle$ in Eq. (10) represents the statistical correction to the transport description. To compute this quantity, we subtract Eq. (10) from Eq. (5) to obtain

$$L\phi=q-M\langle\Psi\rangle+[\langle M\phi\rangle-M\phi], \tag{11}$$

or

$$\phi=L^{-1}(q-M\langle\Psi\rangle)+(B_1-B_2)\phi. \tag{12}$$

Here B_1 is the projection operator defined by

$$B_1\phi=L^{-1}\langle M\phi\rangle=\langle L^{-1}M\phi\rangle, \tag{13}$$

B_2 is the corresponding unprojected operator defined by

$$B_2\phi=L^{-1}M\phi, \tag{14}$$

and the inverse operator L^{-1} is explicitly given by (since ϕ vanishes at $s=0$)

$$L^{-1}\phi(s)=\int_0^s ds'\,\phi(s')\exp\left[-\int_{s'}^s ds''\langle\sigma(s'')\rangle\right]. \tag{15}$$

We rewrite Eq. (12) as

$$(I-B_1+B_2)\phi=L^{-1}(q-M\langle\Psi\rangle), \tag{16}$$

which has the formal Neumann series solution

$$\phi=\sum_{n=0}^{\infty}(-1)^n(B_2-B_1)^nL^{-1}(q-M\langle\Psi\rangle). \tag{17}$$

Operating on Eq. (17) with the operator M and ensemble averaging gives

$$\langle M\phi\rangle=L\sum_{n=0}^{\infty}(-1)^n(\hat{T}_{n+2}-\tilde{T}_{n+2}), \tag{18}$$

where

$$\hat{T}_{n+2}=\langle B_2(B_2-B_1)^nL^{-1}q\rangle,\quad n\geqslant 0, \tag{19}$$

and

$$\tilde{T}_{n+2}=\langle B_2(B_2-B_1)^nB_2\rangle\langle\Psi\rangle,\quad n\geqslant 0. \tag{20}$$

Use of Eq. (18) in Eq. (10) gives

$$L\langle\Psi\rangle+L\sum_{n=0}^{\infty}(-1)^n(\hat{T}_{n+2}-\tilde{T}_{n+2})=\langle S\rangle. \tag{21}$$

Equation (21) is the formally exact transportlike equation for $\langle\Psi\rangle$, the ensemble averaged distribution function. The infinite series in this equation is the statistical correction to the transport description.

From their definitions according to Eqs. (19) and (20), one can easily deduce recurrence relationships for $\hat{T}_n$ and $\tilde{T}_n$ given by

$$\hat{T}_n = \langle (L^{-1}M)^{n-1}L^{-1}q\rangle - \sum_{i=2}^{n-2}\langle (L^{-1}M)^i\rangle \hat{T}_{n-i}, \quad n\geqslant 3, \tag{22}$$

$$\tilde{T}_n = \langle (L^{-1}M)^n\rangle\langle\Psi\rangle - \sum_{i=2}^{n-2}\langle (L^{-1}M)^i\rangle \tilde{T}_{n-i}, \quad n\geqslant 3. \tag{23}$$

These recurrence relationships are initiated by the explicit $n=2$ expressions

$$\hat{T}_2 = \langle L^{-1}ML^{-1}q\rangle, \quad \tilde{T}_2 = \langle L^{-1}ML^{-1}M\rangle\langle\Psi\rangle. \tag{24}$$

From these recurrence relationships one can prove, by induction, that $\hat{T}_n$ and $\tilde{T}_n$ can be written in explicit form as

$$\hat{T}_n = \sum_i a_i \langle (L^{-1}M)^{p_1}\rangle\langle (L^{-1}M)^{p_2}\rangle \cdots \langle (L^{-1}M)^{p_i}L^{-1}q\rangle, \quad n\geqslant 2, \tag{25}$$

$$\tilde{T}_n = \sum_i a_i \langle (L^{-1}M)^{p_1}\rangle\langle (L^{-1}M)^{p_2}\rangle \cdots \langle (L^{-1}M)^{p_i}\rangle\langle\Psi\rangle, \quad n\geqslant 2. \tag{26}$$

The powers p_k can assume any non-negative integer values subject to the constraint

$$p_1 + p_2 + \cdots + p_i = m, \tag{27}$$

where $m = n-1$ for Eq. (25) and $m = n$ for Eq. (26). The sum over i in Eqs. (25) and (26) is over all possible combinations for the powers p_k, and $a_i = +1$ for an odd number of terms in the product involving ensemble averaged operators, and $a_i = -1$ for an even number of terms. As an explicit example, we have

$$\hat{T}_5 = \langle (L^{-1}M)^4L^{-1}q\rangle - \langle (L^{-1}M)^2\rangle\langle (L^{-1}M)^2L^{-1}q\rangle - \langle (L^{-1}M)^3\rangle\langle L^{-1}ML^{-1}q\rangle, \tag{28}$$

$$\tilde{T}_5 = \langle (L^{-1}M)^5\rangle\langle\Psi\rangle - \langle (L^{-1}M)^2\rangle\langle (L^{-1}M)^3\rangle\langle\Psi\rangle - \langle (L^{-1}M)^3\rangle\langle (L^{-1}M)^2\rangle\langle\Psi\rangle. \tag{29}$$

To proceed, we define the nth-order spatial correlations according to

$$\hat{N}_n(s_1,\ldots,s_n) = \langle M(s_1)M(s_2)\cdots M(s_{n-1})q(s_n)\rangle, \tag{30}$$

and

$$\tilde{N}_n(s_1,\ldots,s_n) = \langle M(s_1)M(s_2)\cdots M(s_{n-1})M(s_n)\rangle, \tag{31}$$

and, in analogy to Eq. (4), we define τ_n as the optical depth corresponding to a distance s_n, i.e.,

$$\tau_n = \int_0^{s_n} ds'\sigma(s'). \tag{32}$$

In terms of these definitions, we can write, using Eq. (15) for L^{-1},

$$L\hat{T}_n = \int_0^s ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-2}} ds_{n-1} \times \exp[-(\langle\tau\rangle - \langle\tau_{n-1}\rangle)] \times \sum_i a_i [\tilde{N}_{p_1}\tilde{N}_{p_2}\cdots\tilde{N}_{p_{i-1}}\hat{N}_{p_i}], \tag{33}$$

$$L\tilde{T}_n = \int_0^s ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-2}} ds_{n-1} \times \exp[-(\langle\tau\rangle - \langle\tau_{n-1}\rangle)] \times \sum_i a_i [\tilde{N}_{p_1}\tilde{N}_{p_2}\cdots\tilde{N}_{p_{i-1}}\tilde{N}_{p_i}]\langle\Psi(s_{n-1})\rangle, \tag{34}$$

where the arguments in the product terms involving the $\hat{N}_{p_i}$ and $\tilde{N}_{p_k}$ are $s, s_1, \ldots, s_{n-1}$ in this order. Again, as an explicit example we have

$$L\hat{T}_5 = \int_0^s ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 \int_0^{s_3} ds_4 \exp[-(\langle\tau\rangle - \langle\tau_4\rangle)] \times [\hat{N}_5(s,s_1,s_2,s_3,s_4) - \tilde{N}_2(s,s_1)\hat{N}_3(s_2,s_3,s_4) - \tilde{N}_3(s,s_1,s_2)\hat{N}_2(s_3,s_4)], \tag{35}$$

$$L\tilde{T}_5 = \int_0^s ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 \int_0^{s_3} ds_4 \exp[-(\langle\tau\rangle - \langle\tau_4\rangle)] \times [\tilde{N}_5(s,s_1,s_2,s_3,s_4) - \tilde{N}_2(s,s_1)\tilde{N}_3(s_2,s_3,s_4) - \tilde{N}_3(s,s_1,s_2)\tilde{N}_2(s_3,s_4)]\langle\Psi(s_4)\rangle. \tag{36}$$

To proceed further, one needs to specify a statistical model to compute the spatial correlations $\hat{N}_n$ and $\tilde{N}_n$. We consider one such model in the next section.

To summarize our considerations thus far, Eq. (21) is the formally exact transportlike equation for the ensemble averaged distribution function $\langle\Psi(s)\rangle$, with $\hat{T}_n$ and $\tilde{T}_n$ given by Eqs. (33) and (34). The statistics of the medium enter through the multipoint spatial correlations $\hat{N}_n$ and $\tilde{N}_n$ defined by Eqs. (30) and (31), with q and M in these equations given by $S - \langle S\rangle$ and $\sigma - \langle\sigma\rangle$, respectively. We note that the statistical corrections in Eq. (21), embodied in the infinite series, involve nonlocal (multiple integral) operators. It is clear from Eqs. (19) and (20) that $\hat{T}_n$ and $\tilde{T}_n$ decrease geometrically with n in the smallness parameter characterizing the statistical fluctuations. Accordingly, one can obtain the lowest-order, in this smallness parameter, approximation by keeping only the first term in the infinite series in Eq. (21). We then have, as the small fluctuation approximation, the transportlike equation

$$\frac{d\langle\Psi\rangle}{ds} + \langle\sigma\rangle\langle\Psi\rangle + \int_0^s ds_1 \exp[-(\langle\tau\rangle - \langle\tau_1\rangle)] \times [\langle M(s)q(s_1)\rangle - \langle M(s)M(s_1)\rangle\langle\Psi(s_1)\rangle] = \langle S\rangle. \tag{37}$$

We see that even in this lowest-order approximation, the statistical correction in the transportlike equation involves an integral operator.

One can localize the integral operator in Eq. (37) by employing a Fokker–Planck approximation. Specifically, we approximate $\langle\Psi(s_1)\rangle$ in Eq. (37) by an Nth-order Taylor series expansion about the point s, i.e.,

$$\langle\Psi(s_1)\rangle \approx \sum_{n=0}^{N} \frac{1}{n!}(s_1 - s)^n \frac{d^n\langle\Psi(s)\rangle}{ds^n}. \tag{38}$$

Use of Eq. (38) in Eq. (37) and integrating term by term gives an Nth-order Fokker–Planck approximation to the

small fluctuation equation. To obtain explicit results, we consider the special case of a medium in which $\langle\sigma\rangle$ is a slowly varying (essentially constant) function of position. We then have

$$\langle\tau\rangle - \langle\tau_1\rangle = \langle\sigma\rangle(s - s_1). \tag{39}$$

We further assume that the two-point spatial correlations in Eq. (37) are exponential in form, i.e.,

$$\langle M(s)q(s_1)\rangle = \alpha \exp[-\eta|s - s_1|], \tag{40}$$

$$\langle M(s)M(s_1)\rangle = \beta \exp[-\eta|s - s_1|], \tag{41}$$

where α, β, and η are slowly varying (essentially constant) functions of position. In the next section we present a Markov statistical model for a two-fluid mixture that predicts two-point spatial correlations of precisely this form, and gives explicit expressions for α, β, and η in terms of the parameters in the Markov model. Using Eqs. (38)–(41) in Eq. (37) we find the Nth-order Fokker–Planck approximation to the small fluctuation equation given by

$$\frac{d\langle\Psi\rangle}{ds} + \langle\sigma\rangle\langle\Psi\rangle - \frac{\beta}{\hat{\sigma}}\sum_{n=0}^{N}\left(-\frac{1}{\hat{\sigma}}\frac{d}{ds}\right)^n\langle\Psi\rangle = \langle S\rangle - \frac{\alpha}{\hat{\sigma}}, \tag{42}$$

where we have defined

$$\hat{\sigma} = \langle\sigma\rangle + \eta. \tag{43}$$

In obtaining Eq. (42) from Eq. (37), we have replaced the lower integration limit in Eq. (37) by $s_1 = -\infty$, which means we are neglecting terms of order $\exp(-\hat{\sigma}s)$. This is consistent with $\hat{\sigma}$ being large, which implies rapid convergence of the sum in Eq. (42). We note that the assumption that $\hat{\sigma}$ is large implies in general that η^{-1}, the spatial correlation length, is small. As we shall see in Sec. IV, the small fluctuation result, Eq. (37), and its Fokker–Planck approximation, Eq. (42), can yield nonphysical results if the fluctuations are, in fact, not small.

To summarize the results of this section, we have developed three descriptions of time-independent transport in a purely absorbing statistical medium. These are (1) Eq. (21), which is exact but very formal; (2) Eq. (37), which assumes small fluctuations; and (3) Eq. (42), which assumes small fluctuations, exponential spatial correlations with a small correlation length, and slowly varying spatial properties $\langle\sigma\rangle$, α, β, and η. In the next section we present a Markov statistical model for a two-fluid mixture that yields explicit results for all of the required spatial correlations $\hat{N}_n$ and $\tilde{N}_n$. In particular, this model predicts two-point spatial correlations of the exponential form given by Eqs. (40) and (41).

III. A MARKOV STATISTICAL MODEL

We consider a static turbulent (random) mixture of two immiscible fluids which we denote by fluid A and fluid B. We associate a cross section σ_i and source S_i (i = A,B) with each fluid. As a particle travels through this fluid mixture, it will pass through alternating fluid packets of A and B. We assume that the statistics of this situation can be described by a stationary Markov process in the following sense. Given that a particle is in fluid A at position s, the probability of finding itself (in the absence of absorption) in fluid B at a position $s + ds$ is simply given by ds/λ_A. Similarly, given that a particle is in fluid B at position s, the probability of finding itself (in the absence of absorption) in fluid A at a position $s + ds$ is given by ds/λ_B. We take the σ_i, S_i, and λ_i to be constants, independent of position.

For this two state Markov chain, we define the transition probability function $P_{ij}(s,t)$, i = A,B, as

$$P_{ij}(s,t) = P[X(t) = j | X(s) = i], \quad t \geqslant s, \tag{44}$$

where the rhs of this equation is the conditional probability that the random variable X, which we define to be the state of the fluid, takes on the state j at a distance t (from some defined origin), given that the variable was in state i at a distance s from this origin. Without loss of generality, we assume $t \geqslant s$. Since the probability of transition from fluid i to fluid j in a distance dt is given by dt/λ_i, one can perform a transition balance into and out of a given state, as a function of t for a fixed s. These balance equations are well known as the Chapman–Kolmogorov equations (forward form),[8] and are given by

$$\frac{\partial P_{AB}}{\partial t} = -\frac{P_{AB}}{\lambda_B} + \frac{P_{AA}}{\lambda_A}, \tag{45}$$

$$\frac{\partial P_{AA}}{\partial t} = -\frac{P_{AA}}{\lambda_A} + \frac{P_{AB}}{\lambda_B}, \tag{46}$$

$$\frac{\partial P_{BA}}{\partial t} = -\frac{P_{BA}}{\lambda_A} + \frac{P_{BB}}{\lambda_B}, \tag{47}$$

$$\frac{\partial P_{BB}}{\partial t} = -\frac{P_{BB}}{\lambda_B} + \frac{P_{BA}}{\lambda_A}. \tag{48}$$

The boundary conditions on these differential equations are given by

$$P_{AA}(s,s) = P_{BB}(s,s) = 1, \tag{49}$$

$$P_{AB}(s,s) = P_{BA}(s,s) = 0. \tag{50}$$

It is clear that

$$P_{AB}(s,t) + P_{AA}(s,t) = 1, \tag{51}$$

$$P_{BA}(s,t) + P_{BB}(s,t) = 1, \tag{52}$$

and hence two of the equations in Eqs. (45)–(48) are redundant.

The solution of Eqs. (45) through (50) is

$$P_{AB}(s,t) = (\lambda_A + \lambda_B)^{-1}\lambda_B(1 - e^{-d/\lambda_p}), \tag{53}$$

$$P_{AA}(s,t) = (\lambda_A + \lambda_B)^{-1}(\lambda_A + \lambda_B e^{-d/\lambda_p}), \tag{54}$$

$$P_{BA}(s,t) = (\lambda_A + \lambda_B)^{-1}\lambda_A(1 - e^{-d/\lambda_p}), \tag{55}$$

$$P_{BB}(s,t) = (\lambda_A + \lambda_B)^{-1}(\lambda_B + \lambda_A e^{-d/\lambda_p}), \tag{56}$$

where we have defined

$$\lambda_p^{-1} = \lambda_A^{-1} + \lambda_B^{-1}, \quad d = t - s. \tag{57}$$

We note that these four conditional probabilities are independent of the choice of origin for the position variable; they depend only upon the distance $t - s$ between the points t and s.

We now define $p_i(s)$ as the probability that at any point s the fluid is in state i, i.e.,

$$p_i(s) = P[X(s) = i]. \tag{58}$$

Since the λ_i have been assumed to be independent of position, it is clear that the p_i are also independent of position. That is, the s dependence on the (lhs) of Eq. (58) is redundant. In terms of the p_i, we have for the ensemble averaged cross section and source,

$$\langle\sigma\rangle = p_A\sigma_A + p_B\sigma_B, \tag{59}$$

$$\langle S\rangle = p_A S_A + p_B S_B. \tag{60}$$

The total probabilities p_i are related to the conditional probabilities P_{ij} by

$$p_A(t) = P_{AA}(s,t)p_A(s) + P_{BA}(s,t)p_B(s), \tag{61}$$

with a similar expression for $p_B(t)$ found by interchanging the indices A and B. Equation (61) holds in general, and in particular for our case in which the p_i are independent of position. Use of Eqs. (53) through (56) in Eq. (61) gives

$$p_A(t) = (\lambda_A + \lambda_B)^{-1} \times\{\lambda_A + [\lambda_B p_A(s) - \lambda_A p_B(s)]e^{-d/\lambda_p}\}. \tag{62}$$

For $p_A(t)$ to be constant, independent of t, Eq. (62) implies

$$\lambda_B p_A - \lambda_A p_B = 0. \tag{63}$$

We then deduce

$$p_i = (\lambda_A + \lambda_B)^{-1}\lambda_i, \tag{64}$$

as the relationship between the p_i and the λ_i. We shall shortly see that λ_i, and hence p_i, is proportional to the volume fraction of the ith fluid [see Eqs. (80) and (81)].

We now turn to the calculation of the two-point autocorrelation function for the cross section. We have

$$\begin{aligned}\langle M(s)M(t)\rangle &= \langle[\sigma(s) - \langle\sigma\rangle][\sigma(t) - \langle\sigma\rangle]\rangle \\ &= (\sigma_A - \langle\sigma\rangle)^2 P_{AA}(s,t)p_A + (\sigma_B - \langle\sigma\rangle)^2 P_{BB}(s,t)p_B \\ &\quad + (\sigma_A - \langle\sigma\rangle)(\sigma_B - \langle\sigma\rangle) \\ &\quad \times [P_{AB}(s,t)p_A + P_{BA}(s,t)p_B].\end{aligned} \tag{65}$$

This gives, using Eqs. (53)–(56) for the $P_{ij}(s,t)$,

$$\langle M(s)M(t)\rangle = (\sigma_A - \sigma_B)^2 p_A p_B e^{-d/\lambda_p}, \tag{66}$$

where we recall that d is the distance between the points t and s. A similar calculation for the two-point cross-correlation function between the cross section and the source gives

$$\langle M(s)q(t)\rangle = (\sigma_A - \sigma_B)(S_A - S_B)p_A p_B e^{-d/\lambda_p}. \tag{67}$$

In the notation of the last section [see Eqs. (40) and (41)], we then have

$$\alpha = (\sigma_A - \sigma_B)(S_A - S_B)p_A p_B, \tag{68}$$

$$\beta = (\sigma_A - \sigma_B)^2 p_A p_B, \tag{69}$$

$$\eta = \lambda_p^{-1} = \lambda_A^{-1} + \lambda_B^{-1}, \tag{70}$$

as the constants in the exponential two-point correlations. A similar exponential two-point autocorrelation as given by Eq. (66) was previously reported by Debye and Bueche[9] and Debye, Anderson, and Brumberger[10] within the context of light scattering by an inhomogeneous solid.

The higher-order correlations, $\hat{N}_n$ and $\tilde{N}_n$ for $n > 2$ as defined by Eqs. (30) and (31), can be computed explicitly by an extension of these arguments. For a general n, these algebraic expressions are relatively complex. However, certain linear combinations of products of these higher-order correlations are simple exponentials. Omitting the considerable algebraic detail, one finds

$$\sum_i a_i[\tilde{N}_{p_1}\tilde{N}_{p_2}\cdots\tilde{N}_{p_{i-1}}\hat{N}_{p_i}] = H_n e^{-(s_1 - s_n)/\lambda_p}, \tag{71}$$

$$\sum_i a_i[\tilde{N}_{p_1}\tilde{N}_{p_2}\cdots\tilde{N}_{p_{i-1}}\tilde{N}_{p_i}] = K_n e^{-(s_1 - s_n)/\lambda_p}, \tag{72}$$

where

$$H_n = (\sigma_A - \sigma_B)^{n-1}(S_A - S_B)p_A p_B(p_B - p_A)^{n-2}, \quad n \geqslant 2, \tag{73}$$

$$K_n = (\sigma_A - \sigma_B)^n p_A p_B(p_B - p_A)^{n-2}, \quad n \geqslant 2. \tag{74}$$

Here the spatial points are ordered such that $s_1 \geqslant s_2 \geqslant \cdots \geqslant s_n$, and the arguments in the product terms in Eqs. (71) and (72) involving the $\hat{N}_{p_i}$ and $\tilde{N}_{p_k}$ are $s_1, s_2, \ldots, s_n$ in this order. The coefficients a_i and the subscripts p_k are as discussed in the last section, just below Eq. (27).

The interesting point here is that the lhs's of Eqs. (71) and (72) are precisely of the form needed in the expressions for $\hat{T}_n$ and $\tilde{T}_n$ as introduced in the last section. That is, using Eqs. (71) and (72) in Eqs. (33) and (34) gives the relatively simple results for the nth-order term in Eq. (21) as

$$L\hat{T}_n = \int_0^s ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-2}} ds_{n-1}\, H_n \times \exp[-\hat{\sigma}(s - s_{n-1})], \quad n \geqslant 2, \tag{75}$$

$$L\tilde{T}_n = \int_0^s ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-2}} ds_{n-1}\, K_n \langle\Psi(s_{n-1})\rangle \times \exp[-\hat{\sigma}(s - s_{n-1})], \quad n \geqslant 2, \tag{76}$$

where [see Eqs. (43) and (70)]

$$\hat{\sigma} = \langle\sigma\rangle + \lambda_A^{-1} + \lambda_B^{-1}. \tag{77}$$

In writing Eqs. (75) and (76) we have used an expression analogous to Eq. (39) for $\langle\tau\rangle - \langle\tau_{n-1}\rangle$ since our Markov statistical model is restricted to cases for which $\langle\sigma\rangle$ is independent of position. We note that H_n and K_n, and hence $\hat{T}_n$ and $\tilde{T}_n$, vanish for $n > 2$ in the special case that $p_A = p_B = \frac{1}{2}$. Hence the small fluctuation approximation introduced in the last section, Eq. (37), is, in fact, exact for all size fluctuations when $p_A = p_B = \frac{1}{2}$. For any other values of p_A and p_B, Eq. (37) is only strictly valid for vanishingly small fluctuations. As we shall see shortly, $p_A = p_B = \frac{1}{2}$ implies equal volume fractions of the two fluids A and B.

Let us now address the question as to the physical meaning of our Markov model. Since the probability of transition from fluid i to fluid j in a distance ds is given by ds/λ_i, where λ_i is a constant, the distribution of chord lengths in a fluid packet is a classical Poisson process. That is, the chord length L of a given fluid packet is exponentially distributed, with a probability density function given by

$$f_i(L) = \lambda_i^{-1} e^{-L/\lambda_i}, \quad i = A,B. \tag{78}$$

Equation (78) is implied by the Chapman–Kolmogorov equations by solving these equations after deleting the transition-in terms [the second term on the rhs's of Eqs. (45)–(48)]. The mean of this exponential distribution, $\langle L_i \rangle$, is given by

$$\langle L_i \rangle = \int_0^\infty dL\, L f_i(L) = \lambda_i. \tag{79}$$

Thus the constant λ_i in the Markov model is just the average chord length through a fluid packet of type i. This average chord length is given by the Debye formula[9,10]

$$\lambda_i = 4V_i/S, \tag{80}$$

where V_i is the volume associated with fluid i, and S is the common surface area between the fluid packets of fluids A and B. Using Eq. (80) in Eq. (64) we find

$$p_i = (V_A + V_B)^{-1} V_i. \tag{81}$$

That is, the probability p_i is just the volume fraction of fluid i in the two-fluid stochastic mixture.

We now have the physical interpretation of our Markov model. The statistics of the two-fluid mixture are such that a particle traveling through this fluid sees alternating packets of fluids A and B, with the distance traveled (in the absence of absorption) in any fluid packet being a random variable with an exponential density distribution given by Eq. (78). Further, the parameter λ_i in this distribution is the average chord length through a fluid packet of type i, and is related to the volume fraction of fluid i in this two-fluid mixture through Eqs. (80) and (81). We note, however, that it is not sufficient to know the two volume fractions p_A and p_B. In addition to these volume fractions, one must know one of the λ_i to completely specify the statistics of the two-fluid mixture.

Before leaving this section, we use this Markov model to calculate another quantity which we shall find useful. The optical depth $\tau(s)$ between any two points a distance s apart, say s_0 and $s_0 + s$, is defined by

$$\tau(s) = \int_{s_0}^{s_0+s} ds'\, \sigma(s'). \tag{82}$$

Since σ is a random variable, so is τ. We seek the probability density function for the random variable τ, given a distance s. Since our medium is described by statistics which are independent of position, the point s_0 is irrelevant; the random variable τ is independent of s_0. Since there are two states, A and B, between s_0 and $s_0 + s$, we have

$$\begin{aligned}\tau(s) = \sigma_A \times [&\text{total track length through A in distance } s] \\ &+ \sigma_B \times [\text{total track length through B} \\ &\text{in distance } s].\end{aligned} \tag{83}$$

To obtain the distributions of the total track length through A and B in a distance s, we make use of a problem outline given by Lindley.[11] Let the length a particle travels through in the ith packet of A, before finding itself in fluid B, be denoted by the random variable X_i. Similarly, let the length a particle travels through in the ith packet of B, before finding itself in fluid A, be denoted by the random variable Y_i. We know from Eq. (78) that X_i and Y_i in our model are independent exponentially distributed random variables, and their cumulative distribution functions are given by

$$P(X_i < x) = G(x) = 1 - e^{-x/\lambda_A}, \quad 0 \leqslant x < \infty \tag{84}$$

$$P(Y_i < y) = H(y) = 1 - e^{-y/\lambda_B}, \quad 0 \leqslant y < \infty. \tag{85}$$

We now define

$$G_n(x) = P\left(\sum_{i=1}^{n} X_i < x\right), \quad n \geqslant 1, \tag{86}$$

$$H_n(y) = P\left(\sum_{i=1}^{n} Y_i < y\right), \quad n \geqslant 1, \tag{87}$$

with

$$G_0(x) = H_0(y) = 1. \tag{88}$$

$G_n(x)$ and $H_n(y)$ represent, for $n \geqslant 1$, the distribution of the total track length in fluids A and B, respectively, in n packets of fluid.

We also define the random variable $\beta(s)$ as the total track length of fluid B in the distance s given that the point s_0 is in fluid A. Similarly, we define the random variable $\alpha(s)$ as the total track length of fluid A in the distance s given that the point s_0 is in fluid B. Then, according to Eq. (83) the optical depth as a function of the distance s, $\tau(s)$, is given by one of two expressions, namely,

$$\tau(s) = \sigma_B \beta(s) + \sigma_A [s - \beta(s)], \quad s_0 \in A, \tag{89}$$

or

$$\tau(s) = \sigma_A \alpha(s) + \sigma_B [s - \alpha(s)], \quad s_0 \in B. \tag{90}$$

The cumulative distribution function $F(t,s)$ is the probability that $\tau(s)$ is less than a value t, given a geometric distance s. We have

$$\begin{aligned} F(t,s) &= P[\tau(s) < t] \\ &= P\{\sigma_B \beta(s) + \sigma_A [s - \beta(s)] < t\} P(s_0 \in A) \\ &\quad + P\{\sigma_A \alpha(s) + \sigma_B [s - \alpha(s)] < t\} P(s_0 \in B). \end{aligned} \tag{91}$$

Recalling that

$$P(s_0 \in A) = p_A, \quad P(s_0 \in B) = p_B, \tag{92}$$

and rearranging Eq. (91), we find

$$\begin{aligned} F(t,s) = p_A P\left[\beta(s) > \frac{\sigma_A s - t}{\sigma_A - \sigma_B}\right] \\ + p_B P\left[\alpha(s) < \frac{t - \sigma_B s}{\sigma_A - \sigma_B}\right]. \end{aligned} \tag{93}$$

If we label the fluids such that $\sigma_A > \sigma_B$, Eq. (93) immediately gives, since $0 \leqslant \alpha, \beta \leqslant s$,

$$F(t,s) = \begin{cases} 0, & \tau < \sigma_B s, \\ 1, & \tau > \sigma_A s, \end{cases} \tag{94}$$

which is just the physical statement that in a distance s the minimum optical depth is $\sigma_B s$ and the maximum optical depth is $\sigma_A s$.

To evaluate $F(t,s)$ for $\sigma_B s < t < \sigma_A s$, we need compute the distributions for $\alpha(s)$ and $\beta(s)$. To obtain the distribution for $\beta(s)$, we note that if there are exactly n transitions from state A to state B in a distance $s - x$, then the track length through the n packets of fluid B must lie between 0

and x. The probability of exactly n transitions from state A in a distance $s-x$ is given by

$$P = G_n(s-x) - G_{n+1}(s-x). \tag{95}$$

Thus we may express the distribution for $\beta(s)$ as

$$P[\beta(s) < x] = \sum_{n=0}^{\infty} H_n(x)[G_n(s-x) - G_{n+1}(s-x)]. \tag{96}$$

In a similar fashion, we can deduce the distribution for $\alpha(s)$ as

$$P[\alpha(s) < x] = \sum_{n=0}^{\infty} G_n(x)[H_n(s-x) - H_{n+1}(s-x)]. \tag{97}$$

Now, it is known[12] that the sum of n identically distributed exponential random variables with parameter $1/\lambda$ is given by a gamma distribution with parameters n and $1/\lambda$. Thus we have in our case

$$G_n(x) = \int_0^x dx' \frac{(x'/\lambda_A)^{n-1} e^{-x'/\lambda_A}}{\lambda_A (n-1)!}, \quad n \geqslant 1, \tag{98}$$

$$H_n(y) = \int_0^y dy' \frac{(y'/\lambda_B)^{n-1} e^{-y'/\lambda_B}}{\lambda_B (n-1)!}, \quad n \geqslant 1. \tag{99}$$

From Eqs. (88), (98), and (99) we deduce

$$G_n(s-x) - G_{n+1}(s-x) = \frac{1}{n!}\left(\frac{s-x}{\lambda_A}\right)^n e^{-(s-x)/\lambda_A}, \quad n \geqslant 0,$$

$$H_n(s-x) - H_{n+1}(s-x) = \frac{1}{n!}\left(\frac{s-x}{\lambda_B}\right)^n e^{-(s-x)/\lambda_B}, \quad n \geqslant 0. \tag{100}$$

Thus $P[\beta(s) < x]$, given by Eq. (96), becomes

$$P[\beta(s) < x] = e^{-(s-x)/\lambda_A}\left\{1 + \left(\frac{s-x}{\lambda_A \lambda_B}\right)^{1/2} \times \int_0^x dy \frac{e^{-y/\lambda_B}}{y^{1/2}} I_1\left[2\left(\frac{(s-x)y}{\lambda_A \lambda_B}\right)^{1/2}\right]\right\}, \tag{101}$$

where we have recognized the Taylor series expansion for the modified Bessel function as

$$I_1(z) = \sum_{r=0}^{\infty} \frac{(z/2)^{2r+1}}{r!(r+1)!}. \tag{102}$$

A similar result is found for $P[\alpha(s) < x]$. Using the fact that $P[\beta(s) > x] = 1 - P[\beta(s) < x]$ and inserting these results into Eq. (93) gives the cumulative distribution function in the optical depths range $\sigma_B s < \tau < \sigma_A s$ as

$$F(\tau,s) = p_A\left\{1 - e^{-u}\left[1 + 2\int_0^{(uv)^{1/2}} dx\, I_1(2x) e^{-x^2/u}\right]\right\} + p_B e^{-v}\left[1 + 2\int_0^{(uv)^{1/2}} dx\, I_1(2x) e^{-x^2/v}\right], \quad \sigma_B s < \tau < \sigma_A s, \tag{103}$$

where we have defined

$$u = \frac{1}{\lambda_A}\left(\frac{\tau - \sigma_B s}{\sigma_A - \sigma_B}\right); \quad v = \frac{1}{\lambda_B}\left(\frac{\sigma_A s - \tau}{\sigma_A - \sigma_B}\right). \tag{104}$$

Equations (94) and (103) give the cumulative distribution function for all physically meaningful (namely positive) values of τ; the geometric distance s is simply a parameter in this distribution. We use this distribution function in the next section to obtain the exact solution to a transmission problem.

IV. SOLUTIONS FOR $\langle\Psi(s)\rangle$ AND NUMERICAL RESULTS

As was stated in the Introduction, one way to obtain the solution for $\langle\Psi(s)\rangle$ is to ensemble average the solution $\Psi(s)$ as given by Eq. (3). We carry out the algebraic details of this averaging for the source-free ($S = 0$) problem. In this case Eq. (3) is simply $\Psi(s) = \Psi_0 \exp(-\tau)$, and ensemble averaging this pure exponential, we have

$$\langle\Psi(s)\rangle = \Psi_0\langle\exp(-\tau)\rangle = \Psi_0 \int_0^{\infty} d\tau f(\tau,s) e^{-\tau}, \tag{105}$$

where $f(\tau,s)$ is the probability density function for the optical depth random variable τ, with s a parameter in this distribution function. An integration of Eq. (105) by parts introduces the cumulative distribution function $F(\tau,s)$, and we have

$$\langle\Psi(s)\rangle = \Psi_0\left[e^{-\sigma_A s} + \int_{\sigma_B s}^{\sigma_A s} d\tau F(\tau,s) e^{-\tau}\right], \tag{106}$$

where $F(\tau,s)$ is given by Eq. (103) for our two-fluid Markovian stochastic mixture.

To evaluate the rhs of Eq. (106), we introduce the Laplace transform, with a transform variable p, of $\langle\Psi(s)\rangle$ as $\phi(p)$, i.e.,

$$\phi(p) = \int_0^{\infty} ds\, e^{-ps}\langle\Psi(s)\rangle. \tag{107}$$

Laplace transforming Eq. (105), we then obtain

$$\phi(p) = \Psi_0\left[(\sigma_A + p)^{-1} + \int_0^{\infty} ds \int_{\sigma_B s}^{\sigma_A s} d\tau F(\tau,s) e^{-(ps+\tau)}\right]. \tag{108}$$

We change integration variables in Eq. (108) from (s,τ) to (u,v), where u and v are defined by Eq. (104). The double integral in Eq. (105) then becomes a double integral over the first quadrant of (u,v) space. Inserting Eq. (103) for $F(\tau,s)$ we then have

$$\phi(p) = \Psi_0(\sigma_A + p)^{-1} + \Psi_0 \lambda_A \lambda_B (\sigma_A - \sigma_B) \times \int_0^{\infty} du \int_0^{\infty} dv\, [p_A(1 - e^{-u}) + p_B e^{-v} - 2p_A\, g(u,v) + 2p_B\, g(v,u)] \times \exp\{-[\lambda_A(p_A + \sigma_A)u + \lambda_B(p_B + \sigma_B)v]\}, \tag{109}$$

where we have defined the function $g(u,v)$ as

$$g(u,v) = e^{-u}\int_0^{(uv)^{1/2}} dx\, I_1(2x) e^{-x^2/u}. \tag{110}$$

The difficult integrations on the rhs of Eq. (109) can be written in generic form as

$$I=\int_0^\infty du\int_0^\infty dv\, e^{-u}e^{-(au+bv)}\int_0^{(uv)^{1/2}} dx\, I_1(2x)e^{-x^2/u}, \tag{111}$$

where a and b are positive constants. Interchanging the orders of the x and v integrations in Eq. (111) gives

$$I=\int_0^\infty du\, e^{-(1+a)u}\int_0^\infty dx\, I_1(2x)e^{-x^2/u}\int_{x^2/u}^\infty dv\, e^{-bv}. \tag{112}$$

The integral over v is trivial, and if we change integration variables from u to y according to $y=(1+a)u$, we then have

$$I=\frac{1}{b(1+a)}\int_0^\infty dx\, I_1(2x) \times\int_0^\infty dy\exp\left[-\left(y+\frac{(1+a)(1+b)x^2}{y}\right)\right]. \tag{113}$$

This integral over y can be expressed[13] in terms of the modified Bessel function $K_1(z)$, and we are then left with the single integral over x

$$I=\frac{2}{b}\left(\frac{1+b}{1+a}\right)\int_0^\infty dx\, xI_1(2x) \times K_1\{2[(1+a)(1+b)]^{1/2}x\}. \tag{114}$$

This final integral over x can be expressed[13] as a hypergeometric function $F(2,1;2;z)=(1-z)^{-1}$, and we obtain the relatively simple result

$$I=\{2b(1+a)[(1+a)(1+b)-1]\}^{-1}. \tag{115}$$

Using this generic result to integrate the terms involving $g(u,v)$ and $g(v,u)$ in Eq. (109), we obtain after some algebraic simplification,

$$\phi(p)=\Psi_0\left[\frac{p+\tilde\sigma}{(p+\tilde\sigma)(p+\langle\sigma\rangle)-\beta}\right], \tag{116}$$

where $\langle\sigma\rangle$ is the ensemble averaged cross section given by Eq. (59), β is the coefficient in the two-point autocorrelation function [see Eq. (41)] given by Eq. (69), and $\tilde\sigma$ is defined by

$$\tilde\sigma=p_B\sigma_A+p_A\sigma_B+\lambda_A^{-1}+\lambda_B^{-1}. \tag{117}$$

Laplace inversion of Eq. (116) then gives the exact result for $\langle\Psi(s)\rangle$ in the source-free, two-fluid Markovian mixture as

$$\langle\Psi(s)\rangle=\Psi_0\left(\frac{r_+-\tilde\sigma}{r_+-r_-}\right)e^{-r_+s}+\left(\frac{\tilde\sigma-r_-}{r_+-r_-}\right)e^{-r_-s}, \tag{118}$$

with

$$r_\pm=\tfrac{1}{2}\{\langle\sigma\rangle+\tilde\sigma\pm[(\langle\sigma\rangle-\tilde\sigma)^2+4\beta]^{1/2}\}. \tag{119}$$

For equal volume fractions, i.e., $p_A=p_B=\frac{1}{2}$, Eq. (118) has been obtained earlier by Bourret[14,15] by the method of parastochastic operators in the special case of a dichotomic Markov chain. However, as discussed by Frisch,[4] it is only the $p_A=p_B=\frac{1}{2}$ result which can be obtained by Bourret's method. This is related to the discussion below Eq. (77) in this paper concerning the vanishing of H_n and K_n for $n>2$ when $p_A=p_B=\frac{1}{2}$. Equation (118) has the proper behavior in known limiting cases, namely,

$$\langle\Psi(s)\rangle\underset{\lambda_A\to0}{\to}e^{-\sigma_B s}, \tag{120}$$

$$\langle\Psi(s)\rangle\underset{\lambda_B\to0}{\to}e^{-\sigma_A s}, \tag{121}$$

$$\langle\Psi(s)\rangle\underset{\lambda_A,\lambda_B\to0}{\to}e^{-\langle\sigma\rangle s}, \tag{122}$$

$$\langle\Psi(s)\rangle\underset{\lambda_A,\lambda_B\to\infty}{\to}p_A\,e^{-\sigma_A s}+p_B\,e^{-\sigma_B s}. \tag{123}$$

There is one additional limit that is interesting to consider, namely, $\sigma_B\to0$ and $\sigma_A\to\infty$. This corresponds physically to the case of packets, with an infinite optical thickness, of fluid A imbedded in a vacuum background. In this case Eq. (118) reduces to

$$\langle\Psi(s)\rangle\underset{\substack{\sigma_B\to0\\ \sigma_A\to\infty}}{\to}p_B\,e^{-s/\lambda_B}. \tag{124}$$

The factor p_B on the rhs of Eq. (124) is just the probability that a particle starts in a packet of fluid B, the vacuum. [If it started in fluid A, it would be absorbed at $s=0$ since $\sigma_A=\infty$, and hence not contribute to $\langle\Psi(s)\rangle$.] The exponential term in Eq. (124) merely states the correct physical fact that in this limit the mean free path of a particle is just λ_B, the average distance between packets of fluid A.

We can use the exact result for $\langle\Psi(s)\rangle$ given by Eq. (118) to assess the accuracy of the approximate transport models introduced in Sec. II, namely the small fluctuation description given by Eq. (37), and the Nth-order Fokker–Planck approximation to this small fluctuation equation, given by Eq. (42). In the source-free ($S=0$) case with $\langle\sigma\rangle$ independent of position, Eq. (37) is written, using Eq. (41) for the required two-point spatial correlation with η given by Eq. (70),

$$\frac{d\langle\Psi\rangle}{ds}+\langle\sigma\rangle\langle\Psi\rangle=\beta\int_0^s ds_1\, e^{-\hat\sigma(s-s_1)}\langle\Psi(s_1)\rangle, \tag{125}$$

with β and $\hat\sigma$ given by Eqs. (69) and (77), respectively. The integral in this equation is of the convolution type, and hence Eq. (125) is easily solved by Laplace transforming. The result is

$$\langle\Psi(s)\rangle=\Psi_0\left[\left(\frac{r_+-\hat\sigma}{r_+-r_-}\right)e^{-r_+s}+\left(\frac{\hat\sigma-r_-}{r_+-r_-}\right)e^{-r_-s}\right], \tag{126}$$

where, in this case,

$$r_\pm=\tfrac{1}{2}\{\langle\sigma\rangle+\hat\sigma\pm[(\langle\sigma\rangle-\hat\sigma)^2+4\beta]^{1/2}\}. \tag{127}$$

A comparison of this small fluctuation result [Eqs. (126) and (127)] with the exact result [Eqs. (118) and (119)] shows that they are very similar in form. The only difference is that the small fluctuation result involves $\hat\sigma$, whereas the exact result involves $\tilde\sigma$ in place of $\hat\sigma$. These two results will be identical when $\hat\sigma=\tilde\sigma$, which occurs for $p_A=p_B=\frac{1}{2}$; i.e., equal volume fractions of the two fluids. We previously pointed out [see the discussion below Eq. (77)] that the small fluctuation equation is, in fact, exact for all size fluctuations when $p_A=p_B=\frac{1}{2}$. However, we do not have a physical understanding as to what is special about equal volume fractions for the two fluids which makes the small fluctuation equation exact in this case.

We now consider Eq. (42), the Fokker–Planck approximation to this small fluctuation equation, in the low-order cases $N=0$, 1, and 2. In the source-free ($\langle S\rangle=\alpha=0$) case, the solution is given by the pure exponential

$$\langle\Psi(s)\rangle=\Psi_0 e^{-rs}, \tag{128}$$

where the exponent r is given in these three Fokker–Planck approximations by

$$r=\frac{\hat\sigma}{2}\left\{\left[\left(\frac{\hat\sigma^2}{\beta}+1\right)^2+4\left(\frac{\langle\sigma\rangle\hat\sigma}{\beta}-1\right)\right]^{1/2}-\left(\frac{\hat\sigma^2}{\beta}+1\right)\right\},\quad N=2, \tag{129}$$

$$r=\hat\sigma\frac{\langle\sigma\rangle\hat\sigma-\beta}{\hat\sigma^2+\beta},\quad N=1, \tag{130}$$

$$r=(\langle\sigma\rangle\hat\sigma-\beta)/\hat\sigma,\quad N=0. \tag{131}$$

We note that if we neglect the statistical corrections entirely, we have the so-called "atomic mix" approximation, and the transport equation for $\langle\Psi\rangle$ is simply, in the source-free case,

$$\frac{d\langle\Psi\rangle}{ds}+\langle\sigma\rangle\langle\Psi\rangle=0. \tag{132}$$

This equation again has Eq. (128) as its solution, with $r=\langle\sigma\rangle$ in this case.

To obtain some idea of the accuracy of these various approximate formulations, we present in Tables I and II a few typical numerical results. We have set to unity the incident distribution, i.e., $\Psi_0=1$, and have chosen a length scale such that $\langle\sigma\rangle=1$ for all cases considered. Also, these two tables give $\langle\Psi(s)\rangle$ at $s=\ln 10$, and hence for all cases the atomic mix result is simply $\langle\Psi(s)\rangle=0.1$ since $\langle\sigma\rangle s=\ln 10$. The deviation of our exact result for $\langle\Psi\rangle$ as given by Eq. (118) from 0.1 gives an indication of the importance of properly accounting for the statistical nature of the medium in a transport calculation. The deviation of the small fluctuation equation results, and the corresponding Fokker–Planck approximations, from the exact results gives an indication of the accuracy of these various simplified, but approximate, transport descriptions in a random medium.

Table I presents four different cases, each having $\lambda_A=\lambda_B$, and hence $p_A=p_B=\frac{1}{2}$. As we have already remarked, the small fluctuation equation is exact for all size fluctuations when $p_A=p_B=\frac{1}{2}$. We see from this table, in particular for the last case, the importance of accounting for the statistical nature of the medium. That is, for this case the atomic mix model which completely ignores this statistical nature underestimates $\langle\Psi\rangle$ by a factor in excess of 3. We also see from this table that the lowest-order ($N=0$) Fokker–Planck result is more accurate than the higher-order ($N=1$ and 2) results. This is probably due to extending the lower integration limit in Eq. (37) to $s_1=-\infty$ in deriving the Fokker–Planck approximation given by Eq. (42). This makes the approximation asymptotic in character; keeping more terms in the sum in Eq. (42) does not necessarily improve the accuracy of the result.

In Table II we present five additional cases, but for these cases $\lambda_A\neq\lambda_B$, and hence $p_A\neq p_B\neq\frac{1}{2}$. Here we can assess the accuracy of the small fluctuation approximation. We see, from the last two cases in this table, that the small fluctuation model is completely inadequate when the fluctuations are large and the statistical corrections are important (i.e., one is far from the atomic mix limit). In particular, for the last case $\langle\Psi\rangle$ exceeds unity; the small fluctuation equation is predicting growth rather than decay as the particles traverse the medium. This comes about since r_- as given by Eq. (127) is negative. Such growth also occurs for the second to last case in this table, although in this case $\langle\Psi\rangle$ at $s=\ln 10$ is still less than unity. The "complex" entry in this table means that Eq. (129) gave a value for r which is not real.

Based upon these results and other cases we have con-

TABLE I. $\langle\Psi(\ln 10)\rangle$ for $p_A=p_B=\frac{1}{2}$.

Parameters	Exact	Fokker–Planck $N=2$	Fokker–Planck $N=1$	Fokker–Planck $N=0$
$\lambda_A=0.1$ $\lambda_B=0.1$ $\sigma_A=1.1$ $\sigma_B=0.9$	0.1001	0.1001	0.1001	0.1001
$\lambda_A=10.0$ $\lambda_B=10.0$ $\sigma_A=1.1$ $\sigma_B=0.9$	0.1023	0.1049	0.1036	0.1019
$\lambda_A=0.1$ $\lambda_B=0.1$ $\sigma_A=1.9$ $\sigma_B=0.1$	0.1095	0.1098	0.1097	0.1093
$\lambda_A=10.0$ $\lambda_B=10.0$ $\sigma_A=1.9$ $\sigma_B=0.1$	0.3592	0.6362	0.6194	0.4732

TABLE II. $\langle\Psi(\ln 10)\rangle$ for $p_A\neq p_B$.

Parameters	Exact	Small fluctuation equation	Fokker–Planck $N=2$	Fokker–Planck $N=1$	Fokker–Planck $N=0$
$\lambda_A=0.02$ $\lambda_B=0.08$ $\sigma_A=1.1$ $\sigma_B=0.975$	0.1000	0.1000	0.1000	0.1000	0.1000
$\lambda_A=2.0$ $\lambda_B=8.0$ $\sigma_A=1.1$ $\sigma_B=0.975$	0.1004	0.1004	0.1007	0.1006	0.1004
$\lambda_A=0.02$ $\lambda_B=0.08$ $\sigma_A=4.0$ $\sigma_B=0.25$	0.1083	0.1086	0.1086	0.1086	0.1085
$\lambda_A=2.0$ $\lambda_B=8.0$ $\sigma_A=4.0$ $\sigma_B=0.25$	0.3694	0.9989	1.6656	1.6131	2.4245
$\lambda_A=1.0$ $\lambda_B=9.0$ $\sigma_A=9.1$ $\sigma_B=0.1$	0.5802	9.5438	complex	8.5259	283.90

sidered, it appears that the following two conclusions can tentatively be drawn. First, the small fluctuation equation should only be used when the fluctuations are, in fact, small or when $p_A \approx p_B \approx \frac{1}{2}$. Second, the Fokker–Planck model, since it is an approximation to the small fluctuation equation, should only be used under the same circumstances, and the $N=0$ model seems to be the most accurate.

We conclude this section by obtaining an exact solution for $\langle \Psi(s) \rangle$ in the presence of a source ($S \neq 0$) for our two-fluid Markovian mixture. In this case, we solve the exact transportlike equation for $\langle \Psi(s) \rangle$, namely Eq. (21), as opposed to ensemble averaging Eq. (3). The statistical correction terms in Eq. (21), $\hat{T}_n$ and $\tilde{T}_n$, are given by Eqs. (75) and (76), and can be rewritten as

$$L\hat{T}_n = H_n \int_0^s ds_1\, R(s-s_1) \int_0^{s_1} ds_2\, R(s_1-s_2) \cdots \int_0^{s_{n-2}} ds_{n-1}\, R(s_{n-2}-s_{n-1}), \tag{133}$$

$$L\tilde{T}_n = K_n \int_0^s ds_1\, R(s-s_1) \int_0^{s_1} ds_2\, R(s_1-s_2) \cdots \int_0^{s_{n-2}} ds_{n-1}\, R(s_{n-2}-s_{n-1}) \langle \Psi(s_{n-1}) \rangle, \tag{134}$$

where the kernel $R(s)$ is given by

$$R(s) = \exp(-\hat{\sigma} s). \tag{135}$$

Written in this way, $L\hat{T}_n$ and $L\tilde{T}_n$ can be seen to be multiple convolution integrals, and hence Eq. (21) can be solved by Laplace transforming. If we again define $\phi(p)$ as the Laplace transform of $\langle \Psi(s) \rangle$ according to Eq. (107), then a Laplace transform of Eq. (21) with $L\hat{T}_n$ and $L\tilde{T}_n$ given by Eqs. (133) and (134) gives

$$(p + \langle \sigma \rangle)\phi(p) - \Psi_0 + \phi(p) \sum_{n=0}^{\infty} (-1)^{n+1} K_{n+2} (p+\hat{\sigma})^{-(n+1)} - p^{-1} \sum_{n=0}^{\infty} (-1)^{n+1} H_{n+2} (p+\hat{\sigma})^{-(n+1)} = p^{-1} \langle S \rangle. \tag{136}$$

Using Eqs. (73) and (74) for H_n and K_n in Eq. (136), summing the resulting geometric series, and solving for $\phi(p)$, we find

$$\phi(p) = \frac{\Psi_0 (p+\tilde{\sigma}) + p^{-1}[\langle S \rangle (p+\tilde{\sigma}) - \alpha]}{(p+\tilde{\sigma})(p+\langle \sigma \rangle) - \beta}, \tag{137}$$

where α, β, and $\tilde{\sigma}$ are given by Eqs. (68), (69), and (117), respectively. The Laplace inversion of Eq. (137) gives the exact result, within the context of our Markov model, for the ensemble averaged distribution function $\langle \Psi(s) \rangle$ as

$$\langle \Psi(s) \rangle = \Psi_0 \left[\left(\frac{r_+ - \tilde{\sigma}}{r_+ - r_-} \right) e^{-r_+ s} + \left(\frac{\tilde{\sigma} - r_-}{r_+ - r_-} \right) e^{-r_- s} \right] + \left[\frac{\langle S \rangle (\tilde{\sigma} - r_+) - \alpha}{r_+ (r_+ - r_-)} \right] e^{-r_+ s} - \left[\frac{\langle S \rangle (\tilde{\sigma} - r_-) - \alpha}{r_- (r_+ - r_-)} \right] e^{-r_- s} + \frac{\langle S \rangle \tilde{\sigma} - \alpha}{r_+ r_-}, \tag{138}$$

with $r_\pm$ again given by Eq. (119). We note that in the absence of a source ($\langle S \rangle = \alpha = 0$), Eq. (138) agrees with the result obtained earlier [see Eq. (118)] by ensemble averaging Eq. (3) with $S=0$. We emphasize that Eq. (138) is an exact expression for $\langle \Psi(s) \rangle$, the ensemble averaged distribution function, but only for time-independent transport through a purely absorbing (no scattering) medium with statistics as described in Sec. III. In particular, this statistical model is a Markovian mixture of two immiscible fluids, and further assumes that the Markov statistical parameters λ_i as well as the fluid parameters σ_i and S_i, $i = \text{A,B}$, are all independent of position.

V. CONCLUDING REMARKS

The work summarized in this paper represents our first attempt at developing a general formalism for describing linear transport through a medium composed of two randomly mixed fluids. We have considered only the very simplest situation, that of time-independent transport through a purely absorbing medium for a two-component Markovian mixture, with all parameters λ_i, σ_i, and S_i, $i = \text{A,B}$, independent of position. Clearly, many generalizations suggest themselves. With the inclusion of time dependence and scattering, a generic linear transport equation is given by

$$\frac{1}{v}\frac{\partial \Psi}{\partial t} + \mathbf{\Omega} \cdot \nabla \Psi + (\sigma_a + \sigma_s)\Psi = \int_{4\pi} d\mathbf{\Omega}' \sigma_s(\mathbf{\Omega}' \to \mathbf{\Omega}) \Psi(\mathbf{\Omega}') + S, \tag{139}$$

where $\Psi = \Psi(\mathbf{r}, \mathbf{\Omega}, t)$, and the remaining notation in Eq. (139) is standard. In addition to explicit consideration of time dependence and a scattering contribution, one could investigate other (than Markov) statistical models for the random variables σ_a, σ_s, and S.

With regard to the simplified version of Eq. (139) considered in this paper ($\sigma_s = \partial \Psi / \partial t = 0$), an open question is the physical realizability of our Markov model. Along any given direction s, one can easily envision a mixture of two types of fluid packets, with each packet of fluid i having an exponential chord length distribution with a mean λ_i. However, can one realize such exponential chord length distributions simultaneously in all directions in three-dimensional geometry? In this regard, we note that if the fluid mixture is composed of alternating fluid slabs, with each slab of fluid i infinite in two dimensions and with an exponentially distributed thickness with mean T_i in the third dimension, then one indeed realizes exponential chord length distributions in all directions simultaneously. However, the mean chord length will be direction dependent and given by $\lambda_i = T_i/\mu$, where μ is the cosine of the angle between the particle flight direction and the normal to the slab surfaces. Can any statement concerning physical realizability be made for nonslab geometry, and can one envision any fluid packet geometry which has exponential chord length distributions with the same mean λ_i in all directions? It would also be interesting to investigate the robustness of the results given in this paper to the statistical model used. Specifically, within the context of a two-fluid mixture, how sensitive are the results to the use of an exponential distribution of chord lengths? We note that the expo-

nential distribution contains only one parameter λ_i, and hence the average chord length (which is just λ_i) and the variance (which is just λ_i^2) are not independent. Hence one might ask how sensitive are our results, e.g., Eq. (138), for given average chord lengths of each fluid component, to the variances (and higher moments) of the chord length distributions? Clearly the applicability of the exponential (or any other) distribution must be established from the underlying physics of the particular transport situation under consideration. We mention parenthetically that the exponential distribution appears to be a fairly good description of the distribution of rock fragment sizes, as discussed by Engleman, Jaeger, and Levi.[16] The hope is that relevant transport results are relatively insensitive to the chord length distributions, thus obviating the need for a detailed chord length description.

We hope to address these points, as well as extensions of our analysis to more general transport equations, in future publications.

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Charge operators without local commutativity

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A Goldstone-type theorem is proved for quantum field theories in any $n \geqslant 2$ space-time dimensions, without assuming local commutativity.

I. INTRODUCTION

The problem of associating a symmetry with a conserved current in axiomatic quantum field theory (QFT) has been widely considered in the literature (see, e.g., Refs. 1 and 2 and references therein). Goldstone's theorem[3] plays a distinguished role in this context, inasmuch as it gives equivalent conditions for ensuring an affirmative answer to the above mentioned problem. Postponing its precise formulation to what follows, we want to recall, for the time being, that, besides some assumptions quite usual in relativistic QFT's, this theorem requires locality. It is, therefore, of little use in theories where locality cannot be maintained on the physical subspace—an outstanding example being the Gauss law in any Abelian or non-Abelian gauge theory.

In the present paper we formulate a Goldstone-type theorem that does not require local commutativity. The proof is given in any $n \geqslant 2$ space-time dimensions.

II. CONSTRUCTION OF CHARGES

We start by concisely recalling the procedure generally followed in order to define charge operators without making use of locality.

Let $\{\mathcal{H},(\cdot,\cdot)\}$ be a Hilbert space and $D \subset \mathcal{H}$ a dense set containing a vector Ω (the vacuum) normalized according to

$$(\Omega,\Omega) = 1. \tag{1}$$

A conserved vector current is represented by the operator-valued distributions $\{j_\mu(f): \mu = 0,1,\ldots,n-1, f \in \mathcal{S}(\mathbb{R}^n)\}$ defined on D and satisfying

$$j_\mu(\partial^\mu f)\Phi = 0, \quad \forall \Phi \in D, \tag{2}$$

$$(\Phi, j^0(f)\Psi) = (j^0(\bar{f})\Phi,\Psi), \quad \forall \Phi,\Psi \in D. \tag{3}$$

Without loss of generality one may assume

$$(\Omega, j^0(f)\Omega) = 0. \tag{4}$$

In what follows we postulate that the distribution

$$w_{\mu\nu}(x,y) = (j_\mu(x)\Omega, j_\nu(y)\Omega) \in \mathcal{S}'(\mathbb{R}^{2n}) \tag{5}$$

is translation invariant and Lorentz covariant. Then there exists

$$\omega_{\mu\nu}(x-y) = w_{\mu\nu}(x,y). \tag{6}$$

The distribution $\omega_{\mu\nu}$ is supposed to satisfy the spectral condition, i.e., supp $\omega_{\mu\nu}(p) \subset \overline{V}_+$, $\overline{V}_+$ being the closure of the future light cone. As well known (see, e.g., Ref. 4), for $n \geqslant 3$ (the case $n = 2$ being separately treated in Remark 5 below) our requirements on the current imply the Källen–Lehman representation

$$w_{\mu\nu}(f,g) = \int d\rho(p)(p_\mu p_\nu - g_{\mu\nu}p^2)\bar{\hat{f}}(p)\hat{g}(p) \tag{7}$$

$$= \int d\mu(s) \int d_n p\, \bar{\hat{f}}(p)(p_\mu p_\nu - g_{\mu\nu}p^2)\hat{g}(p)2\pi\Theta(p^0)\delta(p^2 - s). \tag{8}$$

Here $d\rho(p)$ is a positive measure from $\mathcal{S}(\mathbb{R}^n)$ with support in $\overline{V}_+$ and $d\mu(s)$ is a positive tempered measure with support in $[0, +\infty)$, hereafter referred to as the spectral density.

The construction of the charge operator associated with j_μ goes as follows. One first introduces two smearing functions[5]

$$f_R(\mathbf{x}) = f(R^{-1}\mathbf{x}), \quad R \geqslant 1, \quad f \in \mathcal{S}(\mathbb{R}^{n-1}),$$
$$f(\mathbf{x}) = 1, \quad \text{for } |\mathbf{x}| \leqslant 1, \quad f(\mathbf{x}) = 0, \quad \text{for } |\mathbf{x}| \geqslant 2; \tag{9a}$$

$$\alpha_R(x^0) = 2R^{-1}\alpha(2R^{-1}x^0), \quad \alpha \in \mathcal{S}(\mathbb{R}^1),$$
$$\alpha(x^0) = 0, \quad \text{for } |x^0| \geqslant 1, \quad \int dx^0\, \alpha(x^0) = 1; \tag{9b}$$

by which the finite volume charge

$$Q_R = j^0(\alpha_R f_R) \tag{10}$$

is defined. Then the task of giving sense to the formal expression $\int d^{n-1}x\, j^0(x)$ can be accomplished by means of the following lemma, whose proof (see, e.g., Ref. 1) follows from a straightforward application of Riesz's theorem.

Lemma: Assume the following.

(i) $\forall \Phi,\Psi \in D$ there exists the limit

$$\lim_{R\to\infty} (\Phi, Q_R\Psi) = Q(\Phi,\Psi). \tag{11}$$

(ii) The sesquilinear form $Q(\cdot,\cdot)$ is continuous in the first argument, i.e., there exists a $c(\Psi) > 0$, such that

$$|Q(\Phi,\Psi)| \leqslant c(\Psi)\|\Phi\|. \tag{12}$$

Then there exists a symmetric operator Q defined on D and such that $(\Phi, Q\Psi) = Q(\Phi,\Psi)$.

(iii) If, in addition,

$$\lim_{R\to\infty} (\Phi, Q_R\Omega) = 0, \quad \forall \Phi \in D, \tag{13}$$

then

$$Q\Omega = 0. \tag{14}$$

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Following the standard terminology, the validity (violation) of (14) will be referred to as the exactness (spontaneous breaking) of the symmetry to be associated with j_μ. Actually, even when (14) holds, further steps are to be made in order to represent a symmetry group on $\mathscr{H}$. Indeed the lemma provides us with only a symmetric operator Q. The question of existence and uniqueness of a self-adjoint extension of Q will be not touched upon here (see, however, Ref. 1).

Some remarks concerning the assumptions of the lemma are in order.

Remark 1: We note that (11) does not need to hold for any $\Phi\in\mathscr{H}$, but only for $\Phi\in D$. This means that even the weak convergence of the sequence $\{Q_R\Omega\}$ is not required in (13).

Remark 2: Consider the case when there exists a set of fields $\mathscr{B}=\{B_i(f): i=1,...,N; f\in\mathscr{S}(\mathbb{R}^n)\}$ local with respect to j^0 and such that $\mathscr{F}_{\mathscr{B}}\Omega$ is dense in $\mathscr{H}$, $\mathscr{F}_{\mathscr{B}}$ being the polynomial algebra generated by $\mathscr{B}$. Then $D=\mathscr{F}_{\mathscr{B}}\Omega$ automatically satisfies (i) and (ii), provided (13) holds. In *local* QFT's, which precisely enter this framework, one can prove[1-3] the following theorem.

Theorem 1 (Goldstone): A necessary and sufficient condition for the validity of (13) is the absence of discrete zero mass states connected to Ω by j^0.

Remark 3: In the case of gauge theories, i.e., when j_μ obeys a Gauss law, and Q is nontrivial, any set $\mathscr{B}$ such that $\mathscr{F}_{\mathscr{B}}\Omega$ is dense in $\mathscr{H}$, necessarily is nonlocal with respect to j^0 (see Ref. 6).

As a consequence of the last two remarks, the absence of locality leads to the problems P_1: to find a substitute of relative locality from which (i) and (ii) can be deduced; and P_2: to find necessary and sufficient conditions guaranteeing (13).

In our knowledge there is no general solution to P_1. This problem has, however, been successfully faced in four-dimensional massive spinor quantum electrodynamics,[7] by using the specific properties of the model.

In what follows we will be concerned with P_2. More precisely we are looking for sufficient conditions ensuring (13). A first such condition is provided by the following proposition.

Proposition 1: Assume there exists an R-independent constant C such that

$$\|Q_R\Omega\|<C. \tag{15}$$

Let $\mathscr{H}$ carry a unitary representation $U(a)$, $a\in\mathbb{R}^n$, of the translation group in $\mathbb{M}^n$, $n\geqslant 2$, and let Ω be the unique translationally invariant state in $\mathscr{H}$. Then

$$\underset{R\to\infty}{\text{w-lim}}\, Q_R\Omega=0. \tag{16}$$

Proof: Let us introduce the function

$$\eta_R(p)\in\mathscr{S}(\mathbb{R}^n),\quad 0\leqslant\eta_R(p)\leqslant 1,$$
$$\eta_R(p)=\begin{cases}1, & \text{for } |p|^2\equiv p_0^2+p_1^2+\cdots+p_{n-1}^2\leqslant m/R,\\ 0, & \text{for } |p|^2\geqslant 2m/R,\end{cases} \tag{17}$$

with m a positive arbitrary constant. Due to (7) and (10) one has

$$\|Q_R\Omega\|^2=\int_{V_+}d\rho(p)\mathbf{p}^2\left|\hat f(R\mathbf{p})\hat\alpha\left(\frac{1}{2}Rp^0\right)\right|^2 \tag{18a}$$
$$=R^{n-2}\int_{-0}^{+\infty}d\mu(s)g(R^2s), \tag{18b}$$

where -0 means include a possible pure point part of $d\mu$ concentrated at $s=0$ and

$$g(R^2s)=\frac{1}{2}\int d_{n-1}q\,E(R^2s,\mathbf{q})^{-1}$$
$$\times\mathbf{q}^2|\hat f(\mathbf{q})\hat\alpha(\tfrac{1}{2}E(R^2s,\mathbf{q}))|^2>0 \tag{18c}$$

is obtained by integrating with respect to p^0, setting $R\mathbf{p}=\mathbf{q}$ and

$$E(x,\mathbf{y})=(x^2+\mathbf{y}^2)^{1/2}. \tag{19}$$

Note that since $\hat\alpha\in\mathscr{S}(\mathbb{R}^1)$, $g(x)\in C^{n-1}(\mathbb{R}^1)$ and is of fast decrease for $x\to+\infty$. From (18a) one gets

$$\|Q_R\Omega\|^2=J_0+J_m, \tag{20}$$

with

$$J_m=R^{2(n-1)}\int d\rho(p)\mathbf{p}^2\left|\hat f(R\mathbf{p})\hat\alpha\left(\frac{1}{2}Rp^0\right)\right|^2(1-\eta_R(p)) \tag{21a}$$

and

$$J_0=\frac{1}{2}R^{2(n-1)}\int d\mu(s)\int d_{n-1}p\,E(s,\mathbf{p})^{-1}\mathbf{p}^2$$
$$\times|\hat f(R\mathbf{p})\hat\alpha(\tfrac{1}{2}RE(s,\mathbf{p}))|^2\,\eta_R(E(s,\mathbf{p}),\mathbf{p}). \tag{21b}$$

In obtaining the last formula we have again used the representation (18b). Since J_m is positive definite, (15) implies

$$J_0\leqslant C^2. \tag{22}$$

We also claim that $J_m\to 0$ faster than any inverse power of R, as $R\to\infty$. Indeed, noting that $\mathbf{p}^2|\hat f|^2$ is continuous and of fast decrease for $|\mathbf{p}|\to\infty$, one may estimate it by

$$\mathbf{p}^2|\hat f(R\mathbf{p})|^2\leqslant d_M(1+R^2\mathbf{p}^2)^{-M}, \tag{23}$$

with $M\geqslant 0$ an arbitrary integer and $d_M>0$ a suitable constant. Likewise for $|\hat\alpha|^2$, so that for any M there exists a $D_M>0$, such that

$$J_M\leqslant D_{2M}\int d\rho(p)\mathbf{p}^2(1+R^2\mathbf{p}^2)^{-2M}$$
$$\times(1+R^2p_0^2)^{-2M}(1-\eta_R(p)) \tag{24a}$$
$$\leqslant D_{2M}(1+mR)^{-2M}\int d\rho(p)(1+\mathbf{p}^2)^{-M}(1+p_0^2)^{-M}. \tag{24b}$$

In deriving (24b) we have used that $R\geqslant 1$ and the properties of $\eta_R(p)$. Moreover the integral in (24b) is finite for sufficiently large M, since $d\rho(p)$ is of at most polynomial growth. Let now $\mathbf{1}$ denote the identity operator in $\mathscr{H}$ and consider

$$\|(\mathbf{1}-U(a))Q_R\Omega\|^2=2\{\|Q_R\Omega\|^2-\mathrm{Re}(Q_R\Omega,U(a)Q_R\Omega)\}$$
$$=K_0+K_m, \tag{25}$$

with

$$K_m = R^{2(n-1)} \int d\rho(p)\mathbf{p}^2 \left| \hat{f}(R\mathbf{p})\hat{\alpha}\left(\frac{1}{2}Rp^0\right)\right|^2 \times(1-\eta_R(p))2[1-\cos(ap)] \tag{26a}$$

and

$$K_0 = \frac{1}{2} R^{2(n-1)} \int d\mu(s) \int d_{n-1}p\, E(s,\mathbf{p})^{-1} \times\mathbf{p}^2 |\hat{f}(R\mathbf{p})\hat{\alpha}(\tfrac{1}{2}RE(s,\mathbf{p}))|^2 \times\eta_R(E(s,\mathbf{p}),\mathbf{p})2[1-\cos(a^0E(s,\mathbf{p})-\mathbf{a}\cdot\mathbf{p})]. \tag{26b}$$

Due to the inequalities $2(1-\cos x) = \sin^2(\frac{1}{2}x) \leqslant \min\{1,\frac{1}{4}x^2\}$, one, respectively, gets

$$K_m \leqslant J_m, \tag{27}$$

and

$$\eta_R(E(s,\mathbf{p}),\mathbf{p})2\{1-\cos(a^0E(s,\mathbf{p})-\mathbf{a}\cdot\mathbf{p})\} \leqslant |a|^2 m/R,$$

whence

$$K_0 \leqslant |a|^2 m J_0/R \leqslant |a|^2 m C^2/R \to 0, \quad \text{for } R\to\infty, \tag{28}$$

in force of (22). Inserting (27) and (28) into (25), and taking (24) into account, one gets

$$\lim_{R\to\infty} \|(1-U(a))Q_R\Omega\| = 0. \tag{29}$$

Furthermore, (15) implies that $\{Q_R\Omega\}$ admits weakly convergent subsequences. Let $\{Q_{R_k}\Omega\}$ be any one among them and let

$$\text{w-lim}_{k\to\infty} Q_{R_k}\Omega = \Phi. \tag{30}$$

We claim that

$$\Phi = 0, \tag{31}$$

which proves (16), since $\{Q_{R_k}\Omega\}$ is arbitrary. Indeed, consider the matrix element $(\Psi,(1-U(a))\Omega)$, where $\Psi\in\mathscr{H}$ is arbitrary. Taking the limit $k\to\infty$ in the Schwartz inequality

$$|(\Psi,(1-U(a))Q_{R_k}\Omega)| \leqslant \|\Psi\|\,\|(1-U(a))Q_{R_k}\Omega\|$$

and using (29) and (30) one gets

$$\Phi = U(a)\Phi. \tag{32}$$

Equation (32), combined with the unicity of the vacuum, leads to $\Phi = z\Omega$, $z\in\mathbb{C}^1$. Finally, due to (1) and (4),

$$z = (\Omega,z\Omega) = (\Omega,\Phi) = \text{w-lim}_{R\to\infty}(\Omega,Q_R\Omega) = 0,$$

whence (31). This concludes the proof of Proposition 1.

Usually the information one has at one's disposal in the study of models concerns the spectral density $d\mu(s)$. It is, therefore, convenient to translate condition (15) in terms of the spectral measure, i.e., of the integral

$$\mu(s) = \int_{0^-}^{s} d\mu(t)$$

of the spectral density. The following statement holds.

Proposition 2: Let $n\geqslant 3$. The estimate (15) holds if and only if there exist $m>0$ and $K>0$ such that

$$\mu(s) \leqslant Ks^{(1/2)n-1}, \quad \forall s\in[0,m). \tag{33}$$

Condition (33) will be referred to as $(\frac{1}{2}n-1)$-boundedness of the spectral measure.

Proof: Necessity: Since $g(t)$ given by (18c) is positive for any $t\geqslant 0$, there always exists a function $h(t)\in C^0(\mathbb{R}^1)$ with the properties

$$h(t) \leqslant g(t), \quad \forall t\in\mathbb{R}^1, \tag{34a}$$

$$h(t) = \min_{0\leqslant t\leqslant 1} g(t) \equiv g^0 > 0, \quad \text{for } 0\leqslant t\leqslant 1. \tag{34b}$$

Then, due to the positivity of $d\mu$, one has

$$g^0 R^{n-2}\mu(1/R^2) = R^{n-2}\int_{0^-}^{1/R^2} d\mu(s)h(R^2s) \leqslant R^{n-2}\int_{0^-}^{+\infty} d\mu(s)g(R^2s) = \|Q_R\Omega\|^2 < C^2,$$

whence (33) follows on substituting $1/R^2$ with s in the left-hand side.

Sufficiency: Equation (18b) may be written in the form

$$\|Q_R\Omega\|^2 = I_0 + I_m, \tag{35}$$

where

$$I_m = R^{n-2}\int_{m^2}^{+\infty} d\mu(s)g(R^2s), \tag{36a}$$

$$I_0 = R^{n-2}\int_{0^-}^{m^2} d\mu(s)g(R^2s). \tag{36b}$$

In the same way as for J_m one can prove that $I_m\to 0$, for $R\to\infty$ faster than any inverse power of R. Consider now I_0. Since $g\in C^{n-1}(\mathbb{R}^1)$ and is of fast decrease, there always exists a $H(t)\in C^1(\mathbb{R}^1)$ and of fast decrease, such that $g(t)\leqslant H(t)$ and $H'(t)<0$. One can thus estimate

$$\begin{aligned} I_0 &\leqslant R^{n-2}[\mu(m^2)H(m^2R^2) - \mu(0)H(0)] \\ &\quad - R^{n-2}\int_{0^-}^{m^2} ds\, Ks^{(1/2)n-1}R^2H'(R^2s) \\ &= R^{n-2}\mu(m^2)H(m^2R^2) \\ &\quad + K\int_{0^-}^{m^2R^2} d\sigma\,\sigma^{(1/2)n-1}(-H'(\sigma)) \\ &\leqslant R^{n-2}\mu(m^2)H(m^2R^2) \\ &\quad + K\int_{0^-}^{+\infty} d\sigma\,\sigma^{(1/2)n-1}(-H'(\sigma)). \end{aligned} \tag{37a}$$

After integrating by parts, we have used that $\mu(0)=0$, which follows from the assumption (33). Integrating by parts again and going to the limit $R\to\infty$ in (37a) one gets

$$I_0 \leqslant K(\tfrac{1}{2}n-1)\int_{0^-}^{+\infty} d\sigma\,\sigma^{(1/2)n-2}H(\sigma) \leqslant \infty. \tag{37b}$$

Then (15) follows on using (35), (37b), and the decrease property of I_m.

Remark 4: A sufficient condition for the validity of (15) had already been formulated in Ref. 5. It reads

$$\int_{0^-}^{m^2} d\mu(s)s^{1-(1/2)n} < +\infty. \tag{38}$$

We now show that (38) is more restrictive than (33). Indeed let $d\mu(s)$ obey (38). Then in the case under consideration ($n\geqslant 3$),

$$\mu(s) = \int_{0^-}^{s} d\mu(t) t^{1-(1/2)n} t^{(1/2)n-1}$$
$$\leqslant \left[\int_{0^-}^{s} d\mu(t) t^{1-(1/2)n}\right]^{1/2} \times \left[\int_{0^-}^{s} d\mu(t) t^{(1/2)n-1}\right]^{1/2}$$
$$= (\text{const}) \left[\mu(s) s^{(1/2)n-1} - (\tfrac{1}{2}n - 1) \times \int_{0^-}^{s} dt\, \mu(t) t^{(1/2)n-2} \right]^{1/2}$$
$$\leqslant (\text{const}) [\, \mu(s) s^{(1/2)n-1}]^{1/2},$$

where the Hölder inequality and the positivity of $\mu(s)$ have been used. Thus we see that (38) implies (33). On the contrary, the spectral density

$$d\mu(s) = a\Theta(s) s^{(1/2)n-2}\, ds, \quad a > 0, \tag{39}$$

is easily seen to fulfill (33) and to violate (38). The example (39) is not merely academical. Consider the currents

$$j_\mu(f) = i[:\varphi^* \partial_\mu \varphi:(f) - :(\partial_\mu \varphi^*)\varphi:(f)], \tag{40a}$$
$$J_\mu(f) = :\bar{\psi}\gamma_\mu \psi:(f), \tag{40b}$$

where φ and ψ are the free zero mass scalar and spinor fields, respectively, and :···: stands for the standard normal product. A simple computation shows that the spectral densities corresponding to (40a) and (40b) are proportional to (39).

An example of spectral density not fulfilling (33) is provided by

$$d\mu(s) = a\delta(s) ds, \quad a > 0, \quad s \in (0 - \epsilon, 0 + \epsilon). \tag{41}$$

Remark 5: We treat here the case of two-dimensional QFT. In this case the two-point function $\omega_{\mu\nu}$ has two independent tensor structures, namely,

$$\hat{\omega}_{\mu\nu}(p) = (p_\mu p_\nu - g_{\mu\nu} p^2)\rho_1(p) + \epsilon_{\mu\sigma}\epsilon_{\nu\tau} p^\sigma p^\tau \rho_2(p), \tag{42}$$

with $\epsilon_{\mu\nu} = -\epsilon_{\nu\mu}$, $\epsilon_{01} = 1$. Here $\rho_i \in \mathcal{S}'(\mathbb{R}^2)$ are Lorentz invariant and $\operatorname{supp} \rho_i \subset \overline{V}_+$ both for $i = 1$ and 2. For $\mu = \nu = 0$, the two tensor structures in (42) collapse into one and one gets

$$\hat{\omega}_{00}(p) = p^2(\rho_1(p) + \rho_2(p)). \tag{43}$$

Now, combining the positivity of ω_{00} with the just-mentioned properties of ρ_i, one obtains

$$\hat{\omega}_{00}(p) = \int d\mu(s) 2\pi\Theta(p^0) p^2 \delta(p^2 - s), \tag{44}$$

$d\mu(s)$ being a positive tempered measure with support in $[0, +\infty)$. Note that the factor p^2 in the integrand of the right-hand side of (44) removes the arbitrariness (see, e.g., Ref. 8) in the definition of the $\delta(p^2)$ on the tip of the light cone in two dimensions. Equation (44) leads to the representation

$$\|Q_R \Omega\|^2 = \int_{-0}^{m^2} d\mu(s) g(R^2 s) + I_m, \tag{45}$$

where $g(R^2 s)$ and I_m are defined by (18c) and (36a) with $n = 2$, respectively. Now, as in Proposition 1 for J_m, one easily finds that, for $R \to \infty$, $I_m \to 0$. Moreover, since $g(R^2 s)$ is bounded, also the first term in (45) is bounded in R.

In conclusion (16) holds also in two dimensions, under the assumptions of Proposition 1, but without any requirement on the behavior of $\mu(s)$ at $s = 0$. This statement (see, also, Ref. 9) generalizes the Coleman theorem[10] on the absence of Goldstone bosons in two dimensions. We recall, however, that in indefinite metric and/or for translationally noninvariant currents, both of which violate our assumptions, the cited theorem, is, in general, no longer true.[11]

III. CONCLUSIONS

A recapitulation of the presented results is now in order. This is provided by the following chain of implications:

$$(13) \Leftarrow (16) \overset{\text{Pr.1}}{\Leftrightarrow} (15) \overset{\text{Pr.2}}{\Leftrightarrow} (33).$$

Clearly, in general, (13) does not imply (16), but in the specific context of QFT we are not aware of any example where (13) takes place and, at the same time, (16) is violated. Concerning the implication (16)$\Rightarrow$(15), it is a well-known property of the weak topology in Banach spaces (see, e.g., Ref. 12).

The above results and the content of Remark 5 can be also summarized in the form of the following Goldstone-type theorem, which does not require locality.

Theorem 2: Assume that the conserved vector current j_μ is such that conditions (i) and (ii) of the lemma are fulfilled. Then the symmetry corresponding to j_μ (a) is always exact if $n = 2$; and (b) may be spontaneously broken if $n \geqslant 3$ and the corresponding spectral measure $\mu(s)$ is not $(\frac{1}{2}n - 1)$-bounded at $s = 0$. Otherwise the symmetry is exact.

Propositions 1 and 2 and Theorem 2 clarify the relationship between conserved currents and symmetries in field theories where locality cannot be maintained on the physical space. Some applications of the results of this paper concerning gauge theories and more general, identically conserved currents are given in Ref. 13.

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A simple proof of duality for local algebras in free quantum field theory

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New and simple proofs of duality for local von Neumann algebras in free-scalar field models associated with a general class of regions in Minkowski space are presented. The proofs are given for both the massive and massless cases and an abstract result of Araki [H. Araki, J. Math. Phys. **4**, 1343 (1963)] is assumed. The properties of the local algebras are analyzed using the associated real linear manifolds. Duality is proved in the massive models using elementary properties of Sobolev spaces and in the massless model using dilatation covariance. A proof of the factor property and the cyclicity and separability of the vacuum for these local algebras is also given.

I. INTRODUCTION AND STATEMENT OF THE PROBLEM

The duality property for the local algebras of observables associated with free-scalar quantum field theories has been proved by several authors using a variety of techniques, e.g., Refs. 1–8. This paper presents a new and short proof of duality (independent of the Tomita–Takesaki theory) for local von Neumann algebras associated with regular regions in Minkowski space $\mathscr{M}_4$. Proofs are given for both the massive and massless free-scalar field theories. These proofs assume the "abstract" duality property proved by Araki[9] and by Eckmann and Osterwalder.[10] Araki's proof is independent of the Tomita–Takesaki theory,[11(a)] whereas, Eckmann and Osterwalder utilized the results of this theory. The abstract duality theorem states a relation between pairs of strongly closed real linear manifolds and certain von Neumann algebras and their commutants. The proofs of duality for the local algebras presented here are based on an analysis of certain pairs of real linear manifolds in the one-particle subspaces of the Fock spaces for these models.

Preparatory to the discussion of the abstract duality relation and its application, let us recall the general framework of the Fock representation of the canonical commutation relations (CCR) [e.g., Ref. 11(b)]. Let $H_1 \equiv L^2(\mathbb{R}^3)$ be the Hilbert space of one-particle momentum space wave functions and let $(\cdot,\cdot)$ denote the inner product on H_1. Let H_1' be another Hilbert space isometrically isomorphic to H_1. Let $H_0' \equiv \mathbb{C}$ and for $n \geqslant 1$ define $H_n' \equiv \left(\overset{n}{\otimes} H_1' \right)_{\text{sym}}$, the symmetrized n-fold tensor product of H_1' with itself. The Fock space H_F with one-particle subspace $H_1' \cong H_1$ is defined by $H_F \equiv \overset{\infty}{\underset{n=0}{\otimes}} H_n'$. The vector $\{1,0,0,\ldots\} \in H_F$ is denoted by Ω and called the Fock vacuum vector.

The Weyl form of the Fock representation of the CCR on H_F is given by a strongly continuous irreducible unitary projective representation of H_1. This representation is constructed from the creation and annihilation operators as follows. For $f \in H_1$, let $a^\dagger(f)$ denote the usual creation operator that is the closure of an operator defined on the dense domain D_F of finite particle vectors in H_F. This operator is defined such that the map $f \in H_1 \to a^\dagger(f)$ is linear and such that

$$f \in H_1 \mapsto a^\dagger(f)\Omega \in H_1' \tag{1.1}$$

is an isometric isomorphism. The operators $a^\dagger(f)$ and their adjoints, denoted by $a(f)$, satisfy the CCR on D_F. For any $f,g \in H_1$ and $\psi \in D_F$, we have

$$[a(f),a^\dagger(g)]\psi = (f,g)\psi , \tag{1.2a}$$

$$[a(f),a(g)]\psi = 0 . \tag{1.2b}$$

The Segal field operator $\phi_S[f]$, for each $f \in H_1$, is defined to be the unique self-adjoint extension of the operator

$$\hat{\phi}_S[f] \equiv (1/\sqrt{2})\,[a^\dagger(f) + a(f)] \tag{1.3}$$

defined on D_F. The unitary Weyl operators $W_S(f)$ for each $f \in H_1$ are defined by

$$W_S(f) \equiv \exp(i\phi_S[f]) . \tag{1.4}$$

It is checked easily that the map $f \in H_1 \mapsto W_S(f)$ is strongly continuous. These unitary operators satisfy the Weyl form of the CCR:

$$W_S(f)W_S(g) = e^{-i\,\mathrm{Im}(f,g)}W_S(g)W_S(f) \tag{1.5}$$

as is verified easily using (1.2) and the definitions (1.3) and (1.4).

Each strongly closed real linear manifold (RLM) M in H_1, can be associated with a von Neumann algebra $A(M) \subset B(H_F)$ defined by

$$A(M) \equiv \{W_S(f) \,|\, f \in M\}'' , \tag{1.6}$$

where the double prime denotes the double commutant. Because of the strong continuity of the Weyl operators, if $M \subset H_1$ is a RLM and $\overline{M}$ denotes its strong closure, we have

$$A(M) = A(\overline{M}) . \tag{1.7}$$

We associate a RLM M', called the *sympletic complement* of M, to each RLM $M \subset H_1$. The manifold M' is defined by

$$M' \equiv \{f \,|\, \mathrm{Im}(f,g) = 0,\ \forall g \in M\} . \tag{1.8}$$

It is checked easily that M' is weakly and strongly closed and that $M'' = \overline{M}$ (in particular, M'' is weakly closed). It follows from the CCR (1.5) and the definition of M' (1.8) that

$$A(M') \subset A(M)' . \tag{1.9}$$

Moreover, Araki[9] has proved the following theorem.

Theorem 1.1: Let $M \subset H_1$ be a RLM and M' its symplectic complement. Then

$$A(M') = A(\overline{M})' . \tag{1.10}$$

The relation (1.10) is what is referred to here and else-

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where in the literature as *abstract duality*. Araki's proof of (1.10) is independent of Tomita–Takesaki theory. It is based on the unique relationships between $M\subset H_1, H_F$, and $A(M)$ indicated above. These relations characterize the Fock representation of free quantum field models regardless of the spin or mass of the particles. In Ref. 9 Araki established relation (1.10) in the context of proving an isomorphism between a complemented lattice of RLM's in H_1 and von Neumann algebras on H_F. A simpler proof of (1.10) was given by Eckmann and Osterwalder in Ref. 10 and in the unpublished work of Leyland, Roberts, and Testard[7] using the Tomita–Takesaki theory.

We mention that the study of RLM's, associated with a von Neumann algebra with a cyclic and separating vector and its commutant, led Rieffel and van Daele[12] to new proofs of the main results of the Tomita–Takesaki theory using only bounded operators.

We want to apply Theorem 1.1 to prove the duality property for the local von Neumann algebras in free-scalar quantum field models with any mass. As is well known, $H_1\equiv L^2(\mathbb{R}^3)$ carries inequivalent, irreducible, strongly continuous, unitary representations of the Poincaré group indexed by the mass $m\geqslant 0$ (see Ref. 13) (we consider only the spin-0 case). The Poincaré group $P_0\equiv SO_e(3,1)\circledS T_4$, is the semidirect product of the Lorentz group $SO_e(3,1)$ and the four-parameter Abelian group of translations $T_4\cong\mathbb{R}^4$. We write (M,y) for an element of P_0 and $U_m(M,y)$ for the representation on H_1' induced, by means of (1.1), from the representation on H_1. As is standard, we denote by $\Gamma(U_m(M,y))$ the corresponding representation of P_0 on H_F. It is obtained from the action of the n-fold tensor product of $U_m(M,y)$ with itself on H_n'. Consequently, the Fock spaces $H_{F,m}$ for our models are distinguished by the inequivalent representations of P_0 labeled by $m\geqslant 0$. In what follows, each free-field model will be labeled by some fixed $m\geqslant 0$, but we will omit the subscripts for convenience.

A free-scalar quantum field operator $\phi(x)$ can be constructed on H_F, which is linear in the creation and annihilation operators, local, and Poincaré covariant. A standard form for the operator-valued tempered distribution $\phi(x)$ is

$$\phi(x)\equiv(2\pi)^{-3/2}\int_{(\infty)}d\bar{p}(2\omega(\bar{p}))^{-1/2}\times[e^{ix\cdot p}a^\dagger(\bar{p})+e^{-ix\cdot p}a(\bar{p})]\,. \tag{1.11}$$

In (1.11), we write $a^\dagger(\bar{p})$ for the operator-valued distribution defined by $f\in H_1\mapsto a^\dagger(f)$ so that $a^\dagger(f)$ is given symbolically by $\int_{(\infty)}d\bar{p}\,a^\dagger(\bar{p})f(\bar{p})$. We use the notation $x\cdot y\equiv x_4y_4-\bar{x}\cdot\bar{y}$ with $x,y\in\mathbb{R}^4$ and $\bar{x},\bar{y}\in\mathbb{R}^3$; $x^2\equiv x\cdot x$; and $p\cdot x\equiv\omega(\bar{p})x_4-\bar{p}\cdot\bar{x}$ with $\omega(\bar{p})\equiv[|\bar{p}|^2+m^2]^{1/2}$. Locality for the field means that for $x,y\in\mathscr{M}_4$ such that $(x-y)^2<0$:

$$[\phi(x),\phi(y)]=0 \tag{1.12}$$

in the distributional sense on D_F. The field is Poincaré covariant with respect to the representation $\Gamma(U(M,y))$ of the Poincaré group on H_F:

$$\Gamma(U(M,y))\phi(x)\Gamma(U(M,y))^{-1}=\phi(Mx+y)\,. \tag{1.13}$$

Let $\mathcal{O}\subset\mathbb{R}^4$ be any nonempty open set. Let $\mathscr{S}(\mathcal{O})(\mathscr{S}_r(\mathcal{O}))$ denote the vector space of Schwartz test functions (real test functions) with support in $\mathcal{O}$. For $f\in\mathscr{S}_r(\mathbb{R}^4)$, $\phi[f]$ is essentially self-adjoint on D_F and we use the same symbol to denote the closure. It is easy to check that

$$\phi[f]=\phi_S[F]\,, \tag{1.14a}$$

where

$$F(\bar{p})\equiv(2\pi)^{-3/2}\omega(\bar{p})^{-1/2}\tilde{f}(\bar{p},\omega(\bar{p}))\in H_1\,, \tag{1.14b}$$

and $\tilde{f}$ denotes the Fourier transform of f:

$$\tilde{f}(\bar{s},s_4)\equiv\int_{(\infty)}d^4(x)e^{ix\cdot s}f(x)\,. \tag{1.15}$$

We define another family of unitary Weyl operators $W(f)$ on H_F for $f\in\mathscr{S}_r(\mathbb{R}^4)$, by

$$W(f)\equiv\exp(i\phi[f])\,. \tag{1.16}$$

Because of (1.14a), $W(f)=W_S(F)$ and the CCR (1.5) imply that

$$W(f)W(g)=e^{-i\sigma(f,g)}W(g)W(f)\,, \tag{1.17a}$$

for $f,g\in\mathscr{S}_r(\mathbb{R}^4)$. In (1.17a) the bilinear form σ: $\mathscr{S}_r(\mathbb{R}^4)\times\mathscr{S}_r(\mathbb{R}^4)\mapsto\mathbf{R}$ is defined by

$$\sigma(f,g)\equiv-i[\phi[f],\phi[g]]=\mathrm{Im}(F,G)\,, \tag{1.17b}$$

with F and G defined as in (1.14). Note that σ satisfies $\sigma(f,g)=-\sigma(g,f)$.

Definition 1.2: For any $\mathcal{O}\subset\mathbb{R}^4$ nonempty and open, the local von Neumann algebra $R(\mathcal{O})$ is defined by

$$R(\mathcal{O})\equiv\{W(f)\,|\,f\in\mathscr{S}_r(\mathcal{O})\}''\,. \tag{1.18}$$

Two simple consequences of this definition and the above discussion for $R(\mathcal{O})$ are as follows.

(1) *Locality:* if $\mathcal{O}_1$ and $\mathcal{O}_2$ are two strictly spacelike separated open regions, then

$$R(\mathcal{O}_1)\subset R(\mathcal{O}_2)'\,. \tag{1.19}$$

In particular, for $\mathcal{O}\subset\mathbb{R}^4$, we define the spacelike complement $\mathcal{O}^c$ of $\mathcal{O}$ by

$$\mathcal{O}^c\equiv\mathrm{Int}\{x\,|\,(x-y)^2<0,\ \forall y\in\mathcal{O}\} \tag{1.20}$$

and (1.19) implies that

$$R(\mathcal{O}^c)\subset R(\mathcal{O})'\,. \tag{1.21}$$

(2) *Poincaré Covariance:* For $(M,y)\in P_0$ and $\mathcal{O}\subset\mathbb{R}^4$,

$$\Gamma(U(M,y))R(\mathcal{O})\Gamma(U(M,y))^{-1}=R(M\mathcal{O}+y)\,. \tag{1.22}$$

The *duality property* studied here strengthens the locality property (1.21) for suitably regular regions by asserting that

$$R(\mathcal{O}^c)=R(\mathcal{O})'\,. \tag{1.23}$$

As mentioned, this relation has been proved by several authors. In this paper, we prove (1.23) for a large class of regions and for any mass, assuming Theorem 1.1. For the massive models, (1.23) is proved here by verifying an abstract relation between pairs of real linear manifolds in H_1 using elementary properties of Sobolev spaces. For the massless model, the duality relation is established using the dilatation covariance of the theory. Although Araki[1] did not treat the $m=0$ case, arguments similar to his were presented by Benfatto and Nicolò.[6] The use of the dilatation covariance significantly simplifies the proof. The argument using dilatation

covariance given here is similar to the one used in Ref. 7 for the free electromagnetic field (the case of spin-1).

The abstract duality property (1.10) is related to duality for the local algebras $R(\mathcal{O})$ (1.23) as follows. Let $R(\mathcal{O})_{sa}$ be the set of self-adjoint elements of $R(\mathcal{O})$. Then the set $R(\mathcal{O})_{sa}\Omega$ is a RLM in H_F and we set $M(\mathcal{O})_F \equiv \overline{R(\mathcal{O})_{sa}\Omega}$, the strong closure. Let E_1: $H_F \mapsto H_1'$ be the projection onto the one-particle subspace and define

$$M_0(\mathcal{O}) \equiv E_1 M(\mathcal{O})_F . \tag{1.24}$$

This is a strongly closed RLM in H_1', which, by (1.1), corresponds to a strongly closed RLM in H_1 that we denote by $M(\mathcal{O})$. The RLM $M(\mathcal{O}) \subset H_1$ satisfies

$$A(M(\mathcal{O})) = R(\mathcal{O}) . \tag{1.25}$$

From the construction of $R(\mathcal{O})$ (1.18) and from (1.14), we obtain an explicit form for $M(\mathcal{O})$ as a RLM in H_1:

$$M(\mathcal{O}) = \overline{\text{Real span}}\ \{\omega(\bar{p})^{-1/2} f(\bar{p},\omega(\bar{p}))\,|\, f \in \mathcal{S}_r(\mathcal{O})\}, \tag{1.26}$$

where the bar indicates the strong closure of the span and $\tilde{f}$ is defined in (1.15). The RLM $M(\mathcal{O})$ corresponding to $R(\mathcal{O})$ is unique for suppose $M_1, M_2 \subset H_1$ are two RLM's such that $A(M_1) = A(M_2)$. Then from Theorem 1.1, $A(M_2)' = A(M_1')$ and the CCR (1.5) imply that $M_1' \subset M_2'$ and hence, by symmetry, $M_1' = M_2'$ so $\overline{M}_1 = \overline{M}_2$.

We now can reformulate the duality condition (1.23) for the local algebra $R(\mathcal{O})$ in terms of its associated RLM's $M(\mathcal{O})$ and $M(\mathcal{O}^c)$. The abstract duality condition (1.10) and (1.25) imply that

$$R(\mathcal{O})' = A(M(\mathcal{O}))' = A(M(\mathcal{O})') . \tag{1.27}$$

In light of this and the uniqueness of the RLM, the duality condition (1.23),

$$R(\mathcal{O}^c) = A(M(\mathcal{O}^c)) = R(\mathcal{O})' = A(M(\mathcal{O})'), \tag{1.28}$$

will hold if and only if

$$M(\mathcal{O}^c) = M(\mathcal{O})' . \tag{1.29}$$

The locality condition (1.21) implies

$$M(\mathcal{O}^c) \subset M(\mathcal{O})' , \tag{1.30}$$

so the reverse inclusion must be established. It is known[1,7] that this does not hold for arbitrary regions $\mathcal{O}$ so we will restrict the class of regions to those with regular boundaries (see below). This family will include all double cone and wedge regions.

A summary of the contents of this paper is as follows. The duality relation is proved for the massive models in Sec. II and for the massless model in Sec. III. Other properties of the local algebras, in particular, the factor property and the cyclicity and separability of the vacuum, are discussed in Sec. IV.

II. DUALITY FOR THE MASSIVE FREE-SCALAR FIELD

In this section, we consider the local algebras $R(\mathcal{O})$ in the massive free models $m > 0$. The proof of relation (1.29) between the RLM's in H_1 for suitably regular regions $\mathcal{O}$ is based on the following theorem.

Theorem 2.1: Let M_1 and M_2 be two strongly closed RLM's in a complex Hilbert space H satisfying $M_1 \subset M_2'$. Then $M_1 = M_2'$ if and only if $M_1' \cap iM_2' = \{0\}$, which is the case if and only if each vector $h \in H$ has a unique representation of the form $h = g_1 + ig_2$ with $g_1 \in M_1$ and $g_2 \in M_2$.

Proof: (a) First suppose that $M_1 = M_2'$. If $g \in M_1' \cap iM_2' = M_1' \cap iM_1$, it follows from the definition of M' (1.8) that

$$\text{Im}(g, ig) = \|g\|^2 = 0 , \tag{2.1}$$

so $g = 0$.

(b) Second, suppose that $M_1' \cap iM_2' = \{0\}$. If $g \in H$ is orthogonal to $M_1 + iM_2$, then $g \in M_1' \cap iM_2'$, so $g = 0$ and $M_1 + iM_2$ is dense in H. Let $f = \text{s-}\lim_{n\to\infty}(h_n + ig_n)$ with $h_n \in M_1$ and $g_n \in M_2$. Then we have

$$\|h_n + ig_n - h_m - ig_m\|^2 = \|h_n - h_m\|^2 + \|g_n - g_m\|^2 + 2\,\text{Im}(g_n - g_m, h_n - h_m) . \tag{2.2}$$

Because $g_n - g_m \in M_2$ and $h_n - h_m \in M_1 \subset M_2'$, the last term on the right side of (2.2) vanishes and $h_n \to h \in M_1$, $g_n \to g \in M_2$, so $f = h + ig \in M_1 + iM_2$. This representation is unique for if $f = h' + ig'$ also with $h' \in M_1$ and $g' \in M_2$, then $(h' - h) = i(g - g') \in M_1 \cap iM_2 \subset M_2' \cap iM_1' = \{0\}$, so $h' = h$ and $g' = g$.

(c) Finally, let $g \in M_2'$ and write its unique representation as $g = g_1 + ig_2$, $g_1 \in M_1$, and $g_2 \in M_2$. Then, for any $h_2 \in M_2 \subset M_1'$,

$$\text{Im}(g, h_2) = \text{Im}(ig_2, h_2) = 0 , \tag{2.3}$$

so $g_2 \in iM_2'$ and as in (2.1) this implies $g_2 = 0$. Hence, $g = g_1 \in M_1$ and $M_1 = M_2'$. ∎

In light of Theorem 2.1 and (1.30), our strategy is to choose $f \in M(\mathcal{O})' \cap iM(\mathcal{O}^c)'$ and to show, for a suitable family of regions $\mathcal{O} \subset \mathbb{R}^4$, that f is indentically zero. We now describe the family of regions for which the proof is valid. We identify the time-zero hyperplane $\mathcal{S}_o \equiv \{x \,|\, x_4 = 0\}$ in $\mathbb{R}^4$ with $\mathbb{R}^3$. For any open $O \subset \mathbb{R}^3$, we define $\hat{O}$, the open causal span of O in $\mathbb{R}^4$, by

$$\hat{O} \equiv \text{Int}\{x \in \mathbb{R}^4 \,|\, (x - \bar{y})^2 < 0,\ \forall \bar{y} \in O^c \cap \mathcal{S}_0\} . \tag{2.4}$$

We characterize open regions $O \subset \mathbb{R}^3$ in terms of a regularity condition of their boundary.

Definition 2.2: An open set $N \subset \mathbb{R}^3$ has the segment property if there exists a locally finite open cover $\{W_i\}_{i=0}^{\infty}$ of $\overline{N}$ and a set of vectors $\{\bar{y}_i\}_{i=1}^{\infty}$, $\bar{y}_i \in \mathbb{R}^3$, such that

(i) $W_0 \subset N$,

(ii) $W_i \cap \partial N \neq \phi$, $i \geq 1$, where $\partial N \equiv \overline{N} \setminus N$ and for all $\lambda \in (0,1)$ and $\bar{x} \in W_i \cap \overline{N}$, $\bar{x} + \lambda \bar{y}_i \in N$.

We will establish (1.29) for the family $\mathcal{T}$ of nonempty open regions $\mathcal{O} \subset \mathbb{R}^4$ satisfying the following conditions.

Conditions 2.3: (i) $\mathcal{O} = \hat{O}$ for some open $O \subset \mathbb{R}^3$ satisfying Int $\overline{O} = O$; (ii) the region $O \subset \mathbb{R}^3$ and $\sim\overline{O}$ have the segment property.

Remark 2.4: The first condition allows us to work with the time-zero fields. Specifically, let $\phi_0(\bar{x}) \equiv \phi(\bar{x}, 0)$ and $\pi_o(\bar{x}) \equiv (\partial_4 \phi)(\bar{x}, 0)$ be the time-zero fields which are known to be operator-valued distributions on $\mathbb{R}^3$ such that for any $f \in \mathcal{S}_r(\mathbb{R}^3)$, $\phi_0[f]$ and $\pi_0[f]$ are essentially self-adjoint on

D_F. We define two families of unitary operators associated with these fields:

$$U(f)\equiv\exp(i\phi_0[f]) \text{ and } V(g)\equiv\exp(i\pi_0[g]), \quad (2.5)$$

for any $f, g\in\mathscr{S}_r(\mathbb{R}^3)$. For any open $O\subset\mathbb{R}^3$, we define a von Neumann algebra $R_0(O)$ by

$$R_o(O)\equiv\{U(f),V(g)\,|\,f,g\in\mathscr{S}_r(O),\ O\subset\mathbb{R}^3\}''. \quad (2.6)$$

Lemma 2.5: If $\mathscr{O}\subset\mathbb{R}^4$ is open and $\mathscr{O}=\hat{O}$ for some open $O\subset\mathbb{R}^3$ then $R(\mathscr{O})=R_o(O)$.

The proof of this lemma is standard.

Remarks 2.6: (1) The second condition is a mild smoothness property of the boundary of O common in the theory of local Sobolev spaces (e.g., Ref. 14). Regions satisfying the segment property include star-shaped sets and convex sets and they may be bounded or unbounded. The following lemma describes a large class of regions having the segment property.

Lemma 2.7: If $O\subset\mathbb{R}^3$ is open, $\mathrm{Int}\,\overline{O}=O$ and $\partial O=\overline{O}\setminus O$ consists of a union of regular surfaces intersecting transversally, then O and $\sim\overline{O}$ have the segment property.

The proof of this is straightforward and will not be given.

(2) Certain regions satisfying Conditions 2.3 are of particular interest. When $O\subset\mathbb{R}^3$ is a sphere, $\hat{O}$ is a double cone and when O is a half space, $\hat{O}$ is a wedge region. These double cones and wedge regions are obtained by the action of the Poincaré group and the dilatations on the unit-radius double cone centered at the origin $\mathscr{O}_1$ and the "right" wedge region W_R, respectively. The double cone $\mathscr{O}_1$ is defined by

$$\mathscr{O}_1=(V_+-e_4)\cap(V_-+e_4), \quad (2.7)$$

where $e_4\equiv(0,0,0,1)$ and $V_\pm$ are the forward and backward light cones, respectively,

$$V_\pm\equiv\{x\,|\,x\cdot x>0,\ x_4\gtrless 0\}. \quad (2.8)$$

The right wedge W_R is defined by

$$W_R\equiv\{x\,|\,x_3>|x_4|\}. \quad (2.9)$$

(3) The proof of duality for the algebra $R(\mathscr{O})$ with $\mathscr{O}$ satisfying Conditions 2.3 will establish duality for the algebra associated with any region obtained from $\mathscr{O}$ by a Poincaré transformation. This follows from (1.22).

We first characterize $f\in M(\mathscr{O})'\cap iM(\mathscr{O}^c)'$ in terms of the support properties of the initial data of associated tempered distribution solutions to the Klein–Gordon equation. For any $g\in H_1$, we define a positive frequency solution to the Klein–Gordon equation by

$$\phi_+(g;x)\equiv(2\pi)^{-3/2}\int_{(\infty)}d\bar{p}\,\omega(\bar{p})^{-1/2}e^{-ix\cdot p}g(\bar{p}), \quad (2.10a)$$

where $x\cdot p\equiv x_4\omega(\bar{p})-\bar{x}\cdot\bar{p}$, and a real solution by

$$\phi(g;x)=\phi_+(g;x)+\phi_+(g;x)^*. \quad (2.10b)$$

By a simple calculation based on (2.10) and the characterization of $M(\mathscr{O})$ given in (1.26), it is seen that $f\in M(\mathscr{O})'$ is equivalent to the condition that

$$\int_{(\infty)}d^4(x)\,\phi(if;x)g(x)=0, \quad \text{for all } g\in\mathscr{S}(\mathscr{O}). \quad (2.11)$$

Similarly, the condition $if\in M(\mathscr{O}^c)'$ is equivalent to the condition that

$$\int_{(\infty)}d^4(x)\,\phi(f;x)h(x)=0 \quad \text{for all } h\in\mathscr{S}(\mathscr{O}^c). \quad (2.12)$$

It is well known that the tempered distribution solution to the Klein–Gordon equation $\phi(f;x)$ can be expressed as an $\mathscr{S}(\mathbb{R}^3)'$-valued function of t. By using standard approximation arguments, one concludes from (2.11) that the initial data $\phi_o(if;\bar{x})$ and $\pi_o(if;\bar{x})\equiv(\partial_4\phi)(if;x)|_{x_4=0}$, for $\phi(if;x)$ is supported (as distributions) in $\sim O\subset\mathbb{R}^3$ where $\hat{O}=\mathscr{O}$. Similarly, one concludes from (2.12) that the initial data for $\phi(f;x)$ is supported in $\overline{O}$. For brevity, let us write

$$A_i(\bar{x})\equiv\phi_o(g_i;\bar{x}), \quad (2.13a)$$

$$B_i(\bar{x})\equiv\pi_o(g_i;\bar{x}), \quad (2.13b)$$

for $g_1\equiv if$ and $g_2\equiv f$.

With the Fourier transform of h defined by

$$\hat{h}(\bar{p})\equiv(2\pi)^{-3/2}\int_{(\infty)}d\bar{x}\,e^{-i\bar{x}\cdot\bar{p}}h(\bar{x}), \quad (2.14)$$

the initial data (2.13) for $i=1$, for example, can be written as

$$\hat{A}_1(\bar{p})=i\omega(\bar{p})^{-1/2}[f(\bar{p})-(Cf)(\bar{p})], \quad (2.15a)$$

$$\hat{B}_1(\bar{p})=\omega(\bar{p})^{1/2}[f(\bar{p})+(Cf)(\bar{p})]. \quad (2.15b)$$

Here, C denotes the conjugation on H_1 defined by

$$(Cf)(\bar{p})=f(-\bar{p})^*. \quad (2.15c)$$

The Fourier transform of g is real if and only if g is C-invariant. Hence, the inverse Fourier transform of the initial data $\hat{A}_i(\bar{p})$ and $\hat{B}_i(\bar{p})$, $i=1,2$, is real. The Fourier transformed initial data $\hat{A}_i$ and $\hat{B}_i$ in (2.15) is simply related to $\hat{A}_2$ and $\hat{B}_2$ in the following manner:

$$\hat{B}_1(\bar{p})=\omega(\bar{p})\hat{A}_2(\bar{p}), \quad (2.16a)$$

$$\hat{B}_2(\bar{p})=-\omega(\bar{p})\hat{A}_1(p). \quad (2.16b)$$

We call these relations the *coupling relations* between the initial data. Because of the support properties of the initial data, for example, $\mathrm{supp}(B_1)\subset\sim O$ and $\mathrm{supp}(A_2)\subset\overline{O}$, we will show that (2.16) is possible if and only if f is identically zero.

The functions in (2.15) and (2.16) are not necessarily in H_1, but their Fourier transforms (2.13) belong to certain local Sobolev spaces that we now describe. Let μ^τ, $\tau\in\mathbb{R}$, denote the operator defined on the dense set $\mathscr{S}(\mathbb{R}^3)$ of $L^2(\mathbb{R}^3)$ ($\mathbb{R}^3$ identified with coordinate space) in the Fourier transform by

$$(\mu^\tau f)\hat{}\,(\bar{p})=\omega(\bar{p})^\tau\hat{f}(\bar{p}), \quad f\in\mathscr{S}(\mathbb{R}^3). \quad (2.17)$$

Note that $C(\mu^\tau f)\hat{}\,(\bar{p})=\omega(\bar{p})^\tau(C\hat{f})(\bar{p})$. The operator μ^τ is essentially self-adjoint on $\mathscr{S}(\mathbb{R}^3)$ and if $\tau\leqslant 0$, it extends to a bounded operator. Let $D(\mu^\tau)$ denote the domain in $L^2(\mathbb{R}^3)$ on which μ^τ is self-adjoint (we use the same symbol for the closure).

Definition 2.8: H_+ is the Hilbert space consisting of vectors in $D(\mu^{1/2})$ with the inner product

$$(f,g)_+\equiv(\mu^{1/2}f,\mu^{1/2}g). \quad (2.18)$$

The Hilbert space H_- is the completion of $L^2(\mathbb{R}^3)$ in the norm

$$\|f\|_- \equiv \|\mu^{-1/2} f\|_2 , \tag{2.19a}$$

induced by the inner product

$$(f,g)_- \equiv (\mu^{-1/2} f, \mu^{-1/2} g) , \tag{2.19b}$$

for $f,g \in L^2(\mathbb{R}^3)$.

Remark 2.9: The multiplication operator $\omega(\bar{p})^r$ is positive so the inner products (2.18) and (2.19b) are positive definite. The operator $\mu^{1/2}$ on $D(\mu^{1/2})$ is closed. It follows from this and the first inequality in (2.20) below that H_+ is a Hilbert space.

Lemma 2.10: (i) $f,g \in H_+$ and $h,k \in L^2(\mathbb{R}^3) \subset H_-$, the following bounds hold:

$$m|(f,g)| \leqslant |(f,g)_+| \text{ and } |(h,k)_-| \leqslant m^{-1}|(h,k)| . \tag{2.20}$$

(ii) The map $\mu^{1/2}$ is an isometric isomorphism of H_+ onto $L^2(\mathbb{R}^3)$ and of $L^2(\mathbb{R}^3)$ onto H_-.

(iii) The map μ is an isometric isomorphism of H_+ onto H_- with μ^{-1} as the inverse map.

The proof of Lemma 2.10 is trivial. We now define some local Sobolev spaces.

Definition 2.11: Let $O \subset \mathbb{R}^3$ be any measurable set with nonempty interior. We define subspaces $H_\pm(O)$ of $H_\pm$, respectively, by

$$H_+(O) \equiv \{f \,|\, f \in H_+,\ \text{supp}(f) \subset \text{Int}(O)\}^- , \tag{2.21a}$$

$$H_-(O) \equiv \{h \,|\, h \in H_-,\ (\mu^{-1/2} h, \mu^{1/2} f) = 0 , \text{ for all } f \in H_+(\sim O)\} , \tag{2.21b}$$

where the bar in (2.21a) denotes strong closure. With regard to Lemma 2.10, we define two sub-Hilbert spaces of $L^2(\mathbb{R}^3)$ by

$$K_+(O) \equiv \mu^{1/2} H_+(O) , \tag{2.22a}$$

$$K_-(O) \equiv \mu^{-1/2} H_-(O) . \tag{2.22b}$$

Theorem 2.12: Let $O \subset \mathbb{R}^3$ be any measurable subset of $\mathbb{R}^3$ with nonempty interior. Let $K_\pm(O)$ be the closed subsets of $L^2(\mathbb{R}^3)$ defined in (2.22). Then

$$K_+(O)^\perp = K_-(\sim O) , \tag{2.23a}$$

$$K_-(O)^\perp = K_+(\sim O) . \tag{2.23b}$$

Proof: (a) We will use Lemma 2.10 repeatedly. Note that $g \in K_+(O)^\perp \equiv [\mu^{1/2} H_+(O)]^\perp$ if and only if $\mu^{1/2} g \in [\mu H_+(O)]^\perp$ with the latter orthogonal complement taken in H_-. Now $k \in H_-(\sim O)$ if and only if $(\mu^{-1/2} k, \mu^{1/2} f) = 0$, for all $f \in H_+(O)$. This is the case if and only if $(k, \mu f)_- = 0$. Hence,

$$\mu^{1/2} g \in [\mu H_+(O)]^\perp = H_-(\sim O),$$

so $g \in \mu^{-1/2} H_-(\sim O)$.

(b) Because $[\mu^{1/2} H_+(O)]^\perp = \mu^{1/2}[H_+(O)]^\perp$ and because of part (ii) in Lemma 2.10, condition (2.23a) is equivalent to

$$\mu[H_+(O)^\perp] = H_-(\sim O) \tag{2.24}$$

with the orthogonal complement in H_+. Taking the orthogonal complement of both sides of this expression in H_- and recalling part (iii) of Lemma 2.10, we obtain

$$\mu H_+(O) = H_-(\sim O)^\perp . \tag{2.25}$$

Upon replacing O by $\sim O$ in (2.25) and using part (ii) of Lemma 2.10, we obtain (2.23b). ∎

We now return to the initial data A_i and B_i (2.13) for the solutions to the Klein–Gordon equation $\phi(if;x)$ and $\phi(f;x)$ associated with $f \in M(\mathcal{O})' \cap iM(\mathcal{O}^c)'$. We show that this data belongs to the spaces $H_\pm(O)$ and $H_\pm(\sim O)$. This will require that we use the second part of Conditions 2.3 and Lemma 2.7.

Lemma 2.13: Let A_i and B_i be as defined in (2.13). Then

$$\text{(i)} \quad A_1 \text{ and } A_2 \in H_+ \text{ and are real} , \tag{2.26}$$

$$\text{(ii)} \quad B_1 \text{ and } B_2 \in H_- \text{ and are real} , \tag{2.27}$$

$$\text{(iii)} \quad A_1 \in H_+(\sim O) \text{ and } A_2 \in H_+(O) , \tag{2.28}$$

$$\text{(iv)} \quad B_1 \in H_-(\sim O) \text{ and } B_2 \in H_-(O) . \tag{2.29}$$

Proof: (a) Parts (i) and (ii) follow directly from Definition 2.8, formulas (2.15) and (2.16), and the C-invariance of the Fourier transforms of these functions.

(b) We first show that $A_2 \in H_+(O)$. It was proved that $\text{supp}(A_2) \subset \overline{O}$ so we show that A_2 can be approximated by functions in H_+ with support in $\text{Int}(O)$. Let $\{W_i\}_{i=0}^\infty$ be the locally finite open cover of $\overline{O}$ and $\{\bar{y}_i\}_{i=1}^\infty$ the associated vectors guaranteed to exist by the segment property for O, Definition 2.2. Let $\{f_i\}_{i=0}^\infty$ be a partition of unity dominated by the open cover $\{W_i\}_{i=0}^\infty$ and set $A_2(\bar{x}) = \Sigma_{i=0}^\infty A_{2,i}(\bar{x})$ with $A_{2,i} \equiv A_2 f_i$. It suffices to show that each $A_{2,i}(\bar{x}) \in H_+(O)$. For $i=0$, $W_0 \subset O$ so $\text{supp}(A_{2,0}) \subset O$ and $A_{2,0} \in H_+(O)$. For $i \geqslant 1$, the function $A^t_{2,i}(\bar{x}) \equiv A_{2,i}(\bar{x} - t\bar{y}_i)$ has support in $\{\bar{x} + t\bar{y}_i \,|\, \bar{x} \in W_i \cap \overline{O}\} \subset O$, for $t \in (0,1)$ by the segment property. Since translations are unitarily implemented in H_+, $A^t_{2,i} \in H_+(O)$. Moreover, we have

$$\|A_{2,i} - A^t_{2,i}\|_+^2 = \int_{(\infty)} d\bar{p}\, \omega(\bar{p}) |e^{-it\bar{y}_i \cdot \bar{p}} - 1|^2 |\hat{A}_{2,i}(\bar{p})|^2 , \tag{2.30}$$

which converges to zero as $t \to 0$ by the dominated convergence theorem. Hence, $A_{2,i} \in H_+(O)$. The proof that $A_1 \in H_+(\sim O)$ is similar since $\text{supp}(A_1) \subset \sim O$ and $\sim O$ has the segment property by Conditions 2.3.

(c) To prove (2.29), recall that for any $f \in H_+(O)$ there exists a sequence $\{f_n\} \subset H_+(O)$ such that $\text{supp}(f_n) \subset \text{Int}(O)$ and $f_n \to f$ in H_+. Since $\text{supp}(B_1) \subset \sim O$, we have

$$(\mu^{-1/2} B_1, \mu^{1/2} f) = \lim_{n \to \infty} (\mu^{-1/2} B_1, \mu^{1/2} f_n) = \lim_{n \to \infty} B_1[f_n] = 0 , \tag{2.31}$$

where $B_1[f_n]$ denotes the distribution B_1 evaluated at f_n. Hence, $B_1 \in H_-(\sim O)$. The proof for B_2 is similar. ∎

Theorem 2.14: If $f \in M(\mathcal{O})' \cap iM(\mathcal{O}^c)'$, where $\mathcal{O} \subset \mathbb{R}^4$ satisfies Conditions 2.3, then $f = 0$. Consequently, the von Neumann algebra $R(\mathcal{O})$ defined in (1.18) for $m > 0$ satisfies the duality relation

$$R(\mathcal{O})' = R(\mathcal{O}^c) . \tag{2.32}$$

Proof: From the coupling relations (2.16), we have

$$\mu^{-1/2} B_1 = \mu^{1/2} A_2 , \tag{2.33a}$$

$$\mu^{-1/2} B_2 = -\mu^{1/2} A_1 . \tag{2.33b}$$

Lemma 2.13 and Definition 2.11 (2.22a) indicate that $\mu^{1/2}A_2 \in K_+(O)$, whereas $\mu^{-1/2}B_1 \in K_-(\sim O)$. Consequently, by Theorem 2.12 (2.23a), $A_2 = 0 = B_1$ and $f = -Cf$. Similarly, we have $\mu^{-1/2}B_2 \in K_-(O)$ and $\mu^{1/2}A_1 \in K_+(\sim O)$ so Theorem 2.12, (2.23b), and the coupling relation (2.33b) imply that $B_2 = 0 = A_1$ and $f = Cf$. Hence $f = 0$. ∎

III. DUALITY FOR THE MASSLESS FREE-SCALAR FIELD

Relation (1.29) is established for the $m = 0$ case using the dilatation covariance of the model. In this section, we fix $m = 0$ and write $k \equiv (\bar{k}, \kappa)$, $\kappa \equiv |\bar{k}|$, for a lightlike four-vector. The dilatation group on H_1 is the representation of the multiplicative group of the positive reals given by

$$(U_\lambda f)(\bar{k}) \equiv \lambda^{3/2} f(\lambda \bar{k}), \quad \lambda \in \mathbb{R}_+ . \tag{3.1}$$

It is easy to check that this defines a strongly continuous unitary representation. We consider a corresponding family of automorphisms of $\mathscr{S}(\mathbb{R}^4)$ defined by

$$f(x) \mapsto f_\lambda(x) \equiv \lambda^{-3} f(\lambda^{-1}x), \quad \lambda \in \mathbb{R}_+ . \tag{3.2}$$

Note that for any $f \in \mathscr{S}(\mathbb{R}^4)$ we have $\phi[f_\lambda]\Omega = \phi_S[U_\lambda F]\Omega$, where ϕ_S and F are defined in (1.14).

For any $\mathscr{O} \subset \mathbb{R}^4$, let $\mathscr{O}_\lambda$ denote the set $\{\lambda x | x \in \mathscr{O}\}$. Then the automorphisms defined in (3.2) implement the scaling:

$$\mathscr{S}(\mathscr{O}) \mapsto \mathscr{S}_\lambda(\mathscr{O}) \equiv \{f_\lambda | f \in \mathscr{S}(\mathscr{O})\} = \mathscr{S}(\mathscr{O}_\lambda) . \tag{3.3}$$

In particular, for regions of the form $\mathscr{O} = \hat{O}$, $O \subset \mathbb{R}^3$, as discussed in Condition 2.3 and (2.4), we find

$$\mathscr{S}_\lambda(\mathscr{O}) = \mathscr{S}(\hat{O}_\lambda) , \tag{3.4}$$

where $O_\lambda \equiv \{\lambda \bar{x} | \bar{x} \in O\}$. In this section, we restrict our discussion to those nonempty open regions $\mathscr{O} \subset \mathbb{R}^4$ belonging to the set of regions $\mathscr{T}_0$ satisfying the following conditions.

Conditions 3.1: (i) $\mathscr{O} = \hat{O}$ for some open $O \subset \mathbb{R}^3$ with $\hat{O}$ defined in (2.4); (ii) $O \subset \mathbb{R}^3$ satisfies the scaling property $O_\lambda \subset O$, $\lambda \in (0,1)$, and $\lim_{\lambda \to 1} O_\lambda = O$. Condition 3.1 (ii) will allow the approximation of functions in $\mathscr{S}(O)$ by those in $\mathscr{S}(O_\lambda)$ in an appropriate norm.

A general class of regions satisfying Condition 3.1 (ii) with $c = 1$ consists of regions which are star-shaped with respect to the origin. This set of regions includes double cones whose base O is a ball centered at the origin.

We remark that the methods outlined below extend to other regions provided that they possess a scaling property similar to Condition 3.1 (ii) and that the field is covariant with respect to this scaling. For example, we consider the right wedge W_R and the scaling by translations in the x_3 direction. For $\lambda > 0$, set

$$W_\lambda \equiv \{x | x_3 - \lambda > |x_4|\} = W_R + \lambda e_3 .$$

The base in $\mathbb{R}^3$ is $W_{0,\lambda} = \{\bar{x} | x_3 > \lambda\}$ and $\lim_{\lambda \to 0} \hat{W}_{0,\lambda} = W_R$.

Let $\mathscr{O} \in \mathscr{T}_0$ and let $R(\mathscr{O})$ be the von Neumann algebra defined in Definition 1.2 with $m = 0$. We define three strongly closed RLM's in H_1, for $\lambda \in (0,1)$, associated with the algebras $R(\mathscr{O}_\lambda^c)$, $R(\mathscr{O}_\lambda^c)'$, and $R(\mathscr{O}_\lambda)$, respectively, by

$$K_o(\lambda) \equiv M(\mathscr{O}_\lambda^c) , \tag{3.5a}$$

$$K_i(\lambda) \equiv K_o(\lambda)' , \tag{3.5b}$$

$$R_i(\lambda) \equiv M(\mathscr{O}_\lambda) , \tag{3.5c}$$

where $M(\mathscr{O})$ is defined in (1.26). Note that $(\mathscr{O}^c)_\lambda = (\mathscr{O}_\lambda)^c$.

The results of Bisognano and Wichmann[15] suggest that $K_o(\lambda)$, the RLM associated with the "outside" algebra, and $K_i(\lambda)$ are the appropriate pair of RLM's to study. From Theorem 1.1, the duality relation (1.23) will be established by showing that $R_i(1) = K_i(1)$. By locality, $R_i(\lambda) \subset K_i(\lambda)$ and we will show that $K_i(\lambda) \subset R_i(1)$. We first characterize the elements of $K_i(\lambda)$ and, second, we show how these elements can be strongly approximated by elements in $R_i(\lambda')$ for slightly larger λ'.

We associate with each $f \in H_1$ a classical positive frequency solution to the wave equation as in (2.10a) with $\omega(\bar{p})$ replaced by $|\bar{k}| \equiv \kappa$ and $x \cdot p$ by $x \cdot k \equiv x_4\kappa - \bar{x} \cdot \bar{k}$. The corresponding real solution is constructed as in (2.10b).

Lemma 3.2: $f \in K_i(\lambda)$ if and only if the real solution to the wave equation constructed from $-if$ as in (2.10) vanishes as a distribution for all $x \in (O_\lambda)^c$.

Proof: For any $g \in \mathscr{S}(\mathbb{R}^4)$ write $g \equiv g_1 + ig_2$ with g_i real. A simple calculation shows that

$$\frac{1}{2}\int_{(\infty)} d^4(x)\, \phi(-if;x) g(x) = \mathrm{Im}(G_1, f) + i\,\mathrm{Im}(G_2, f) \tag{3.6a}$$

with

$$G_i(\bar{k}) \equiv (2\pi)^{-3/2}(\kappa)^{-1/2}\tilde{g}_i(\bar{k}, \kappa) . \tag{3.6b}$$

If $f \in K_i(\lambda)$, then the right side of (3.6a) vanishes for all $g \in \mathscr{S}((O_\lambda)^c)$. Conversely, if the left side vanishes for all such g, then $f \in K_o(\lambda)'$ since the elements of the form (3.6b) are dense in $K_o(\lambda)$. ∎

We replace each $f \in K_i(\lambda)$ by an approximation function such that the initial data for the corresponding real solution ϕ is smooth. Let $c \in \mathscr{S}(\mathbb{R}^3)$ be a smooth non-negative function supported in the unit ball integrating to 1. Set $c_\epsilon(\bar{x}) \equiv \epsilon^{-3} c(\epsilon^{-1}\bar{x})$, $\epsilon > 0$, and $\check{f}_\epsilon(\bar{x}) \equiv (\check{f} * c_\epsilon)(\bar{x})$ with $\check{f}$ defined by

$$\check{f}(\bar{x}) \equiv (2\pi)^{-3/2} \int_{(\infty)} d\bar{k}\, e^{i\bar{k}\cdot\bar{x}} f(\bar{k}) , \tag{3.7}$$

for $f \in H_1$. Obviously,

$$f_\epsilon = (2\pi)^{3/2} f \hat{c}_\epsilon \in L^2(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) .$$

Lemma 3.3: Let $f \in K_i(\lambda)$.

(i) $\phi(-if_\epsilon;x) = 0$ for all $x \in (O_\lambda + B_\epsilon(0))^c$, where $B_\epsilon(0)$ is the ball of radius ϵ centered at the origin.

(ii) The initial value data (IVD) for $\phi(-if_\epsilon;x)$ is given by

$$\phi_o(-if_\epsilon;\bar{x}) = (c_\epsilon * \phi_o^f)(\bar{x}) \equiv h_1(\bar{x}) , \tag{3.8a}$$

$$\pi_o(-if_\epsilon;\bar{x}) = (c_\epsilon * \pi_o^f)(\bar{x}) \equiv h_2(\bar{x}) , \tag{3.8b}$$

where ϕ_o^f and π_o^f are the IVD for $\phi(-if;x)$. The functions h_1 and h_2 are real elements of $C^\infty(\mathbb{R}^3)$ supported in $O_\lambda + B_\epsilon(0)$. If O is bounded, $h_1, h_2 \in \mathscr{S}(\mathbb{R}^3)$.

Proof: Part (i) follows from Lemma 3.2 and the construction of f_ϵ. The form of h_1 and h_2 is obtained by trivial calculation. It is clear that these functions are C^∞. If O is bounded, they have compact support. The Fourier transforms of h_1 and h_2 are

$$\hat{h}_1(\bar{k}) = -i(2\pi)^{3/2}(\kappa)^{-1/2}[f(\bar{k}) - (Cf)(\bar{k})]\hat{c}_\epsilon(\bar{k}), \tag{3.9}$$

$$\hat{h}_2(\bar{k}) = -(2\pi)^{3/2}(\kappa)^{1/2}[f(\bar{k}) + (Cf)(\bar{k})]\hat{c}_\epsilon(\bar{k}), \tag{3.10}$$

where C is defined in (2.15c). Since $\hat{h}_1$ and $\hat{h}_2$ are C invariant, the functions h_1 and h_2 are real. ■

If the region O is unbounded, we must approximate h_1 and h_2 by smooth functions of compact support in $O_\lambda + B_\epsilon(0)$. The following lemma provides a sufficient means of approximation. We extend Definition 2.8 to the massless case and define Hilbert spaces $H_\pm$ to be the completion of $\mathscr{S}(\mathbb{R}^3)$ in the norms

$$\|f\|_\pm^2 \equiv \int_{(\infty)} d\bar{k}\, \kappa^{\pm 1}|\hat{f}(\bar{k})|^2 . \tag{3.11}$$

Lemma 3.4: Let $h\in\mathscr{D}_r(\mathbb{R}^3)$, $\mathrm{supp}(h)\subset B_1(0)$, $h\geqslant 0$, and $h(\bar{x}) = 1$, for $|\bar{x}| < \frac{1}{2}$. Set $h_\sigma(\bar{x}) \equiv h(\sigma\bar{x})$. For $f\in H_-$ and $g\in H_+$, set $f_\sigma \equiv h_\sigma f$, $g_\sigma \equiv h_\sigma g$. Then $f_\sigma\in H_-$, $g_\sigma\in H_+$, f_σ, and g_σ have compact support, and $f_\sigma\to f$, $g_\sigma\to g$ weakly as $\sigma\to 0$ in H_- and H_+, respectively.

Proof: (a) By a straightforward calculation (e.g., Ref. 6), it can be shown that for $\eta\in\mathscr{S}(\mathbb{R}^3)$ and $f\in H_+$ there is a constant $K_\eta \geqslant 0$ such that

$$\|\eta f\|_+ \leqslant K_\eta \|f\|_+ , \tag{3.12a}$$

and for h_σ as above,

$$\|h_\sigma f\|_+ \leqslant K\|f\|_+ , \tag{3.12b}$$

with K independent of σ. The dual space of H_+ is naturally isomorphic to H_- by the pairing

$$T\in H_-, f\in H_+ : T[f] \equiv (\mu_o^{-1/2} T, \mu_o^{1/2} f), \tag{3.13a}$$

where $(\mu_o^r f)\hat{}\,(\bar{k}) \equiv \kappa^r \hat{f}(\bar{k})$. Note that

$$|T[f]| \leqslant \|T\|_- \|f\|_+ . \tag{3.13b}$$

For $\eta\in\mathscr{S}(\mathbb{R}^3)$ and $T\in H_-$, it is easy to check that $\eta T\in H_-$ and for $f\in H_+$,

$$\eta T[f] = T[\eta^* f] . \tag{3.14a}$$

Consequently, from (3.12a) and (3.13),

$$|\eta T[f]| \leqslant K_{\eta^*}\|T\|_-\|f\|_+ , \tag{3.14b}$$

so it follows that

$$\|\eta T\|_- \leqslant K_{\eta^*}\|T\|_- , \tag{3.14c}$$

and multiplication by $\mathscr{S}(\mathbb{R}^3)$ is continuous on H_-. Applying this to h_σ, it follows from (3.12b) and (3.14) that

$$\|h_\sigma T\|_- \leqslant K\|T\|_- . \tag{3.15}$$

(b) Let $g_\sigma \equiv 1 - h_\sigma$. For h, $\ell\in\mathscr{S}(\mathbb{R}^3)$, we have

$$(h, g_\sigma \ell)_- = \frac{1}{2\pi^2}\int_{(\infty)} d\bar{x}\, d\bar{y}\, h(\bar{x})^* |\bar{x} - \bar{y}|^{-2} g_\sigma(\bar{y})\ell(\bar{y}) , \tag{3.16}$$

and $|(h, g_\sigma\ell)_-| \leqslant (1 + K)\|h\|_-\|\ell\|_-$ by (3.15). Since

$$H(\bar{y}) \equiv \int_{(\infty)} d\bar{x}|\bar{x} - \bar{y}|^{-2} h(\bar{x})^* \in L^2(\mathbb{R}^3)\cap C^\infty ,$$
$$\ell H\in L^1(\mathbb{R}^3) .$$

Since $g_\sigma|\ell H| \leqslant |\ell H|$, it follows from the dominated convergence theorem that $\lim_{\sigma\to 0}(h, g_\sigma\ell)_- = 0$. It is easy to show that weak convergence follows from this, the bound (3.15), and the density of $\mathscr{S}(\mathbb{R}^3)$ in H_-.

(c) Finally, for any $T\in H_-$ and $f\in H_+$, we have, from (b),

$$\lim_{\sigma\to 0} g_\sigma T[f] = \lim_{\sigma\to 0}(g_\sigma T, \mu_\sigma f)_-$$
$$= \lim_{\sigma\to 0}(\mu_o^{-1} T, g_\sigma f)_+ = 0 . \tag{3.17}$$

Since μ_o^{-1}: $H_-\to H_+$ is an isomorphism, $g_\sigma f$ converges weakly to zero in H_+. ■

Lemma 3.5: (i) The strong limit as $\lambda\to 1$ *of* $K_i(\lambda)$ is $K_i \equiv K_i(1)$.

(ii) For any $\lambda\in(0,1)$ we have

$$K_i(\lambda)\subset R_i(1)\subset K_i , \tag{3.18}$$

i.e., $K_i = R_i(1)$.

Proof: (a) We have the formula $K_o(\lambda) = U_\lambda K_o(1)$ from the dilatation covariance of the field and the strong continuity of U_λ. For definition (3.5b), we have

$$K_i(\lambda) = (U_\lambda K_o(1))' = U_\lambda K_i(1) , \tag{3.19}$$

which proves (i).

(b) For $\lambda\in(0,1)$, we can choose $\epsilon > 0$ such that $\overline{O_\lambda + B_\epsilon(0)}\subset O_1$. By the analog of Lemma 2.5 for the $m = 0$ case, $R_i(\lambda)$ is the closure of real linear span of functions of the form $i\kappa^{1/2}\hat{h}(\bar{k})$ and $\kappa^{-1/2}\hat{g}(\bar{k})$ with g, $h\in\mathscr{S}_r(O_\lambda)$. We first suppose O is bounded. Choose any $f\in K_i(\lambda)$. From Lemma 3.3, the IVD h_1 and h_2 for the real solution $\phi(-if_\epsilon; x)$ belongs to $\mathscr{S}_r(O_\lambda + B_\epsilon(0))$. Hence, h_1 and h_2 can be used to smear the time-zero fields:

$$\phi_o[h_2] = (2\pi)^{-3/2}\int_{(\infty)} d\bar{k}(2\kappa)^{-1/2}\hat{h}_2(\bar{k})a^\dagger(\bar{k}) , \tag{3.20a}$$

$$\pi_o[h_1] = i(2\pi)^{-3/2}\int_{(\infty)} d\bar{k}\left(\frac{\kappa}{2}\right)^{1/2}\hat{h}_1(\bar{k})a^\dagger(\bar{k}) , \tag{3.20b}$$

so $\kappa^{-1/2}\hat{h}_2, i\kappa^{1/2}\hat{h}_1\in R_i(1)$. From the form of $\hat{h}_1$ and $\hat{h}_2$ in (3.9) and (3.10), it follows that $f(\bar{k})\hat{c}_\epsilon(\bar{k})\in R_i(1)$. Since this function converges strongly to f, $f\in R_i(1)$.

(c) If O is unbounded, define $h_{1,\sigma}$ and $h_{2,\sigma}$ as in Lemma 3.4. In particular, $h_{1,\sigma}, h_{2,\sigma}\in\mathscr{D}_r((O_\lambda + B_\epsilon(0))\cap B_\sigma(0))$ and $\kappa^{1/2}\hat{h}_{1,\sigma}, \kappa^{-1/2}\hat{h}_{2,\sigma}\in H_1$. Given any $g\in H_1$, we have

$$\lim_{\sigma\to 0}\left|\int_{(\infty)} d\bar{k}\,[\kappa^{1/2}\hat{h}_{1,\sigma}(\bar{k}) - \kappa^{1/2}\hat{h}_1(\bar{k})]^* g(\bar{k})\right|$$
$$= \lim_{\sigma\to 0}\left|(h_{1,\sigma} - h_1, G)_+\right| = 0 , \tag{3.21}$$

by Lemma 3.4, where $G \equiv \mu_o^{-1/2}\check{g}\in H_+$. Consequently, w-$\lim_{\sigma\to 0}\kappa^{1/2}\hat{h}_{1,\sigma} = \kappa^{1/2}\hat{h}_1$ in H_1. A similar calculation establishes that w-$\lim_{\sigma\to 0}\kappa^{-1/2}\hat{h}_{2,\sigma} = \kappa^{-1/2}\hat{h}_2$ in H_1. It follows from the argument in part (b) that $i\kappa^{1/2}\hat{h}_{1,\sigma}, \kappa^{-1/2}\hat{h}_{2,\sigma}\in R_i(1)$. Since the RLM $R_i(1)$ is weakly closed in H_1, we obtain $i\kappa^{1/2}\hat{h}_1, \kappa^{-1/2}\hat{h}_2\in R_i(1)$ and hence $f\in R_i(1)$ as above. ■

Theorem 3.6: If $\mathcal{O} \subset \mathbb{R}^4$ satisfies Conditions 3.1, then the RLM's $M(\mathcal{O}^c)'$ and $M(\mathcal{O})$, defined in (3.5), are equal. Consequently, the von Neumann algebra $R(\mathcal{O})$ defined in (1.18) for $m = 0$ satisfies the duality relation

$$R(\mathcal{O})' = R(\mathcal{O}^c) .$$

IV. OTHER PROPERTIES OF THE LOCAL ALGEBRAS

We now discuss some other properties of the local algebras, namely, the cyclic and separating properties of the vacuum and the factor property. Returning to the general setting of Sec. I, we formulate these properties in terms of real linear manifolds in H_1.

Theorem 4.1: Let M and M' be a complementary pair of strongly closed RLM's in H_1 and let $A(M)$ and $A(M')$ be the associated von Neumann algebras on H_F as in (1.6). Then we have the following.

(i) Ω is cyclic and separating for $A(M)$ [and hence for $A(M)' = A(M')$] if and only if $M \cap iM = \{0\} = M' \cap iM'$.

(ii) $A(M)$ is a factor if and only if $M \cap M' = \{0\}$.

Proof: (a) Let $M^\perp$ be the complex orthogonal complement of M in H_1. It is easy to show that $M^\perp = M' \cap iM'$. Similarly, one shows that $(M')^\perp = M \cap iM$. Consequently, the condition in (i) guarantees the cyclicity of Ω for $A(M)$ and $A(M)'$, and hence the separability.

(b) We note that for strongly closed RLM's M_1, $M_2 \subset H_1$, it is easy to show that $A(M_1 + M_2) = A(M_1) \vee A(M_2)$, where $M_1 + M_2$ is the real linear span of all elements in M_1 and M_2 [see (1.7)]. The center of $A(M)$ is $A(M) \cap A(M)' = A(M) \cap A(M') \equiv Z(M)$ by Theorem 1.1. Since

$$[A(M_1) \vee A(M_2)]' = A[(M_1 + M_2)']$$

and

$$(M_1 + M_2)' = M_1' \cap M_2',$$

we obtain

$$Z(M) = [A(M) \cap A(M')]'' = [A(M) \vee A(M')]'$$
$$= A[(M + M')'] = A(M \cap M')$$

and the result follows. ■

Theorem 4.2: Let $\mathcal{O} \in \mathcal{T}$ for $m > 0$ or $\mathcal{O} \in \mathcal{T}_0$ for $m = 0$ and further suppose that $\mathcal{O}^c$ is nonempty. Then the vacuum vector Ω is cyclic and separating for $R(\mathcal{O})$.

Proof: Let $f \in M(\mathcal{O}) \cap iM(\mathcal{O})$, where $M(\mathcal{O}) \subset H_1$ is the RLM constructed in (1.26). Let $\phi_+(f;x)$ be the positive frequency solution associated with f as in (2.10a) [replace $\omega(\bar{p})$ by $|\bar{p}|$ for $m = 0$]. By an argument similar to that in Sec. II, we conclude that for any $g \in \mathcal{S}(\mathcal{O}^c)$:

$$\int_{(\infty)} d^4(x)\phi(if;x)g(x) = 0 = \int_{(\infty)} d^4(x)\phi(f;x)g(x) , \tag{4.1}$$

and consequently, $\phi_+(f;x) = 0$ for $x \in \mathcal{O}^c$ as a distribution. Now $\phi_+(f;x)$ is the boundary value of a function analytic on $T_{-i} \equiv \{x - iy | x \in \mathbb{R}^4,\ y \in V_+\}$ so by the edge-of-the-wedge theorem,[16] $\phi_+(f;x) = 0$ everywhere which implies $f = 0$. A similar argument applies for

$$M(\mathcal{O})' \cap iM(\mathcal{O})' = M(\mathcal{O}^c) \cap iM(\mathcal{O}^c)$$

(by duality) so by Theorem 4.1 part (i) the result follows. ■

Theorem 4.3: Let $\mathcal{O} \in \mathcal{T}$ for $m > 0$ or $\mathcal{O} \in \mathcal{T}_0$ for $m = 0$. Then $\mathcal{O} = \hat{O}$ and assume that the Lebesgue measure of $\partial O = \overline{O} \setminus O$ is zero. Then $R(\mathcal{O})$ is a factor.

Proof: (a) Let $f \in M(\mathcal{O}) \cap M(\mathcal{O})' = M(\mathcal{O}) \cap M(\mathcal{O}^c)$ by duality. It follows by arguments similar to those leading to (2.11) and (2.12) that (regardless of the mass)

$$\int_{(\infty)} d^4(x)\phi(if;x)h(x) = 0, \quad \forall h \in \mathcal{S}(\mathcal{O}) \cup \mathcal{S}(\mathcal{O}^c) , \tag{4.2}$$

and hence the distribution $\phi(if;x)$ is supported in $\partial\mathcal{O}$. The IVD for $\phi(if;x)$, denoted by $\phi_o(if;\bar{x}) \equiv h_1(\bar{x})$ and $\pi_o(if;\bar{x}) \equiv h_2(\bar{x})$, is supported on ∂O, where $\mathcal{O} = \hat{O}$, and has the form

$$\hat{h}_1(\bar{p}) = i\omega(\bar{p})^{-1/2}[f(\bar{p}) - (Cf)(\bar{p})] , \tag{4.3a}$$

$$\hat{h}_2(\bar{p}) = \omega(\bar{p})^{1/2}[f(\bar{p}) + (Cf)(\bar{p})] , \tag{4.3b}$$

where here and below $p \equiv |\bar{p}|$ replaces $\omega(\bar{p})$ for $m = 0$. It follows that $h_1 \in H_+$ and $h_2 \in H_-$ and that h_1 and h_2 are real tempered distributions supported in ∂O.

(b) Let $\mathcal{D} \equiv \mathcal{S}(O) + \mathcal{S}[\mathrm{Int}(\sim O)] \subset L^2(\mathbb{R}^3)$. We denote by $\hat{\mathcal{D}}$ the subspace of Fourier transformed functions in H_1. Since the Lebesgue measure of $\partial O \equiv \overline{O} \setminus O$ is zero, standard arguments show that $\mathcal{D}$ is dense in $L^2(\mathbb{R}^3)$ (and hence $\hat{\mathcal{D}}$ is dense in H_1). Let $g \in \mathcal{D}$ so that by considering h_i, $i = 1,2$, as real tempered distributions supported in ∂O:

$$0 = h_i[g] = \int_{(\infty)} d\bar{p}\ \hat{h}_i(\bar{p})^* \hat{g}(\bar{p})$$
$$= \int_{(\infty)} d\bar{p}\ \omega(\bar{p})^{\pm 1/2} \hat{h}_i(\bar{p})^* [\omega(\bar{p})^{\mp 1/2} \hat{g}(\bar{p})] , \tag{4.4}$$

where we choose the upper signs for $i = 1$ and the lower for $i = 2$. We show $\omega^{\pm 1/2}\hat{h}_i = 0$, so $f = 0$ and the result then follows from part (ii) of Theorem 4.1

(c) The operators (multiplication by) $\omega^{\pm 1/2}$ are self-adjoint on their natural domain in H_1 and $\hat{\mathcal{D}}$ is a core for these operators. We show that $\mathrm{Ran}(\omega^{\pm 1/2} \restriction \hat{\mathcal{D}})$ is dense in H_1 so that from (4.4) we conclude $\omega^{\pm 1/2}\hat{h}_i = 0$. If $\ell \in \mathrm{Ran}(\omega^{\pm 1/2} \restriction \hat{\mathcal{D}})^\perp$, then $\ell \in \ker[(\omega^{\pm 1/2} \restriction \hat{\mathcal{D}})^*]$. Since $(\omega^{\pm 1/2} \restriction \hat{\mathcal{D}})^* = \omega^{\pm 1/2}$ on its natural domain, $\|\omega^{\pm 1/2}\ell\| = 0$ so $\ell = 0$. ■

Corollary 4.4: If $\mathcal{O} = \mathbb{R}^4$, then $R(\mathbb{R}^4) = B(H_F)$.

Remark 4.5: Theorem 4.2 also follows from an application of the Reeh–Schlieder theorem[16] to the models studied here since the local algebras are generated by the free fields.

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Yang–Mills cohomology in four dimensions

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The local polynomial cohomology space of the Yang–Mills BRS operator in four dimensions is computed. In order to simplify the analysis, without omitting the physically interesting cases, the investigation is limited to polynomials whose Fadeev–Popov charge and UV naive dimensions have upper bounds. Furthermore the results are used to compute, *á la* Stora, the local functional Yang–Mills anomalies, from which the uniqueness of the Adler–Bardeen–Jackiw anomaly follows.

I. INTRODUCTION

The Yang–Mills (YM) model[1] has been proposed at the very origin of relativistic quantum field theory (QFT) as a contact point of quantum mechanics and geometry, in order to try a unification of nuclear forces.

This initial idea proved quite fruitful in the unification program of weak and electromagnetic forces, and it encourages hopes of getting, in the near future, a scenario in which all the physical interactions will be described by a single theory.

However, in the last decade the necessity has emerged of adopting the language of differential geometry within the QFT framework. One of the most important steps in this direction was the Becchi–Rouet–Stora (BRS)[2] treatment of gauge theories, which outlined the cohomological aspects of the renormalization program and emphasized the need for a systematic approach to the computation of the cohomology spaces of the BRS differential operators.

Much work has been done in this direction,[3] but no general treatment has, up to now, appeared in the literature.

In this paper we investigate the cohomology space of the YM semisimple models following the method of the spectral sequences, first introduced in QFT by Dixon,[4] and later refined by Bandelloni.[5]

We shall obtain explicitly the cohomology space of the BRS operator in the class of local polynomials, already first found by Joglekar and Lee.[3]

Furthermore we treat the problem of the BRS cohomology in the class of local integrated polynomials (local functional space) and the uniqueness of the Adler–Bardeen–Jackiw gauge anomaly is recovered.

In Sec. II we shall focus the problem and recall some notation.

In Sec. III we shall solve the BRS local polynomials cohomology.

In Sec. IV we use the results of the previous section to solve the local functional cohomology.

Appendix A is devoted to a fast guide to spectral sequences techniques.

Appendices B, C, and D contain technical aspects of results given in Sec. III.

II. THE PROBLEM AND SOME NOTATION

Let us consider a semisimple pure Yang–Mills model in a four-dimensional space based on a connection $A^a_\mu(x)$ with UV dimensions equal to 1 and a dimensionless Fadeev–Popov ($\Phi\Pi$) ghost anticommuting field $C^a(x)$ obeying the BRS infinitesimal transformation laws

$$\delta A^a_\mu(x) = [\partial_\mu C^a(x) + f^{abc} A^b_\mu(x) C^c(x)] = [D^{ab}_\mu C^b(x)], \tag{2.1}$$

$$\delta C^a(x) = -[\tfrac{1}{2} f^{abc} C^b(x) C^c(x)], \tag{2.2}$$

with

$$f^{abc} f^{cdg} C^b(x) C^d(x) C^g(x) = 0, \tag{2.3a}$$

$$f^{abc} f^{abd} = C(2)/2\delta^{cd}, \tag{2.3b}$$

and the field $C^a(x)$ carries a $\Phi\Pi$ charge equal to 1, while the connection $A^a_\mu(x)$ is $\Phi\Pi$ neutral.

The above transformation laws lead to the nilpotent differential operator

$$\delta = \int d^4x \left[D^{ab}_\mu C^b(x) \frac{\delta}{\delta A^a_\mu(x)} - \frac{1}{2} f^{abc} C^b(x) C^c(x) \frac{\delta}{\delta C^a(x)} \right], \tag{2.4}$$

which, at the classical level, defines the symmetric polynomial action functional Γ^{cl} satisfying the Slavnov identity $\delta\Gamma^{cl} = 0$. The renormalization program consists of finding, at an arbitrary order of the loop perturbative expansion, an action functional that maintains the gauge symmetry.

If one tries to implement this program with counterterms derived through a subtraction procedure, one realizes that the Slavnov identity is modified into $\delta\Gamma = \Delta^1$ and anomalies $\Delta^1 = \int \Delta^1_4(x)$ appear [such that $\delta\Delta^1 = 0$ and $\Delta^1_4(x)$ is a local polynomial with $\Phi\Pi$ charge equal to 1] and the consistency condition $\delta\Delta^1_4(x) + d\Delta^2_3(x) = 0$ holds.

As pointed out by Stora,[6] if we label with p the value of the $\Phi\Pi$ charge, we can, in general, characterize the charged p cohomology sector by the system

$$\delta\Delta^p_4(x) + d\Delta^{p+1}_3(x) = 0, \tag{2.5a}$$

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$$\delta\Delta_3^{p+1}(x) + d\Delta_2^{p+2}(x) = 0\,, \tag{2.5b}$$

$$\delta\Delta_2^{p+2}(x) + d\Delta_1^{p+3}(x) = 0\,, \tag{2.5c}$$

$$\delta\Delta_1^{p+3}(x) + d\Delta_0^{p+4}(x) = 0\,, \tag{2.5d}$$

$$\delta\Delta_0^{p+4}(x) = 0\,. \tag{2.5e}$$

In particular the case $p = 0$ corresponds to the class of the Lagrangian densities, and if $p = 1$ we find the anomalies sector.

Moreover the validity of the quantum action principle limits the dimensionality of the anomalies, and the sectors with a physical relevance are those with $p = 0,1$.

For this reason we are interested here in the cohomology classes satisfying the conditions

$$(\dim + Q_{\Phi\Pi})\Delta_r^p(x) \leqslant 5\Delta_r^p(x)\,, \tag{2.6a}$$

$$\dim \Delta_r^p(x) \leqslant 4\Delta_r^p(x)\,, \tag{2.6b}$$

where dim is the naive dimension counting operator, and $Q_{\Phi\Pi}$ is the $\Phi\Pi$ charge operator defined by

$$\dim \Delta_r^p(x) = r\Delta_r^p(x)\,, \tag{2.7a}$$

$$Q_{\Phi\Pi}\ \Delta_r^p(x) = p\Delta_r^p(x)\,. \tag{2.7b}$$

We shall follow the general strategy of solving first the equation $\delta\Delta_r^p(x) = 0$ for generic p and r.

Notice that a more rigorous treatment requires the introduction of classical external fields (with negative $\Phi\Pi$ charge) coupled to $\delta A_\mu^a(x)$ and $\delta C^a(x)$.

For the sake of computational simplicity here we shall avoid this step; however, it can be proven that for $p = 0,1$ these fields do not contribute to the cohomology spaces.

III. SOLUTION OF THE BRS LOCAL POLYNOMIALS COHOMOLOGY

In this section we solve the equation

$$\delta\Delta_r^p(x) = \sum_n \Big[[D_{\alpha(n)}(\partial_\mu C^a(x) + f^{abc}A_\mu^b(x)C^c(x))] \times \frac{\partial}{\partial D_{\alpha(n)}A_\mu^a(x)} - \frac{1}{2}\Big[D_{\alpha(n)}(f^{abc}C^b(x)C^c(x)) \times \frac{\partial}{\partial D_{\alpha(n)}C^a(x)}\Big]\Big]\Delta_r^p(x) = 0\,, \tag{3.1}$$

where $\Delta_r^p(x)$ is a local polynomial obeying the constraints [Eqs. (2.6)], and

$$D_{\alpha(n)}A_\mu^a(x) = \partial_{\alpha(1)}\partial_{\alpha(2)}\cdots\partial_{\alpha(n)}A_\mu^a(x)\,.$$

It is well known that the most general solution has the form

$$\Delta_r^p(x) = \overline{\Delta}_r^p(x) + \delta\hat{\Delta}_r^{p-1}(x)\,, \tag{3.2}$$

with $\hat{\Delta}_r^{p-1}(x)$ arbitrary and $\overline{\Delta}_r^p(x)$ is the general element of the cohomology space $H(\delta)$ for the operator δ.

We compute the space $H(\delta)$ using the spectral sequences method, introduced by Dixon,[4] to which Appendix A is devoted.

This method allows us to calculate $H(\delta)$ by successive approximations, defined (up to isomorphisms) by a sequence of spaces $H(d(s))$ $(s = 0,1,2,\ldots)$, where the operators $d(s)$ are induced by the filtration $\delta(s)$ of the operator δ obtained by means of a self-adjoint operator ν as

$$[\nu,\delta] = \sum_{s=0} s\delta(s)\,. \tag{3.3}$$

However, the construction of the operators $d(s)$ is not straightforward and the isomorphisms are not obvious; the first difficulty is overcome by showing that the system

$$\delta(s)\,\overline{\Delta}_r^p(x) = 0\,, \tag{3.4a}$$

$$\delta^+(s)\overline{\Delta}_r^p(x) = 0\,, \qquad s = 0,1,2,3,\ldots\,, \tag{3.4b}$$

will also identify the space $H(\delta)$, up to isomorphisms, as shown in Ref. 5, where it is also found, by studying the local polynomials diffeomorphism cohomology, that a filtration induced by the counting operator of the ghost fields and their space-time derivatives reduces the isomorphism to the identity.

This result, which was interpreted there as an accident (for the isomorphism in general depends "*a priori*" on the differential null square operator, too), is proved to hold in the present case, too. This occurrence brings into doubt that this is not an accident, but a general property due to the particular filtration. Anyhow, we are not able to give any argument in support of this conclusion.

We shall use here the same derivative notation as in Ref. 5 (instead of the one employed by Dixon); so we shall define an adjoint operator by the procedure that replaces monomials in the fields and their space-time derivatives with the partial derivatives with respect the same quantities and vice-versa. As counting operator we shall use

$$\nu = \sum_{n=0}(1+n)D_{\alpha(n)}C^a(x)\frac{\partial}{\partial D_{\alpha(n)}C^a(x)}\,, \tag{3.5}$$

and the filtration of the operator δ gives the results

$$\delta(1) = \sum_{n=0} f^{abc}\Big[C^c(x)D_{\alpha(n)}A_\mu^b(x)\frac{\partial}{\partial D_{\alpha(n)}A_\mu^b(x)} - \frac{1}{2}[D_{\alpha(n)}(C^b(x)C^c(x))]\frac{\partial}{\partial D_{\alpha(n)}C^a(x)}\Big]\,, \tag{3.6a}$$

$$\delta(2) = \partial_\mu C^a(x)\Big[\frac{\partial}{\partial A_\mu^a(x)} + \sum_{n=0} nf^{cba}D_{\alpha(n-1)}A_\nu^b(x)\frac{\partial}{\partial\partial_\mu D_{\alpha(n-1)}A_\nu^c(x)}\Big]\,, \tag{3.6b}$$

$$\delta(s) = D_{\alpha(s-1)}C^c(x)\sum_{n>s-1}\binom{n}{s-1}f^{abc}D_{\alpha(n-s+1)}A_\nu^b(x)\frac{\partial}{\partial D_{\alpha(n)}A_\nu^a(x)} + D_{\alpha(s-2)}\partial_\mu C^a(x)\frac{\partial}{\partial D_{\alpha(s-2)}A_\mu^a(x)} \quad (s = 3,4,\ldots)\,, \tag{3.6c}$$

and their adjoints

$$\delta^+(1)=\sum_{n=0}\left[f^{abc}\left[D_{\alpha(n)}A^a_\mu(x)\frac{\partial}{\partial D_{\alpha(n)}A^b_\mu(x)}\frac{\partial}{\partial C^c(x)}-\frac{1}{2}D_{\alpha(n)}C^a(x)\frac{\partial}{\partial D_{\alpha(n)}(C^c(x)C^b(x))}\right]\right], \tag{3.6d}$$

$$\delta^+(2)=\left[A^a_\mu(x)+\sum_{n=0}nf^{abc}\partial_\mu D_{\alpha(n-1)}A^c_\nu(x)\frac{\partial}{\partial D_{\alpha(n-1)}A^b_\nu(x)}\right]\frac{\partial}{\partial\partial_\mu C^a(x)}, \tag{3.6e}$$

$$\delta^+(s)=\sum_{n=0}\left[\binom{n}{s-1}f^{abc}D_{\alpha(n)}A^a_\nu(x)\frac{\partial}{\partial D_{\alpha(n-s+1)}A^b_\nu(x)}\right]\frac{\partial}{\partial D_{\alpha(s-1)}C^c(x)}$$
$$+D_{\alpha(s-2)}A^a_\mu(x)\frac{\partial}{\partial D_{\alpha(s-2)}\partial_\mu C^a(x)}\quad(s=3,4,\ldots)\,. \tag{3.6f}$$

Now we have to find the functions $\bar{\Delta}^\rho_\tau(x)$, which are solutions of the systems

$$\delta(1)\,+\bar{\Delta}^\rho_\tau(x)=0\,, \tag{3.7a1}$$
$$\delta^\dagger(1)\,\bar{\Delta}^\rho_\tau(x)=0\,, \tag{3.7a2}$$
$$\delta(2)\,\bar{\Delta}^\rho_\tau(x)=0\,, \tag{3.7b1}$$
$$\delta^\dagger(2)\,\bar{\Delta}^\rho_\tau(x)=0\,, \tag{3.7b2}$$
$$\delta(s)\,\bar{\Delta}^\rho_\tau(x)=0\,, \tag{3.7c1}$$
$$\delta^\dagger(s)\,\bar{\Delta}^\rho_\tau(x)=0,\quad s>2\,. \tag{3.7c2}$$

With a short algebra it is easy to see that $\delta^2(1)=0$ so the system in Eq. (3.7) identifies the cohomology $H(\delta(1))$ of the operator $\delta(1)$, since the whole space F admits the Hodge decomposition

$$F=\mathrm{Im}\,\delta(1)+\mathrm{Im}\,\delta^\dagger(1)+H(\delta(1)) \tag{3.8}$$

and the spectral sequences method is at our disposal to find the functions that belong to $H(\delta(1))$. The detailed analysis is carried out in Appendix B and the result is that the functions $\bar{\Delta}^\rho_\tau(x)$ satisfy

$$\frac{\partial}{\partial D_{\alpha(n)}C^a(x)}\bar{\Delta}^\rho_\tau(x)=0\,, \tag{3.9}$$
$$\text{for } n>1,\quad \text{if } \bar{\Delta}^\rho_\tau(x)\in H(\delta(1))\,,$$

i.e., they do not depend on the ghost field space-time derivatives of order greater than 2; and the following conditions hold:

$$g^c(1)\,\bar{\Delta}^\rho_\tau(x)=0\,, \tag{3.10a}$$
$$h^c(1)\,\bar{\Delta}^\rho_\tau(x)=0\,, \tag{3.10b}$$

where

$$g^c(1)=\sum_{n=0}f^{abc}\left[D_{\alpha(n)}A^b_\mu(x)\frac{\partial}{\partial D_{\alpha(n)}A^a_\mu(x)}+\partial_\rho C^b(x)\frac{\partial}{\partial\partial_\rho C^a(x)}\right], \tag{3.11a}$$

$$h^c(1)=f^{abc}C^b(x)\frac{\partial}{\partial C^a(x)}, \tag{3.11b}$$

which imply that the functions $\bar{\Delta}^\rho_\tau(x)$ have the form

$$\bar{\Delta}^\rho_\tau(x)=I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x);\partial_\rho C^c(x))T(C^d(x))\,, \tag{3.12}$$

with $I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x);\partial_\rho C^c(x))$ and $T(C^d(x))$ invariant under $g^c(1)$ and $h^c(1)$, respectively.

The power counting conditions in Eqs. (2.7) suggest the decomposition

$$I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x);\partial_\rho C^c(x))$$
$$=I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x)),+\partial_\rho C^a(x)I^\rho_a(A^c_\mu(x),$$
$$D_{\alpha(n)}A^b_\nu(x))+\partial_\rho C^a(x)\partial_\sigma C^b(x)$$
$$\times I^{\rho\sigma}_{ab}(A^c_\mu(x),D_{\alpha(n)}A^b_\nu(x))\,, \tag{3.13}$$

with

$$\dim I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x))\leqslant 5I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x))\,, \tag{3.14a}$$

$$\dim I^\rho_a(A^c_\mu(x),D_{\alpha(n)}A^b_\nu(x))\leqslant 3I^\rho_a(A^c_\mu(x),D_{\alpha(n)}A^b_\nu(x)), \tag{3.14b}$$

$$\dim I^{\rho\sigma}_{ab}(A^c_\mu(x),D_{\alpha(n)}A^d_\nu(x))\leqslant I^{\rho\sigma}_{ab}(A^c_\mu(x),D_{\alpha(n)}A^d_\nu(x))\,. \tag{3.14c}$$

A very elementary argument that we shall use repeatedly eliminates the dependence of $I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x);\partial_\rho C^c(x))$ from the function $I^{\rho\sigma}_{ab}(A^c_\mu(x),D_{\alpha(n)}A^d(x))$. Indeed the condition (3.14c) implies the form

$$\partial_\rho C^a(x)\partial_\sigma C^b(x)\,I^{\rho\sigma}_{ab}(A^c_\mu(x),D_{\alpha(n)}A^d_\nu(x))$$
$$=[O^{\rho\sigma\mu}_{abc}A^c_\mu(x)+O^{\rho\sigma}_{ab}]\partial_\rho C^a(x)\partial_\sigma C^b(x)\,. \tag{3.15}$$

Now, the above expression must be a Lorentz scalar and a global gauge invariant, so we get $O^{\rho\sigma}_{ab}=\delta_{ab}\delta^{\rho\sigma}$, and the impossibility of building a Lorentz-invariant tensor with an odd number of indices in four dimensions implies $O^{\rho\sigma\mu}_{abc}=0$.

Furthermore a detailed analysis of the equation $\delta^\dagger(2)\bar{\Delta}^\rho_\tau(x)=0$, carried out in Appendix C, eliminates the term $\partial_\rho C^a(x)I^\rho_a(A^c_\mu(x),D_{\alpha(n)}A^d_\nu(x))$.

Now the polynomial $I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x))$ (which has UV naive dimensions $\leqslant 4$) has the general expression

$$I(A^a_\mu(x),D_{\alpha(n)}A^b_\nu(x))$$
$$=L^{abcd}_{\mu\nu\rho\sigma}A^a_\mu(x)A^b_\nu(x)A^c_\rho(x)A^d_\sigma(x)$$
$$+M^{abc}_{\mu\nu\rho\sigma}A^a_\mu(x)A^b_\nu(x)\partial_\rho A^c_\sigma(x)$$
$$+R^{ab}_{\mu\nu\rho\sigma}\partial_\mu\partial_\nu A^a_\rho(x)A^b_\sigma(x)+T^a_{\mu\nu\rho\sigma}\partial_\mu\partial_\nu\partial_\rho A^a_\sigma(x)$$
$$+N^{ab}_{\mu\nu\rho\sigma}\partial_\mu A^a_\nu(x)\partial_\rho A^b_\sigma(x)+S^a_{\mu\nu}\partial_\mu A^a_\nu(x)$$
$$+R^{ab}_{\mu\nu}A^a_\mu(x)A^b_\nu(x)+K\,, \tag{3.16}$$

where K is a constant and $L^{abcd}_{\mu\nu\rho\sigma}, M^{abc}_{\mu\nu\rho\sigma}, N^{ab}_{\mu\nu\rho\sigma}, S^a_{\mu\nu}, R^{ab}_{\mu\nu\rho\sigma}$,

$R^{ab}_{\mu\nu}$, and $T^{a}_{\mu\nu\rho\sigma}$ are tensors invariant under Lorentz and global gauge transformations separately, and the terms involving tensors with odd numbers of Lorentz indices are not included since they obviously vanish.

The global gauge invariance now enforces $T^{a}_{\mu\nu\rho\sigma}=0$ and $S^{a}_{\mu\nu}=0$ (since they have only one index in the gauge group) and

$$R^{ab}_{\mu\nu}=r\delta_{\mu\nu}\delta^{ab}, \tag{3.17a}$$

$$N^{ab}_{\mu\nu\rho\sigma}=\delta^{ab}(m_{\mu\nu\rho\sigma})$$
$$=\delta^{ab}(a\delta_{\mu\nu}\delta_{\rho\sigma}+b\delta_{\mu\rho}\delta_{\nu\sigma}+c\delta_{\mu\sigma}\delta_{\nu\rho}+d\epsilon_{\mu\nu\rho\sigma}). \tag{3.17b}$$

Now the equation $\delta(2)\,\overline{\Delta}^{p}_{r}(x)=0$ implies the conditions $R^{ab}_{\mu\nu\rho\sigma}=0$, since this tensor appears in the coefficient of the sole term containing a second-order derivative in the gauge field, and

$$4L^{abcd}_{\mu\nu\rho\sigma}+f^{arb}M^{rcd}_{\mu\nu\rho\sigma}=0, \tag{3.18a}$$

$$M^{abc}_{\mu\nu\rho\sigma}+f^{brc}N^{ra}_{\rho\sigma\mu\nu}=0, \tag{3.18b}$$

$$R^{ab}_{\mu\nu}+R^{ba}_{\nu\mu}=0, \tag{3.18c}$$

from which we derive

$$r=0, \tag{3.19a}$$

$$M^{abc}_{\mu\nu\rho\sigma}=f^{abc}m_{\mu\nu\rho\sigma}, \tag{3.19b}$$

$$L^{abcd}_{\mu\nu\rho\sigma}=\tfrac{1}{4}f^{abr}f^{rcd}m_{\mu\nu\rho\sigma}. \tag{3.19c}$$

From the symmetry condition

$$M^{abc}_{\mu\nu\rho\sigma}=M^{bac}_{\nu\mu\rho\sigma}, \tag{3.20}$$

we get

$$a=0, \tag{3.21a}$$

$$b=-c, \tag{3.21b}$$

so finally we have

$$I(A^{a}_{\mu}(x),\partial_{\nu}A^{b}_{\rho}(x))$$
$$=bG^{a}_{\mu\nu}(x)G^{a}_{\mu\nu}(x)+d\epsilon_{\mu\nu\rho\sigma}G^{a}_{\mu\nu}(x)G^{a}_{\rho\sigma}(x)+K, \tag{3.22}$$

where

$$G^{a}_{\mu\nu}(x)=\partial_{\mu}A^{a}_{\nu}(x)-\partial_{\nu}A^{a}_{\mu}(x)+f^{abc}A^{b}_{\nu}(x)A^{c}_{\mu}(x). \tag{3.23}$$

Hence we find that the polynomial $\overline{\Delta}^{p}_{r}(x)$ has the well-known form

$$\overline{\Delta}^{p}_{r}(x)=(K+aG^{a}_{\mu\nu}(x)G^{a}_{\mu\nu}(x)$$
$$+d\epsilon_{\mu\nu\rho\sigma}G^{a}_{\mu\nu}(x)G^{a}_{\rho\sigma}(x))T(C^{d}(x)), \tag{3.24}$$

which coincides with the solution already found by Joglekar and Lee[3] in 1975. It is straightforward to show that the above polynomial also verifies the equations $\delta^{+}(s)\overline{\Delta}^{p}_{r}(x)=0$ $(s=3,4,5,\ldots)$.

Furthermore the expression (3.24) satisfies the condition $\delta(3)\overline{\Delta}^{p}_{r}(x)=0$ due to the antisymmetry properties of the $G^{a}_{\mu\nu}(x)$ field and the equations $\delta(s)\overline{\Delta}^{p}_{r}(x)=0$ $(s>3)$ by direct computation.

Notice that the problem has been fully solved by considering the actions of the operators associated only with the first and the second filtration, as pointed out by Dixon.[4]

IV. SOLUTION OF THE LOCAL FUNCTIONAL COHOMOLOGY

In this section we shall solve the system [Eqs. (2.5)] for $p=1$ starting from the cocycle condition [Eq. (2.5e)] and then going backward to Eq. (2.5a).

Taking into account the result of the preceding section, Eq. (2.5e) has the general solution

$$\Delta^{5}_{0}(x)=4p\,\mathrm{Tr}[(\lambda^{a}\lambda^{b}\lambda^{c}\lambda^{d}\lambda^{g})C^{a}(x)C^{b}(x)C^{c}(x)C^{d}(x)C^{g}(x)]+\delta\hat{\Delta}^{4}_{0}(x), \tag{4.1}$$

where λ^{a} is in the adjoint representation of the global group, such that

$$\lambda^{a}\lambda^{b}=q\delta^{ab}+f^{abc}\lambda^{c}+d^{abc}\lambda^{c}. \tag{4.2}$$

Now

$$\mathrm{Tr}(\lambda^{a}\lambda^{b}\lambda^{c}\lambda^{d}\lambda^{g})=2q(f^{abc}+d^{abc})\delta^{dg}+f^{ars}f^{rbc}f^{sdg}+f^{ars}d^{rbc}f^{sdg}+d^{ars}f^{rbc}f^{sdg}+f^{ars}f^{rbc}d^{sdg}$$
$$+f^{ars}d^{rbc}d^{sdg}+d^{ars}d^{rbc}f^{sdg}+d^{ars}d^{rbc}d^{sdg}, \tag{4.3}$$

so that, taking into account the anticommutativity of the ghost fields, we get

$$\Delta^{5}_{0}(x)=pd^{abc}C^{a}(x)\delta C^{b}(x)\delta C^{c}(x)+\delta\hat{\Delta}^{4}_{0}(x). \tag{4.4}$$

It is now a matter of a lengthy algebraic computation, already pointed out in Refs. 7, to go backward to Eq. (2.5a).

The result of the previous section says that the gauge cohomology admits nonzero elements only for polynomials of naive dimensions 0 or 4.

Using the Jacobi identity, it is easy to show that

$$d\Delta^{5}_{0}(x)=\partial_{\mu}\Delta^{5}_{0}(x)\,dx^{\mu}=pd^{abc}[dC^{a}(x)\delta C^{b}(x)\delta C^{c}(x)+2C^{a}(x)\delta dC^{b}(x)\delta C^{c}(x)]+d\delta\hat{\Delta}^{4}_{0}(x)$$
$$=pd^{abc}\delta[-C^{a}(x)\partial_{\mu}C^{b}(x)\delta C^{c}(x)dx^{\mu}+2\delta(A^{a}_{\mu}(x)C^{b}(x)\delta C^{c}(x))dx^{\mu}]+d\delta\hat{\Delta}^{4}_{0}(x), \tag{4.5}$$

so

$$\Delta^{4}_{1}(x)=pd^{abc}C^{a}(x)\partial_{\mu}C^{b}(x)\delta C^{c}(x)\,dx^{\mu}+d\hat{\Delta}^{4}_{0}(x)+\delta\hat{\Delta}^{3}_{1}(x). \tag{4.6}$$

The next step is performed along the same lines: indeed

$$d\Delta_1^4(x) = 2pd^{abc}(\partial_\nu C^a(x)\partial_\mu C^b(x)\delta C^c(x))\,dx^\mu \wedge dx^\nu + d\delta\,\hat{\Delta}_1^3(x)$$
$$= -2pd^{abc}\delta[C^a(x)\partial_\nu C^b(x)\partial_\mu C^c(x)]\,dx^\mu \wedge dx^\nu + d\delta\hat{\Delta}_1^3(x)\,, \tag{4.7}$$

so that

$$\Delta_2^3(x) = 2pd^{abc}(C^a(x)\partial_\nu C^b(x)\partial_\mu C^c(x))\,dx^\mu \wedge dx^\nu + d\,\hat{\Delta}_1^3(x) + \delta\hat{\Delta}_2^2(x)\,. \tag{4.8}$$

Furthermore

$$d\Delta_2^3(x) = 2pd^{abc}(\partial_\rho C^a(x)\partial_\nu C^b(x)\partial_\mu C^c(x))dx^\mu \wedge dx^\nu \wedge dx^\rho + d\delta\hat{\Delta}_2^2(x)$$
$$= 2pd^{abc}\delta(A_\rho^a(x)\partial_\nu C^b(x)\partial_\mu C^c(x))dx^\mu \wedge dx^\nu \wedge dx^\rho + d\delta\hat{\Delta}_2^2(x)\,,$$

using again the Jacobi identity, so

$$\Delta_3^2(x) = -2pd^{abc}(A_\rho^a(x)\partial_\nu C^b(x)\partial_\mu C^c(x))dx^\mu \wedge dx^\nu \wedge dx^\rho + d\hat{\Delta}_2^2(x) + \delta\hat{\Delta}_3^1(x)\,. \tag{4.9}$$

The last step is quite tedious, but every person who has some experience in gauge theory has done it (even if in the opposite direction), since

$$d\Delta_3^2(x) = 2pd^{abc}\partial_\sigma A_\rho^a(x)\partial_\nu C^b(x)\partial_\mu C^c(x)dx^\mu \wedge dx_\nu^2 \wedge dx^\rho \wedge dx^\sigma + d\delta\hat{\Delta}_1^3(x)$$
$$= -2p\delta[d^{abc}\partial_\sigma A_\rho^a(x)\,A_\nu^b(x)] + \tfrac{1}{12}(d^{bcd}f^{dlm} + d^{cld}f^{dmb} + d^{cmd}f^{dbl})\,A_\sigma^b(x)\,A_\rho^l(x)\,A_j^m(x)]$$
$$\times\partial_\mu C^c(x)dx^\mu \wedge dx^\nu \wedge dx^\rho \wedge dx^\sigma + d\delta\hat{\Delta}_3^1(x)\,,$$

so that

$$\Delta_4^1(x) = 2p[d^{abc}\partial_\sigma A_\rho^a(x)\,A_\nu^b(x) + \tfrac{1}{12}(d^{bcd}f^{dlm} + d^{cld}f^{dmb} + d^{cmd}f^{dbl})\,A_\sigma^b(x)\,A_\rho^l(x)\,A_\nu^m(x)]$$
$$\times\partial_\mu C^c(x)dx^\mu \wedge dx^\nu \wedge dx^\rho \wedge dx^\sigma + d\hat{\Delta}_3^1(x) + \delta\hat{\Delta}_4^0(x)\,,$$

and the uniqueness of the ABJ anomaly is recovered.

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APPENDIX A: THE SPECTRAL SEQUENCES METHOD

In this Appendix we present a short mathematical guide to the spectral sequences method. Let F be the whole vector space, in which an inner product is defined: $(x,y)\in R$ for all $x,y\in F$. Suppose that on F two linear operators δ and ν act such that

$$\delta^2 = 0\,,\quad \nu = \nu^\dagger\,, \tag{A1}$$

and the eigenvalues of the Hermitian operator are the integers.

Let $G(p)$ be the eigenspace belonging to the eigenvalue p of ν, that is, $x(p) = px(p)$ if $x(p)\in G(p)$.

Consequently,

$$F = \sum_{p=0} G(p) \tag{A2}$$

and if $x(p)\in G(p)$, then $(x(p),x(q)) = 0$ for $p\neq q$.

Define the Hilbert spaces

$$F(p) = \sum_{q>p} G(q)\,,\quad F(p) > F(p+1)\,, \tag{A3}$$

$$E(p,r) = [F(p)\cap\delta^{-1}F(p+r)]\,[\delta F(p-r+1)\cap F(p) + \delta^{-1}F(p+r)\cap F(p+1)]^{-1}\,, \tag{A4}$$

where $x\in\delta^{-1}F(p+r)$ if $\delta x\in F(p+r)$, and the nested ones

$$E(r) = \left\{\cup_p E(p,r)\,;\ -\infty < p < +\infty\right\}. \tag{A5}$$

The following theorem, due to Leray, holds.

Theorem: Suppose that the space F is decomposed by a finite number of filtrations, that is, an m exists such that $G(p) = 0$ for all $p > m$. Then

(i) $E(p,r) = 0$ unless $0 < p < m$,

(ii) $E(m) = E(m+1) = \cdots = E(\infty)$,

(iii) $E(r+1)\simeq H(E(r),d(r))$ $(0 < r < p)$,

where $\simeq$ denotes isomorphism and $H(E(r),d(r))$ is the cohomology space on $E(r)$ of $d(r)$ that is induced by δ. Also,

(iv) $E(\infty)\simeq \mathrm{Gr}\{H(F,\delta)\}$,

where

$$\mathrm{Gr}\{H(F,\delta)\} = \left[\cup_p H(F(p),\delta),\ -\infty < p < +\infty\right],$$

which means that the space $E(\infty)$ is isomorphic to the cohomology space of the operator δ on F, and is approximated, by successive iterations, by the spaces $E(r)$ [which are the cohomology spaces of the operators $d(r)$ for each r].

Now a suitable procedure for the construction of the operators $d(r)$ is needed, and this, as stressed by Dixon, is nontrivial. To overcome this difficulty we have found, in Ref. 5, a different characterization of the spaces $E(r)$ using a trick introduced in the topological analysis by Zeeman,[8] and we showed the isomorphism

$$E(p,r+1)\simeq\{E(p,r)\cap(\delta^{-1}F(p+r+1))\}\times\{E(p,r)\cap(\delta F(p-r))\}^{-1}\,, \tag{A6}$$

so if the operator δ admits the decomposition

$$\delta = \sum_{p=0} \delta(p) , \tag{A7}$$

where

$$[\nu,\delta(p)] = p\delta(p) , \tag{A8}$$

an algebraic characterization of the spaces $E(p,r+1)$ can be given by the following theorem, proved in Ref. 5.

Theorem: If $x(p)\in E(p,r)$, then the same $x(p)\in E(p,r+1)$ if

$$\delta(r)x(p) = 0 , \tag{A9a}$$

$$\delta^{\dagger}(r)x(p) = 0 . \tag{A9b}$$

So, recalling the definition of $E(r)$, it is easy to show that if $x\in E(r)$, then the same $x\in E(r+1)$ if

$$\delta(r)x = 0 , \tag{A10a}$$

$$\delta^{\dagger}(r)x = 0 , \tag{A10b}$$

for each r.

APPENDIX B

In this Appendix we want to discuss the cohomology space of the operator

$$\delta(1) = \sum_{n=0} \left[f^{abc} C^c(x) D_{\alpha(n)} A^b_\mu(x) \frac{\partial}{\partial D_{\alpha(n)} A^a_\mu(x)} + \frac{1}{2} D_{\alpha(n)} (C^b(x) C^c(x)) \frac{\partial}{\partial D_{\alpha(n)} C^a(x)} \right] \tag{B1}$$

using the spectral sequences method, on the space of functions bounded by the conditions Eq. (3.6a) and (3.6b) $(\dim + Q_{\Phi\Pi})\overline{\Delta}^p_r(x) \leqslant 5$ and $\dim \overline{\Delta}^p_r(x) \leqslant 4$.

Filtering $\delta(1)$ with the counting operator

$$\nu = C^a(x) \frac{\partial}{\partial C^a(x)} ,$$

we get

$$\delta(1) = \frac{1}{2} \sum_{n>r>1} \binom{n}{r} f^{abc} D_{\alpha(n)} C^b(x) D_{\alpha(n-r)} C^c(x) \times \frac{\partial}{\partial D_{\alpha(n)} C^a(x)} , \tag{B2a}$$

$$\delta^1(1) = C^c(x) \sum_n f^{abc} \left[D_{\alpha(n)} A^b_\mu(x) \frac{\partial}{\partial D_{\alpha(n)} A^a_\mu(x)} + \partial_\mu C^b(x) \frac{\partial}{\partial \partial_\mu C^a(x)} \right] - \frac{1}{2} f^{abc} C^b(x) C^c(x) \frac{\partial}{\partial C^a(x)} = C^a(x)[h^a(1) + g^0(1)] . \tag{B2b}$$

So we have to solve

$$\Delta(\delta^0(1))\overline{\Delta}^p_r(x) = \{\delta^{0+}(1),\delta^0(1)\}\overline{\Delta}^p_r(x) = 0 , \tag{B3a}$$

$$\Delta(\delta^1(1))\overline{\Delta}^p_r(x) = \{\delta^{1+}(1),\delta(1)\}\overline{\Delta}^p_r(x) = 0 . \tag{B3b}$$

Equation (B3a), after some calculations, gives

$$\Delta(\delta^0(1))\overline{\Delta}^p_r(x) = \frac{1}{4} \left[\sum_{n>r,s>1} \binom{n}{r}\binom{n}{s} f^{abc} f^{alp} \left[D_{\alpha(r)} C^b(x) D_{\alpha(n-r)} \times C^c(x) \frac{\partial}{\partial D_{\alpha(n-s)} C^p(x) D_{\alpha(s)} C^l(x)} \right] + C(2) D_{\alpha(n)} C^a(x) \frac{\partial}{\partial D_{\alpha(n)} C^a(x)} \right] \overline{\Delta}^p_r(x) = 0 , \tag{B4}$$

which implies

$$\sum_{n\geq 2} \left\langle \frac{\partial}{\partial D_{\alpha(n)} C^a(x)} \overline{\Delta}^p_r(x) \middle| \frac{\partial}{\partial D_{\alpha(n)} C^a(x)} \overline{\Delta}^p_r(x) \right\rangle = 0 , \tag{B5}$$

and taking into account Eq. (2.6a) we can easily derive that the function $\overline{\Delta}^p_r(x)$ does not depend on the derivatives of the field $C^a(x)$ of order greater than 2.

Concerning Eq. (B3b), the calculation is easily carried out taking into account the identities

$$g^{c^+}(1) = -g^c(1) , \tag{B6a}$$

$$h^{c^+}(1) = -h^c(1) , \tag{B6b}$$

and yields

$$\Delta(\delta^1(1))\overline{\Delta}^p_r(x) = [g^{c^+}(1)g^c(1) + 2h^{c^+}(1)g^c(1) + 2h^{c^+}(1)h^c(1)]\overline{\Delta}^p_r(x) = [(g^{c^+}(1) + h^{c^+}(1))(g^c(1) + h^c(1)) + h^{c^+}(1)h^c(1)]\overline{\Delta}^p_r(x) = 0 ,$$

which means

$$[h^c(1) + g^c(1)]\overline{\Delta}^p_r(x) = 0 , \quad h^c(1)\Delta^p_r(x) = 0 ,$$

that is,

$$h^c(1)\overline{\Delta}^p_r(x) = 0 , \quad g^c(1)\overline{\Delta}^p_r(x) = 0 .$$

So $\overline{\Delta}^p_r(x)$ has to be a polynomial with the general form

$$\overline{\Delta}^p_r(x) = I(D_{\alpha(n)} A^a_\mu(x), \partial_\nu C^b_\rho(x)) T(C^c(x)) ,$$

where the functions $I(D_{\alpha(n)} A^a_\mu(x), \partial_\nu C^b_\rho(x))$ and $T(C^c(x))$ are invariant under $g^c(1)$ and $h^c(1)$, respectively.

APPENDIX C: THE EQUATION $\delta^+(2)\overline{\Delta}^p_r(x) = 0$

We want to discuss here Eq. (3.7b2),

$$\delta^+(2)\overline{\Delta}^p_r(x) = \left[A^a_\mu(x) + f^{abc}\partial_\mu A^c_\nu(x) \frac{\partial}{\partial A^b_\nu(x)} + 2f^{abc}\partial_\rho\partial_\mu A^c_\nu(x) \frac{\partial}{\partial \partial_\rho A^b_\nu(x)} \right] \times \frac{\partial}{\partial \partial_\mu C^a(x)} \overline{\Delta}^p_r(x) = 0 , \tag{C1}$$

and to show that no solution that contains first-order derivatives of the $C^a(x)$ fields will exist.

Indeed the general expression for

$$I^\rho_c(A^a_\mu(x), D_{\alpha(n)} A^b_\nu(x))\partial_\rho C^c(x)$$

(bounded by the conditions [Eqs. (2.6)]) is

$$
\begin{aligned}
I^{\rho}_{c}(A^{a}_{\mu}(x), D_{\alpha(n)} A^{b}_{\nu}(x))\partial_{\rho} C^{c}(x) \\
&= L^{abc}_{\mu\nu\rho\sigma}\partial_{\nu} A^{a}_{\mu}(x)\partial_{\rho} C^{b}(x) A^{c}_{\sigma}(x) \\
&\quad + M^{abcd}_{\mu\nu\rho\sigma} A^{a}_{\mu}(x) A^{b}_{\nu}(x) A^{d}_{\sigma}(x)\partial_{\rho} C^{c}(x) \\
&\quad + K^{ab}_{\mu\nu\rho}\partial_{\mu} A^{b}_{\nu}(x)\partial_{\rho} C^{a}(x) \\
&\quad + N^{abc}_{\mu\nu\rho} A^{c}_{\mu}(x) A^{b}_{\nu}(x)\partial_{\rho} C^{c}(x) \\
&\quad + R^{ab}_{\mu\nu} A^{a}_{\mu}(x)\partial_{\nu} C^{b}(x) + S^{a}_{\rho}\partial_{\rho} C^{a}(x) \\
&\quad + M^{ab}_{\mu\nu\rho\sigma}\partial_{\mu}\partial_{\nu} A^{a}_{\sigma}(x)\partial_{\rho} C^{b}(x) , \qquad \text{(C2)}
\end{aligned}
$$

where all the tensors are separately invariant under Lorentz and global gauge groups.

Since no Lorentz-invariant tensor with an odd number of indices exists in four-dimensional space, then

$$
K^{ab}_{\mu\nu\rho} = N^{abc}_{\mu\nu\rho} = V^{abc}_{\mu\nu\rho} = S = 0 . \qquad \text{(C3)}
$$

If we now directly compute Eq. (C1), it is easy to derive that (i) $L^{abc}_{\mu\nu\rho\sigma} = 0$, since it appears in the sole term having the structure

$$
\partial_{\mu}\partial_{\nu} A^{a}_{\rho}(x) A^{d}_{\sigma}(x) f^{dbc} L^{abc}_{\mu\nu\rho\sigma} ;
$$

(ii) $M^{ab}_{\mu\nu\rho\sigma} = 0$, since it appears in the sole term of the form

$$
f^{abc} M^{ab}_{\mu\nu\rho\sigma}\partial_{\mu}\partial_{\nu}\partial_{\rho} A^{c}_{\sigma}(x) ;
$$

and (iii) $M^{abcd}_{\mu\nu\rho\sigma} = 0$, since it gives the only contribution of the kind

$$
M^{abcd}_{\mu\nu\rho\sigma} A^{a}_{\mu}(x) A^{b}_{\nu}(x) A^{c}_{\rho}(x) A^{d}_{\sigma}(x) .
$$

So, at last, it is easy to derive $R^{ab}_{\mu\nu} = 0$.

We have so proved that no term containing derivatives on $C^{a}(x)$ can satisfy Eq. (3.7b).

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Traveling-wave solutions and the coupled Korteweg–de Vries equation

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Some coupled nonlinear equations are considered for studying traveling-wave solutions. By introducing a stream function Ψ it is shown that if one of the solutions is of the form $v \equiv v(x-ct)$, the other also must be of the form $u \equiv u(x-ct)$. In addition, the possibility of including cubic nonlinear terms has been considered and such a system, assuming that the solutions are of the traveling-wave type, has been solved.

I. INTRODUCTION

Some time ago, Ito[1] had proposed the following coupled nonlinear wave equations:

$$u_t = u_{xxx} + 6uu_x + 2vv_x, \tag{1a}$$

$$v_t = 2(uv)_x. \tag{1b}$$

An interesting characteristic of this couple is that it reduces to the familiar Korteweg–de Vries equation when $v = 0$. Moreover the symmetries associated with it generate a hierarchy of coupled equations each of which is a Hamiltonian system with infinitely many constants of motion.

Recently, Kawamoto[2] has shown that of all the particular solutions obtainable from (1), the traveling-wave solutions of the type

$$u \equiv u(x-ct), \quad v \equiv v(x-ct) \tag{2}$$

(c being a constant) are necessarily cusplike in nature. It may be noted that Kawamoto had considered a more general version of (1), namely,

$$u_t + \alpha v v_x + \beta u u_x + \delta u_{xxx} = 0, \tag{3a}$$

$$v_t + \gamma (uv)_x = 0, \tag{3b}$$

where the parameters α, β, δ, and γ were kept arbitrary. The purpose of this work is twofold.

(i) First, we show that if one of the solutions of (3) is of the traveling-wave form, say $v \equiv v(x-ct)$, then the other solution also must exhibit the same form, i.e., u must also be of the form $u \equiv u(x-ct)$.

(ii) Second, even if one introduces cubic nonlinearity in (3) and modifies (3a) to make it assume the form

$$u_t + \alpha (v^3)_x + \beta (u^3)_x + \lambda (u^2)_x + \delta u_{xxx} = 0, \tag{4a}$$

$$v_t + \gamma (uv)_x = 0, \tag{4b}$$

the conclusion in (i) remains unchanged. For completeness, we also have solved (4) postulating that the functions u and v are of the traveling-wave type (2).

II. TRAVELING-WAVE SOLUTIONS

We begin by writing (3a) in the form

$$u_t + ((\beta/2)u^2 + (\alpha/2)v^2 + \delta u_{xx})_x = 0.$$

This enables us to introduce an arbitrary function $\Psi = \Psi(x,t)$ [which may be called the stream function of the system (3)] such that

$$u\,dx - \left(\frac{\beta}{2}u^2 + \frac{\alpha}{2}v^2 + \delta u_{xx}\right)dt = d\Psi = \frac{\partial \Psi}{\partial x}dx + \frac{\partial \Psi}{\partial t}dt.$$

On comparison, one finds

$$\frac{\partial \Psi}{\partial x} = u, \tag{5a}$$

and

$$-\frac{\partial \Psi}{\partial t} = \frac{\beta}{2}u^2 + \frac{\alpha}{2}v^2 + \delta u_{xx}. \tag{5b}$$

Substituting (5a) into (5b), v can be expressed as, let us say,

$$v^2 = -(2/\alpha)(\Psi_t + (\beta/2)\Psi_x^2 + \delta \Psi_{xxx}) \equiv (2/\alpha)\Phi(x,t). \tag{6}$$

One of the advantages of introducing a stream function is that the two coupled equations in (3) may be combined to yield a single relation in Ψ. Solving then for Ψ, one can immediately obtain u and v through the connection (5). Combining (3b), (5a), and (6) we get

$$\Phi_t + \gamma \Psi_x \Phi_x + 2\gamma \Psi_{xx} \Phi = 0, \tag{7}$$

where Φ may be represented in terms of Ψ using the definition in (6).

Let us assume that v is a function of $(x-ct)$ only. Then it may be asserted that

$$c\Phi_x + \Phi_t = 0.$$

Replacing Φ_t by Φ_x, we have from (7)

$$(c - \gamma \Psi_x)\Phi_x = 2\gamma \Psi_{xx} \Phi. \tag{8}$$

On integrating (8), Φ may be obtained in a closed form

$$\Phi = (K^2(t)/(\gamma \Psi_x - c)^2),$$

where $K(t)$ is an arbitrary function of time.

Since Φ is a function of $(x-ct)$ only, we can write without any loss of generality

$$(\gamma \Psi_x - c)^2 = K^2(t) f^2(x-ct),$$

where $f(x-ct)$ is another function of $(x-ct)$. Thus

$$\Psi_x = (1/\gamma)[c + K(t) f(x-ct)]. \tag{9}$$

In order to show that Ψ_x (and hence u) is a function of $(x-ct)$ only, we need to prove that $K(t)$ must necessarily be a constant, i.e., $K(t)$ must be independent of t.

To this end, we substitute (9) in (6) to obtain

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$$\Phi(x-ct) = -\Psi_t - (\delta/\gamma)K(t)f''(x-ct) - (\beta/2\gamma^2)[c+K(t)f(x-ct)]^2,$$

where dashes denote derivatives (partial) with respect to (w.r.t.) x only. Expanding and rearranging the right-hand side (rhs) of the above expression, one can express Ψ_t in the form

$$\Psi_t = -\Phi(x-ct) - K(t)A(x-ct) - K^2(t)B(x-ct) - (\beta c^2/2\gamma^2). \tag{10}$$

It may be noted that Ψ_t can be obtained also from (9), first, by integrating (partially) (9) w.r.t. x and then differentiating (partially) the result w.r.t. t. In this way one arrives at

$$\Psi = \frac{c}{\gamma}x + \frac{K(t)}{\gamma}g(x-ct) + \frac{\lambda(t)}{\gamma},$$

where $\lambda(t)$ is an arbitrary function of time and $g(x-ct)$ stands[3] for the quantity $\int f(x-ct)dx$. Consequently,

$$\Psi_t = \frac{\dot{K}(t)}{\gamma}g(x-ct) - \frac{cK(t)}{\gamma}h(x-ct) + \frac{\dot{\lambda}(t)}{\gamma}, \tag{11}$$

where dots represent derivatives (partial) w.r.t. t and $h(x-ct) = g_t(x-ct)$, assuming that $g_t(x-ct)$ is not a constant.

On comparison of (10) and (11), we have therefore,

$$\Phi(x-ct) = -K(t)A(x-ct) - K^2(t)B(x-ct) - \frac{\dot{K}(t)}{\gamma}g(x-ct) + \frac{cK(t)}{\gamma}h(x-ct) - \frac{\beta c^2}{2\gamma^2} - \frac{\dot{\lambda}(t)}{\gamma}. \tag{12}$$

Since the lhs of (12) is a function of $(x-ct)$ alone while the rhs is a product of functions of time and $(x-ct)$, it follows that $K(t)$ and $\dot{\lambda}(t)$ must reduce to a constant value. Accordingly, Ψ_x (and therefore u) must be a function of $(x-ct)$ only.

III. INCLUSION OF CUBIC NONLINEAR TERMS

We now turn to Eqs. (4a) and (4b). Here instead of (10) and (11) we have

$$\Psi_t = -\Phi(x-ct) - K(t)A(x-ct) - K^2(t)B(x-ct) - K^3(t)D(x-ct) - \frac{c^2}{\gamma^2}\left(\frac{c\beta}{\gamma}+\lambda\right) \tag{10'}$$

and

$$\Psi_t = \frac{\dot{K}(t)}{\gamma}g(x-ct) - \frac{cK(t)}{\gamma}h(x-ct) + \frac{\dot{\lambda}(t)}{\gamma}. \tag{11'}$$

Comparing (10') and (11'), we can write

$$\Phi(x-ct) = -K(t)A(x-ct) - K^2(t)B(x-ct) - K^3(t)D(x-ct) - \frac{\dot{K}(t)}{\gamma}g(x-ct) + \frac{cK(t)}{\gamma}h(x-ct) - \frac{c^2}{\gamma^2}\left(\frac{c\beta}{\gamma}+\lambda\right) - \frac{\dot{\lambda}(t)}{\gamma}. \tag{12'}$$

Applying the arguments similar to those given before, we can claim that here too u must be a function of $(x-ct)$ only.

IV. TRAVELING-WAVE SOLUTIONS IN THE PRESENCE OF CUBIC NONLINEAR TERMS

In order to extract traveling-wave solutions of (4), let us write

$$u = u(\rho), \quad v = v(\rho),$$

where

$$\rho = (x-t).$$

Then (4a) and (4b) become

$$-u_\rho + \alpha(v^3)_\rho + \beta(u^3)_\rho + \lambda(u^2)_\rho + \delta u_{\rho\rho\rho} = 0 \tag{13a}$$

and

$$-v_\rho + \gamma(uv)_\rho = 0. \tag{13b}$$

Integrating (13b), one obtains

$$v = c_1/(\gamma u - 1), \tag{14}$$

where c_1 is an arbitrary constant of integration. Substituting (14) in (13a) and integrating twice w.r.t. ρ, it is easy to obtain

$$\frac{\delta}{2}(u_\rho)^2 = c_3 + c_2 u + \frac{1}{2}u^2 - \frac{\lambda}{3}u^3 - \frac{\beta}{4}u^4 + \frac{1}{2}\frac{\alpha c_1^3}{\gamma}\frac{1}{(\gamma u-1)^2}, \tag{15}$$

where c_2 and c_3 are again constants of integration. The above Eq. (15) can be expressed in a compact form as

$$\frac{z\,dz}{\sqrt{az^6+bz^5+cz^4+dz^3+ez^2+g}} = \frac{1}{\sqrt{2}}d\rho, \tag{16}$$

where the parameters a, b, c, d, e, and g are given by

$$a = -\frac{\beta}{\delta\gamma^2},$$

$$b = -4\gamma^2\left(\frac{\beta}{\delta\gamma^4}+\frac{\lambda}{3\delta\gamma^3}\right),$$

$$c = -4\gamma^2\left(\frac{\lambda}{\delta\gamma^3}-\frac{1}{2\delta\gamma^2}+\frac{3\beta}{2\delta\gamma^4}\right),$$

$$d = -4\gamma^2\left(\frac{\beta}{\delta\gamma^4}-\frac{c_2}{\delta\gamma}-\frac{1}{\delta\gamma^2}+\frac{\lambda}{\delta\gamma^3}\right),$$

$$e = -4\gamma^2\left(\frac{\beta}{4\delta\gamma^4}+\frac{\lambda}{3\delta\gamma^3}-\frac{c_3}{\delta}-\frac{c_2}{\delta\gamma}-\frac{1}{2\delta\gamma^2}\right),$$

$$g = \frac{2\alpha c_1^3\gamma}{\delta}.$$

Knowing the precise values of the parameters, (16) may be either integrated in a closed form or evaluated numerically.

In the following, we consider the particular case when the parameters b and d vanish.[4] Equation (16) then reduces to a convenient form

$$\frac{1}{2}\left(\frac{d\tau}{d\rho}\right)^2 = a\tau^3 + c\tau^2 + e\tau + g \equiv f(\tau) \tag{17}$$

or

$$\int \frac{d\tau}{\sqrt{a\tau^3 + c\tau^2 + e\tau + g}} = \sqrt{2}\,\rho + c_4, \qquad (17')$$

where c_4 is a constant of integration.

V. NATURE OF THE SOLUTIONS

Without going into the nature of the parameters a, c, e, and g, one can make some qualitative remarks,[5] about the possible solutions of (17).

We first of all note that a real bounded solution τ is permitted when $(d\tau/d\rho)^2 \geqslant 0$. Moreover, at the vanishing points of $f(\tau)$, either $d\tau/d\rho$ should change sign or tend to zero as $\rho \to \pm\infty$. To examine this, let τ_1 be a simple zero of $f(\tau)$. Then

$$\left(\frac{d\tau}{d\rho}\right)^2 = 2f'(\tau_1)(\tau - \tau_1) + \text{higher-order terms.}$$

On integration, the above yields

$$\tau = \tau_1 + \tfrac{1}{2}f'(\tau_1)(\rho - \rho_1)^2 + \text{higher-order terms,}$$

where $\rho = \rho_1$ when $\tau = \tau_1$. Thus τ has a simple minimum or maximum τ_1 at ρ_1, according as $df/d\rho$ at τ_1 is positive or negative, respectively.

If, however, τ_1 is a double zero of $f(\tau)$, then

$$\left(\frac{d\tau}{d\rho}\right)^2 = f''(\tau_1)(\tau - \tau_1)^2 + \text{higher-order terms.}$$

Obviously, the validity of such a zero is possible only when $f''(\tau_1) > 0$.

Moreover, it also follows that

$$\tau - \tau_1 \sim \text{const} \times \exp[\pm\sqrt{f''(\tau_1)}\,\rho]$$

as $\rho \to \mp\infty$ in order that τ be bounded. The crucial point to note is that τ attains the maximum value τ_1 exponentially over an infinite range ρ. This may be recognized as the typical case of a solitary wave.

In addition to the solitary waves, it is possible to find the cnoidal wave also. The solution may be expressed in terms of three distinct real zeros of $f(\tau)$, namely, τ_1, τ_2, and τ_3, as

$$\rho = \rho_3 + \int_{\tau_3}^{\tau} \frac{d\tau}{\pm\sqrt{2f(\tau)}}$$

$$= \rho_3 + \int_{\tau_3}^{\tau} \frac{d\tau}{\pm\sqrt{2(\tau - \tau_1)(\tau - \tau_2)(\tau - \tau_3)}},$$

where τ_3 is a simple minimum of $f(\tau)$ and $\tau_3 < \tau_2 < \tau_1$. Therefore,

$$\tau = \tau_2 - (\tau_2 - \tau_3)\,\mathrm{cn}^2[\sqrt{\tfrac{1}{2}(\tau_1 - \tau_3)}\,(\rho - \rho_3)|m],$$

where the parameter "m" of the Jacobian elliptic function cn is given by

$$m = (\tau_2 - \tau_3)/(\tau_1 - \tau_3).$$

Noting that the period of cn for $0 \leqslant m < 1$ is given by $4\bar{K}(m)$, where

$$\bar{K}(m) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{(1 - m\sin^2\theta)}},$$

one may define the period of τ as

$$2\bar{K}(m)\sqrt{2/(\tau_1 - \tau_3)}\,.$$

Now if the wavelength of a nonlinear cnoidal wave be represented by $2\pi/K$, then we must have

$$K = \pi\sqrt{\tau_1 - \tau_3}/\sqrt{2}\cdot\bar{K}(m),$$

which yields the frequency (ω) of the cnoidal wave as

$$\omega = \pi c\sqrt{\tau_1 - \tau_3}/\sqrt{2}\cdot\bar{K}(m).$$

VI. LIMITING CASES OF CNOIDAL WAVES

We next consider the two important limiting cases of cnoidal waves.

Case 1: $m \to 0$. When $m \to 0$, $\tau_3 \to \tau_2$ and $c \to [-a(\tau_1 + 2\tau_2)]$. Thus

$$\tau(\rho) \to \tau_2 - (\tau_2 - \tau_3)\cos^2[\sqrt{\tfrac{1}{2}(\tau_1 - \tau_2)}\,(\rho - \rho_3)]$$

$$\to \tau_2 - A\cos[K(\rho - \rho_3)],$$

where

$$A = \tfrac{1}{2}(\tau_2 - \tau_3) \quad \text{and} \quad K = \sqrt{2(\tau_1 - \tau_2)}\,,$$

which is the solution for infinitesimal waves.

Case 2: $m \to 1$. When $m \to 1$, $\tau_2 \to \tau_1$ and $c \to [-a(2\tau_1 + \tau_3)]$. As a result

$$\tau(\rho) \to \tau_1 - (\tau_1 - \tau_3)\,\mathrm{sech}^2[\sqrt{\tfrac{1}{2}(\tau_1 - \tau_3)}\,(\rho - \rho_3)],$$

which is similar to the Boussinesq–Rayleigh solution for the solitary wave.

VII. CONCLUDING REMARKS

In this paper we have considered some coupled nonlinear equations that involve two variables $u(x,t)$ and $v(x,t)$. We have found that if one of these is a function of $(x - ct)$, the other must exhibit the same dependence of variables. In addition, we have generalized the works of Ito and Kawamoto to include cubic nonlinearity in one of the basic equations. Assuming that the functions $u(x,t)$ and $v(x,t)$ are of the traveling-wave type, we have solved such a system and considered some interesting particular cases. For instance, inclusion of nonlinear cubic terms in the equation has been found to lead to the possibility of cnoidal waves. Some limiting cases of such waves also have been considered.

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[3] It may be noted that the integration has been done treating t as a constant. Any arbitrary function of time that results from the constants of integration has been lumped with $\lambda(t)$.

[4] For "b" to vanish, the required condition is $\beta = -\frac{1}{3}\lambda\gamma$ whereas for "d" to vanish the condition is $\beta = \gamma(\gamma^2 c_2 + \gamma - \lambda)$. Thus, both "$b$" and "$d$" will vanish simultaneously if $\beta = -\frac{1}{3}\lambda\gamma$ and $c_2 = (2\lambda - 3\gamma)/3\gamma^2$.

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Exact localized solutions of a family of two-dimensional nonlinear spinor fields

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The classical equations of motion for two-dimensional nonlinear spinor fields are investigated. Explicit solutions for monomial and logarithmic self-interactions are presented. Furthermore properties of these classical solutions are discussed.

I. INTRODUCTION

It has been known for a long time that nonlinear field equations possess classical solutions with particlelike properties.[1] There is also much interest in finding explicit finite-energy solutions that can be used as representations of extended particles. There are several studies in quantization around such classical localized solutions[2–5] and for certain two-dimensional field theories this procedure is worked out, e.g., the Thirring model and the Gross–Neveu model.[6–9] Moreover classical field theory is, at least, the order-zero approximation to quantum field theory. Thus classical field equations form a starting point for quantum theories of extended particles such as hadrons. Therefore it is interesting to study certain properties of the classical solutions of nonlinear field equations.

Here we investigate the equations of motion for the classical Dirac field with a general class of self-interaction terms in one space and one time dimension. To our knowledge explicit solutions have been determined only for interactions of the form $L_I = (\bar\psi \Gamma \bar\psi)^2$ (see Refs. 10–13). By using a different approach we are able to present explicit solutions for arbitrary monomial self-interactions and for the logarithmic self-interaction. General steps of this method are done in Sec. II. In Sec. III, exact, explicit localized solutions for specific models are worked out and certain properties of them are investigated by exact computation or general estimates. In Sec. IV, we derive relations between the solutions for the different types of interactions (scalar, vector, and pseudoscalar interactions) in the case of monomial nonlinearities.

In Sec. V, we investigate nonlinear scalar fields obtained as a Klein–Gordon limit of the nonlinear spinor fields of Sec. III. Also some explicit solutions are presented.

Furthermore we mention some relations of spinor field theories to the sine–Gordon equation.

II. THE GENERAL METHOD

We study the following Lagrangian:

$$\mathcal{L}_D = (i/2)\,[\bar\psi\gamma^\mu\,\partial_\mu\psi - (\partial_\mu\bar\psi)\gamma^\mu\psi] - m\bar\psi\psi + G(\bar\psi\Gamma\psi), \tag{2.1}$$

where m is a positive constant and G a real-valued function with $G(0) = 0$.

We choose the following representation of the γ matrices:

$$\gamma^0 = \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$
$$\gamma^1 = -i\sigma^1 = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \tag{2.2}$$
$$\gamma^5 = \gamma^0\gamma^1 = \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

We are looking for stationary solutions of the form

$$\psi(x,t) = e^{-i\omega t}\varphi(x)\,,$$

which are localized, that is, with the boundary condition

$$\lim_{x\to\pm\infty} \varphi(x) = 0\,,$$

such that the physical quantities are finite.

The field equations are

$$i\gamma^\mu\,\partial_\mu\psi - m\psi + \frac{\partial G}{\partial\bar\psi} = 0 \tag{2.3}$$

(resp.

$$i\gamma^1\frac{d\varphi}{dx} - m\varphi + \gamma^0\omega\varphi + \frac{\partial G}{\partial\bar\varphi} = 0)\,. \tag{2.3'}$$

We require φ to be real and define

$$\varphi(x) = \begin{pmatrix} v(x) \\ u(x) \end{pmatrix}, \quad z^2(x) = \bar\varphi(x)\Gamma\varphi(x)$$

and we set

$$H = \tfrac{1}{2}[G(z^2) - m(v^2 - u^2) + \omega(v^2 + u^2)]\,. \tag{2.4}$$

Then we are lead to the following system:

$$\frac{du}{dx} = \frac{\partial H}{\partial v}, \quad \frac{dv}{dx} = -\frac{\partial H}{\partial u}\,. \tag{2.5}$$

Thus H is a constant of motion and using the boundary condition we have $H = 0$. Therefore localized solutions only exist if (0,0) is not isolated in the set $\{(u,v)\,|H = 0\}$.

The strategy is as follows: We define $q(x) := u(x)/v(x)$. Let us remark that $\theta(x) := \arctan q(x)$ is the phase between the two components of the solution. Then we derive differential equations for $q(x)$ and $z(x)$ from the system (2.5) and try to decouple them by using $H = 0$.

In the next section three types of interactions are worked out:

(i) scalar interaction S,
(ii) vector interaction V,
(iii) pseudoscalar interaction P.

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In addition we make a brief investigation of combinations of the different interactions S, V, and P.

III. EXACT SOLUTIONS OF SPECIFIC MODELS AND THEIR PROPERTIES

In the sequel, G is assumed to be differentiable on $\mathbb{R}\setminus\{0\}$ and $G(0)=0$. We denote the derivative of G by g.

A. Scalar interaction

In this case the system (2.5) reads

$$\begin{aligned}\frac{du_s}{dx}&=v_s(g(v_s^2-u_s^2)-(m-\omega)),\\ \frac{dv_s}{dx}&=u_s(g(v_s^2-u_s^2)-(m+\omega)).\end{aligned}\tag{3.1}$$

Using $H=0$ we obtain for $q_s=u_s/v_s$ and $z_s=(v_s^2-u_s^2)^{1/2}$ the following equations:

$$\frac{dq_s/dx}{1-q_s^2}=g(z_s^2)-\frac{G(z_s^2)}{z_s^2},\tag{3.2}$$

$$\frac{dz_s}{dx}=-2\omega\frac{q_s}{1-q_s^2}z_s\,.\tag{3.3}$$

Equation (3.3) is very interesting because it does not depend on the particular form of the interaction term G, but is only related to the type of interaction.

In addition, the relation $H=0$ reads

$$\frac{G(z_s^2)}{z_s^2}=m+\omega-\frac{2\omega}{1-q_s^2}\,.\tag{3.4}$$

Now we have to express $g(z_s^2)$ in terms of the right-hand side of (3.4). Putting this into Eq. (3.2) leads to an ordinary first-order differential equation that can be easily solved in a lot of cases.

Example 1 [$g(x)=\lambda x^p$, $p>0,\lambda>0$]: Here q_s satisfies

$$\frac{dq_s}{dx}=p[(m-\omega)-(m+\omega)q_s^2]\,,\tag{3.5}$$

which has the solution [choosing $q(0)=0$]

$$q_s(x)=\alpha\tanh(p\beta x)\,,\tag{3.6}$$

with $\alpha=((m-\omega)/(m+\omega))^{1/2}$, $\beta=(m^2-\omega^2)^{1/2}$. We see that $\omega<m$ corresponds to a confined solution.

By (3.2),

$$z_s^{2p}(x)=\frac{(m-\omega)(p+1)}{\lambda}\frac{1-\tanh^2(p\beta x)}{1-\alpha^2\tanh^2(p\beta x)}\,.$$

Using the tranformations $u_s=z_sq_s(1-q_s)^{-1/2}$, $v_s=z_s(1-q_s^2)^{-1/2}$,

$$u_s(x)=\left(\frac{(p+1)(m-\omega)}{\lambda}\right)^{1/2p}\alpha\frac{\tanh(p\beta x)}{(1-\alpha^2\tanh^2(p\beta x))^{1/2}}\times\left(\frac{1-\tanh^2(p\beta x)}{1-\alpha^2\tanh^2(p\beta x)}\right)^{1/2p},\tag{3.7a}$$

$$v_s(x)=\left(\frac{(p+1)(m-\omega)}{\lambda}\right)^{1/2p}\times\frac{(1-\tanh^2(p\beta x))^{1/2p}}{(1-\alpha^2\tanh^2(p\beta x))^{1/2p+1/2}}\,.\tag{3.7b}$$

Example 2 [$g(x)=k\log x$, $k>0$]: Because of $G(x)=k(-x+x\log x)$, (3.2) reduces to

$$\frac{dq_s}{dx}=k(1-q_s^2)\,.\tag{3.8}$$

The solution is

$$q_s(x)=\tanh kx\tag{3.9}$$

By (3.3),

$$z_s(x)=\exp\left(\frac{m+k}{2k}\right)\exp\left[-\frac{\omega}{2k}\cosh 2kx\right].$$

Thus we obtain the solutions

$$u_s(x)=\exp\left(\frac{m+k}{2k}\right)\sinh(kx)\exp\left[-\frac{\omega}{2k}\cosh 2kx\right],\tag{3.10a}$$

$$v_s(x)=\exp\left(\frac{m+k}{2k}\right)\cosh(kx)\exp\left[-\frac{\omega}{2k}\cosh 2kx\right].\tag{3.10b}$$

The energy eigenvalue ω is determined by the normalization condition

$$\int_{\mathbb{R}}\varphi^{+}\varphi\,dx=1\,.$$

It is easy to see that for the solutions of example 1, $\omega(\lambda)$ is a decreasing function and $\omega\to m$ for $\lambda\to 0$.

The "expectation value" of the classical Hamiltonian given by

$$\langle\mathscr{H}\rangle=m\int_{\mathbb{R}}\bar{\varphi}\varphi\,dx$$

is clearly bounded above by m in view of the estimate

$$\omega(v_s^2+u_s^2)<m(v_s^2-u_s^2)$$

for the solutions of example 1 we have $\langle\mathscr{H}\rangle\to m$ for $\lambda\to 0$.

Hence in the zero-coupling limit the expectation corresponds to a free, massive fermion while for finite values of λ the bound state requirement holds.

In Ref. 12 these values have been computed for the special case $g(x)=\lambda x$:

$$\omega=m\cdot(1+\lambda^2/4)^{-1/2}\,,\tag{3.11}$$

$$\langle\mathscr{H}\rangle=(2m/\lambda)\operatorname{arcsinh}(\lambda/2)\,.\tag{3.12}$$

In order to get an estimation of the size of the localized solutions we prove the following lemma.

Lemma 3.1: Suppose $G(v_s^2-u_s^2)\geqslant 0$. Then

$$\langle x^2\rangle:=\frac{\int(v_s^2+u_s^2)x^2\,dx}{\int v_s^2+u_s^2\,dx}\geqslant\frac{1}{4\beta^2}\,.\tag{3.13}$$

Proof: Multiplying the first equation of (3.1) by $u\cdot x$ and the second by $v\cdot x$ and subtracting yield

$$-\frac{x}{2}\frac{d}{dx}(v_s^2-u_s^2)=2\omega u_sv_s\cdot x\,.\tag{3.14}$$

Integration leads to

$$\frac{1}{2}\int v_s^2-u_s^2\,dx=2\omega\int u_sv_sx\,dx\,.\tag{3.15}$$

Then by the Cauchy–Schwarz inequality

$$\int v_s^2 x^2\,dx \geqslant \frac{1}{16\omega^2}\frac{(\int v_s^2 - u_s^2\,dx)^2}{\int u_s^2\,dx},$$

$$\int u_s^2 x^2\,dx \geqslant \frac{1}{16\omega^2}\frac{(\int v_s^2 - u_s^2\,dx)^2}{\int v_s^2\,dx}.$$

Thus

$$\frac{\int (v_s^2+u_s^2)x^2\,dx}{\int v_s^2+u_s^2\,dx} \geqslant \frac{1}{16\omega^2}\frac{(\int v_s^2-u_s^2\,dx)^2}{(\int u_s^2\,dx)(\int v_s^2\,dx)} = \frac{1}{4\omega^2}\frac{(\int v_s^2-u_s^2\,dx)^2}{(\int v_s^2+u_s^2\,dx)^2-(\int v_s^2-u_s^2\,dx)^2}. \quad (3.16)$$

Now (3.13) follows using the inequality $v_s^2+u_s^2<(m/\omega)(v_s^2-u_s^2)$.

In the case $g(x)=\lambda x$ one obtains a better bound under the assumption of normalization by using (3.16) directly. In combination with (3.11) and (3.12), we see

$$\langle x^2\rangle \geqslant \frac{1}{4m^2}\frac{((2/\lambda)^2+1)(\operatorname{arcsinh}(\lambda/2))^2}{1-(2/\lambda)^2(\operatorname{arcsinh}(\lambda/2))^2}. \quad (3.17)$$

This bound shows that there are no confined solutions for $\lambda\to 0$ and $\lambda\to\infty$.

Remark 1: The solutions of the $(1+1)$-dimensional scalar-interaction problem correspond precisely to the asymptotic forms of the $(1+3)$-dimensional equations.[13] There are no analytic solutions in $(1+3)$ dimensions, so that the exact solutions in $(1+1)$ dimensions get an additional importance. The existence of localized solutions for classical nonlinear Dirac fields in $(1+3)$ dimensions has been proved when $G(x)$ is strictly convex on $\mathbf{R}_0^+$, $G(0)=g(0)=0$ and $\lim_{x\to\infty} g(x)=\infty$ (see Ref. 14).

Remark 2: Lemma 3.1 exhibits the existence of a minimal radius x_0 of the classical solutions. Similar investigations were only done for solutions in three space dimensions. See, for example, Ref. 15. A numerical computation of $\langle x^2\rangle$ when $g(x)=\lambda x$ is given in the Appendix.

Remark 3: The assumption on $G(v_s^2-u_s^2)$ in Lemma 3.1 is made not only for technical reasons. For the logarithmic self-interaction a numerical computation shows that $\langle x^2\rangle$ can be arbitrary small (see the Appendix).

B. Vector Interaction

By (2.4) and (2.5) we are lead to the equations

$$\frac{du_v}{dx} = v_v(g(v_v^2+u_v^2)-(m-\omega)),$$
$$\frac{dv_v}{dx} = -u_v(g(v_v^2+u_v^2)+(m+\omega)). \quad (3.18)$$

Analogous to the scalar case we obtain for $q_v=u_v/v_v$ and $z_v=(v_v^2+u_v^2)^{1/2}$

$$\frac{dq_v/ux}{1+q_v^2} = g(z_v^2)-\frac{G(z_v^2)}{z_v^2}, \quad (3.19)$$

$$\frac{dz_v}{dx} = -2m\frac{q_v}{1+q_v^2}z_v. \quad (3.20)$$

Again we have an equation that does not depend on the nonlinearity G. Identity (3.4) is replaced by

$$\frac{G(z_v^2)}{z_v^2} = -(m+\omega)+\frac{2m}{1+q_v^2}. \quad (3.21)$$

Now we take the same examples as in the scalar-interaction case.

Example 1 $[g(x)=\lambda x^p,\ \lambda>0,\ p>0]$: We see that q_v satisfies (3.5) and therefore

$$q_v(x)=q_s(x)=\alpha\tanh(p\beta x). \quad (3.22)$$

Computing

$$z_v^{2p}(x)=\frac{(p+1)(m-\omega)}{\lambda}\frac{1-\tanh^2(p\beta x)}{1+\alpha^2\tanh^2(p\beta x)}$$

and using $u_v=z_v q_v(1+q_v^2)^{-1/2}$ and $v_v=z_v(1+q_v^2)^{-1/2}$, we obtain the following explicit solutions:

$$u_v(x)=\alpha\left(\frac{(p+1)(m-\omega)}{\lambda}\right)^{1/2p}\frac{\tanh(p\beta x)}{(1+\alpha^2\tanh^2(p\beta x))^{1/2}} \times\left(\frac{1-\tanh^2(p\beta x)}{1+\alpha^2\tanh^2(p\beta x)}\right)^{1/2p}, \quad (3.23a)$$

$$v_v(x)=\left(\frac{(p+1)(m+\omega)}{\lambda}\right)^{1/2p} \times\frac{(1-\tanh^2(p\beta x)^{1/2p}}{(1+\alpha^2\tanh^2(p\beta x))^{1/2p+1/2}}. \quad (3.23b)$$

We see that again $\omega\to m$ as $\lambda\to 0$ for ω determined by the normalization condition $\int\varphi^+\varphi\,dx=1$. Moreover $\langle\mathscr{H}\rangle\to m$ as $\lambda\to 0$, so that the solutions exhibit a bound state behavior.

For $p=1$ the exact results are well known[12]:

$$\omega = m\cos(\lambda/2),$$
$$\langle\mathscr{H}\rangle = (2m/\lambda)\sin(\lambda/2). \quad (3.24)$$

The first identity imposes $\lambda\leqslant\pi$ to have positive-energy fermion states.

Lemma 3.1 is replaced by the following lemma.

Lemma 3.2: Suppose $G(v_v^2+u_v^2)>0$. Then for a localized solution of (3.18) the following estimate holds:

$$\langle x^2\rangle \geqslant 1/4\beta^2. \quad (3.25)$$

Proof: Multiplying the first equation of (3.18) by $u\cdot x$ and the second by $v\cdot x$ leads after addition to

$$-\frac{x}{2}\frac{d}{dx}(v_v^2+u_v^2)=2mu_v v_v x.$$

Integration yields

$$\frac{1}{2}\int_{\mathbf{R}} v_v^2+u_v^2\,dx = 2m\int_{\mathbf{R}} u_v v_v x\,dx.$$

As in the proof of Lemma 3.1 we use the Cauchy–Schwarz inequality and obtain

$$\frac{\int(v_v^2+u_v^2)x^2\,dx}{\int v_v^2+u_v^2\,dx}\geqslant\frac{1}{16m^2}\frac{(\int v_v^2+u_v^2\,dx)^2}{(\int v_v^2\,dx)(\int u_v^2\,dx)}\geqslant\frac{1}{4\beta^2}. \quad \square$$

For $g(x)=\lambda x$ we obtain the better bound

$$\langle x^2\rangle\geqslant\frac{1}{4m^2}\frac{1}{(1-(4/\lambda^2)\sin^2(\lambda/2))}, \quad (3.26)$$

which shows that for $\lambda\to 0$ there is no confined solution. A numerical computation of $\langle x^2\rangle$ is given in the Appendix.

Example 2 [$g(x) = k \log x$]: There will be no localized solution for this interaction. For q_v we immediately obtain the simple equation

$$\frac{dq_v}{dx} = k(1 + q_v^2) .$$

The solution is

$$q_v(x) = \tan kx .$$

Then

$$\frac{dz_v}{dx} = -2m \frac{\tan kx}{1 + \tan^2 kx} z_v = -m \sin(2kx) z_v .$$

Integration leads to

$$\log[z_v(x)/z_v(0)] = -(m/k)\sin^2 kx ,$$

with

$$z_v(0) = \exp((m - \omega)/2k + \tfrac{1}{2}) .$$

Thus we found an oscillating solution.

C. Pseudoscalar interaction

The equations of motion are

$$\frac{du_p}{dx} = u_p g(2u_p v_p) - v_p(m - \omega) ,$$

$$\frac{dv_p}{dx} = -v_p g(2u_p v_p) - u_p(m + \omega) . \tag{3.27}$$

As before we derive one equation for $q_p = u_p/v_p$,

$$\frac{1}{2q_p}\frac{dq_p}{dx} = g(z_p^2) - \frac{G(z_p^2)}{z_p^2} , \tag{3.28}$$

using $z_p := (2u_p v_p)^{1/2}$ the relation $H = 0$ reads

$$\frac{G(z_p^2)}{z_p^2} = \frac{m}{2}\frac{1 - q_p^2}{q_p} - \frac{\omega}{2}\frac{1 + q_p^2}{q_p} \tag{3.29}$$

and we obtain an ordinary differential equation in terms of q_p for a certain class of nonlinearities G.

Example 1 [$g(x) = \lambda x^p, \lambda > 0, p > 0$]: Again we obtain for the quotient of the solutions

$$q_p(x) = \alpha \tanh(p\beta x) .$$

This yields

$$z_p^{2p}(x) = \frac{(p + 1)}{2\lambda p}\beta \frac{1}{\cosh(p\beta x)\sinh(p\beta x)} .$$

Using the transformations $u_p = (1/\sqrt{2}) z_p q_p^{1/2}$ and $v_p = (1/\sqrt{2}) z_p q_p^{-1/2}$, the solutions are given by

$$u_p(x) = \frac{\sqrt{\alpha}}{\sqrt{2}}\left(\frac{p + 1}{2\lambda}\beta\right)^{1/2p} \frac{\tanh^{1/2}(p\beta x)}{(\cosh(p\beta x)\sinh(p\beta x))^{1/2p}} , \tag{3.30a}$$

$$v_p(x) = \sqrt{\frac{1}{2\alpha}}\left(\frac{p + 1}{2\lambda}\beta\right)^{1/2p} \times \frac{1}{\tanh^{1/2}(p\beta x)(\cosh(p\beta x)\sinh(p\beta x))^{1/2p}} . \tag{3.30b}$$

Since the upper spinor component possesses a nonintegrable singularity at $x = 0$ the obtained solutions are not normalizable.

Thus in contrast to scalar and vector interaction localized solutions do not exist contradicting the result in Ref. 12.

Example 2 [$g(x) = k \log x, k > 0$]: We find

$$\frac{dq_p}{dx} = 2kq_p ,$$

which has the solution $q(x) = q(0)e^{2kx}$.

The general equation for z_p that is independent on the nonlinearity g is

$$\frac{dz_p}{d\lambda} + \frac{z_p}{2}\frac{1}{q_p}[(m - \omega) + (m + \omega)q_p^2] = 0 .$$

Thus there is no localized solution.

D. Combination of different types of interaction

By simple extensions of the methods presented above it is also possible to find explicit solutions of Lagrangians that contain different types of couplings, e.g., scalar and vector interaction. We will not give a complete discussion of all possible combinations, but we illustrate the procedure for a particular case: Suppose the Lagrangian of interaction possesses a scalar and a vector interaction term, i.e.,

$$L_I = G(\bar{\psi}\psi) + F(\bar{\psi}\gamma^1\psi) , \tag{3.31}$$

where G, F satisfy the assumptions made at the beginning of this section. If f and g denote the derivatives of F (resp. G) the equations of motion are

$$\frac{du}{dx} = v(g(v^2 - u^2) + f(v^2 + u^2) - (m - \omega)) ,$$

$$\frac{dv}{dx} = u(g(v^2 - u^2) - f(v^2 + u^2) - (m + \omega)) . \tag{3.32}$$

For localized solutions we have

$$H(u,v) = \tfrac{1}{2}[G(v^2 - u^2) + F(v^2 + u^2) - m(v^2 - u^2) + \omega(v^2 + u^2)] , \tag{3.33}$$

which is equivalent to ($q = u/v$)

$$(1 - q^2)\frac{G(v^2 - u^2)}{v^2 - u^2} + (1 + q^2)\frac{F(v^2 + u^2)}{v^2 + u^2} = m(1 - q^2) - \omega(1 + q^2) , \tag{3.34}$$

where q satisfies the differential equation

$$\frac{dq}{dx} = (1 - q^2)\left[g(v^2 - u^2) - \frac{G(v^2 - u^2)}{v^2 - u^2}\right] + (1 + q^2)\left[f(v^2 + u^2) - \frac{F(v^2 + u^2)}{v^2 + u^2}\right] . \tag{3.35}$$

We consider the following example: $g(x) = \lambda x^p$, $f(x) = \mu x^p$. Again we obtain $q(x) = \alpha \tanh \beta x$. Then (3.35) and the fact that

$$(v^2 + u^2) = [(1 + q^2)/(1 - q^2)](v^2 - u^2)$$

leads to

$$(v^2 - u^2)^p = (p + 1)(m - \omega)(1 - \tanh^2 p\beta x) \times (1 - \alpha^2 \tanh^2 p\beta x)^p \times [\lambda(1 - \alpha^2 \tanh^2 p\beta x)^{p+1} + \mu(1 + \alpha^2 \tanh^2 p\beta x)^{p+1}]^{-1} . \tag{3.36}$$

Thus we obtain the solution using

$$u = (v^2 - u^2)^{1/2} \cdot q \cdot (1 - q^2)^{-1/2},$$
$$v = (v^2 - u^2)^{1/2} \cdot (1 - q^2)^{-1/2}.$$

Clearly we have (3.7a) and (3.7b) if $\mu = 0$ and (3.23a) and (3.23b) if $\lambda = 0$.

Let us remark that if $p = 1$ the total solution for classical Fermi interactions is given by (3.36): For scalar interaction we have $\mu = 0$ while $\lambda = 0$ in the vector case. For pseudoscalar interaction we get $\mu = -\lambda$. In addition other types of interaction are all equivalent with vector interaction.

IV. RELATIONS BETWEEN THE SOLUTIONS FOR THE DIFFERENT TYPES OF INTERACTION

In this section we will only consider the monomial interaction $g(x) = \lambda x^p$ because we know the explicit solutions for the three types of interaction.

At first we see that the phase between upper and lower components does not depend on the type of interaction. It is solely determined by m and ω. This reads

$$q_s = q_v = q_p . \tag{4.1}$$

This was first observed in Ref. 12 for $g(x) = \lambda x$. Relation (4.1) is based on the following relation for the Lagrangian of interaction:

$$\bar\psi \frac{\partial G(\bar\psi\Gamma\psi)}{\partial\bar\psi} = (p+1)G(\bar\psi\Gamma\psi),$$
$$\frac{\partial G(\bar\psi\Gamma\psi)}{\partial\psi}\psi = (p+1)G(\bar\psi\Gamma\psi). \tag{4.2}$$

See Ref. 12 for the details.

Remember

$$z_s^{2p}(x) = \frac{(m-\omega)(p+1)}{\lambda}\frac{1-\tanh^2(p\beta x)}{1-\alpha^2\tanh^2(p\beta x)},$$
$$z_s^2 = v_s^2 - u_s^2,$$
$$z_v^{2p}(x) = \frac{(m-\omega)(p+1)}{\lambda}\frac{1-\tanh^2(p\beta x)}{1+\alpha^2\tanh^2(p\beta x)},$$
$$z_v^2 = v_v^2 - u_v^2,$$
$$z_p^p(x) = \frac{(m-\omega)(p+1)}{\lambda}\frac{1}{2\alpha\sinh(p\beta x)\cosh(p\beta x)},$$
$$z_p^2 = 2u_p v_p .$$

Thus we have the following relation between the different types of interaction:

$$z_s^{-4p} + z_p^{-4p} = z_v^{-4p}. \tag{4.3}$$

By computing the Hamiltonian densities $\mathscr{H}$ and the charge densities $\mathscr{Q}$ we obtain

$$\mathscr{H}_s^{-\rho} + \mathscr{H}_p^{-\rho} = \mathscr{H}_v^{-\rho}, \quad \rho = 2p/(p+1), \tag{4.4}$$
$$\mathscr{Q}_s^{-\rho} + \mathscr{Q}_p^{-\rho} = \mathscr{Q}_v^{-\rho}, \quad \rho = 2p/(p+1). \tag{4.5}$$

Equation (4.5) was observed also in Ref. 12 for $g(x) = \lambda x$.

As a consequence of (4.1) we see

$$\frac{\mathscr{H}_s}{\mathscr{Q}_s} = \frac{\mathscr{H}_v}{\mathscr{Q}_v} = \frac{\mathscr{H}_p}{\mathscr{Q}_p} = \frac{1-q_s^2}{1+q_s^2}. \tag{4.6}$$

V. NONLINEAR SCALAR FIELD EQUATIONS IN ONE DIMENSION

At the beginning of this section we restrict ourselves to the scalar interaction.

Applying $i\gamma^\nu\partial_\nu$ to (2.3) one gets an equation similar to the Klein–Gordon equation. Considering only the upper spinor component we obtain the Klein–Gordon limit. This was done in Ref. 16 for (1 + 3) dimensions. Here we have to investigate the equation

$$\frac{d^2v}{dx^2} = (m^2-\omega^2)v - 2mg(v^2)v + g(v^2)g(v^2)v, \tag{5.1}$$

which gives

$$\frac{d^2v}{dx^2} = (m^2-\omega^2)v - 2m\lambda v^{2p+1} + \lambda^2 v^{4p+1} \tag{5.2}$$

for the monomial interaction $g(x) = \lambda x^p$.

Using the transformation $v(x) = (\beta/\lambda^2)^{1/4p}\varphi(\beta x)$ and defining $\epsilon = 2m\beta^{-1}$ we obtain (denote the derivative with respect to $r = \beta \times g$ by a prime)

$$\varphi'' = \varphi - \epsilon\varphi^{2p+1} + \varphi^{4p+1}. \tag{5.3}$$

Now by a well-known existence and also uniqueness theorem (see, e.g., Ref. 17) localized solutions exist if and only if

$$\epsilon > 2(p+1)(2p+1)^{-1/2}$$
$$= 2(1 + p^2/(2p+1))^{1/2}. \tag{5.4}$$

Condition (5.4) is equivalent to the requirement

$$(\omega/m) > p/(p+1). \tag{5.5}$$

Example: Consider the Fermi interaction $g(x) = \lambda x$ and let ω be determined by the normalization condition [see (3.11)]. Then the associated Klein–Gordon equation has only confined solutions if

$$\lambda < 2\sqrt{3}. \tag{5.6}$$

In general it is difficult to compute the solution explicitly but it is possible in this case. We see that the explicit solution of the scalar equation is given by

$$\varphi(r) = (4/\epsilon)^{1/2}[1 + (1 - 16/3\epsilon^2)^{1/2}\cosh 2r]^{-1/2}.$$

For the logarithmic nonlinearity $g(x) = k\log x$, (5.1) leads to

$$\frac{d^2v}{dx^2} = (m^2-\omega^2)v - 2mk(\log v^2)v + k^2(\log v^2)^2 v. \tag{5.7}$$

Setting $v(x) = a\phi(bx)$, $a = \exp[(m+k)/2k]$, $b = k$, and

$$\delta = 1 - (\omega/k),$$

we obtain

$$\varphi'' = \delta\phi + 2\phi\log\phi^2 + \phi(\log\phi^2)^2. \tag{5.8}$$

The potential associated to the above equation is

$$F(\phi) = -\tfrac{1}{2}\phi^2[\delta + (\log\phi^2)^2].$$

Thus there are no solutions if $\delta \geqslant 0$. For $\delta < 0$ we find by direct integration

$$\phi(r) = \exp(-\tfrac{1}{2}\sqrt{-\delta}\cosh 2r), \tag{5.9}$$

which is

$$v(x) = \exp\left(\frac{m+k}{2k}\right)\exp\left(-\frac{1}{2k}\sqrt{\omega^2-k^2}\cosh 2kx\right) \tag{5.10}$$

in the old variables.

Applying the same procedure to the vector interaction case one obtains the following scalar field equation:

$$\frac{d^2v}{dx^2} = (m^2-\omega^2)v - 2\omega g(v^2)v - g(v^2)g(v^2)v\,. \tag{5.11}$$

For $g(x) = \lambda x^p$ this reads

$$\frac{d^2v}{dx^2} = (m^2-\omega^2)v - 2\omega\lambda v^{2p+1} - \lambda^2 v^{4p+1}\,. \tag{5.12}$$

This equation always admits a confined solution.

Here we want to discuss an important particular case related to the massive Thirring model. We are interested in solutions for which $\omega = 0$. Remember that there are localized solutions for the nonlinear Dirac equation. (This is different from the scalar interaction case where $\omega = 0$ produces no localized solution.) The related Klein–Gordon equation is

$$\frac{d^2v}{dx^2} = m^2v - \lambda^2 v^{4p+1}\,. \tag{5.13}$$

The solution of this equation is given by

$$v(x) = (\gamma\cosh 2pmx)^{-1/2p}\,,$$

where

$$\gamma^2 = [1/(2p+1)]\lambda^2/m^2\,.$$

Thus v has the same asymptotic behavior as the spinor solutions for $\omega = 0$ and v^2 is proportional to the charge density of the spinor field or, more precisely,

$$v^2 = (\sqrt{2p+1}/(p+1))^{1/p}(v_v^2+u_v^2)!$$

As remarked in Ref. 12 the phase $\theta(x) = \arctan v(x)$ satisfies the sine–Gordon equation

$$\frac{d^2\theta}{dx^2} = -(pm)^2\sin 4\theta\,.$$

Furthermore the classical solution of the massive Thirring model ($p = 1$) and $\Phi = 4\theta$ satisfy the Coleman correspondence equations.[18] In some sense also the related scalar field equation (5.13) is connected with the sine–Gordon equation, because

$$\tau_\mu(x) = \mu\arccos(v/\gamma)^2,\quad \mu>0\,,$$

satisfies

$$\frac{d^2\tau_\mu}{dx^2} = -2\mu m^2\sin\frac{2}{\mu}\tau_\mu\,.$$

Moreover we see that the logarithmic scalar interaction (see example 2 in Sec. III A) is—at least formally—related to the sine–Gordon equation. The phase $\theta(x) = \arctan\tanh kx$ does not depend on ω and m, and $\phi = 4\theta$ satisfies

$$\frac{d^2\phi}{dx^2} = -4k^2\sin\phi\,,$$

where k is the coupling constant of the interaction. But up to the present time we do not have any physical interpretation of these facts.

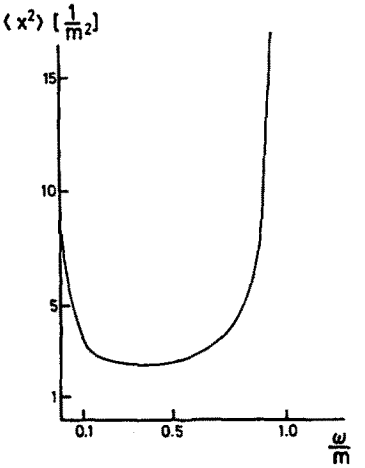

FIG. 1. In units of $1/m^2$, $\langle x^2\rangle$ is plotted as a function of ω/m.

Note added: A few days after this work was finished we got the November issue of J. Phys. A, in which Mathieu[19] studied soliton solutions for $(1+1)$-dimensional Dirac equations with nonlinearities satisfying the homogeneity relation (4.2) of our paper. Using this property he obtained a nice formula finding explicit solutions for general types of interaction, while we treated general nonlinearities in particular types of interaction, although only for homogenous self-interactions and for the logarithmic self-interaction are explicit solutions presented. Nevertheless our approach allows us to determine such soliton solutions in more general cases. Furthermore the existence conditions of Mathieu coincide with our results in Secs. II and III.

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APPENDIX: NUMERICAL COMPUTATION OF $\langle x^2\rangle$ FOR CERTAIN EXAMPLES

We compute the integrals numerically by Simpson's rule with the use of the HP-67 programmable pocket calculator.

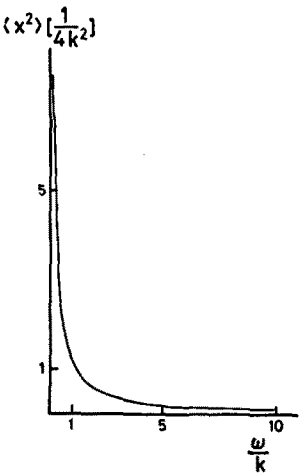

FIG. 2. In units of $1/4k^2$, $\langle x^2\rangle$ is plotted as a function of ω/k.

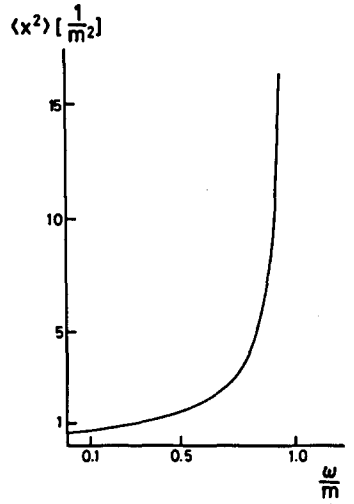

FIG. 3. In units of $1/m^2$, $\langle x^2\rangle$ is plotted as a function of ω/m.

1. Scalar Fermi interaction ($g(x) = \lambda x$)

Using

$$\int_{\mathbf{R}} v_s^2 + u_s^2\, dx = \frac{4}{\lambda}\frac{\alpha}{1-\alpha^2}$$

we obtain

$$\langle x^2\rangle = \frac{1}{m^2}\frac{(1+\alpha^2)(1-\alpha^2)}{2\alpha^2} I(\alpha)\,, \tag{A1}$$

where

$$I(\alpha) = \int_0^\infty \frac{(1-\tanh^2 r)(1+\alpha^2\tanh^2 r)}{(1-\alpha^2\tanh^2 r)^2}\, r^2\, dr$$

is the integral we compute numerically.

In Fig. 1, $\langle x^2\rangle$ in units of $1/m^2$ is plotted as a function of ω/m.

The minimum value $\langle x_0^2\rangle = 2.3875 \cdot (1/m^2)$ is attained for $\omega = 0.371$.

2. Logarithmic scalar interaction

We have

$$\langle x^2\rangle = \frac{1}{4k^2}\frac{\int_0^\infty r^2 \cosh r \cdot \exp[-(\omega/k)\cosh r]dr}{\int_0^\infty \cosh r \cdot \exp[-(\omega/k)\cosh r]dr}. \tag{A2}$$

Thus $\langle x^2\rangle$ depends on the absolute value of k and the quotient ω/k but not on m. This is different from the case before. Figure 2 exhibits $\langle x^2\rangle$ in units of $1/4k^2$ as a function of ω/k. We see that there is no minimum value of $\langle x^2\rangle$. Therefore the positivity of the interaction is somewhat essential for Lemma 3.1.

3. Vector Fermi Interaction

Using

$$\int_{\mathbf{R}} u_v^2 + v_v^2\, dx = \frac{2}{\lambda}\arccos\frac{\omega}{m},$$

we find after simple calculation

$$\langle x^2\rangle = \frac{1}{m^2}\frac{1+\alpha^2}{\alpha}\frac{1}{\arccos(\omega/m)} \times \int_0^\infty \frac{r^2\, dr}{1+(1+\alpha^2)\sinh^2 r}. \tag{A3}$$

If one restricts to positive energy fermion states $\langle x^2\rangle = 0{,}617 \cdot (1/m^2)$ is a lower bound attained in the zero-energy limit (i.e., $\omega = 0$). (See Fig. 3.)

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The action of a general gauge field theory: Minimum or stationary. II

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In a previous paper the author has shown that for a gauge field theory with positive definite Cartan–Killing metric $C_{\alpha\beta}$ and space metric g_{ij} the action functional is locally strictly minimum provided that the critical point and the variation both satisfy the gauge condition $A^{\alpha}_{i,i}=0$. This result is now extended so that no assumption is needed about gauge conditions.

I. INTRODUCTION

The action functional of a general gauge field theory is

$$S[A]=\frac{1}{4}C_{\alpha\beta}\int_{\Omega}(A^{\alpha}_{[h,j]}+C^{\alpha}_{\epsilon\lambda}A^{\epsilon}_{j}A^{\lambda}_{h})(A^{\beta}_{[k,l]}+C^{\beta}_{\mu\nu}A^{\mu}_{l}A^{\nu}_{k})g^{hk}g^{jl}\,d^{n}x\,, \tag{1}$$

where the $A^{\alpha}_{i}(x)$ are gauge potentials. The notation, etc. is fully described in a previous paper[1], where it was argued that when both the Cartan–Killing metric ($C_{\alpha\beta}$) and the space metric (g_{ij}) are positive definite, a solution of the field equations always represents a strict local minimum of the action ("local" in the sense that the domain Ω must be sufficiently small). In order to prove this assertion it was necessary to assume that both the critical point A and the variation $\overline{A}=A+\epsilon$ satisfy the Lorentz gauge condition $A^{\alpha}_{i,i}=0$. Of course there exists a gauge transformation $\mu^{\alpha}(x)$ so that $A(\mu)^{\alpha}_{i,i}=0$, but it is not in general true that also $\overline{A}(\mu)^{\alpha}_{i,i}=0$. In this paper strict local minimality of the action will be proved without any assumptions being made about gauge conditions.

II. CALCULATION

Suppose that $A^{\alpha}_{i}(x)$ is a critical point of the action functional (1) and that $\overline{A}^{\alpha}_{i}(x)=A^{\alpha}_{i}(x)+\epsilon\mathscr{A}^{\alpha}_{i}(x)$ is a variation [so that on the boundary $\partial\Omega$, $\mathscr{A}^{\alpha}_{i}(x)=0$]. The Cartan–Killing metric $C_{\alpha\beta}$ and the space metric g_{ij} are positive definite. Gauge transformations μ to A and ν to $\overline{A}$ are made so that, in Ω,

$$A(\mu)^{\alpha}_{i,i}=\overline{A}(\nu)^{\alpha}_{i,i}=0\,, \tag{2}$$

and, on $\partial\Omega$, $\mu,\nu=0$. It was shown in Sec. IV of Ref. 1 that such μ, ν exist and are unique when Ω is small enough. It should also be noted that the difference $\mu-\nu$ is of order ϵ. Define

$$\epsilon\mathscr{A}(\mu,\nu)^{\alpha}_{i}=\overline{A}(\nu)^{\alpha}_{i}-A(\mu)^{\alpha}_{i}\,, \tag{3}$$

so that

$$\mathscr{A}(\mu,\nu)^{\alpha}_{i,i}=0\,. \tag{4}$$

By expressing $A(\mu)$ and $\overline{A}(\nu)$ in terms of A, $\overline{A}$, μ, and ν it follows that[2]

$$\epsilon\mathscr{A}(\mu,\nu)^{\alpha}_{i}=\epsilon\mathscr{A}^{\alpha}_{i}+C^{\alpha}_{\beta\epsilon}(\nu^{\beta}\overline{A}^{\epsilon}_{i}-\mu^{\beta}A^{\epsilon}_{i})-(\nu^{\alpha}-\mu^{\alpha})_{,i}\,, \tag{5}$$

which on the boundary $\partial\Omega$ simplifies to

$$\epsilon\mathscr{A}(\mu,\nu)^{\alpha}_{i}=(\mu^{\alpha}-\nu^{\alpha})_{,i}\,. \tag{6}$$

Thus, in general, on the boundary $\partial\Omega$ $\mathscr{A}(\mu,\nu)^{\alpha}_{i}$ is nonzero, but the component tangential to the boundary is zero.

The action functional is gauge invariant so that $S[A(\mu)]=S[A]$ and $S[A(\mu)+\epsilon\mathscr{A}(\mu,\nu)]=S[A+\epsilon\mathscr{A}]$. Expansion in powers of ϵ implies that $S^{(2)}[A(\mu),\mathscr{A}(\mu,\nu)]=S^{(2)}[A,\mathscr{A}]$. Thus minimality is proved by showing that at a critical point A, $S^{(2)}[A(\mu),\mathscr{A}(\mu,\nu)]>0$, for all nonzero $\mathscr{A}(\mu,\nu)^{\alpha}_{i}$ whose tangential component is zero on the boundary $\partial\Omega$. Under this condition and condition (4) it follows that

$$\|\mathscr{A}(\mu,\nu)^{\alpha}_{[k,j]}\|^{2}=\tfrac{1}{2}\|\mathscr{A}(\mu,\nu)^{\alpha}_{k,j}\|^{2}\,. \tag{7}$$

In other words, Lemma 5.1 of Ref. 1 remains valid under the weakened conditions used here. For notational convenience $\mathscr{A}(\mu,\nu)$ will now be written as $\mathscr{B}$. The proof of Eq. (7) proceeds as in Ref. 1 to obtain

$$\|\mathscr{B}^{\alpha}_{[k,j]}\|^{2}-\|\mathscr{B}^{\alpha}_{(k,j)}\|^{2}=\sum_{\alpha}\int_{\partial\Omega}-\mathscr{B}^{\alpha}_{j}\mathscr{B}^{\alpha}_{k,j}n_{k}\,d^{n-1}x+\sum_{\alpha}\int_{\Omega}\mathscr{B}^{\alpha}_{k}(\mathscr{B}^{\alpha}_{k,k})_{,j}\,d^{n}x\,. \tag{8}$$

The second term is zero by condition (4). The first term is evaluated by using coordinates such that at a given point $P\in\partial\Omega$, $n_{k}=(1,0,\ldots,0)$. Then, as $\mathscr{B}$ has zero tangential component, $\mathscr{B}^{\alpha}_{i}=(\mathscr{B}^{\alpha}_{1},0,\ldots,0)$ at points in $\partial\Omega$ at or near P. At P, $\mathscr{B}^{\alpha}_{2,2}=\mathscr{B}^{\alpha}_{3,3}=\cdots=0$, so that by (4) $\mathscr{B}^{\alpha}_{1,1}=0$. The first term on the right-hand side of (8) is therefore also zero and the proof of Eq. (7) is completed as in Ref. 1.

As in Ref. 1 it may be shown that

$$S^{(2)}_{\Omega}[A,\mathscr{B}]\geq k\|\mathscr{B}^{\alpha}_{j,k}\|^{2}+O(\|\mathscr{B}\|^{2},\|\mathscr{B}\|\,\|\nabla\mathscr{B}\|)\,. \tag{9}$$

Unfortunately Poincaré's inequality cannot be applied because $\mathscr{B}$ is not zero in $\partial\Omega$. However an extension of Poincaré's inequality can be used[3]: Given a bounded Lipschitz domain Ω and a vector function $\mathbf{u}(x)$ such that at all points in the boundary $\partial\Omega$ at which $\exists$ a unique normal, the tangential component of $\mathbf{u}(x)$ vanishes. Then $\exists$ c, independent of $\mathbf{u}(x)$, such that

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$$\int_\Omega |\mathbf{u}|^p \, dx \leqslant c \int_\Omega |\nabla \mathbf{u}|^p \, dx \,. \tag{10}$$

Further, if Ω is changed in size by means of a linear map then the value of the constant c behaves as R^p, where R is the radius of the smallest ball containing Ω.

Use of the above theorem then shows that for Ω small enough $S_\Omega^{(2)}[A, \mathscr{B}] > 0$ (if $\mathscr{B} \neq 0$) so that the critical point A is a strict local minimum of the action.

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The geometrical interpretation of the Faddeev–Popov determinant in Polyakov's theory of random surfaces

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In the context of Polyakov's theory the geometrical approach, in which the functional measure is defined as a formal volume ∞-form, is developed. The special version of the Fubini theorem on manifolds is derived, which provides the geometrical interpretation of the Faddeev–Popov method. The conformal gauge is studied within this framework. As a result, the explicit form of functional measure in effective Liouville quantum field theory is obtained.

I. INTRODUCTION

In Polyakov's method of averaging,[1] the sum over the random surfaces can be reduced to the two-dimensional quantum field theory, which is determined by the effective action and the resulting functional measure. This action is well known (as the Liouville action[1–3]) in contrast to the measure, the explicit form of which remains unclear.[2,4,5] In principle the exact form of this measure can be derived by application of the Faddeev–Popov method. At the starting point of Polyakov's considerations[1] the functional measures are introduced as Riemannian measures on an infinite-dimensional manifold. Thus it is clear that the Faddeev–Popov procedure is related to a certain version of the Fubini theorem on manifolds. Such a geometrical approach to the functional integration in the quantum field theory is not new. In a hidden form it can be found in the earlier papers on quantum gravity.[6] More recently these geometrical ideas have appeared in the context of Yang–Mills theory. It is known that the quotient of the space of connections by the group of gauge transformations is a principal nontrivial fibration.[7–9] Moreover, the gauge orbit manifold has a natural Riemannian structure[7,10] and the associated formal volume element gives rise to the Faddeev–Popov determinant.[10,11] In this paper, we will apply this geometrical approach to a discussion of the Faddeev–Popov procedure in Polyakov's theory. Our analysis will be performed on the algebraic level, i.e., the problems connected with the topology and differential structure of functional manifolds under consideration will be omitted. Such a restriction is in a way justifiable. There exist well-defined functional measures on infinite-dimensional manifolds (e.g., Gaussian measures on abstract Wiener manifolds[12]) that, in many cases, are insufficient for the quantum field theory, however. So, in physics the commonly used approach to functional integration is the heuristic one based on analogy with the finite-dimensional case. From this analogy only the algebraic structure of the formal calculus of functional measures can be derived. It seems that this structure should be, in general, preserved in future corrected theory. The present geometrical approach, in which the functional measure is introduced by means of a volume ∞-form, has some advantages. The invariance of the measure easily can be studied as the invariance of the underlying Riemannian metric. Moreover, various versions of the Fubini theorem seem to be powerful tools not only in those cases in which the volume of the gauge group must be extracted (the change of variable can be seen in fact as a special case of this theorem[13]). After this brief motivation of methods used in this paper, let us summarize its content.

In Sec. II the formal definition of functional measure in the spirit of Riemannian geometry is introduced. As examples, invariant measures on the space of scalar functions on an m-dimensional manifold and on the group of diffeomorphisms are studied. Some simple relations that immediately follow from definitions are obtained.

In Sec. III a version of the Fubini theorem on finite-dimensional manifolds is derived. The result is particularly appropriate in Polyakov's theory, but it can be applied to other gauge theories as well.

In Sec. IV the results of Secs. II and III are applied to a detailed discussion of the Faddeev–Popov procedure in Polyakov's theory. The exact form of the functional measure of the effective Liouville quantum field theory is derived.

II. FORMAL FUNCTIONAL MEASURES

The Riemannian measure induced by the Riemannian metric g on an m-dimensional manifold M can be defined by means of a volume m-form $d\omega^g$, which at the point $x\in M$ is determined by

$$d\omega^g_x = d\omega^1_x \wedge \cdots \wedge d\omega^m_x, \tag{2.1}$$

where $d\omega^i_x$ $(i=1,\ldots,m)$ form the basis dual to the orthonormal one $\{\delta\omega_{ix}\}_{i=1}^m$ in the tangent space T_xM at x:

$$g(\delta\omega_{ix},\delta\omega_{jx}) = \delta_{ij}, \tag{2.2}$$

$$d\omega^i_x(\delta\omega_{jx}) = \delta^i_j. \tag{2.3}$$

Since the formula (2.1) is independent of the choice of an oriented orthonormal basis in T_xM, this definition is correct.

We introduce Riemannian functional measures by means of volume ∞-forms, which are defined by formal extension of the formulas (2.1)–(2.3) to infinite-dimensional manifolds. Let us start with the simplest case of a constant metric on a vector space. We consider the space Φ_M of real functions on the compact m-dimensional Riemannian manifold (M,g); we introduce the constant metric on Φ_M:

$$G^g_\phi(\delta\phi,\delta\phi') = \int \sqrt{g}\, d^m z\, \delta\phi(z)\delta\phi'(z),$$

where $\phi\in\Phi_M$ and $\delta\phi',\delta\phi\in T_\phi\Phi_M\simeq\Phi_M$. In the space tangent

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to Φ_M one can choose the countable basis $\{\delta\phi_k\}_{k=1}^{\infty}$ for which the extension of formula (2.2) has the form

$$G^g(\delta\phi_k,\delta\phi_l)=\delta_{kl},\quad k,l\in\mathbb{N}.$$

However, such a basis is inconvenient (e.g., in the calculation of the determinant of elliptic operators it is convenient to use their integral kernels). Therefore we introduce the external orthonormal basis

$$G^g(\delta\phi_x,\delta\phi_y)=\delta(x-y)/\sqrt{g_0} \tag{2.4}$$

and the dual one

$$d\phi_x(\delta\phi_y)=\delta(x-y)/\sqrt{g_0}, \tag{2.5}$$

where g_0 is the additional Riemannian metric on M. The correct definition of an external basis in Φ_M (as distributions on a manifold M) requires some scalar product in Φ_M. In our case this product is defined by

$$(\phi,\phi')=\int\sqrt{g_0}\,d^m z\,\phi(z)\phi'(z).$$

The expressions on the right-hand side of Eqs. (2.4) and (2.5) play the role of Kronecker's delta in Eqs. (2.2) and (2.3). So it is clear that under global diffeomorphism of M considered as a change of the chart of a functional manifold Φ_M, g_0 remains unchanged.

Now we are ready to introduce the formal volume ∞-form related to the metric G^g

$$d\Omega^{G^g}=\bigwedge_{x\in M}d\phi_x. \tag{2.6}$$

In our approach, the well-known formal expression

$$\prod_x d\phi(x)$$

can be interpreted as the volume ∞-form related to the metric

$$\int dz^m\,\delta\phi(z)\delta\phi'(z).$$

The advantage of the definition (2.6) (which, of course, is completely formal) is that by analogy with Riemannian measures on finite-dimensional manifolds we are able to build a formal calculus of such functional measures. Now we use the analogy mentioned above to find the relation between $d\Omega^{G^g}$ and $d\Omega^{G^{g'}}$.

Let $\{\delta\omega_{ix}\}_{i=1}^m$, $\{\delta\omega'_{ix}\}_{i=1}^m$ be the orthonormal bases in T_xM with respect to metrics g and g'. If $A_{ij}(x)$ is the transition matrix from the $\{\delta\omega'_{ix}\}_{i=1}^m$, to the $\{\delta\omega_{ix}\}_{i=1}^m$ basis,

$$\delta\omega_{ix}=A_{ij}(x)\delta\omega'_{jx},$$

then

$$d\omega_x^{g'}=\det A(x)\cdot d\omega_x^g. \tag{2.7}$$

The external orthonormal bases $\{\delta\phi_x\}_{x\in M}$, $\{\delta\phi'_x\}_{x\in M}$ of metrics $G^g,G^{g'}$ have the form

$$\delta\phi_x(y)=\delta(x-y)/(g_0\,g)^{1/4},$$
$$\delta\phi'_x(y)=\delta(x-y)/(g_0\,g')^{1/4},$$

and therefore,

$$\delta\phi_x(y)=\left(\frac{g'}{g}\right)^{1/4}(x)\delta\phi'_x(y)$$
$$=\int\sqrt{g_0}\,dz^m\left(\frac{g'}{g}\right)^{1/4}(x)\,\frac{\delta(x-z)}{\sqrt{g_0}}\,\delta\phi'_z(y).$$

Applying the formula (2.7) in its extended version, we have

$$d\Omega^{G^{g'}}=\exp\left(\frac{1}{4}\int\ln\frac{g'}{g}\,\delta(0)dz^m\right)d\Omega^{G^g}. \tag{2.8}$$

Note that $\delta(0)$ cannot be extracted from the integral without breaking coordinate invariance. Now we consider the nonconstant metric on Φ_M:

$$\tilde{G}^g_\phi(\delta\phi,\delta\phi')=\int e^{\phi(z)}\sqrt{g}\,dz^m\,\delta\phi(z)\delta\phi'(z). \tag{2.9}$$

Applying our method, it is easy to obtain the following relation:

$$d\Omega^{\tilde{G}^g}_\phi=\exp\left(\frac{1}{2}\int\phi\delta(0)dz^m\right)d\Omega^{G^g}_\phi, \tag{2.10}$$

where $d\Omega^{\tilde{G}^g}_\phi$ ($d\Omega^{G^g}_\phi$) is the volume ∞-form related to the metric $\tilde{G}^g$ (G^g) at the point $\phi\in\Phi_M$.

Now we consider left-invariant measures on the infinite-dimensional Lie group. In the finite-dimensional case the left-invariant measures can be constructed as a Riemannian metric on the group manifold, which are completely determined by their values in the tangent space at a neutral group element. Without referring to a serious mathematical theory, we can assume in our heuristic approach that all that we have mentioned above remains valid in the infinite-dimensional case, too. As an example, we consider the group $\mathscr{D}_M$ —the connected component of neutral element of the group of diffeomorphisms of M on M. We assume that on $\mathscr{D}_M$ exists a topological structure such that $\mathscr{D}_M$ can be thought of as an infinite-dimensional Lie group with a Lie algebra containing all vector fields on M (for M without boundary). The problem of finding such a structure we leave aside in this paper: however, this question is nontrivial (e.g., $\mathscr{D}_M$ with the compact–open topology is not a Lie group). Let us introduce on the space $\mathscr{V}_M$ of all vector fields on M the scalar product H^g:

$$H^g(\delta V,\delta V')=\int\sqrt{g}\,dz^m\,g_{ab}\delta V^a\delta V'^b, \tag{2.11}$$

where $\delta V,\delta V'\in\mathscr{V}_M\simeq T_{\mathrm{id}}\mathscr{D}_M$. We define the external orthonormal basis $\{\delta V\}_{i=1,\dots,m,\ x\in M}$:

$$H^g(\delta V_{ix},\delta V_{jy})=g_{0ij}(x)\left[\delta(x-y)/\sqrt{g_0}\right]$$

and the dual one

$$dV^i_x(\delta V_{jy})=\delta^i_j\left[\delta(x-y)/\sqrt{g_0}\right].$$

We define the left-invariant volume ∞-form $d\Omega^{H^g}$ by its value at the identity diffeomorphism

$$d\Omega^{H^g}_{\mathrm{id}}=\bigwedge_{x\in M}dV^1_x\wedge\cdots\wedge dV^m_x.$$

Now we will seek a relation between $d\Omega^{H^g}$ and $d\Omega^{H^{g'}}$. Let $e^a_i(x),e'^b_j(x)$ be "m-beins" of metric g,g' with respect to the metric g_0:

$$g_{ab}(x)e_i^a(x)e_j^b(x) = g_{oij}(x),$$
$$g'_{ab}(x)e_i'^a(x)e_j'^b(x) = g_{oij}(x).$$

Then the orthonormal bases have the form

$$\delta V_{yi}^a(x) = e_i^a(x)[\delta(x-y)/(g\cdot g_0)^{1/4}],$$
$$\delta V_{yi}'^a(x) = e_i'^a(x)[\delta(x-y)/(g'\cdot g_0)^{1/4}],$$

and

$$\delta V_{yi}^a(x) = \left(\frac{g'}{g}\right)^{1/4} e_j^a(e'^{-1})_b^j \delta V_{yi}'^b(x).$$

Finally we obtain

$$d\Omega^{H^g} = \exp\left(\frac{2+m}{4}\int \ln\frac{g'}{g}\,\delta(0)dz^m\right)d\Omega^{H^g}. \quad (2.12)$$

III. THE SPECIAL VERSION OF THE FUBINI THEOREM

In this section we will consider the version of the Fubini theorem that (after formal generalization to the infinite-dimensional case) gives the geometrical interpretation of the Faddeev–Popov procedure.

Let τ be a homomorphism of a compact n-dimensional Lie group G into the group of isometries of an m-dimensional ($m>n$) Riemannian manifold (M,g). We consider the integral

$$\int_M f\,d\omega^g, \quad (3.1)$$

where f is a G-invariant function on M [i.e., $f(\tau_a x) = f(x)$ for $a\in G$] and $d\omega^g$ is the volume m-form on M related to the metric g. For simplicity we assume that isotropy subgroups at every point of M are trivial (i.e., $H_x = \{e\}$). The canonical projection $p' = M\to M/G$ induces on M the structure of locally trivial fibration (M,V,p') over the space of orbits $V = M/G$ with a typical fiber G. We assume further that fibration (M,V,p') is trivial, so a global cross section σ: $V\to M$ exists. It is convenient to consider instead of (M,V,p') the fibration $(M,\Sigma=\sigma(V), p=\sigma\circ p')$, which is, in fact, the principal fiber bundle with the structure group G. Since the fiber bundle (M,Σ,p) is trivial, for every point $x\in M$ the unique $a\in G$ and $u\in\Sigma$ for which $x=\tau_a u$ exist.

Our aim is to rewrite the integral (3.1) in terms of integrals with respect to suitable Riemannian measures on the group G and the submanifold Σ.

The first step in our derivation is the construction of a suitable expression of the volume m-form $d\omega^g$ as an exterior product of two forms on M. Let us introduce in the bundle (M,Σ,p) the family of global cross sections $\{\sigma_a\}_{a\in G}$, obtained by the action of the group G on the cross section $\sigma_e = \mathrm{id}$:

$$\sigma_a\colon\ \Sigma\ni u\to\sigma_a(u) = \tau_a u\in M.$$

By means of these cross sections we can construct a G-invariant decomposition of the tangent space at every point $x=\tau_a u\in M$:

$$T_xM = W_x^{\perp}\oplus W_x'', \quad (3.2)$$

where W_x'' is the space tangent to the submanifold $\Sigma_a = \sigma_a(\Sigma)\subset M$ at x and $W_x^{\perp}$ is the orthogonal complement of W_x'' (with respect to the metric g). It is possible to choose at every point $x\in M$ an orthonormal basis $\{\delta\omega_{ix}\}_{i=1}^m$ in T_xM such that vectors $\delta\omega_{ix}$ ($i=1,\ldots,n$) form G-invariant vector fields $\delta\omega_i$ on M, and $\{\delta\omega_{ix}\}_{i=1}^n$ is a basis of $W_x^{\perp}$ for every $x\in M$. Using the dual basis $\{d\omega_x^i\}_{i=1}^m$ we can write the following expression of the form $d\omega^g$:

$$d\omega_x^g = d\omega_x^1\wedge\cdots\wedge d\omega_x^m. \quad (3.3)$$

Now we will construct another m-form on M. Let us introduce the family of maps $\{\tau^u\}_{u\in\Sigma}$,

$$\tau^u\colon\ G\ni a\to\tau^u(a) = \tau_a u\in p^{-1}(u),$$

and a family of left-invariant Riemannian metrics on G, $\{h^u\}_{u\in\Sigma}$. Let $\{\delta s_i^u\}_{i=1}^n$ be a set of orthonormal (with respect to the metric h^u) left-invariant vector fields on G. If h^u depends smoothly on u, those fields can be chosen in such a way that the fields $\{\delta t_i\}_{i=1}^n$ defined at the point $x=\tau_a u\in M$ by the formula

$$\delta t_{ix} = \tau_*^u\,\delta s_{ia}^u,\quad i=1,\ldots,n,$$

are smooth, G-invariant vector fields on M. Let us complete $\{\delta t_{ix}\}_{i=1}^n$ to the basis $\{\delta t_{ix}\}_{i=1}^m$ in T_xM by adding the vectors

$$\delta t_{ix} = \delta\omega_{ix},\quad i=n+1,\ldots,m.$$

Using the dual basis $\{dt_x^i\}_{i=1}^m$ we can construct G-invariant forms on M:

$$d\omega_x^{\perp} = dt_x^1\wedge\cdots\wedge dt_x^n,$$
$$d\omega_x'' = dt_x^{n+1}\wedge\cdots\wedge dt_x^m, \quad (3.4)$$
$$d\omega = d\omega^{\perp}\wedge d\omega''.$$

For these forms the following relations are true:

$$d\omega^{\perp}{}_{|p^{-1}(u)} = (\tau^u)^{-1*}d\omega^{h^u}, \quad (3.5)$$
$$d\omega'' = p^*\,d\omega^{\Sigma}, \quad (3.6)$$

where $d\omega^{h^u}$ is the volume n-form on G related to the metric h^u and $d\omega^{\Sigma}$ is the volume $(m-n)$-form on the submanifold Σ related to the induced metric.

The transition matrix $[A_{ij}(x)]$ from the basis $\{\delta\omega_{ix}\}_{i=1}^m$ to the basis $\{\delta t_{ix}\}_{i=1}^m$ has the following form:

$$[A_{ij}(x)] = \begin{bmatrix}\Delta(x) & [g(\delta t_{ix},\delta\omega_{jx})]\\ 0 & 1\end{bmatrix},$$

where $\Delta(x)$ is an $n\times n$ matrix with elements

$$\Delta_{ij}(x) = g(\delta t_{ix},\delta\omega_{jx}),\quad i,j=1,\ldots,n.$$

The relation between forms $d\omega^g$ (3.3) and $d\omega$ (3.4) can be easily computed [see formula (2.7)] with the result

$$d\omega^g = \det\Delta\cdot d\omega.$$

Using Eq. (3.6) we have

$$d\omega^g = \det\Delta\cdot d\omega^{\perp}\wedge p^*\,d\omega^{\Sigma}. \quad (3.7)$$

Now we will elaborate a more convenient form of $\det\Delta$. From the G invariance of $g,\delta t_i,\delta\omega_j$ ($i,j=1,\ldots,n$) the G invariance of $\det\Delta$ follows. So, $\det\Delta$ as a function on Σ can be interpreted as the determinant of the linear operator

$$\Delta_u\colon\ T_eG\equiv\mathcal{G}\to W_u^{\perp}\subset T_uM,$$
$$\Delta_u = P_u^{\perp}\circ\tau_{*e}^u, \quad (3.8)$$

calculated in the orthonormal bases of the spaces $\mathcal{G}$ and

$W_u^\perp$. In the definition (3.8), $P_u^\perp$ denotes the projection on the subspace $W_u^\perp$ [see decomposition (3.2)] and $\mathcal{G}$ is the Lie algebra of G. We introduce an adjoint operator Δ_u^*, usually defined as

$$h_e^u(\Delta_u^*\delta\omega,\delta s) = g_u(\delta\omega,\Delta_u\delta s), \tag{3.9}$$

where $\delta\omega\in W_u^\perp$, $\delta s\in\mathcal{G}$. Since

$$\det\Delta(u) = (\det(\Delta^T\Delta)(u))^{1/2} = (\det\Delta_u^*\Delta_u)^{1/2},$$

we can interpret $\det\Delta(u)$ as a square root of determinant of the linear operator $\Delta_u^*\Delta_u:\mathcal{G}\to\mathcal{G}$.

Using the decomposition (3.7) we can apply the Fubini theorem on the manifold[10] to the integral (3.1):

$$\begin{aligned}\int_M f\,d\omega^g &= \int_M f\cdot\det\Delta\cdot d\omega^\perp\wedge p^*\,d\omega^\Sigma\\ &= \int_\Sigma f\cdot\det\Delta\cdot\left(\int_{p^{-1}(u)} d\omega^\perp\right)\cdot d\omega^\Sigma\\ &= \int_\Sigma f\cdot\det\Delta\cdot\left(\int_G d\omega^{h^u}\right)\cdot d\omega^\Sigma \end{aligned}\tag{3.10}$$

[the last equality follows from Eq. (3.5) and from the change of variable]. Finally, introducing a left-invariant reference metric h on G, we have the following version of the Fubini theorem:

$$\int_M f\,d\omega^g = \int_G d\omega^u\cdot\int_\Sigma f(\det\Delta_u^*\Delta_u)^{1/2}\left(\frac{h^u}{h}\right)^{1/2} d\omega^\Sigma. \tag{3.11}$$

This formula can be interpreted as the finite-dimensional version of the Faddeev–Popov procedure. If we choose the family of metrics $\{h^u\}_{u\in\Sigma}$ such that $h^u = h$ for every $u\in\Sigma$, Eq. (3.11) has the more familiar form

$$\int_M f\,d\omega^g = \int_G d\omega^h\cdot\int_\Sigma f(\det\Delta_u^*\Delta_u)^{1/2}\,d\omega^\Sigma. \tag{3.12}$$

In Ref. 11 a similar formula has been derived in which integration goes over the space of orbits. The advantage of the formula (3.12) is that the integration is performed over the gauge slice, parametrization of which is explicitly known. Moreover, the measure $d\omega^\Sigma$ can be obtained easily as one related to the induced metric on Σ.

IV. APPLICATIONS TO POLYAKOV'S MODEL OF A BOSONIC STRING

Let us briefly recall the basic concepts of Polyakov's method for calculating averages of functionals defined on surfaces. Such averages generally can be expressed in symbolic form as follows:

$$\int_{\mathcal{S}} d\Omega\,F[s]e^{-W[s]}, \tag{4.1}$$

where $\mathcal{S}$ denotes some space of surfaces embedded in $\mathbb{R}^d$ and endowed with the intrinsic Riemannian metric. The surface $s\in\mathcal{S}$ can be described by its parametrization (x,g), where x is the embedding of some fixed two-dimensional manifold M in $\mathbb{R}^d$ and g is the Riemannian metric on M. It is easy to see that if ψ is a diffeomorphism of M, then the parametrizations (x,g), $(x\circ\psi,\psi^*g)$ describe an identical surface in $\mathbb{R}^d$ with its intrinsic metric $x^{-1*}g$. Therefore we can write

$$\mathcal{S} = \mathcal{P}_M/\mathcal{D}_M = (\mathcal{M}_M\times\chi_M)/\mathcal{D}_M = (\mathcal{M}_M/\mathcal{D}_M)\chi_M,$$

where $\mathcal{P}_M$ is the space of the parametrizations, $\mathcal{M}_M$ is the space of Riemannian metrics on M, χ_M is the space of embeddings of M into $\mathbb{R}^d$, and $\mathcal{D}_M$ is the group of diffeomorphisms (see Sec. II). It is clear that the integral (4.1) can be defined by means of the integral

$$\int_{\mathcal{M}_M} d\Omega^{\mathcal{M}}\int_{\chi_M} d\Omega^\chi\,F[x,g]\exp^{-W[x,g]},$$

provided that the measures $d\Omega^{\mathcal{M}}$, $d\Omega^\chi$ and the action $W[x,g]$ are $\mathcal{D}_M$ invariant. Polyakov's proposal is to introduce $d\Omega^{\mathcal{M}}$ and $d\Omega^\chi$ as the volume ∞-forms related to the Riemannian metrics $G^{\mathcal{M}}$ on $\mathcal{M}_M$ and G^χ on χ_M:

$$\begin{aligned}&G_g(\delta g,\delta g')\\ &\quad= \int\sqrt{g}\,d^2z\left[\frac{1}{2}(g^{ac}g^{bd}+g^{ad}g^{bc}-g^{ab}g^{cd})\right.\\ &\qquad\left.+ug^{ab}g^{cd}\right]\delta g_{ab}\,\delta g'_{cd}\end{aligned}$$

($\delta g,\delta g'\in T_g\mathcal{M}_M$, u is an arbitrary positive real number),

$$G_x^\chi(\delta x,\delta x') = \int\sqrt{g}\,d^2z\,\delta x^\mu(z)\delta x'^\mu(z)$$

($\delta x,\delta x'\in T_x\chi_M$). These metrics are covariantly defined: this ensures the formal $\mathcal{D}_M$ invariance of $d\Omega^{\mathcal{M}}$ and $d\Omega^\chi$. In different physical applications various spaces of surfaces and various actions are used.[2,4] For our purpose it is sufficient to consider the integral over closed surfaces

$$\begin{aligned}z = &\int_{\mathcal{M}_M} d\Omega^{\mathcal{M}}\int_{\chi_M} d\Omega^\chi\\ &\times\exp\left(-\frac{1}{2}\int_M\sqrt{g}\,d^2z\,g^{ab}\,\partial_a x^\mu\partial_b x^\mu-\mu\int\sqrt{g}\,dz^2\right).\end{aligned}$$

Let us notice that the volume ∞-form $d\Omega^\chi$ depends on $g\in\mathcal{M}_M$ so the integration over χ_M must be performed first. In our case this integral is Gaussian and

$$\begin{aligned}&\int_{\mathcal{M}_M} d\Omega^\chi\exp\left(-\frac{1}{2}\int_M\sqrt{g}\,d^2z\,g^{ab}\,\partial_a x^\mu\,\partial_b x^\mu\right)\\ &\quad= (\det\mathcal{L}_g^0)^{-d/2},\end{aligned}$$

where $\mathcal{L}_g^0$ denotes the Laplace–Beltrami differential operator

$$\mathcal{L}_g^0 = -(1/\sqrt{g})\partial_a\sqrt{g}g^{ab}\,\partial_b$$

acting on the space Φ_M of scalar real functions on M. From the $\mathcal{D}_M$ invariance of the action and $d\Omega^\chi$ it follows that $\det\mathcal{L}_g^0$ can be treated as a $\mathcal{D}_M$-invariant functional on $\mathcal{M}$. Therefore we can apply the Faddeev–Popov method to the integral

$$z = \int_{\mathcal{M}_M} d\Omega^{\mathcal{M}}(\det\mathcal{L}_g^0)^{-d/2}. \tag{4.2}$$

The first step is to introduce some gauge fixing conditions. In the conformal gauge proposed by Polyakov[1] the gauge slice is the subspace of metrics conformal to some fixed metric $\hat{g}$ on M, i.e., gauge fixing condition has the form

$$g = e^\phi\hat{g}, \tag{4.3}$$

where $\phi\in\Phi_M$. However, in this gauge some problems connected with the global topological structure of manifold M arise. If the Euler characteristic of M is non-negative, then the continuous group of diffeomorphisms (the so-called conformal group of M) exists. The action of a diffeomorphism from this group on $e^{\phi}\hat{g}$ is equivalent to the change in the conformal factor e^{ϕ}, so Eq. (4.3) does not fix the gauge completely. If the Euler characteristic of M is nonpositive, then there exist gauge slices that cannot be transformed into one another by any diffeomorphism of M. Such nonequivalent slices are parametrized by the so-called Teichmüller parameters. Because the dimension of the conformal group as well as the dimension of space of Teichmüller parameters in every topological sector is finite, all problems mentioned above can be treated separately (for details see Ref. 2). These remarks justify the assumption that the conformal gauge is a good, global one, i.e., that the representation of every $g\in\mathscr{M}_M$,

$$g=\psi^*(e^{\phi}\hat{g}),\quad \psi\in\mathscr{D}_M,\quad \phi\in\Phi_M,$$

is unique. Let us denote by $\Sigma\hat{g}$ the gauge slice defined by Eq. (4.3) and introduce the map

$$\Pi\colon\ \mathscr{M}_M\ni g=\psi^*(e^{\phi}\hat{g})\to\Pi(g)=e^{\phi}\hat{g}\in\Sigma\hat{g}.$$

According to our assumptions the fiber bundle $(\mathscr{M}_M,\Sigma\hat{g},\Pi)$ is trivial and the analogy between the integral (4.2) and the integral (3.1) becomes complete, so the results of Sec. III can be used.

First of all we must construct a $\mathscr{D}_M$-invariant orthonormal decomposition of the space $\mathscr{T}_{\phi}$ tangent to $\mathscr{M}_M$ at every point $e^{\phi}\hat{g}\in\Sigma\hat{g}$. The space $\mathscr{T}_{\gamma}$ is the space of all second-order symmetric covariant tensors on M. Let us introduce the subspace of traceless tensors

$$\mathscr{H}_{\phi}=\{\delta g\in\mathscr{T}_{\phi}\colon\ \hat{g}^{ab}\delta g_{ab}=0\},$$

and the subspace tangent to $\Sigma\hat{g}$

$$\mathscr{K}_{\phi}=\{\delta g\in T_{\phi}\colon\ \delta g_{ab}=\delta\phi e^{\phi}\hat{g}_{ab},\ \delta\phi\in\Phi_M\}.$$

The spaces $\mathscr{H}_{\phi}$ and $\mathscr{K}_{\phi}$ are the orthogonal one to another with respect to the metric $G^{\mathscr{M}}$ and the decomposition

$$\mathscr{T}_{\phi}=\mathscr{H}_{\phi}\oplus\mathscr{K}_{\phi}$$

is the required one.

Next, we introduce the family of left-invariant metrics $\{H^g\}_{g\in\Sigma\hat{g}}$ on the group $\mathscr{D}_M$ [see formula (2.11)]. In the case under consideration, the operator Δ [see formula (3.8)] has the form

$$\Delta_{\phi}\colon\ \mathscr{V}_M\to\mathscr{H}_{\phi},$$
$$(\Delta_{\phi}\delta V)_{ab}(z)=(g_{ac}\nabla_b+g_{bc}\nabla_a-2g_{ab}\nabla_c)\delta V^c(z),$$

where $g=e^{\phi}\hat{g}$ and ∇ is the covariant derivative defined by g. The operator $\mathscr{L}_{\phi}=\Delta_{\phi}^{*}\Delta_{\phi}\colon\ \mathscr{V}_M\to\mathscr{V}_M$ can be derived from the equation

$$G^{M}_{e^{\phi}\hat{g}}(\Delta_{\phi}\,\delta V,\Delta_{\phi}\,\delta V')=H^{g}_{\mathrm{id}}(\delta V,\mathscr{L}_{\phi}\,\delta V'),$$

which can be rewritten in the following form:

$$\int\sqrt{g}\,dz^2\,\frac{1}{2}\,(g^{ac}g^{bd}+g^{ad}g^{bc}-g^{ab}g^{cd})\times(\Delta_{\phi}\delta V)_{ab}(z)(\Delta_{\phi}\delta V')_{cd}(z)=\int\sqrt{g}\,dz^2\,g_{ab}(\mathscr{L}_{\phi}\,\delta V)^a(z)\delta V'^b(z).$$

After simple calculations one gets

$$(\mathscr{L}_{\phi}\delta V)^a(z)=-2(\nabla_c\nabla^c\delta^a_b+[\nabla_b,\nabla^a])\delta V^b(x).$$

This is exactly the same operator which appears in Polyakov's consideration.[1] The determinant of $\mathscr{L}_{\phi}$ (as well as the determinant of $\mathscr{L}^0_{\phi}$) can be evaluated by the conformal anomaly method up to terms independent of the conformal factor.[2,3]

Now we are able to explain usefulness of the construction involving the family of metrics $\{H^g\}_{g\in\Sigma\hat{g}}$ on the gauge group $\mathscr{D}_M$. If we fix some metric in $\mathscr{D}_M$, for example $H^{\hat{g}}$, then in order to extract the volume of $\mathscr{D}_M$ from the integral (4.2) according to the formula (3.11), we must calculate the determinant of the operator $\hat{\mathscr{L}}$ defined by the following formula:

$$\hat{\mathscr{L}}_{\phi}=e^{2\phi}\mathscr{L}\phi.$$

However, it is difficult to obtain full information about ϕ independence of $\det\hat{\mathscr{L}}_{\phi}$.

According to Eq. (3.10) the integral (4.2) can be rewritten in the following form:

$$\int_{\Sigma_{\hat{g}}}\left(\int_{\mathscr{D}_M}d\Omega^{\phi}\right)(\det\mathscr{L}^0_{\phi})^{-d/2}(\det\mathscr{L}_{\phi})^{1/2}\,d\Omega^{\Sigma_{\hat{g}}},\qquad(4.4)$$

where the abbreviations $d\Omega^{\phi}=d\Omega^{H^{e^{\phi}\hat{g}}}$, $\mathscr{L}^0_{\phi}=\mathscr{L}^0_{e^{\phi}\hat{g}}$ are used and $d\Omega^{\Sigma_{\hat{g}}}$ denotes the volume ∞-form on $\Sigma_{\hat{g}}$ related to the metric $\hat{G}$ on $\Sigma_{\hat{g}}$ induced by the metric $G^{\mathscr{M}}$. For $\delta g=\delta\phi e^{\phi}g$, $\delta g'=\delta\phi' e^{\phi}\hat{g}\in\mathscr{K}_{\phi}$, we have

$$\hat{G}_{e^{\phi}\hat{g}}(\delta g,\delta g')=G^{\mathscr{M}}_{e^{\phi}\hat{g}}(\delta\phi e^{\phi}\hat{g},\delta\phi' e^{\phi}\hat{g})=4u\int e^{\phi}\sqrt{\hat{g}}\,dz^2\,\delta\phi(z)\,\delta\phi'(z).$$

Therefore by change of variables in the integral (4.4) we obtain the following expression:

$$\int_{\Phi_M}\left(\int_{\mathscr{D}_M}d\Omega^{\phi}\right)(\det\mathscr{L}^0_{\phi})^{-d/2}(\det\mathscr{L}_{\phi})^{1/2}\,d\Omega^{\tilde{G}^{\hat{g}}},$$

where the volume ∞-form $d\Omega^{\tilde{G}^{\hat{g}}}$ is that defined in Sec. II. Now, applying the relations (2.10) and (2.12) we have

$$z=\int_{\mathscr{D}_M}d\Omega^{H^{\hat{g}}}\int_{\Phi_M}d\Omega^{G^{\hat{g}}}\left[\exp(-S_L[\phi,\hat{g}])\times\exp\left(\frac{3}{2}\int_M\phi(z)\delta(0)dz^2\right)\right],$$

where $S_L[\phi,\hat{g}]=(d/2)\ln\det\mathscr{L}^0_{\phi}-\frac{1}{2}\ln\det\mathscr{L}_{\phi}$. In order to obtain the "physical" partition function we must choose some metric on M to normalize the volume of the gauge group $\mathscr{D}_M$. It is natural to choose the metric g_0 used in Sec. II in the definition of the external basis [see formulas (2.4) and (2.5)]. Applying the relation (2.10) once again, we have finally

$$z_{\text{phys}} = \int_{\Phi_M} d\Omega^{G^{\hat{g}}} \left[\exp(-S_L[\phi,\hat{g}]) \exp\left(\frac{3}{2} \int_M \phi(z)\delta(0)dz^2 + \int \ln \frac{\hat{g}}{g_0} \delta(0)dz^2 \right) \right].$$

For completeness, let us rewrite the last formula applying the explicit form of the Liouville action $S_L[\phi,\hat{g}]$, which has been derived in its general form by Alvarez in Ref. 2:

$$z_{\text{phys}} = \int_{\Phi_M} d\Omega^{G^{\hat{g}}} \left[\exp\left(-\frac{26-d}{48\pi} \left(\frac{1}{2} \int_M \sqrt{g}\, d^2 z\, g^{ab} \partial_a \phi\, \partial_b \phi + \int_M \sqrt{\hat{g}}\, dz^2\, \hat{R}\phi \right) \right) \right.$$
$$\left. \times \exp\left(-\mu \int_M \sqrt{\hat{g}}\, d^2 z\, e^{\phi} + S[\hat{g}] \right) \exp\left(\frac{3}{2} \int_M \phi(z)\, \delta(0)\, dz^2 + \int \ln \frac{\hat{g}}{g_0} \delta(0)\, dz^2 \right) \right],$$

where $S[\hat{g}]$ denotes the part of $S_L[\phi,\hat{g}]$ independent of ϕ. In other words, one can say that the effective quantum field theory in Polyakov's method of averaging is determined by the Liouville action $\mathscr{S}_L[\phi,\hat{g}]$ and by the functional measure related to the nonconstant metric:

$$G_{\phi}(\delta\phi,\delta\phi') = \int \sqrt{\hat{g}}\, dz^2\, e^{3\phi} \left(\frac{\hat{g}}{g_0} \right)^2 \delta\phi\delta\phi',$$

where

$$\phi \in \Phi_M, \quad \delta\phi,\delta\phi' \in T_{\phi}\Phi_M \simeq \Phi_M.$$

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Basis states for relativistic three-body calculations of particles with spin

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Using a linear combination of the three-body helicity states constructed by Wick, a new set of basis states is constructed that can be used to perform three-body calculations with relativistic treatment of the spin. These states are diagonal in the usual angular momentum quantum numbers of a pair $l_i S_i j_i$, where l_i is the orbital angular momentum, S_i the spin, and j_i the total angular momentum of the pair jk. These states are used to write down the relativistic Faddeev equations obtaining two sets of uncoupled integral equations that are identified as corresponding to the states of positive and negative parity. It is also shown, by means of some simple examples, that the relativistic recoupling coefficients reduce to the usual nonrelativistic ones if one neglects the effects of relativity. Some possible applications involving particles off the mass shell are discussed.

I. INTRODUCTION

The existing controversy in recent years regarding the polarization observables of the pion–deuteron system in the energy region of the P_{33} resonance[1–8] has given us a clear indication of the need for a careful treatment of the spin variables in the relativistic three-body problem.[9] Such a treatment is obviously more necessary in the case of polarization observables, since for these the spin degrees of freedom are the most relevant variables. Of course, in the case of spin-averaged quantities like differential cross sections, these new effects will tend to be washed out to a large extent by the averaging procedure, and the standard method that treats the spin nonrelativistically may give reasonable results for these quantities.[10–13]

The relativistic Faddeev equations are normally written in the three-body c.m. frame, in terms of two-body amplitudes which are known only in the two-body c.m. frame of each pair. Thus, it becomes necessary to express the three-body equations in terms of relative coordinates of the pairs both for the space and spin variables. In the case of the space variables this is a well understood procedure,[10,12] although this is not so for the spin part. The problem with the treatment of the spin in a relativistic theory is that the spin projection of a particle is defined only with respect to its rest frame.[14] Thus, the quantum number ν, which represents the projection of the spin in the three-body c.m. frame, actually means the projection that one will measure if one goes from the three-body c.m. frame to the rest frame of the particle. Similarly, the quantum number λ, which represents the projection of the spin in the two-body c.m. frame, also means the projection that one will measure if one goes from the two-body c.m. frame to the rest frame of the particle. Thus, if one wishes to express the spin variables defined in the three-body c.m. frame in terms of spin variables defined in the two-body c.m. frame, one must perform a well defined procedure that, however, is rather complicated if the spin projections are taken with respect to a fixed set of axes.[15,16] This transformation on the other hand, is very simple if the spin projections are taken with respect to the direction of motion of the particle, which corresponds to the helicity convention. Thus, the quantum numbers λ and ν represent in this case the helicities of the particle in the two-body and three-body c.m. frames, respectively. The reason why the transformation is simple in the helicity convention is that the helicity quantum number is invariant under Lorentz transformations along the direction of motion of the particle as well as under rotations.[14,17] The transformation of the spin variables in the helicity basis is given simply as

$$|s\lambda\rangle = \sum_{\nu} d^{s}_{\nu\lambda}(\beta)|s\nu\rangle, \tag{1}$$

where $d^{s}_{\nu\lambda}(\beta)$ is a Wigner rotation matrix and the argument β is the angle between the velocities of the two-body and three-body c.m. frames as seen from the rest frame of the particle.[18]

As we will show in this paper, the relativistic Faddeev equations can be partial-wave decomposed including the transformation of the spin given in Eq. (1), by using a linear combination of the three-body helicity states constructed by Wick.[18] The resulting integral equations have the same degree of complexity as the nonrelativistic ones and decouple into two sets that correspond to the states of positive and negative parity. They resemble even more their nonrelativistic counterparts in the fact that they contain explicitly the familiar quantum numbers of a pair $l_i S_i j_i$, where l_i is the orbital angular momentum, S_i the spin, and j_i the total angular momentum of the pair.

We review briefly in Sec. II the three-body helicity formalism developed by Wick[18] and in Sec. III introduce the new set of basis states that contain the familiar quantum numbers $l_i S_i j_i$. In Sec. IV we write down the integral equations for the three-body problem using these basis states and show that the equations decouple into two independent sets according to their parity. In Sec. V we make the connection between these states and the nonrelativistic ones for some simple examples, and show that for these cases the relativistic states have the correct nonrelativistic limit. Finally, in Sec. VI we discuss the application of this formalism for some

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problems involving particles off the mass shell.

II. WICK'S THREE-BODY HELICITY STATES

The helicity quantum number is the projection of the spin along the direction of motion of the particle.[17,18] The helicity basis states for three free particles have been constructed by Wick[18] as

$$
\begin{aligned}
&|q_i\nu_i JMp_i\lambda_j\lambda_k\, j_i m_i\rangle \\
&\quad = \eta_{j_i}\eta_J e^{-i\pi s_k}\int \sin\theta_i\, d\theta_i\, d^{\,j_i}_{m_i,\lambda_j-\lambda_k}(\theta_i) \\
&\qquad \times \sum_{\nu_j\nu_k} d^{\,s_j}_{\nu_j\lambda_j}(\beta_j) d^{\,s_k}_{\nu_k\lambda_k}(\beta_k)\int d\varphi_i \sin\theta_i'\, d\theta_i'\, d\varphi_i' \\
&\qquad \times \mathscr{D}^{J}_{m_i-\lambda_i,M}(\varphi_i,\theta_i',\varphi_i')|\mathbf{k}_i\nu_i\mathbf{k}_j\nu_j\mathbf{k}_k\nu_k\rangle, \qquad (2)
\end{aligned}
$$

where s_i, s_j, s_k are the spins of the three particles, and $\mathbf{k}_i,\mathbf{k}_j,\mathbf{k}_k$ and ν_i,ν_j,ν_k are the momenta and helicities of the three particles measured in the three-body c.m. frame,

$$\mathbf{k}_i+\mathbf{k}_j+\mathbf{k}_k=0. \qquad (3)$$

The relative momentum between particle i and the center of mass of the pair jk measured in the three-body c.m. frame is of course $\mathbf{q}_i=-\mathbf{k}_i$, which has the polar components $(q_i,\theta_i',\varphi_i')$, while the relative momentum between particles j and k measured in the two-body c.m. frame is $\mathbf{p}_i$, which has the polar coordinates (p_i,θ_i,φ_i). The quantum numbers ν_i, J, and M are the helicity of particle i, the total angular momentum of the system, and its magnetic projection, all of which are measured in the three-body c.m. frame, while the quantum numbers λ_j,λ_k,j_i, and m_i are the helicities of particles j and k, the total angular momentum of the pair, and its magnetic projection, which are all measured in the two-body c.m. frame. The functions $d^{\,s_j}_{\nu_j\lambda_j}(\beta_j)$ and $d^{\,s_k}_{\nu_k\lambda_k}(\beta_k)$ are the matrix elements of the unitary transformation (1) that transforms the helicity spinors from the three-body c.m. frame to the two-body c.m. frame, while the constants η_J are given by

$$\eta_J=((2J+1)/4\pi)^{1/2}. \qquad (4)$$

The states (2) were constructed by Wick, by starting with the state $|p_i\lambda_j\lambda_k\rangle$ of particles j and k in the c.m. frame of the pair in which particle j has helicity λ_j and momentum p_i in the positive Z direction, while particle k has helicity λ_k and momentum p_i in the negative Z direction. To obtain a two-body state in an arbitrary reference frame, first an operator $R_{0\theta\rho}$ is applied, where $R_{0\theta\rho}=e^{-i\theta J_y}$ produces a rotation along the Y axis, that is,

$$R_{0\theta\rho}|p_i\lambda_j\lambda_k\rangle=e^{-i\pi s_k}|\mathbf{p}_i\lambda_j\lambda_k\rangle, \qquad (5)$$

where now $\mathbf{p}_i$ is a vector in the ZX plane at an angle θ_i from the Z axis, and the phase $e^{-i\pi s_k}$ is necessary in order to define consistently the helicity state of particle k in the "south pole" $\theta_i=\pi$. Next, a Lorentz operator Z is applied that transforms the state (5) into a state with total momentum $\mathbf{q}_i=\mathbf{k}_j+\mathbf{k}_k$ along the positive Z axis, that is,

$$
\begin{aligned}
&ZR_{0\theta\rho}|p_i\lambda_j\lambda_k\rangle \\
&\quad = e^{-i\pi s_k}\sum_{\nu_j\nu_k} d^{\,s_j}_{\nu_j\lambda_j}(\beta_j)\, d^{\,s_k}_{\nu_k\lambda_k}(\beta_k)|\mathbf{k}_j\nu_j\mathbf{k}_k\nu_k\rangle, \qquad (6)
\end{aligned}
$$

and finally to the state (6) the operator $e^{-i\varphi_i J_z}$ is applied to get a state where $\mathbf{p}_i=(p_i,\theta_i,\varphi_i)$, since $\varphi_{\mathbf{k}_j}=\varphi_{\mathbf{p}_i}$. If now a rotation operator $R_{\varphi_i'\theta_i'0}=e^{-i\varphi_i' J_z}e^{-i\theta_i' J_y}$ is applied to the state (6), one obtains a state with total momentum $\mathbf{q}_i=(q_i,\theta_i',\varphi_i')$, so that multiplying this state by the single-particle state $|\mathbf{k}_i\nu_i\rangle=|-\mathbf{q}_i\nu_i\rangle$ corresponding to the third particle i with momentum $-\mathbf{q}_i$ and helicity ν_i, and taking the partial-wave projection, the state (2) is obtained.

III. BASIS STATES CONTAINING THE ORBITAL ANGULAR MOMENTUM AND SPIN OF A PAIR

One of the most attractive features of the three-body helicity states (2) is that the quantum numbers of the two-body subsystem jk are all defined in the c.m. frame of the pair and therefore the matrix elements of a two-body operator in the three-body basis space can be related directly to the two-body matrix elements in their own subspace. In most cases, however, for which a three-body relativistic formalism is required, the two-body amplitudes are given not in terms of helicity quantum numbers but in terms of the orbital angular momentum and spin quantum numbers of the pairs. Therefore, it is necessary, for physical applications, to introduce a new set of basis states that are a linear combination of the states (2) such that they are eigenstates of the familiar operators $\mathbf{l}_i$ and $\mathbf{S}_i$, where $\mathbf{l}_i$ is the relative orbital angular momentum of the pair and $\mathbf{S}_i$ its spin.

Since a two-body state in the $l_iS_i\,j_i$ representation can be expressed as a linear combination of two-body helicity states of the form[17]

$$
\begin{aligned}
&|l_iS_i\,j_im_i\rangle \\
&\quad = \sum_{\lambda_j\lambda_k}\left(\frac{2l_i+1}{2j_i+1}\right)^{1/2} C^{l_iS_ij_i}_{0,\lambda_j-\lambda_k}\, C^{s_js_kS_i}_{\lambda_j-\lambda_k}|\lambda_j\lambda_k\, j_im_i\rangle, \qquad (7)
\end{aligned}
$$

if we take the same linear combination of three-body helicity states (2), we get the new states

$$
\begin{aligned}
&|q_i\nu_i JMp_il_iS_i\,j_im_i\rangle \\
&\quad = \sum_{\lambda_j\lambda_k}\left(\frac{2l_i+1}{2j_i+1}\right)^{1/2} C^{l_iS_ij_i}_{0,\lambda_j-\lambda_k}\, C^{s_js_kS_i}_{\lambda_j-\lambda_k}\eta_{j_i}\eta_J e^{-i\pi s_k} \\
&\qquad \times\int \sin\theta_i\, d\theta_i\, d^{\,j_i}_{m_i,\lambda_j-\lambda_k}(\theta_i) \\
&\qquad \times\sum_{\nu_j\nu_k} d^{\,s_j}_{\nu_j\lambda_j}(\beta_j)\, d^{\,s_k}_{\nu_k\lambda_k}(\beta_k) \\
&\qquad \times\int d\varphi_i \sin\theta_i'\, d\theta_i'\, d\varphi_i'\, \mathscr{D}^{J}_{m_i-\lambda_i,M}(\varphi_i,\theta_i',\varphi_i') \\
&\qquad \times|\mathbf{k}_i\nu_i\mathbf{k}_j\nu_j\mathbf{k}_k\nu_k\rangle, \qquad (8)
\end{aligned}
$$

which contain the desired quantum numbers.

If we normalize the single-particle helicity states invariantly in the mass shell as

$$\langle\mathbf{k}_i'\nu_i'|\mathbf{k}_i\nu_i\rangle=2\omega_i(k_i)\delta(\mathbf{k}_i'-\mathbf{k}_i)\delta_{\nu_i'\nu_i}, \qquad (9)$$

where

$$\omega_i(k)=(m_i^2+k^2)^{1/2}, \qquad (10)$$

then we have that for states $|\mathbf{k}_i\nu_i\mathbf{k}_j\nu_j\mathbf{k}_k\nu_k\rangle$ which satisfy the condition (3), we can write

$$\langle \mathbf{k}_i'\nu_i'\mathbf{k}_j'\nu_j'\mathbf{k}_k'\nu_k' | \mathbf{k}_i\nu_i\mathbf{k}_j\nu_j\mathbf{k}_k\nu_k\rangle = \frac{8W_i(p_iq_i)\omega_i(q_i)\omega_j(p_i)\omega_k(p_i)}{\omega(p_i)}\delta(\mathbf{p}_i'-\mathbf{p}_i) \times\delta(\mathbf{q}_i'-\mathbf{q}_i)\,\delta_{\nu_i'\nu_i}\delta_{\nu_j'\nu_j}\delta_{\nu_k'\nu_k}, \tag{11}$$

where

$$\omega(p_i) = (m_j^2+p_i^2)^{1/2} + (m_k^2+p_i^2)^{1/2}, \tag{12}$$

$$W_i(p_iq_i) = [\omega^2(p_i)+q_i^2]^{1/2}, \tag{13}$$

$$W(p_iq_i) = (m_i^2+q_i^2)^{1/2} + [\omega^2(p_i)+q_i^2]^{1/2}. \tag{14}$$

If we apply Eq. (11) together with the orthogonality relations of the rotation matrices and of the Clebsch–Gordan coefficients, it is easy to see that the basis states (8) are normalized as

$$\langle q_i'\nu_i'J'M'p_i'l_i'S_i'j_i'm_i'|q_i\nu_iJMp_il_iS_ij_im_i\rangle = \frac{8W_i(p_iq_i)\omega_i(q_i)\omega_j(p_i)\omega_k(p_i)}{\omega(p_i)} \times\frac{1}{p_i^2}\delta(p_i'-p_i)\frac{1}{q_i^2}\delta(q_i'-q_i)\delta_{\nu_i'\nu_i} \times\delta_{J'J}\,\delta_{M'M}\delta_{l_i'l_i}\delta_{S_i'S_i}\delta_{j_i'j_i}\delta_{m_i'm_i}, \tag{15}$$

so that they form a complete set such that

$$1 = \sum_{\substack{\nu_iJM\\ l_iS_ij_im_i}}\int p_i^2\,dp_i\,q_i^2\,dq_i\,\frac{\omega(p_i)}{8W_i(p_iq_i)\omega_i(q_i)\omega_j(p_i)\omega_k(p_i)} \times|q_i\nu_iJMp_il_iS_ij_im_i\rangle\langle q_i\nu_iJMp_il_iS_ij_im_i|. \tag{16}$$

The recoupling coefficients between a state (8) of type i and a state of type j can be obtained by applying Wick's result for the states (2) [see Eq. (35) of Ref. 18] and the transformation (7), so as to get in our normalization

$$\langle q_i\nu_iJ'M'p_il_iS_ij_im_i|q_j\nu_jJMp_jl_jS_jj_jm_j\rangle = \delta_{J'J}\,\delta_{M'M}\,\delta[W(p_iq_i)-W(p_jq_j)] \times H(1-\cos^2\chi)\frac{4\omega(p_i)\omega(p_j)}{p_iq_ip_jq_j} \times\langle q_i\nu_ip_il_iS_ij_im_i|q_j\nu_jp_jl_jS_jj_jm_j\rangle_J, \tag{17}$$

where $W(p_iq_i)$ is the total energy of the system as given by Eq. (14), H is the step function, and the reduced recoupling coefficients are given by

$$\langle q_i\nu_ip_il_iS_ij_im_i|q_j\nu_jp_jl_jS_jj_jm_j\rangle_J = (2l_i+1)^{1/2}(2l_j+1)^{1/2}d^J_{m_j-\nu_j,m_i-\nu_i}(\chi) \times\sum_{\lambda_i\lambda_k\lambda_k'\lambda_i'}C^{l_iS_ij_i}_{0,\lambda_j-\lambda_k}C^{s_js_kS_i}_{\lambda_j-\lambda_k}C^{l_jS_jj_j}_{0,\lambda_k'-\lambda_i'} \times C^{s_ks_jS_j}_{\lambda_k'-\lambda_i'}(-)^{s_j-\nu_j+s_k+\lambda_k'}d^{j_i}_{m_i,\lambda_j-\lambda_k}(\theta_i) \times d^{j_j}_{m_j,\lambda_k'-\lambda_i'}(\theta_j)d^{s_i}_{\lambda_i',\nu_i}(-\beta_i)d^{s_j}_{\nu_j\lambda_j}(\beta_j)d^{s_k}_{\lambda_k'\lambda_k}(\rho_k). \tag{18}$$

The arguments of the rotation matrices in Eq. (18) are the angles of the Wick triangle shown in Fig. 1, where the distances oi and oj represent the velocities of particles i and j in the three-body c.m. frame, the distances aj and ak represent the velocities of particles j and k in the two-body c.m. frame

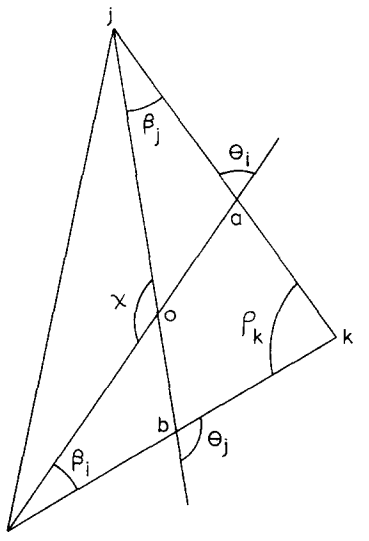

FIG. 1. The Wick triangle.

of the pair jk, etc. Since the distances in Fig. 1 are defined in a non-Euclidean space, the sum of the internal angles of a triangle is smaller than π. We give in Appendix A the necessary formulas to construct the angles of Fig. 1 as a function of the relative variables p_i, q_i, p_j, and q_j.

IV. PARTIAL-WAVE DECOMPOSITION OF THE RELATIVISTIC FADDEEV EQUATIONS

As an example of the usefulness of the basis states constructed in the previous section, we will carry out the partial-wave decomposition of the relativistic generalization of the Faddeev equations proposed by Aaron, Amado, and Young[19] with the modification introduced by Garcilazo and Mathelitsch[20,21] so as to use them also in the bound-state problem. These equations have the standard Faddeev form

$$T_i = t_i + \sum_{j\neq i} t_iG_0T_j, \tag{19}$$

where an invariant phase space must be used, and G_0 is the Green's function for three free particles which is obtained by putting the three particles on their mass shells and performing a dispersion integral in the total energy of the system $\sqrt{S}$ or in the total energy squared S as proposed by Blankenbecler and Sugar,[22] so as to get in each case

$$G_0(\sqrt{S};p_iq_i) = \frac{1}{\sqrt{S}-W(p_iq_i)+i\epsilon}, \tag{20a}$$

$$G_0(S;p_iq_i) = \frac{2W(p_iq_i)}{S-W^2(p_iq_i)+i\epsilon}, \tag{20b}$$

where we have used Eq. (14) to express the total energy in terms of the relative variables p_i and q_i.

The two-body amplitudes t_i taken between basis states (8) are given in the case of central interactions (the generalization to the case of noncentral interactions is straightforward) as

$$\langle q_i'\nu_i'J'M'p_i'l_i'S_i'j_i'm_i'|t_i|q_i\nu_iJMp_il_iS_ij_im_i\rangle = \delta_{\nu_i'\nu_i}\,\delta_{J'J}\,\delta_{M'M}\,\delta_{l_i'l_i}\,\delta_{S_i'S_i}\,\delta_{j_i'j_i} \times\delta_{m_i'm_i}\,2\omega_i(q_i)(1/q_i^2)\delta(q_i'-q_i)\,t_i^{l_iS_ij_i}(p_i',p_i;q_i), \tag{21}$$

where the partial-wave amplitudes $t_i^{l_i S_i j_i}$ are obtained by solving the two-body Kadyshevski equation[23]

$$t_i^{l_i S_i j_i}(p_i'', p_i'; q_i) = V_i^{l_i S_i j_i}(p_i'', p_i') + \int_0^\infty p_i^2\, dp_i \frac{\omega(p_i)}{4W_i(p_i q_i)\omega_j(p_i)\omega_k(p_i)} \times V_i^{l_i S_i j_i}(p_i'', p_i) \frac{1}{\sqrt{S} - W(p_i q_i) + i\epsilon} \times t_i^{l_i S_i j_i}(p_i, p_i'; q_i), \tag{22}$$

where the phase factors are defined in Eqs. (9)–(14). The motivation[20] for constructing the two-body amplitudes with the Kadyshevski equation[23] instead of with the customary Blankenbecler–Sugar equation[22] (both equations satisfy the necessary discontinuity relation, which is the only condition imposed by Aaron, Amado, and Young[19]) is to make the theory applicable also in the case of the bound-state problem, since with the first choice the relativistic Faddeev equations possess spurious bound-state solutions and in some special cases can give rise to unphysical behavior even in the scattering region.[20,21]

If we now introduce complete sets of states (16) into Eq. (19) and use Eq. (21), we see that the three-body amplitudes satisfy the set of two-dimensional coupled integral equations

$$\begin{aligned}\langle q_i \nu_i JMp_i l_i S_i j_i m_i | T_i | \phi_0 \rangle &= \langle q_i \nu_i JMp_i l_i S_i j_i m_i | t_i | \phi_0 \rangle \\ &+ \sum_{j \neq i} \sum_{\nu_j l_j S_j j_j m_j} \frac{1}{q_i} \int_0^\infty q_j\, dq_j \int_{p_j-}^{p_j+} p_j\, dp_j \\ &\times \frac{\omega^2(p_j)}{8W_j(p_j q_j)\omega_j(q_j)\omega_k(p_j)\omega_i(p_j)} \\ &\times t_i^{l_i S_i j_i}(p_i, p_i'; q_i) G_0(p_i' q_i) \\ &\times \langle q_i \nu_i p_i' l_i S_i j_i m_i | q_j \nu_j p_j l_j S_j j_j m_j \rangle_J \\ &\times \langle q_j \nu_j JMp_j l_j S_j j_j m_j | T_j | \phi_0 \rangle,\end{aligned} \tag{23}$$

where the variable p_i' is given in terms of the variables q_i, q_j, and p_j as

$$p_i' = \left\{ \frac{[s_i(q_i q_j p_j) - (m_j + m_k)^2][s_i(q_i q_j p_j) - (m_j - m_k)^2]}{4s_i(q_i q_j p_j)} \right\}^{1/2}, \tag{24}$$

$$s_i(q_i q_j p_j) = [W(p_j q_j) - \omega_i(q_i)]^2 - q_i^2, \tag{25}$$

and the limits of integration $p_{j\pm}$ in Eq. (23) are

$$p_{j\pm} = \left\{ \frac{[s_{j\pm}(q_i q_j) - (m_k + m_i)^2][s_{j\pm}(q_i q_j) - (m_k - m_i)^2]}{4s_{j\pm}(q_i q_j)} \right\}^{1/2}, \tag{26}$$

$$s_{j\pm}(q_i q_j) = [W_\pm(q_i q_j) - \omega_j(q_j)]^2 - q_j^2, \tag{27}$$

$$W_\pm(q_i q_j) = \omega_i(q_i) + \omega_j(q_j) + \omega_k(q_i \pm q_j). \tag{28}$$

Finally, we will show that Eqs. (23) decouple into two sets of integral equations that correspond to the two cases of positive and negative parity. In order to do this, we first show in Appendix B that the reduced recoupling coefficients (18) obey the parity relation

$$\langle q_i \nu_i p_i l_i S_i j_i m_i | q_j \nu_j p_j l_j S_j j_j m_j \rangle_J = (-)^{l_i + s_j + s_k - j_i} \langle q_i - \nu_i p_i l_i S_i j_i - m_i | q_j - \nu_j p_j l_j S_j j_j - m_j \rangle_J (-)^{l_j + s_k + s_i - j_j}, \tag{29}$$

so that using Eqs. (23) and (29), one sees that the amplitudes

$$(-)^{l_i + s_j + s_k - j_i} \langle q_i - \nu_i JMp_i l_i S_i j_i - m_i | T_i | \phi_0 \rangle$$

also obey Eq. (23). Thus, if we define the two linear combinations of amplitudes that are also solutions of Eq. (23) as

$$\begin{aligned}&\langle q_i \nu_i JMp_i l_i S_i j_i m_i | T_i | \phi_0 \rangle_\pm \\ &= \langle q_i \nu_i JMp_i l_i S_i j_i m_i | T_i | \phi_0 \rangle \pm (-)^{J - s_i - s_j - s_k} (-)^{l_i + s_j + s_k - j_i} \langle q_i - \nu_i JMp_i l_i S_i j_i - m_i | T_i | \phi_0 \rangle \\ &= \langle q_i \nu_i JMp_i l_i S_i j_i m_i | T_i | \phi_0 \rangle \pm (-)^{J + l_i - s_i - j_i} \langle q_i - \nu_i JMp_i l_i S_i j_i - m_i | T_i | \phi_0 \rangle,\end{aligned} \tag{30}$$

they obviously obey the parity relation

$$\langle q_i \nu_i JMp_i l_i S_i j_i m_i | T_i | \phi_0 \rangle_\pm = \pm (-)^{J + l_i - s_i - j_i} \langle q_i - \nu_i JMp_i l_i S_i j_i - m_i | T_i | \phi_0 \rangle_\pm, \tag{31}$$

so that only approximately half of them are linearly independent, with the remaining ones given by Eq. (31). Thus, for example, if particle i has spin-$\frac{1}{2}$, only the amplitudes with $\nu_i = \frac{1}{2}$, $m_i = -j_i, -j_i + 1, \ldots, +j_i$ are linearly independent, while those with $\nu_i = -\frac{1}{2}$, $m_i = -j_i, -j_i + 1, \ldots, +j_i$ can be obtained by using Eq. (31). The integral equations for the $+$ and $-$ amplitudes (30), are completely decoupled and they differ from Eq. (23) in that now the recoupling coefficients are

$$\begin{aligned}&\langle q_i \nu_i p_i' l_i S_i j_i m_i | q_j \nu_j p_j l_j S_j j_j m_j \rangle_{J\pm} \\ &= \langle q_i \nu_i p_i' l_i S_i j_i m_i | q_j \nu_j p_j l_j S_j j_j m_j \rangle_J \pm (-)^{J + l_j - s_j - j_j} \langle q_i \nu_i p_i' l_i S_i j_i m_i | q_j - \nu_j p_j l_j S_j j_j - m_j \rangle_J,\end{aligned} \tag{32}$$

and the sum over the magnetic quantum numbers ν_j, m_j in Eq. (23) goes only over the set of linearly dependent ones.

In order to see that the amplitudes (30) correspond to the two cases of positive and negative parity, we expand these amplitudes in terms of a new set of basis states that contain explicitly the orbital angular momentum between particle i and the two-body subsystem jk. If we use the fact that the quantum numbers j_i and m_i represent the spin and helicity of the pair jk, we can use the inverse of the transformation (7) to expand our states (8) as

$$|q_i\nu_i JMp_i l_i S_i j_i m_i\rangle = \sum_{L_i Z_i} \left(\frac{2L_i+1}{2J+1}\right)^{1/2} C^{L_i Z_i J}_{0,\nu_i - m_i} C^{s_i j_i Z_i}_{\nu_{p_i} - m_i} \times |q_i L_i Z_i JMp_i l_i S_i j_i\rangle, \tag{33}$$

where L_i is the orbital angular momentum between particle i and the pair jk, and Z_i its effective total spin. From Eq. (33), we see that

$$|q_i - \nu_i JMp_i l_i S_i j_i - m_i\rangle = \sum_{L_i Z_i} (-)^{L_i - J + s_i + j_i} \left(\frac{2L_i+1}{2J+1}\right)^{1/2} C^{L_i Z_i J}_{0,\nu_i - m_i} C^{s_i j_i Z_i}_{\nu_{p_i} - m_i} \times |q_i L_i Z_i JMp_i l_i S_i j_i\rangle, \tag{34}$$

so that using Eqs. (33) and (34) into Eq. (30), we get that

$$\langle q_i\nu_i JMp_i l_i S_i j_i m_i | T_i | \phi_0\rangle_{\pm} = \sum_{L_i Z_i} [1 \pm (-)^{l_i + L_i}] \left(\frac{2L_i+1}{2J+1}\right)^{1/2} C^{L_i Z_i J}_{0,\nu_i - m_i} \times C^{s_i j_i Z_i}_{\nu_{p_i} - m_i} \langle q_i L_i Z_i JMp_i l_i S_i j_i | T_i | \phi_0\rangle, \tag{35}$$

which clearly shows that the amplitudes (30) possess the correct parity behavior.

V. EXAMPLES ILLUSTRATING THE RELATIVISTIC TRANSFORMATION OF THE SPIN

The basis states that we are discussing in this paper differ from the usual nonrelativistic ones apart from the use of relativistic kinematics, essentially in that they take into account the relativistic transformation of the spin between the two-body and three-body c.m. frames. This effect is contained totally in the recoupling coefficients (18), so that by comparing these coefficients with the corresponding nonrelativistic ones in some simple cases, one can isolate the effects due to the transformation of the spin.

The recoupling coefficients similar to those defined by Eqs. (32) and (18) are in the nonrelativistic case[24] given by

$$\begin{aligned}\langle q_i L_i s_i J_i p_i l_i S_i j_i | q_j L_j s_j J_j p_j l_j S_j j_j\rangle_J &= [(2j_i+1)(2j_j+1)(2J_i+1) \times (2J_j+1)(2S_i+1)(2S_j+1)]^{1/2} \\ &\times \sum_{LS} (-)^{S_j + s_j - S}(2S+1) \\ &\times \begin{Bmatrix} l_i & L_i & L \\ S_i & s_i & S \\ j_i & J_i & J \end{Bmatrix} \begin{Bmatrix} l_j & L_j & L \\ S_j & s_j & S \\ j_j & J_j & J \end{Bmatrix} \\ &\times W(s_j s_k S s_i; S_i S_j) A^{l_i L_i l_j L_j}_{ij,L}(p_i q_i p_j q_j),\end{aligned} \tag{36}$$

$$\begin{aligned}A^{l_i L_i l_j L_j}_{ij,L}(p_i q_i p_j q_j) &= (4\pi)^2 \sum_{M m_i m_j} C^{l_i L_i L}_{m_i, M - m_i} C^{l_j L_j L}_{m_j, M - m_j} Y^*_{l_i m_i}(\hat{p}_i) \\ &\times Y^*_{L_i, M - m_i}(\hat{q}_i) Y_{l_j m_j}(\hat{p}_j) Y_{L_j, M - m_j}(\hat{q}_j),\end{aligned} \tag{37}$$

where the order of the coupling is indicated by the $9j$ symbols.

As a first example let us consider the case of three particles of spin-$\frac{1}{2}$ such that the total angular momentum of the system is $J = \frac{1}{2}$, while the quantum numbers of the pair jk are $l_i = S_i = j_i = 0$ and similarly those of the pair ki are $l_j = S_j = j_j = 0$. This corresponds for example to the configuration of the triton in which the nucleon pairs jk and ki are both in the $^1S_0$ channel. The recoupling coefficients for the cases of positive and negative parity correspond, respectively, to having $L_i = L_j = 0$ and $L_i = L_j = 1$, and from Eqs. (36) and (37) one finds that they are given by

$$\langle q_i 0 \tfrac{1}{2}\tfrac{1}{2} p_i 000 | q_j 0 \tfrac{1}{2}\tfrac{1}{2} p_j 000\rangle_{1/2} = -\tfrac{1}{2}, \tag{38a}$$

$$\langle q_i 1 \tfrac{1}{2}\tfrac{1}{2} p_i 000 | q_j 1 \tfrac{1}{2}\tfrac{1}{2} p_j 000\rangle_{1/2} = -\tfrac{1}{2}\hat{q}_i \cdot \hat{q}_j = -\tfrac{1}{2}\cos\chi. \tag{38b}$$

In the case of our relativistic basis states, we find from Eqs. (32) and (18) that the positive and negative parity recoupling coefficients for these states are

$$\begin{aligned}\langle q_i \tfrac{1}{2} p_i 0000 | q_j \tfrac{1}{2} p_j 0000\rangle_{1/2\pm} &= \langle q_i \tfrac{1}{2} p_i 0000 | q_j \tfrac{1}{2} 0000\rangle_{1/2} \\ &\pm \langle q_i \tfrac{1}{2} p_i 0000 | q_j - \tfrac{1}{2} 0000\rangle_{1/2} \\ &= -\tfrac{1}{2}[d^{1/2}_{(1/2)(1/2)}(\chi) d^{1/2}_{(1/2)(1/2)}(\beta_i + \rho_k + \beta_j) \\ &\pm d^{1/2}_{(1/2)-(1/2)}(\chi) d^{1/2}_{(1/2)-(1/2)}(\beta_i + \rho_k + \beta_j)].\end{aligned} \tag{39}$$

The recoupling coefficients (39) are different from the corresponding coefficients (38) even if one uses relativistic kinematics to calculate the angles in (38). In particular, the positive parity coefficient (38a) is still equal to a constant, while the corresponding coefficient (39) depends on the angles of Fig. 1, which are functions of the relative momenta p_i, q_i, p_j, and q_j. The difference between the coefficients (38) and (39) is due precisely to the effect of the so-called Wigner rotation of the spin in a Lorentz transformation,[14,18] which is the difference between π and the sum of the internal angles of a triangle in Fig. 1. We can see this easily, by using nonrelativistic kinematics to calculate the angles in Eq. (39), so that the Wick triangle becomes an ordinary triangle and the sum of the internal angles of the triangles ijo and ijk in Fig. 1 are both equal to π and therefore $\beta_i + \rho_k + \beta_j = \chi$, so that the recoupling coefficients (39) become

$$\begin{aligned}\langle q_i \tfrac{1}{2} p_i 0000 | q_j \tfrac{1}{2} p_j 0000\rangle_{1/2\pm} &\underset{NR}{\to} -\tfrac{1}{2}\{[d^{1/2}_{(1/2)(1/2)}(\chi)]^2 \pm [d^{1/2}_{(1/2)-(1/2)}(\chi)]^2\} \\ &= -\tfrac{1}{2}[\tfrac{1}{2}(1+\cos\chi) \pm \tfrac{1}{2}(1-\cos\chi)] \\ &= -\frac{1}{2}\begin{Bmatrix} 1 \\ \cos\chi \end{Bmatrix},\end{aligned} \tag{40}$$

which are precisely the results (38).

As a second example let us consider the case when particles i and j have spin-$\frac{1}{2}$ and particle k has spin-0 and the

orbital angular momentum of both pairs $l_i = l_j = 0$, so that $S_i = j_i = S_j = j_j = \frac{1}{2}$, while the total angular momentum is $J = 0$. The positive and negative parity recoupling coefficients for the nonrelativistic case correspond to having $L_i = L_j = 0$ and $L_i = L_j = 1$, respectively, which from Eq. (36) are given by

$$\langle q_i 0 \tfrac{1}{2}\tfrac{1}{2} p_i 0 \tfrac{1}{2}\tfrac{1}{2} | q_j 0 \tfrac{1}{2}\tfrac{1}{2} p_j 0 \tfrac{1}{2}\tfrac{1}{2}\rangle_0 = -1, \tag{41a}$$

$$\langle q_i 1 \tfrac{1}{2}\tfrac{1}{2} p_i 0 \tfrac{1}{2}\tfrac{1}{2} | q_j 1 \tfrac{1}{2}\tfrac{1}{2} p_j 0 \tfrac{1}{2}\tfrac{1}{2}\rangle_0 = \hat{q}_i \cdot \hat{q}_j = \cos\chi. \tag{41b}$$

In the case of the relativistic basis states, we find from Eqs. (32) and (18) that the positive and negative parity recoupling coefficients for these states are

$$\begin{aligned}
&\langle q_i \tfrac{1}{2} p_i 0 \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2} | q_j \tfrac{1}{2} p_j 0 \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle_{0\pm} \\
&\quad = \langle q_i \tfrac{1}{2} p_i 0 \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2} | q_j \tfrac{1}{2} p_j 0 \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle_0 \\
&\qquad \mp \langle q_i \tfrac{1}{2} p_i 0 \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2} | q_j -\tfrac{1}{2} p_j 0 \tfrac{1}{2} -\tfrac{1}{2}\rangle_0 \\
&\quad = -[d^{1/2}_{(1/2)\,(1/2)}(\theta_i - \beta_j)\, d^{1/2}_{(1/2)\,(1/2)}(\pi - \theta_j - \beta_i) \\
&\qquad \mp d^{1/2}_{(1/2)\,-(1/2)}(\theta_i - \beta_j) \\
&\qquad \times d^{1/2}_{-(1/2)\,(1/2)}(\pi - \theta_j - \beta_i)] \\
&\quad = -d^{1/2}_{(1/2)\,(1/2)}(\theta_i - \beta_j \mp \pi \pm \theta_j \pm \beta_i).
\end{aligned} \tag{42}$$

The recoupling coefficients (42) are again different than the coefficients (41) even if one uses relativistic kinematics to calculate the angles in Eq. (41). Again, it is easy to see that if we use nonrelativistic kinematics, then the sum of the internal angles in the triangles of Fig. 1 is equal to π, so that $\theta_j + \beta_i = \chi = \pi - \theta_i + \beta_j$ and

$$\begin{aligned}
&\langle q_i \tfrac{1}{2} p_i 0 \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2} | q_j \tfrac{1}{2} p_j 0 \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\rangle_{0\pm} \\
&\quad \underset{NR}{\to} \begin{Bmatrix} -d^{1/2}_{(1/2)\,(1/2)}(0) \\ -d^{1/2}_{(1/2)\,(1/2)}(2\pi - 2\chi) \end{Bmatrix} = \begin{Bmatrix} -1 \\ \cos\chi \end{Bmatrix},
\end{aligned} \tag{43}$$

which are identical to the results (41).

In the general case of arbitrary angular momentum and spins of the particles, we have checked numerically that the recoupling coefficients given by Eqs. (32) and (18), reduce to the nonrelativistic ones if one calculates the angles of the Wick triangle with nonrelativistic kinematics.

VI. APPLICATIONS WITH PARTICLES OFF THE MASS SHELL

We will discuss, in this section, the use of Wick's three-body states for processes in which a pion or a nucleon is allowed to go off the mass shell. These two cases are the most relevant ones in the few-body problems that one encounters in medium energy physics.

As a first example let us consider the process $N\Delta \to N\Delta$

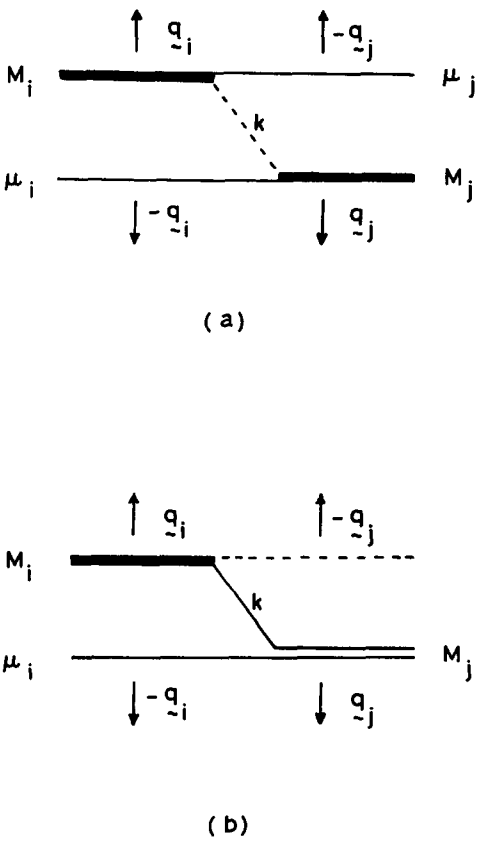

FIG. 2. (a) The process $N\Delta \to N\Delta$. (b) The process $\pi d \to N\Delta$.

shown in Fig. 2(a), where a pion is exchanged between two deltas. This diagram is given by

$$\begin{aligned}
&F_{M_i \mu_i M_j \mu_j}(\mathbf{q}_i, \mathbf{q}_j) \\
&\quad = \bar{u}_{\mu_i} k_\nu W^\nu_{M_j} [-1/(t - m_\pi^2 + i\epsilon)]\, \bar{W}^\eta_{M_i} k_\eta u_{\mu_j},
\end{aligned} \tag{44}$$

where $t = k^\nu k_\nu$ is the invariant mass squared of the off-shell pion, u_{μ_j} is a spinor of helicity μ_j, and $W^\nu_{M_j}$ is a Rarita–Schwinger spinor of helicity M_j. The partial-wave projection of the amplitude (44) with angular momentum J is

$$\begin{aligned}
&F^J_{M_i \mu_i M_j \mu_j} \\
&\quad = \int_{-1}^{1} d\cos\theta\, d^J_{M_j - \mu_j, M_i - \mu_i}(\theta) F_{M_i \mu_i M_j \mu_j}(\mathbf{q}_i, \mathbf{q}_j).
\end{aligned} \tag{45}$$

If we use our basis states to calculate this partial-wave amplitude, we would proceed as

$$\begin{aligned}
F^J_{M_i \mu_i M_j \mu_j} = &\sum_{\substack{\nu_i J' M' \\ l_i S_i j_i m_i}} \sum_{\substack{\nu_j J'' M'' \\ l_j S_j j_j m_j}} \int p_i^2\, dp_i\, q_i'^2\, dq_i'\, p_j^2\, dp_j\, q_j'^2\, dq_j' \frac{\omega(p_i)}{8 W_i(p_i q_i')\omega_i(q_i')\omega_j(p_i)\omega_k(p_i)} \\
&\times \frac{\omega(p_j)}{8 W_j(p_j q_j')\omega_j(q_j')\omega_k(p_j)\omega_i(p_j)} \langle JMM_i\mu_i | q_i' \nu_i J' M' p_i l_i S_i j_i m_i\rangle \frac{\omega_k}{[\sqrt{S} - \omega_i(q_i') - \omega_j(q_j')]^2 - \omega_k^2 + i\epsilon} \\
&\times \langle q_i' \nu_i J' M' p_i l_i S_i j_i m_i | q_i' \nu_j J'' M'' p_j l_j S_j j_j m_j\rangle \langle q_j' \nu_j J'' M'' p_j l_j S_j j_j m_j | JMM_j \mu_j\rangle,
\end{aligned} \tag{46}$$

where

$$\omega_k = W(p_i q_i') - \omega_i(q_i') - \omega_j(q_j'), \tag{47}$$

and the vertex function is

$$\langle JMM_i\,\mu_i|q_i'\nu_i J'M' p_i l_i S_i j_i m_i\rangle = \delta_{JJ'}\,\delta_{MM'}\,\delta_{M_i m_i}\,\delta_{\mu_i\nu_i}\,\delta_{l_i 1}\,\delta_{S_i(1/2)}\delta_{j_i(3/2)}\,2\omega_i(q_i) \times \frac{1}{q_i^2}\delta(q_i - q_i')p_i\left[\frac{\omega_j(p_i)+m_j}{3m_j}\right]^{1/2}. \tag{48}$$

We found numerically that Eqs. (44) and (45) and (46)–(48) give identical results provided one evaluates the kinematics (10)–(14) and the angles in Appendix A, using for the mass of the pion not the physical mass squared m_π^2, but the off-shell mass squared t. The same result is obtained if one replaces in Fig. 2(a) one or both deltas by nucleons. Thus, Wick's formalism can be used whenever the particle that is going off mass shell is spinless, one only has to remember to use the off-shell mass to calculate the kinematics [except when evaluating the function (47), where the physical mass must be used]. Thus one could use this formalism, for example, to include the fully off mass shell pion in the three-body treatment of nucleon–nucleon scattering proposed by Kloet *et al.*[25–27]

As a second example let us consider the process $\pi d \to N\Delta$ shown in Fig. 2(b), where a nucleon is exchanged between a deuteron and a delta. This diagram is given by

$$F_{M_i\mu_i M_j}(\mathbf{q}_i,\mathbf{q}_j) = \bar{v}_{\mu_i}\left[q_i^\nu \epsilon_\nu^{M_j} A(t) + \gamma^\nu \epsilon_\nu^{M_j} B(t)\right] \times \frac{\gamma^\eta k_\eta + M}{t - M^2 + i\epsilon}\, q_{j\mu}\, W_{M_i}^{\mu}, \tag{49}$$

where $\bar{v}_{\mu_i}$ is a conjugated spinor with helicity μ_i, $\epsilon_\nu^{M_j}$ is a spin-1 spinor for the deuteron with helicity M_j, and $A(t)$ and $B(t)$ are the NNd form factors that, in the nonrelativistic limit, can be related to the S- and D-wave components of the deuteron wave functions φ_0 and φ_2, as[28]

$$A(t) = (p^2 + MB_d)\left[\varphi_0(p) + (1/\sqrt{2})\varphi_2(p)\right], \tag{50}$$

$$B(t) = (p^2 + MB_d)\{-(3M/p^2)(1/\sqrt{2})\varphi_2(p) + (1/2M)\left[\varphi_0(p) + (1/\sqrt{2})\varphi_2(p)\right]\}, \tag{51}$$

where B_d is the binding energy of the deuteron, and p is the magnitude of the relative three-momentum of the two nucleons in the deuteron rest frame which is given in terms of t as

$$p^2 = (m_d^2 + M^2 - t)^2/4m_d^2 - M^2. \tag{52}$$

In order to use Wick's helicity states to try to evaluate the process of Fig. 2(b), we first write the numerator of the nucleon propagator as

$$\gamma^\nu k_\nu + M = \gamma^0(k_0 - \omega_k) + \gamma^0\omega_k - \boldsymbol{\gamma}\cdot\mathbf{k} + M = \gamma^0(k_0 - \omega_k) + 2m\sum_{\mu_k} u_{\mu_k}\bar{u}_{\mu_k}, \tag{53}$$

and neglect the first term in the right-hand side of Eq. (53). This approximation effectively replaces in the numerator of the nucleon propagator, a particle with four-momentum $(k^0,\mathbf{k})$ which is off the mass shell by an on mass shell particle with four-momentum $(\omega_k,\mathbf{k})$. Thus, with this approximation we can now use Wick's states to evaluate the process of Fig. 2(b) using Eq. (46), where the NNd vertex function is given by

$$\langle q_j'\nu_j J''M''p_j l_j S_j j_j m_j|JMM_j\rangle = \delta_{JJ'}\,\delta_{MM'}\,\delta_{M_j m_j}\,\delta_{0\nu_j}\,\delta_{S_j 1}\,\delta_{j_j 1}\,2\omega_j(q_j)\,(1/q_j^2) \times \delta(q_j - q_j')2\sqrt{2}(p_j^2 + MB_d)\varphi_{l_j}(p_j). \tag{54}$$

We show in Fig. 3 the partial-wave amplitudes for this process $F^J_{(1/2)\,(1/2),0}$, which have been calculated with the deuteron wave function of the Paris potential.[29] The solid lines are the exact amplitudes given by Eqs. (45) and (49), and the dashed lines the results obtained using Eq. (46) and the approximation (53). As we see, the results obtained with Wick's states are quite close to the exact results in the energy region considered. The dotted lines in Fig. 3 are the results of Eq. (46) when the kinematics is calculated not with the physical mass squared M^2, but with the off-shell mass squared t.

Thus, we can conclude from this discussion that Wick's states provide also a good approximation to describe off mass shell particles at medium energies.

APPENDIX A: KINEMATICS OF THE WICK TRIANGLE

In order to find the angles of the Wick triangle shown in Fig. 1, one must first calculate the sides of the triangle where

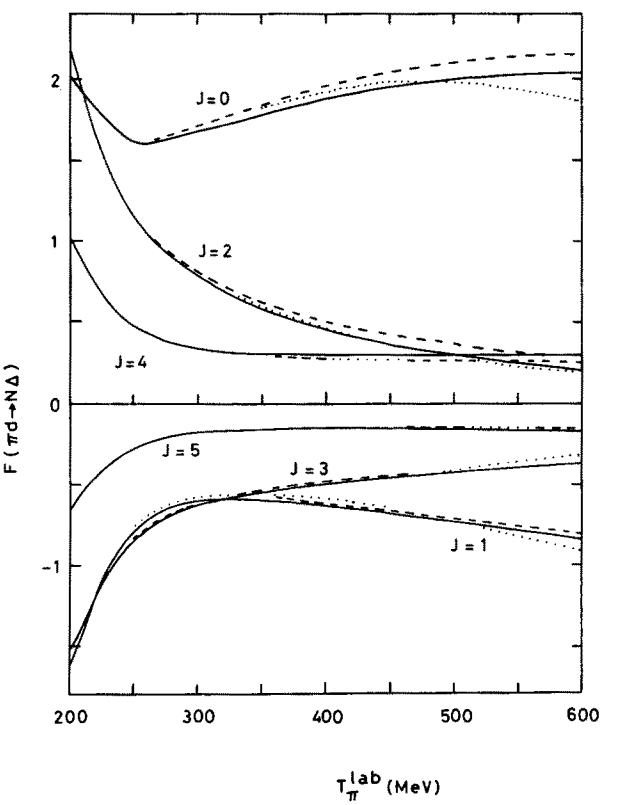

FIG. 3. Partial-wave amplitudes $F^J_{(1/2)\,(1/2),0}$ for the process $\pi d \to N\Delta$. The solid lines are the exact results, the dashed lines the results of Eq. (46), and the dotted lines the results of Eq. (46) using the off-shell mass squared t to calculate the kinematics.

the segments between points represent relative velocities, so that in terms of the definitions (10), (12), and (13) we have that

$$v_{ib} = p_j/\omega_i(p_j), \tag{A1}$$

$$v_{bk} = p_j/\omega_k(p_j), \tag{A2}$$

$$v_{ja} = p_i/\omega_j(p_i), \tag{A3}$$

$$v_{ak} = p_i/\omega_k(p_i), \tag{A4}$$

$$v_{io} = q_i/\omega_i(q_i), \tag{A5}$$

$$v_{jo} = q_j/\omega_j(q_j), \tag{A6}$$

$$v_{oa} = q_i/W_i(p_i q_i), \tag{A7}$$

$$v_{ob} = q_j/W_j(p_j q_j). \tag{A8}$$

The larger segments are calculated using Einstein's addition law for velocities, as

$$v_{ik} = (v_{ib} + v_{bk})/(1 + v_{ib}v_{bk}), \tag{A9}$$

$$v_{jk} = (v_{ja} + v_{ak})/(1 + v_{ja}v_{ak}), \tag{A10}$$

$$v_{ia} = (v_{io} + v_{oa})/(1 + v_{io}v_{oa}), \tag{A11}$$

$$v_{jb} = (v_{jo} + v_{ob})/(1 + v_{jo}v_{ob}). \tag{A12}$$

Finally, the angles of the Wick triangle are obtained by using the cosines law for this non-Euclidean space, as

$$\cos\beta_i = \frac{1}{v_{ia}v_{ik}}\left[1 - \frac{(1-v_{ia}^2)^{1/2}(1-v_{ik}^2)^{1/2}}{(1-v_{ak}^2)^{1/2}}\right], \tag{A13}$$

$$\cos\beta_j = \frac{1}{v_{jb}v_{jk}}\left[1 - \frac{(1-v_{jb}^2)^{1/2}(1-v_{jk}^2)^{1/2}}{(1-v_{bk}^2)^{1/2}}\right], \tag{A14}$$

$$\cos\rho_k = \frac{1}{v_{ik}v_{ak}}\left[1 - \frac{(1-v_{ik}^2)^{1/2}(1-v_{ak}^2)^{1/2}}{(1-v_{ia}^2)^{1/2}}\right], \tag{A15}$$

$$\cos\theta_i = \frac{1}{v_{ia}v_{ak}}\left[1 - \frac{(1-v_{ia}^2)^{1/2}(1-v_{ak}^2)^{1/2}}{(1-v_{ik}^2)^{1/2}}\right], \tag{A16}$$

$$\cos\theta_j = \frac{1}{v_{ib}v_{ob}}\left[1 - \frac{(1-v_{ib}^2)^{1/2}(1-v_{ob}^2)^{1/2}}{(1-v_{io}^2)^{1/2}}\right], \tag{A17}$$

$$\cos(\pi-\chi) = \frac{1}{v_{io}v_{ob}}\left[1 - \frac{(1-v_{io}^2)^{1/2}(1-v_{ob}^2)^{1/2}}{(1-v_{ib}^2)^{1/2}}\right]. \tag{A18}$$

APPENDIX B: DERIVATION OF EQ. (29)

We will show here that the recoupling coefficients (18) obey the parity relation (29). In order to show this, we first notice that the Clebsch–Gordan coefficients obey

$$C^{l_i S_i j_i}_{0,\lambda_j-\lambda_k}\, C^{s_j s_k S_i}_{\lambda_j-\lambda_k} = (-)^{l_i+s_j+s_k-j_i} C^{l_i S_i j_i}_{0,-\lambda_j+\lambda_k}\, C^{s_j s_k S_i}_{-\lambda_j,\lambda_k}, \tag{B1}$$

$$C^{l_j S_j j_j}_{0,\lambda'_k-\lambda'_i}\, C^{s_k s_i S_j}_{\lambda'_k,-\lambda'_i} = (-)^{l_j+s_k+s_i-j_j} C^{l_j S_j j_j}_{0,-\lambda'_k+\lambda'_i}\, C^{s_k s_i S_j}_{-\lambda'_k,\lambda'_i}, \tag{B2}$$

while from the property of the rotation matrices

$$d^{j}_{\mu\nu}(\theta) = (-)^{\mu-\nu} d^{j}_{-\mu,-\nu}(\theta) = (-)^{\nu-\mu} d^{j}_{-\mu,-\nu}(\theta), \tag{B3}$$

we get that

$$\begin{aligned} &d^{J}_{m_i-\nu_i,m_j-\nu_j}(\chi)\, d^{j_i}_{m_i,\lambda_j-\lambda_k}(\theta_i)\, d^{j_j}_{m_j,\lambda'_k-\lambda'_i}(\theta_j) \\ &\quad\times d^{s_i}_{\lambda'_i,\nu_i}(-\beta_i) d^{s_j}_{\nu_j,\lambda_j}(\beta_j) d^{s_k}_{\lambda'_k,\lambda_k}(\rho_k) \\ &\quad= (-)^{2\nu_j-2\lambda'_k} d^{J}_{-m_i+\nu_i,-m_j+\nu_j}(\chi) \\ &\quad\times d^{j_i}_{-m_i,-\lambda_j+\lambda_k}(\theta_i) d^{j_j}_{-m_j,-\lambda'_k+\lambda'_i}(\theta_j) \\ &\quad\times d^{s_i}_{-\lambda'_i,-\nu_i}(-\beta_i)\, d^{s_j}_{-\nu_j,-\lambda_j}(\beta_j)\, d^{s_k}_{-\lambda'_k,-\lambda_k}(\rho_k), \end{aligned} \tag{B4}$$

so that substituting Eqs. (B1), (B2), and (B4) into Eq. (18) and noticing that

$$(-)^{s_j-\nu_j+s_k+\lambda'_k}(-)^{2\nu_j-2\lambda'_k} = (-)^{s_j+\nu_j+s_k-\lambda'_k}, \tag{B5}$$

we get immediately Eq. (29).

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Differential and integral methods for multidimensional inverse scattering problems

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A layer stripping procedure for solving three-dimensional Schrödinger equation inverse scattering problems is developed. This procedure operates by recursively reconstructing the Radon transform of the potential from the jump in the Radon transform of the scattered field at the wave front. This reconstructed potential is then used to propagate the wave front and scattered field differentially further into the support of the potential. The connections between this differential procedure and integral equation procedures are then illustrated by the derivations of two well known exact integral equation procedures using the Radon transform and a generalized Radon transform. These procedures, as well as the layer stripping procedure, are then reduced to the familiar Born approximation result for this problem by neglecting multiple scattering events. This illustrates the central role of the Radon transform in both exact and approximate inversion procedures.

I. INTRODUCTION

The inverse scattering problem for the Schrödinger equation in three dimensions with a time-independent, local, nonspherically symmetric potential has a wide variety of applications. In particular, the inverse seismic problem of reconstructing the density and wave speed of an inhomogeneous isotropic acoustic medium from surface measurements of the medium response to an excitation can be formulated as a Schrödinger equation inverse scattering problem, as was done by Coen *et al.*[1] Other applications include quantum mechanical particle scattering problems, in which particles are treated as wave functions,[2] and the propagation of electromagnetic waves in the ionosphere.[3]

There are several methods available for solving the inverse scattering problem. The most important of the *exact* methods are generalized Gel'fand–Levitan and Marchenko integral equation procedures of Newton,[4] and the coupled integral equation procedure of Moses.[5] Newton's Marchenko integral equation procedure has been applied to an inverse seismic problem in (Ref. 1). Moses[5] gave the first exact (in principle) solution to the inverse scattering problem, but Moses's procedure cannot be implemented in closed form. Other exact methods have been given in Refs. 6–12; this paper focuses on the exact procedures given in Refs. 4 and 5.

An alternative approach is to use the *first Born approximation*, in which the wave field inside the support of the potential is approximated by the incident field being used to probe the potential. This approach has been applied to the variable-velocity wave equation by Cohen and Bleistein,[13] Devaney,[14] and others.

All of these methods have shortcomings. Newton's integral equation procedure requires that the scattering amplitude (the far-field response) be measured for all incident and outgoing directions and all frequencies. This makes it unsuitable for inverse seismic problems, for which data are only available in the near field and in backscattered directions. Furthermore, the complete specification of the scattering amplitude results in an overdetermined problem, so that a slight corruption of the data may result in an inadmissible scattering amplitude. Moses's coupled integral equations cannot be solved in closed form; power series expansions are required for various quantities, and as a result a considerable amount of computation is required to determine each higher-order correction term. The Born approximation methods, although requiring less computation, employ a single scattering approximation, and thus are only valid for problems with weakly scattering potentials.

A completely different approach to solving the Schrödinger equation inverse scattering problem is *layer stripping*. Layer stripping is a *differential* procedure, in contrast to the above *integral* equation procedures. A layer stripping algorithm works by recursively reconstructing the potential as the probing wave penetrates it. By employing causality and the inherent structure of an inverse scattering problem, a layer stripping algorithm requires much less computation than the integral equation procedures of Newton and Moses. It also requires only near-field, backscattered data, making it ideal for applications to inverse seismic problems, and avoiding the overdetermined problem to which Newton's procedure is applicable. A layer stripping algorithm has been proposed in Yagle and Levy[15]; however, this algorithm is numerically untested.

The objectives of this paper are twofold: (1) to present a new layer stripping algorithm for solving the Schrödinger equation inverse scattering problem; and (2) to present an approach, based on the Radon transform, for interpreting all of the various methods mentioned above for solving the inverse scattering problem. We thus show, for the first time, how the integral-equation methods of Newton and Moses, the Born approximation approach, and the layer stripping method presented in this paper are all related to each other. In this way, the common basis of all of these seemingly unrelated approaches is exposed, resulting in new insight into their operation.

The paper is organized as follows. The Radon transform

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is quickly reviewed in Sec. II, including a generalized Radon transform noted in Rose *et al.*[9] The basic Schrödinger equation inverse scattering problem that is the subject of this paper is set up in Sec. III, and the basic integral equation procedures of Newton and Moses for solving this problem are specified. In Sec. IV a new layer stripping procedure for solving this problem is presented and discussed. In Sec. V the same basic equations used in deriving the layer stripping algorithm are used to derive the integral equation procedures of Newton and Moses. This illustrates that all three procedures have a common basis. The basic Born approximation result is also derived from all three procedures by neglecting multiple scattering events. Finally, Sec. VI concludes by summarizing the results of the paper and noting directions in which further research is needed.

II. THE RADON TRANSFORM

The Radon transform of a function in three-dimensional space is the integral of the function over a plane. It is thus a slice or sample of the function. Specifically, the Radon transform $\mathscr{R}\{f(\mathbf{x})\}$ of a function $f(\mathbf{x})$ is given by

$$\mathscr{R}\{f(\mathbf{x})\} = \hat{f}(\tau,\mathbf{e}) = \int f(\mathbf{x})\delta(\tau - \mathbf{e}\cdot\mathbf{x})d\mathbf{x}. \tag{2.1}$$

Given the projections $\hat{f}(\tau,\mathbf{e})$ for all τ and all angles $\mathbf{e}$, the function $f(\mathbf{x})$ may be recovered by the inverse Radon transform

$$f(\mathbf{x}) = \mathscr{R}^{-1}\{\hat{f}(\tau,\mathbf{e})\}$$
$$= -(8\pi^2)^{-1}\int_{S^2}\frac{\partial^2}{\partial\tau^2}\hat{f}(\tau = \mathbf{e}\cdot\mathbf{x},\mathbf{e})d^2\mathbf{e}, \tag{2.2}$$

where S^2 is the unit sphere in R^3. This result is originally due to Radon[16]; a good treatment is Deans.[17]

Following Rose *et al.*,[9] a *generalized Radon transform* can be defined from the fact that the solutions of the Schrödinger equation in the absence of bound states form a complete set. If $u(\mathbf{x},k,\mathbf{e})$ is a solution of the Schrödinger equation, where $\mathbf{e}$ is the direction of initial probing, and $f(\mathbf{x})$ is square integrable, then we may write

$$f(\mathbf{x}) = (2\pi)^{-3}\int_0^\infty\int_{S^2} u(\mathbf{x},k,\mathbf{e})$$
$$\times\int u^*(\mathbf{y},k,\mathbf{e})f(\mathbf{y})d\mathbf{y}\,d^2\mathbf{e}k^2\,dk, \tag{2.3}$$

and if $u(\mathbf{x},k,\mathbf{e})$ is extended to negative k by $u(\mathbf{x},-k,\mathbf{e}) = u^*(\mathbf{x},k,\mathbf{e})$ then an inverse Fourier transform from k to t

$$u(\mathbf{x},t,\mathbf{e}) = \mathscr{F}^{-1}\{u(\mathbf{x},k,\mathbf{e})\} = \frac{1}{2\pi}\int_{-\infty}^{\infty} u(\mathbf{x},k,\mathbf{e})e^{ikt}\,dk \tag{2.4}$$

results in

$$f(\mathbf{x}) = -(8\pi^2)^{-1}\int_{-\infty}^{\infty}\int_{S^2}\int u(\mathbf{x},t,\mathbf{e})$$
$$\times\frac{\partial^2}{\partial t^2}u(t,\mathbf{e},\mathbf{y})f(\mathbf{y})d\mathbf{y}\,d^2\mathbf{e}\,dt, \tag{2.5}$$

which can be written as the pair of equations

$$\hat{f}(t,\mathbf{e}) = \mathscr{G}\{f(\mathbf{x})\} = \int u(\mathbf{y},t,\mathbf{e})f(\mathbf{y})d\mathbf{y}, \tag{2.6a}$$

$$f(\mathbf{x}) = \mathscr{G}^{-1}\{\hat{f}(t,\mathbf{e})\}$$
$$= -(8\pi^2)^{-1}\int_{-\infty}^{\infty}\int_{S^2} u(\mathbf{x},t,\mathbf{e})\frac{\partial^2}{\partial t^2}\hat{f}(t,\mathbf{e})d^2\mathbf{e}\,dt, \tag{2.6b}$$

which is the generalized Radon transform pair.

In the particular case where $u(\mathbf{x},t,\mathbf{e})$ is chosen to be the impulse $\delta(t - \mathbf{e}\cdot\mathbf{x})$, then it is clear that the generalized Radon transform pair (2.6) reduces to the standard Radon transform pair (2.1) and (2.2). This explains why (2.6) is termed a generalized Radon transform.

III. THE INVERSE SCATTERING PROBLEM

The inverse scattering problem considered in this paper is as follows. The wave field $u(\mathbf{x},k)$ satisfies the Schrödinger equation

$$(\Delta + k^2 - V(\mathbf{x}))\,u(\mathbf{x},k) = 0, \tag{3.1}$$

where the potential $V(\mathbf{x})$ is real-valued, smooth, and has compact support. It is also assumed that $V(\mathbf{x})$ does not induce bound states; a sufficient condition for this is for $V(\mathbf{x})$ to be non-negative.

Scattering solutions of (3.1) are given by the Lippman–Schwinger equation

$$u(\mathbf{x},k,\mathbf{e}_i) = e^{-ik\mathbf{e}_i\cdot\mathbf{x}} - \int (4\pi|\mathbf{x}-\mathbf{y}|)^{-1}$$
$$\times e^{-ik|\mathbf{x}-\mathbf{y}|}V(\mathbf{y})u(\mathbf{y},k,\mathbf{e}_i)d\mathbf{y}, \tag{3.2}$$

where the incident field is an impulsive plane wave propagating in the direction of the unit vector $\mathbf{e}_i$. Letting $\mathbf{x} = |\mathbf{x}|\mathbf{e}_s$ and taking $|\mathbf{x}|\to\infty$ we have, in the far field,

$$u(\mathbf{x},k,\mathbf{e}_i) = e^{-ik\mathbf{e}_i\cdot\mathbf{x}} + (e^{-ik|\mathbf{x}|}/4\pi|\mathbf{x}|)$$
$$\times A(k,\mathbf{e}_s,\mathbf{e}_i) + O(|\mathbf{x}|^{-2}), \tag{3.3}$$

where

$$A(k,\mathbf{e}_s,\mathbf{e}_i) = -\int e^{ik\mathbf{e}_s\cdot\mathbf{y}}V(\mathbf{y})u(\mathbf{y},k,\mathbf{e}_i)d\mathbf{y} \tag{3.4}$$

is the *scattering amplitude* for incident direction $\mathbf{e}_i$ and scattered direction $\mathbf{e}_s$.

An inverse Fourier transform of (3.1) yields the *plasma wave equation*

$$\left(\Delta - \frac{\partial^2}{\partial t^2} - V(\mathbf{x})\right)u(\mathbf{x},t) = 0. \tag{3.5}$$

This equation models the propagation of electromagnetic waves in the ionosphere.[3] An inverse Fourier transform of (3.3) results in

$$u(\mathbf{x},t,\mathbf{e}_i) = \delta(t - \mathbf{e}_i\cdot\mathbf{x}) + (4\pi|\mathbf{x}|)^{-1}$$
$$\times R(t - \mathbf{e}_s\cdot\mathbf{x},\mathbf{e}_s,\mathbf{e}_i) + O(|\mathbf{x}|^{-2}), \tag{3.6}$$

where $R(t,\mathbf{e}_s,\mathbf{e}_i)$ is the inverse Fourier transform of $A(k,\mathbf{e}_s,\mathbf{e}_i)$. Since $R(\cdot)$ represents the time response in the far field to the probing impulse $\delta(t - \mathbf{e}_i\cdot\mathbf{x})$, it is termed the impulse response.

Exact solutions to this inverse scattering problem have been given by Newton[4] and Moses[5] (and others as well).

Both of these methods involve the solution of integral equations. Newton's method is to solve the *Marchenko integral equation*

$$u_s(\mathbf{x},t,\mathbf{e}_i) = \int_{S^2}\int_{-\mathbf{e}_s\cdot\mathbf{x}}^{\infty} M(t+\tau,\mathbf{e}_s,\mathbf{e}_i)u_s(\mathbf{x},\tau,-e_s) \times d\tau\, d^2\mathbf{e}_s + \int_{S^2} M(t-\mathbf{e}_s\cdot\mathbf{x},\mathbf{e}_s,\mathbf{e}_i)d^2\mathbf{e}_s \tag{3.7}$$

for the scattered field $u_s(\mathbf{x},t,\mathbf{e}_i)$, which is defined by

$$u(\mathbf{x},t,\mathbf{e}_i) = \delta(t-\mathbf{e}_i\cdot\mathbf{x}) + u_s(\mathbf{x},t,\mathbf{e}_i). \tag{3.8}$$

In (3.7) the quantity $M(t,\mathbf{e}_s,\mathbf{e}_i)$ is obtained from the scattering data using

$$M(t,\mathbf{e}_s,\mathbf{e}_i) = -\frac{1}{8\pi^2}\frac{\partial}{\partial t}R(t,\mathbf{e}_s,\mathbf{e}_i). \tag{3.9}$$

Finally, the potential $V(\mathbf{x})$ is recovered from the scattered field using the *miracle* equation[4]

$$V(\mathbf{x}) = -2\mathbf{e}_i\cdot\nabla u_s(\mathbf{x},t=\mathbf{e}_i\cdot\mathbf{x},\mathbf{e}_i). \tag{3.10}$$

Note the redundancy in this equation. Newton[4] notes that the right side of this equation characterizes admissible scattering amplitudes: only a subset of all possible $A(k,\mathbf{e}_s,\mathbf{e}_i)$ (five independent variables) can result from all possible $V(\mathbf{x})$ (three independent variables). Thus the inverse scattering problem solved by this method is overdetermined; clearly there is a great amount of unnecessary computation to reconstruct $V(\mathbf{x})$. In addition, the use of far-field data and transmission data makes this procedure unsuitable for solving inverse seismic problems, as noted in (Ref. 1).

Moses's method is to solve the coupled set of integral equations:

$$T(\mathbf{k},\mathbf{k}') = V(\mathbf{k},\mathbf{k}') + \int V(\mathbf{k},\mathbf{k}'') \times\gamma(k'^2-k''^2)T(\mathbf{k}'',\mathbf{k}')d\mathbf{k}'', \tag{3.11}$$

$$W(\mathbf{k}) = b(\mathbf{k}) + \int T(-\mathbf{k},\mathbf{k}')[1(k)\gamma^*(k'^2-k^2) + 1(-k)\gamma(k'^2-k^2)]T^*(\mathbf{k},\mathbf{k}')d\mathbf{k}', \tag{3.12}$$

$$V(\mathbf{k},\mathbf{k}') = W((\mathbf{k}'-\mathbf{k})/2), \tag{3.13}$$

where $b(\mathbf{k})$ is the backscattering amplitude

$$b(\mathbf{k}) = b(k,\mathbf{e}) = A(k,-\mathbf{e},\mathbf{e}), \quad k\geqslant 0, \tag{3.14}$$

$1(k)$ is the Heaviside or unit step function, and $\gamma(k)$ is defined by

$$\gamma(k) = -i\pi\delta(k) + P/k = \lim_{\epsilon\to+0}(1/k+i\epsilon), \tag{3.15}$$

which is the Fourier transform of $1(t)$ (P denotes the Cauchy principal value). The potential $V(\mathbf{x})$ is recovered from $W(\mathbf{k})$ using the inverse Fourier transform

$$V(\mathbf{x}) = (2\pi)^{-3}\int W(\mathbf{k})e^{-2i\mathbf{k}\mathbf{x}}d\mathbf{k}. \tag{3.16}$$

Note that Moses's method is not overdetermined, since only the backscattering amplitude $b(\mathbf{k})$, not the entire scattering amplitude $A(k,\mathbf{e}_s,\mathbf{e}_i)$, is used to reconstruct the potential $V(\mathbf{x})$. However, the coupled integral equations cannot be solved in closed form. Moses[5] employs power series expansions for $T(\mathbf{k},\mathbf{k}')$, $V(\mathbf{k},\mathbf{k}')$, and $W(\mathbf{k})$; clearly an easier procedure for solving this problem is desirable. However, Moses's approach has been suggested for solving an inverse seismic problem in (Ref. 18).

An alternative to these integral equation methods is a differential or layer stripping approach. Such an approach was used to derive a layer stripping algorithm in (Ref. 15). A different layer stripping algorithm, employing the Radon transform, is derived below.

IV. A LAYER STRIPPING SOLUTION TO THE INVERSE SCATTERING PROBLEM

A *layer stripping* procedure recursively reconstructs the potential as the probing wave penetrates it. It is thus a *differential* procedure, in contrast to the *integral* equation procedures described above. By taking full advantage of the inherent structure of the inverse scattering problem, and of time causality, a layer stripping algorithm requires significantly less computation to reconstruct a scattering potential than the above methods. This is important in a three-dimensional inverse problem, since the number of points to be reconstructed in a discretized potential increases as the cube of the number of discrete points in a single dimension.

The essence of a layer stripping procedure is to differentially reconstruct the Radon transform of $V(\mathbf{x})$ from the jump in the scattered field at the wave front, and then use this reconstructed slice of $V(\mathbf{x})$ to propagate the wave front and scattered field differentially further. The jump in the scattered field at the new location of the wave front yields another slice of $V(\mathbf{x})$, which can be used to propagate the wave front and scattered field still further. This differential, layer-by-layer reconstruction contrasts with the batch operation of the integral equation approach.

There are several advantages to using a layer stripping technique. Only one direction of probing is required, and only backscattered data in the near field is used. This makes the procedure more applicable to inverse seismic problems than the integral equation procedures, which require far-field data and, in Newton's[4] procedure, transmission data. The procedure is in principle exact, since all multiple reflection, refraction, and diffraction effects are accounted for. Approximation is inherent only in the discretization necessary to implement the algorithm numerically, and data at all frequencies are used. However, the applicability of this approach to problems with bound states is not clear at present.

The layer stripping concept has been used to obtain fast algorithm solutions for the one-dimensional Schrödinger equation inverse scattering problem by Corones *et al.*,[19] Symes,[20] Bruckstein *et al.*,[21] and Yagle and Levy.[22] This approach has also been applied to various one-dimensional inverse seismic problems by Bube and Burridge,[23] and Yagle and Levy.[24–26] Similar approaches have been used by other authors. Results of computer runs of these one-dimensional problem algorithms have been encouraging (see Bube and Burridge[23] and Yagle[27]). The numerical performance of the multidimensional problem algorithms proposed in Yagle and Levy[15] and this paper are unknown at present, but are subjects of current research.

The layer stripping procedure given in this section

differs from that of Ref. 15 in the use of the Radon transform. To use this transform, we operate in the time domain. Recall from Sec. III that an inverse Fourier transform of the Schrödinger equation results in the plasma wave equation

$$\left(\Delta - \frac{\partial^2}{\partial t^2} - V(\mathbf{x})\right) u(\mathbf{x},t) = 0 \tag{4.1}$$

and the scattered field $u_s(\mathbf{x},t,\mathbf{e}_i)$ is defined by

$$u(\mathbf{x},t,\mathbf{e}_i) = \delta(t - \mathbf{e}_i \cdot \mathbf{x}) + u_s(\mathbf{x},t,\mathbf{e}_i). \tag{4.2}$$

Taking the Radon transform of (4.1) results in

$$\left\{\frac{\partial^2}{\partial \tau^2} - \frac{\partial^2}{\partial t^2}\right\} U(\tau,t,\mathbf{e}) = \mathscr{R}\{V(\mathbf{x})u(\mathbf{x},t)\}, \tag{4.3}$$

where $U(\tau,t,\mathbf{e})$ is the Radon transform of $u(\mathbf{x},t,\mathbf{e}_i)$, and the parametric dependence on the direction of probing $\mathbf{e}_i$ is no longer listed. Equation (4.3) may be written as the coupled first-order system

$$\left(\frac{\partial}{\partial \tau} + \frac{\partial}{\partial t}\right) U(\tau,t,\mathbf{e}) = Q(\tau,t,\mathbf{e}), \tag{4.4a}$$

$$\left(\frac{\partial}{\partial \tau} - \frac{\partial}{\partial t}\right) Q(\tau,t,\mathbf{e}) = \mathscr{R}\{V(\mathbf{x})u(\mathbf{x},t)\}. \tag{4.4b}$$

The crucial step is to recognize that the scattered field $u_s(\mathbf{x},t,\mathbf{e}_i)$ is *causal*: until the probing impulsive plane wave $\delta(t - \mathbf{e}_i \cdot \mathbf{x})$ reaches $\mathbf{x}$, the scattered field at $\mathbf{x}$ is zero. This can be written explicitly as

$$u(\mathbf{x},t,\mathbf{e}_i) = \delta(t - \mathbf{e}_i \cdot \mathbf{x}) + u_s(\mathbf{x},t,\mathbf{e}_i)1(t - \mathbf{e}_i \cdot \mathbf{x}). \tag{4.5}$$

Taking the Radon transform of (4.5) and considering only $\mathbf{e} = \mathbf{e}_i$ gives

$$U(\tau,t,\mathbf{e} = \mathbf{e}_i) = \delta(t - \tau) + U_s(\tau,t,\mathbf{e} = \mathbf{e}_i)1(t - \tau). \tag{4.6}$$

A mental picture of the Radon transform will make the meaning of (4.6) clear: Since the Radon transform is being taken over planes parallel to the probing impulsive plane wave ($\mathbf{e} = \mathbf{e}_i$), it must be zero if t is less than τ, since in this case the plane lies entirely with the region that the probing impulsive plane wave has not yet penetrated. From the form of (4.4a) it may be seen that $Q(\tau,t,\mathbf{e} = \mathbf{e}_i)$ is also causal. Specifically,

$$Q(\tau,t,\mathbf{e} = \mathbf{e}_i) = Q_s(\tau,t,\mathbf{e} = \mathbf{e}_i)1(t - \tau). \tag{4.7}$$

Inserting (4.5)–(4.7) into the coupled system (4.4) results in

$$\left(\frac{\partial}{\partial \tau} + \frac{\partial}{\partial t}\right) U_s(\tau,t,\mathbf{e}) = Q_s(\tau,t,\mathbf{e}), \tag{4.8a}$$

$$\left(\frac{\partial}{\partial \tau} - \frac{\partial}{\partial t}\right) Q_s(\tau,t,\mathbf{e}) = \mathscr{R}\{V(\mathbf{x})u_s(\mathbf{x},t)\}, \tag{4.8b}$$

$$\mathscr{R}\{V(\mathbf{x})\} = -2Q_s(\tau,t = \tau,\mathbf{e}), \tag{4.8c}$$

where equating the coefficients of $\delta(t - \tau)$ in (4.4b) has been used to obtain (4.8c), and $\mathbf{e} = \mathbf{e}_i$ throughout.

Equations (4.8) suggest a *recursive procedure for reconstructing* $V(\mathbf{x})$: Starting with known $U_s(\tau = 0,t,\mathbf{e} = \mathbf{e}_i)$ and $Q_s(\tau = 0,t,\mathbf{e} = \mathbf{e}_i)$, propagate Eqs. (4.8) recursively in increasing τ, yielding $\mathscr{R}\{V(\mathbf{x})\}$ recursively in τ. Once $\mathscr{R}\{V(\mathbf{x})\}$ has been computed for all τ, and for a hemisphere of angles of probing $\mathbf{e}_i$, then the inverse Radon transform (2.2) can be used to compute $V(\mathbf{x})$ [only a hemisphere of incident directions is needed, since $V(\tau,-\mathbf{e}) = V(-\tau,\mathbf{e})$].

However, there is a complication: The right side of (4.8b) seems to require that $u_s(\mathbf{x},t)$ and $V(\mathbf{x})$ be computed recursively as well. Since it is assumed in (4.8) that $\mathbf{e} = \mathbf{e}_i$, there is insufficient information to compute these quantities, since the inverse Radon transform requires projection at all angles, not just the angle of probing $\mathbf{e}_i$, and it also requires knowledge for all positive τ.

The solution to this problem is to recognize that (4.8b) requires not $u_s(\mathbf{x},t)$, but only $\mathscr{R}\{V(\mathbf{x})u_s(\mathbf{x},t)\}$. Writing this out gives

$$\mathscr{R}\{V(\mathbf{x})u_s(\mathbf{x},t)\} = -\frac{1}{8\pi^2}\int_{S^2}\int \frac{\partial^2}{\partial \tau_1^2} U_s(\tau_1 = \mathbf{e}_1 \cdot \mathbf{x},\mathbf{e}_1) \times \frac{\partial^2}{\partial \tau_2^2} V(\tau_2 = \mathbf{e}_2 \cdot \mathbf{x},\mathbf{e}_2) \times \delta(\tau - \mathbf{e}_i \cdot \mathbf{x})d\mathbf{x}\, d^2\mathbf{e}_1 d^2\mathbf{e}_2. \tag{4.9}$$

Note that this quantity is only required for $\mathbf{e} = \mathbf{e}_i$ and for a specific value of τ. The integrand is nonzero only for $\mathbf{x}$ such that $\tau = \mathbf{e}_i \cdot \mathbf{x}$, and $U_s(\tau,\mathbf{e})$ and $V(\tau,\mathbf{e})$ are only required for $\tau_1 = \mathbf{e}_1 \cdot \mathbf{x}$ and $\tau_2 = \mathbf{e}_2 \cdot \mathbf{x}$. These three planes intersect in a point unless at least two of them coincide; virtually all of the contribution to the integral occurs when all three planes coincide (this point is made and discussed in Ref. 28). Fortunately, those values of $U_s(\tau,\mathbf{e})$ that make this contribution are precisely those available at each recursion: $U_s(\tau = \mathbf{e}_i \cdot \mathbf{x}, \mathbf{e} = \mathbf{e}_i)$. Similar comments hold for $V(\mathbf{x})$; however, since $V(\mathbf{x})$ is independent of the direction of probing $\mathbf{e}_i$, it can be completely reconstructed using the inverse Radon transform (2.2) once the algorithm is complete. The second partial derivatives required in the inverse Radon transforms can be implemented numerically.

The procedure is initialized as follows. Assume without loss of generality that the support of $V(\mathbf{x})$ is contained inside a sphere of radius R, and that the backscattered field $u_s(\mathbf{x},t,\mathbf{e}_i)$ is measured on the plane $R = -\mathbf{e}_i \cdot \mathbf{x}$. Then it is possible to compute $U_s(\tau = -R,t,\mathbf{e}_i)$, and from this compute $Q_s(\tau = R,t,\mathbf{e}_i)$, and then propagate the algorithm in increasing τ from $-R$ to R. Since the support of $V(\mathbf{x})$ lies inside a sphere of radius R, $\mathscr{R}\{V(\mathbf{x})\}$ is zero for $\tau \geqslant R$.

The layer stripping procedure can be summarized as follows. (1) *Initialize* the procedure by computing

$$U_s(\tau = -R,t,\mathbf{e}_i) = \mathscr{R}\{u_s(\tau = -R,t,\mathbf{e} = \mathbf{e}_i)\} \tag{4.10}$$

from measurements of the backscattered field on the plane $-R = \mathbf{e}_i \cdot \mathbf{x}$, which by hypothesis lies outside the support of $V(\mathbf{x})$. Compute $Q_s(\tau = -R,t,\mathbf{e}_i)$ from $R_s(\tau = -R,t,\mathbf{e}_i)$ using (4.8a) above.

(2) *Recursively* compute $U_s(\cdot)$ and $Q_s(\cdot)$ in τ using (4.8) above, for each $\mathbf{e}_i$, yielding $\mathscr{R}\{V(\mathbf{x})\}$ on the plane $t = \tau = \mathbf{e}_i \cdot \mathbf{x}$ from (4.8c) at each recursion. This is used along with $U_s(\cdot)$ in (4.9) to compute the right-hand side of (4.8b). The recursion in τ runs from $-R$ to R.

(3) After the recursion is complete, an inverse Radon transform may be used to reconstruct $V(\mathbf{x})$, since its support lies inside a sphere of radius R.

Some comments are in order here. First, note that the recursive, layer-by-layer (in τ) reconstruction of $V(\mathbf{x})$ sharply contrasts with the batch reconstructions of the integral equation procedures. Newton's[4] procedure first recon-

structs the scattered field for *all* angles of probing *all at once* [note the coupling in $\mathbf{e}_i$ in (3.7)]. Computationally, this is a tremendous undertaking. The layer stripping procedure decouples the computations for different angles of probing, so that they can be run concurrently on an array processor, and results from different angles are combined only in (2.2).

Second, note that the simpler form of the layer stripping algorithm is a result of the exploitation of *causality* and the structure of the inverse scattering problem. By examining the jump in the scattered field at the wave front, which is measured by the first nonzero value of the causal quantity $Q_s(\cdot)$, we avoid problems with multiple scattering events, which aids in recovering values of $V(\mathbf{x})$. This structure is manifested by the Hankel structure of the kernel of the Marchenko integral equation (3.7); but this structure can be exploited more directly by appealing to the physical nature of the problem. The concept of exploiting the jump in the scattered field at the wave front in order to determine the potential has been noted in Morawetz,[29] and is the basis of the *miracle* equation of Newton[4] [Eq. (3.10) above] and the *fundamental identity* of Rose *et al.*[9] This is discussed in more detail below.

Finally, note that the layer stripping algorithm uses only near-field, backscattered data, unlike the integral equation procedures. This makes it more suitable for solving inverse seismic problems, since for these problems data are measured in the near field and transmission data are not available. In Yagle and Levy,[15] a layer stripping algorithm is applied to an inverse seismic problem formulated in Coen *et al.*[1] The issue of overdetermination arising in Newton's procedure also does not arise in the present procedure since only backscattered data are used.

V. INTEGRAL EQUATION METHODS AND THE RADON TRANSFORM

In this section it is shown that the same basic equations that led to the layer stripping procedure in Sec. IV also lead to the integral equation procedures of Moses and Newton described in Sec. III. This shows that the layer stripping and integral equation approaches are related to each other. Similar connections between layer stripping and integral equation approaches were demonstrated for the one-dimensional inverse problem in Bruckstein *et al.*[21] It is also demonstrated in this section that basic Born approximation results may be derived easily from all three methods by employing a single scattering approximation. The results of this section are not intended to be rigorous derivations; they are heuristic derivations that illustrate why the equations have the forms they have. They are intended to aid in understanding and interpreting the various inverse problem solution procedures.

A. The integral equation procedure of Moses

In Moses,[5] $T(\mathbf{k}',\mathbf{k})$ is defined as [Eq. (5.12) in Ref. 5]

$$T(\mathbf{k}',\mathbf{k}) = \int e^{-i\mathbf{k}'\mathbf{x}} V(\mathbf{x}) u(\mathbf{x},\mathbf{k}) d\mathbf{x}, \tag{5.1}$$

where $\mathbf{k} = k\mathbf{e}_i$, so that $u(\mathbf{x},\mathbf{k}) = u(\mathbf{x},k,\mathbf{e}_i)$. Therefore, $T(\mathbf{k}',\mathbf{k})$ can be interpreted as a *generalized scattering amplitude* [Eq. (5.1) reduces to the definition (3.4) of scattering amplitude if $|\mathbf{k}| = |\mathbf{k}'|$]. In addition, if we write $\mathbf{k} = |\mathbf{k}|\mathbf{e}_i = k\mathbf{e}_i$ and $\mathbf{k}' = |\mathbf{k}'|\mathbf{e}_s = k'\mathbf{e}_s$, and extend k and k' to negative values by writing $\mathbf{k} = (-k)(-\mathbf{e}_i)$ and $\mathbf{k}' = (-k')(-\mathbf{e}_s)$, then we may regard $T(\mathbf{k}',\mathbf{k})$ as the double Fourier transform of $\mathscr{R}\{V(\mathbf{x})u(\mathbf{x},t,\mathbf{e}_i)\}$:

$$\begin{aligned} T(\mathbf{k}',\mathbf{k}) &= \mathscr{F}\mathscr{F}\{\mathscr{R}\{V(\mathbf{x})u(\mathbf{x},t,\mathbf{e}_i)\}\} \\ &= \int\int\int V(\mathbf{x})u(\mathbf{x},t,\mathbf{e}_i)\delta(\tau - \mathbf{e}_s\cdot x) \\ &\quad \times e^{-ikt}e^{-ik'\tau}\,d\mathbf{x}\,dt\,d\tau. \end{aligned} \tag{5.2}$$

Using this observation, taking the double Fourier transform of the Radon transform (4.3) of the plasma wave equation (4.1) gives

$$(k^2 - k'^2)u(\mathbf{k}',\mathbf{k}) = T(\mathbf{k}',\mathbf{k}), \tag{5.3}$$

which leads to

$$u_s(\mathbf{k}',\mathbf{k}) = \gamma(k^2 - k'^2)T(\mathbf{k}',\mathbf{k}), \tag{5.4}$$

where $\gamma(\cdot)$ is defined by (3.15). In Moses[5] (5.4) was derived directly from the definition (3.4) of the scattering amplitude, but this lends no insight into *why* (5.3) has the form it does, whereas the present derivation shows that (5.3) is a direct consequence of the application of the Radon transform to the plasma wave equation. Multiplying the trivial definition (4.2) of the scattered field $u_s(\cdot)$ by $V(\mathbf{x})$ and taking the double Fourier transform from t to k and $\mathbf{x}$ to $\mathbf{k}' = k'\mathbf{e}_s$ (recall $\mathbf{e}_s = \mathbf{x}/|\mathbf{x}|$) results in

$$\begin{aligned} T(\mathbf{k}',\mathbf{k}) &= V(\mathbf{k}',\mathbf{k}) + \int V(\mathbf{k}',\mathbf{k}'')u_s(\mathbf{k}'',\mathbf{k})\,d\mathbf{k}'' \\ &= V(\mathbf{k}',\mathbf{k}) + \int V(\mathbf{k}',\mathbf{k}'') \\ &\quad \times \gamma(k^2 - k''^2)T(\mathbf{k}'',\mathbf{k})\,d\mathbf{k}'', \end{aligned} \tag{5.5}$$

where $V(\mathbf{k}',\mathbf{k})$ is defined by

$$V(\mathbf{k}',\mathbf{k}) = \int V(\mathbf{x})e^{i(\mathbf{k}-\mathbf{k}')\mathbf{x}}\,d\mathbf{x}, \tag{5.6}$$

and (5.4) has been used. Note that (5.5) is the same as (3.11), the first of the coupled integral equations of Moses's procedure.

The other equations of Moses's procedure may be derived using the *generalized Radon transform* (2.6) and a Fourier transform $\mathscr{F}$ that takes time t into k'', where $\mathbf{k}'' = k''\mathbf{e}$ and k'' is extended to negative values as before. We may write

$$\begin{aligned} &V(\mathbf{x})e^{-i\mathbf{k}'\mathbf{x}} \\ &\quad = (\mathscr{F}\mathscr{G})^{-1}(\mathscr{F}\mathscr{G})\{V(\mathbf{x})e^{-i\mathbf{k}'\mathbf{x}}\} \\ &\quad = (\mathscr{F}\mathscr{G})^{-1}\{T(\mathbf{k}',\mathbf{k}'')\} \\ &\quad = \int_{S^2}\int_0^\infty T(\mathbf{k}',\mathbf{k}'')u^*(\mathbf{x},\mathbf{k}'')k''^2\,d^2\mathbf{e}\,dk'' \\ &\quad = \int T(\mathbf{k}',\mathbf{k}'')u^*(\mathbf{x},\mathbf{k}'')\,d\mathbf{k}'' \end{aligned} \tag{5.7}$$

and a Fourier transform taking $\mathbf{x}$ into $\mathbf{k}$ results in

$$V(\mathbf{k}',\mathbf{k}) = \int T(\mathbf{k}',\mathbf{k}'')u^*(\mathbf{k},\mathbf{k}'')\,d\mathbf{k}''. \tag{5.8}$$

Taking a double Fourier transform of (4.2), inserting into (5.8), and setting $\mathbf{k}' = -\mathbf{k}$ results in

$$W(\mathbf{k}) = V(-\mathbf{k},\mathbf{k}) = T(-\mathbf{k},\mathbf{k}) + \int T(-\mathbf{k},\mathbf{k}'')\gamma^*(k''^2 - k^2)T^*(\mathbf{k},\mathbf{k}'')d\mathbf{k}''. \tag{5.9}$$

Using (3.14), $T(-\mathbf{k},\mathbf{k})$ can be obtained from the backscattering amplitude $A(k,-\mathbf{e},\mathbf{e})$ for $k \geqslant 0$. For $k \leqslant 0$, replace k with $-k$ in (5.9). This equation, combined with (5.9), gives (3.12), the second of Moses's equations. The last of the coupled integral equations (3.13) follows immediately from the definition of $W(\mathbf{k})$ in (5.9).

Thus it may be seen that the coupled integral equations (3.11)–(3.13) of Moses[5] may be interpreted as merely various Fourier and Radon transforms of elementary equations like (4.1) and (4.2). Note that at no point in the above derivations was time causality used. Indeed, this solution procedure does not exploit the structure of the inverse scattering problem at all. This is why the layer stripping algorithm, which does exploit this structure, is simpler.

B. The integral equation procedure of Newton

The generalized Radon transform may also be used to derive Newton's Marchenko integral equation (3.7). Let $u^+(\mathbf{x},t,\mathbf{e}_i)$ be a solution of the Schrödinger equation (3.1) with an outgoing radiation condition, and let $u^-(\mathbf{x},t,\mathbf{e}_i)$ be a solution with an incoming radiation condition. By reversing time we have that

$$u^-(\mathbf{x},t,\mathbf{e}_i) = u^+(\mathbf{x},-t,-\mathbf{e}_i). \tag{5.10}$$

Consider

$$\mathcal{G}\{u^+(\mathbf{x},t,\mathbf{e}_i) - u^-(\mathbf{x},t,\mathbf{e}_i)\} = \int u^-(\mathbf{y},\tau,\mathbf{e}_s)(u^+(\mathbf{y},t,\mathbf{e}_i) - u^-(\mathbf{y},t,\mathbf{e}_i))d\mathbf{y}. \tag{5.11}$$

We show first that this quantity can only depend on the time difference $t-\tau$. To do this, we apply a double Fourier transform taking t into k and τ into k' to the right side of (5.11). The result is shown to be the product of some function and $\delta(k+k')$. Since

$$\mathcal{F}^{-1}\{\mathcal{F}^{-1}\{\hat{f}(k)\delta(k+k')\}\} = f(t-\tau), \tag{5.12}$$

this will demonstrate that the right side of (5.11) depends only on the difference $t-\tau$.

Proceeding as discussed above, the double Fourier transform of (5.11) is

$$\mathcal{F}\{\mathcal{F}\{\mathcal{G}\{u^+ - u^-\}\}\} = \int u^-(\mathbf{y},k',\mathbf{e}_s)(u^+(\mathbf{y},k,\mathbf{e}_i) - u^-(\mathbf{y},k,\mathbf{e}_i))d\mathbf{y}. \tag{5.13}$$

We know that $u^+(\mathbf{y},k,\mathbf{e}_i)$ and $u^-(\mathbf{y},k,\mathbf{e}_i)$ are related by some *scattering operator* S by[4]

$$u^+(\mathbf{y},k,\mathbf{e}_i) = u^-(\mathbf{y},k,\mathbf{e}_i)S, \tag{5.14}$$

where the application of the operator S has the form[4]

$$u^+(\mathbf{y},k,\mathbf{e}_i) = \int u^-(\mathbf{y},k,\mathbf{e})S(k,\mathbf{e},\mathbf{e}_i)d^2\mathbf{e}. \tag{5.15}$$

Note that only the *existence* of the operator S is being used here; nothing need be known about it except that its inverse operator S^{-1} also exists. Using (5.14) in (5.13) along with the double Fourier transform of (5.10) results in

$$\mathcal{F}\{\mathcal{F}\{\mathcal{G}\{u^+ - u^-\}\}\} = \int u^{+*}(\mathbf{y},k',-\mathbf{e}_s)u^+(\mathbf{y},k,\mathbf{e}_i)(I - S^{-1})d\mathbf{y} = \delta(k\mathbf{e}_i + k'\mathbf{e}_s)(I - S^{-1}), \tag{5.16}$$

where I is the identity operator and the last equality follows from the completeness property of the solutions $u^+(\mathbf{y},k,\mathbf{e}_i)$.[8,9] Equation (5.16) has the form of the left side of (5.12); hence (5.11) depends only on $t-\tau$. In point of fact we have[4]

$$S - I = (k/2\pi i)A, \tag{5.17}$$

where A is the scattering amplitude operator defined similarly to (5.15), and S is Hermitian. Although these facts are not used here, they explain the use of $u^+ - u^-$ and the presence of $R(t,\mathbf{e}_s,\mathbf{e}_i)$ below.

Next, we evaluate (5.11) using this time invariance property. Without loss of generality, we may let t and τ approach infinity. Then the field in the vicinity of the scatterer will have decayed to zero, and virtually all of the contribution to the integral (5.11) will be in the far field. The incoming wave $u^-(\mathbf{y},\tau,\mathbf{e}_s)$ is simply the probing plane wave $\delta(\tau - \mathbf{e}_s\cdot\mathbf{y})$, and the outgoing wave is given by (3.6). Inserting these into (5.11), defining $\mathbf{e}_y = y/|y|$, and noting that $d\mathbf{y} = |\mathbf{y}|^2\, d|\mathbf{y}|\, d^2\mathbf{e}_y$ gives

$$\begin{aligned}\mathcal{G}\{u^+(\mathbf{x},t,\mathbf{e}_i) - u^-(\mathbf{x},t,\mathbf{e}_i)\} &= \int \delta(\tau - \mathbf{e}_s\cdot\mathbf{y})\frac{R(t-|\mathbf{y}|,\mathbf{e}_y,\mathbf{e}_i)}{4\pi|\mathbf{y}|}|\mathbf{y}|^2\, d|\mathbf{y}|\, d^2\mathbf{e}_y \\ &= \frac{1}{4\pi}\int_{S^2}\int_0^\infty \delta\left(\frac{\tau}{|y|} - \mathbf{e}_s\cdot\mathbf{e}_y\right) \times R(t-|\mathbf{y}|,\mathbf{e}_y,\mathbf{e}_i)d|\mathbf{y}|\, d^2\mathbf{e}_y \\ &= \int_0^{t-\tau} R(t-\tau-|\mathbf{y}|,\mathbf{e}_s,\mathbf{e}_i)d|\mathbf{y}|.\end{aligned} \tag{5.18}$$

The final equality in (5.18) is a result of letting $\tau, |\mathbf{y}| \to \infty$: the scattered field is significant only in the vicinity of the wave front $\tau = |\mathbf{y}|$ (the speed of propagation is unity) so that the only contribution to the integral occurs for $\tau/|\mathbf{y}| = 1$. Note that the upper limit at the end of (5.18) results from the causality of $R(\cdot)$.

Taking an inverse generalized Radon transform of both sides results in

$$\begin{aligned}u^+(\mathbf{x},t,\mathbf{e}_i) - u^-(\mathbf{x},t,\mathbf{e}_i) &= -\left(\frac{1}{8\pi^2}\right)\int_{S^2}\int_{-\infty}^{\infty} u^-(\mathbf{x},\tau,\mathbf{e}_s)\frac{\partial^2}{\partial\tau^2} \times \int_0^{t-\tau} R(t-\tau-|\mathbf{y}|,\mathbf{e}_s,\mathbf{e}_i)d|\mathbf{y}|\, d^2\mathbf{e}_s \\ &= -\left(\frac{1}{8\pi^2}\right)\int_{S^2}\int_{-\infty}^{\infty} u^-(\mathbf{x},\tau,\mathbf{e}_s)\frac{\partial}{\partial t} \times R(t-\tau,\mathbf{e}_s,\mathbf{e}_i)d\tau\, d^2\mathbf{e}_s,\end{aligned} \tag{5.19}$$

which is (4.16) in Ref. 9. Using (3.8) and (5.10) in (5.19), and noting that $u^+(\mathbf{x},t,\mathbf{e}_i)$ is zero for $t \leqslant \mathbf{e}_i\cdot\mathbf{x}$ yields the Mar-

chenko integral equation (3.7). Thus this integral equation is essentially an inverse generalized Radon transform. This interpretation of the Marchenko integral equation differs greatly from the functional analysis derivation in Newton[4] and Rose *et al.*,[9] and the representation theorem derivation in Rose *et al.*[30]

To recover the potential from the scattered field, we simply insert (4.5), which expresses the causality of the scattered field, into the plasma wave equation (4.1). Equating the coefficient of $\delta(t-\mathbf{e}_i\cdot\mathbf{x})$ to zero gives the miracle equation (3.10), since $(\partial/\partial t)u_s(\mathbf{x},t,\mathbf{e}_i)$ does not jump at the wave front. In Rose *et al.*[9] (3.10) is called the *fundamental identity*, and it is pointed out that this equation and the miracle equation are identical. An inverse Radon transform of (4.8c), from the layer stripping algorithm, also gives this equation. In all three cases, this equation is used to recover the potential from the jump in the scattered field at the wave front. However, the methods used to recover the scattered field itself differ widely.

Solving the Marchenko integral equation (3.7) is very difficult, due to the coupling between the $u_s(\mathbf{x},t,\mathbf{e}_i)$ in $\mathbf{e}_i$—it is necessary to solve for all of the scattered fields, due to probings in all directions, in one huge batch operation. The reason for this can be found by noting from (5.2) that knowledge of the complete Radon transform of $V(\mathbf{x})u(\mathbf{x},t,\mathbf{e}_i)$ is equivalent to knowledge of the generalized scattering amplitude $T(\mathbf{k},\mathbf{k}')$. However, this quantity is known only for $|\mathbf{k}|=|\mathbf{k}'|$, so that the scattering amplitude for one direction of probing $\mathbf{e}_i$ is not sufficient to reconstruct the scattered field for that $\mathbf{e}_i$. It is necessary to utilize the scattering amplitude for *all* $\mathbf{e}_i$ to reconstruct the scattered field for *any* $\mathbf{e}_i$.

C. The Born approximation

The (first) Born approximation is a *single scattering* approximation that greatly simplifies the solution to the inverse scattering problem. It consists of approximating the total wave field $u(\mathbf{x},t)$ inside the support of $V(\mathbf{x})$ by the probing impulse $\delta(t-\mathbf{e}_i\cdot\mathbf{x})$ alone—the scattered field $u_s(\mathbf{x},t)$ is neglected. This amounts to neglecting all multiple scattering events, an assumption that is reasonable for weak potentials or large values of k. Applying this approximation to the definition (3.4) of scattering amplitude and taking an inverse Fourier transform from k to t yields

$$\int V(\mathbf{x})\delta(t-(\mathbf{e}_s-\mathbf{e}_i)\cdot\mathbf{x})d\mathbf{x} = \mathscr{R}\{V(\mathbf{x})\}|_{\mathbf{e}=(\mathbf{e}_s-\mathbf{e}_i)} = -R^B(t,\mathbf{e}_s,\mathbf{e}_i), \tag{5.20}$$

where $R^B(\cdot)$ is the impulse response in the Born approximation. Thus the potential $V(\mathbf{x})$ can be recovered by an inverse Radon transform of the impulse response.

It is elucidating to note how the three exact methods discussed in this paper all reduce to this result when a single scattering approximation is imposed on each of them. This illustrates where multiple scattering events are being accounted for in each method, and thus further illuminates their operation.

D. Moses's integral equation procedure

In Moses's procedure the second term on the right side of (3.12) accounts for multiple scattering events. To see this, note that if this term is neglected (3.12) reduces to

$$W(\mathbf{k}) = W(k,\mathbf{e}_i) = \int V(\mathbf{x})e^{-2ike_i\cdot\mathbf{x}}d\mathbf{x} = -b(k,\mathbf{e}_i) = -A^B(k,-\mathbf{e}_i,\mathbf{e}_i) \tag{5.21}$$

and an inverse Fourier transform from k to t (with k extended to negative values in the usual way) results in (5.20) with $\mathbf{e}_s=-\mathbf{e}_i$. Note that this is sufficient information to invert the Radon transform; backscattered data alone suffices.

E. Newton's integral equation procedure

The Born approximation applied to Newton's procedure amounts to neglecting the first term in the Marchenko integral equation (3.7). This leaves

$$u_s(\mathbf{x},t,\mathbf{e}_i) = -\frac{1}{8\pi^2}\int\frac{d}{dt}R^B(t-\mathbf{e}_s\cdot\mathbf{x},\mathbf{e}_s,\mathbf{e}_i)d^2\mathbf{e}_s. \tag{5.22}$$

Applying the miracle equation (3.10), which we write here as

$$V(\mathbf{x}) = -2\mathbf{e}_i\cdot\nabla u_s(\mathbf{x},t=\mathbf{e}_i\cdot\mathbf{x},\mathbf{e}_i) + 2\frac{\partial}{\partial t}u_s(\mathbf{x},t=\mathbf{e}_i\cdot\mathbf{x},\mathbf{e}_i) \tag{5.23}$$

(recall that the second term is zero) results in

$$V(\mathbf{x}) = -\frac{1}{8\pi^2}\int\frac{\partial^2}{\partial t^2}\times R^B(t=(\mathbf{e}_i-\mathbf{e}_s)\mathbf{x},\mathbf{e}_s,\mathbf{e}_i)|\mathbf{e}_i-\mathbf{e}_s|^2d^2\mathbf{e}_s = \mathscr{R}^{-1}\{-R^B(t,\mathbf{e}_s,\mathbf{e}_i-\mathbf{e}_s)\} \tag{5.24}$$

and a Radon transform of both sides results in (5.20).

F. Layer stripping procedure

In the layer stripping procedure the coupling in the system of equations (4.8) accounts for multiple scattering events. To see this, neglect this coupling, so that the algorithm becomes simply (4.8c), backpropagated to the far field as

$$\mathscr{R}\{V(\mathbf{x})\} = -2Q_s(\tau,t=\tau,\mathbf{e}) = -2Q_s(-R,t=2\tau+R,\mathbf{e}). \tag{5.25}$$

Taking the Radon transform of (3.6) and utilizing the definition (4.8a) of $Q_s(\cdot)$ in terms of $U_s(\cdot)$ yields (5.20).

VI. CONCLUSION

A layer stripping algorithm for solving Schrödinger equation inverse scattering problems has been proposed. This algorithm is differential in nature, in contrast to the other integral equation procedures discussed. By exploiting the inherent structure of the inverse scattering problem (time causality), this algorithm appears to require much less computation time than the integral equation procedures, which reconstruct the potential in one huge batch operation without taking advantage of the structure of the problem. In addition, this algorithm requires near-field, backscattered data, making it more suitable for inverse seismic problems

and other situations in which transmission data are not available.

The proposed algorithm differs from that of Yagle and Levy[15] in its use of the Radon transform. While this makes the reconstruction of $V(\mathbf{x})$ more complicated, it also simplifies the propagation of the scattered field, since the transverse Laplacian required at each step of the algorithm in Ref. 15 is no longer required. Both algorithms are in principle exact, with approximation inherent only in the discretization needed to implement them.

A significant consequence of the use of the Radon transform in this algorithm is that it made direct mathematical comparison between the layer stripping and integral equation procedures possible, which was not the case in Ref. 15. Indeed, the integral equation procedures of Newton and Moses were *derived* heuristically using the Radon transform and the generalized Radon transform. In addition, it was shown how all three inversion procedures reduce to the Born approximation when single scattering approximations are made. This showed the important role these transforms play in both exact and approximate procedures.

Considerable work remains to be done in making the layer stripping procedure a practical method for solving inverse scattering problems. Their numerical performance on synthetic data is a subject of current research. Other topics on which research is needed include numerical performance on noisy data, improved ways of implementing Eq. (4.9), and investigation of the applicability of this procedure to problems with bound states.

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Gravitational mass in an expanding universe

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A test for the Hawking definition of mass is given in a Tolman–Bondi model that asymptotically approaches the open Friedmann universe. An expanding universe filled with dustlike matter of zero pressure is considered. The matter distribution is spherically symmetric but nonhomogeneous. With appropriate boundary conditions, the calculation yields a finite and nonzero value for the Hawking mass, measured as a deviation from a "renormalized" zero mass in the unperturbed Friedmann model. These boundary conditions are more restrictive than those found for a model with gravitational radiation.

I. INTRODUCTION

There is no well defined gravitational energy density in general relativity. Gravitational energy cannot be localized and there does not exist a stress-energy tensor for the gravitational field. The total energy of a gravitational system therefore cannot be expressed as a simple integral over a spacelike three-surface of a local energy density.

For an isolated system in general relativity, i.e., an asymptotically flat space-time, there is a well defined total energy of the system. By asymptotic flatness we mean that the curvature vanishes both at large spacelike distances and at large null distances from the source.[1] The Arnowitt–Deser–Misner (ADM) mass[2] is defined asymptotically at spatial infinity and represents the total energy of the system. At null infinity the asymptotically defined Bondi mass[3] represents the remaining energy of the system at some retarded time u after radiation has been emitted. Thus for a radiating system the Bondi mass is a decreasing function of u and is equal to the ADM mass in the past limit $u\to-\infty$ at future null infinity, $\mathscr{I}^+$ (see Ref. 4).

Hawking has provided a definition of mass at $\mathscr{I}^+$ in a space-time that is asymptotically an open Friedmann model.[5] We have reason to assume that our universe is described by one of the Friedmann models, and current observations indicate that we live in an open universe.[6] Hawking defined a quantity $\tilde{M}$ that can be divided into two pieces $\tilde{M}_1$ and $\tilde{M}_2$, where $\tilde{M}_1$ is infinite and $\tilde{M}_2$ is zero in the unperturbed open Friedmann model. He then considered outgoing gravitational radiation from a bounded source in a model that asymptotically approaches that of the open Friedmann model. It was shown that the piece $\tilde{M}_2$, which is vanishing in the background metric, might be interpreted as the total mass of the source and the disturbance. In asymptotically flat space the Hawking definition of mass agrees with the Bondi mass. Hawking also showed that $\tilde{M}_2$ obeys a conservation law similar to that of the Bondi mass in asymptotically flat space.

In this paper we shall test $\tilde{M}_2$ as a definition of mass in a model that asymptotically goes over to the open Friedmann universe. We shall do so by considering a spherically symmetric, not necessarily homogeneous, model of a universe filled with dustlike matter. Such models are commonly called Tolman–Bondi models in the literature.[7] If the falloff behavior of the matter fields is chosen such that the effective gravitational mass gets a constant added to it asymptotically, we can show that $\tilde{M}_2$ gives a finite and nonzero mass of the disturbance, as measured from the unperturbed Friedmann model.

II. THE HAWKING MASS

We employ the Newman–Penrose formalism where $\{l^a,n^a,m^a,\bar{m}^a\}$ is a tetrad of null vectors.[8] The vectors satisfy the orthonormality relations

$$\begin{aligned} &l_a l^a = n_a n^a = m_a m^a = \bar{m}_a \bar{m}^a = 0, \\ &l_a n^a = -m_a \bar{m}^a = 1, \quad l_a m^a = n_a m^a = 0, \end{aligned} \tag{2.1}$$

and, as a consequence of these,

$$g^{ab} = l^a n^b + n^a l^b - m^a \bar{m}^b - \bar{m}^a m^b. \tag{2.2}$$

The vector l^a is taken to be orthogonal to a family of null hypersurfaces designated by $u=$ const, that is, $l_a = u_{;a}$. An affine parameter r along the null geodesics in the surfaces $u=$ const is introduced such that $r_{;a} l^a = 1$. Since l^a is null it is also a tangent vector to these null geodesics and we have

$$l^a = \frac{dx^a}{dr} = g^{ab} u_{;b}. \tag{2.3}$$

We define the vector n^a to be the ingoing null vector orthogonal to the two-surfaces of constant u and r. The vectors m^a and $\bar{m}^a$ are complex conjugate null vectors that lie in these two-surfaces.

Hawking defined the quantity[5]

$$M(S) = (4\pi)^{-3/2}\left(\int dS\right)^{1/2}\int (-\Psi_2 - \sigma\lambda + \Phi_{11} + \Lambda)\,dS, \tag{2.4}$$

where S is a spacelike two-sphere of constant u and r. The quantities in the integrand are

$$\begin{aligned} &\Psi_2 = -\tfrac{1}{2} C_{abcd}(l^a n^b l^c n^d - l^a n^b m^c \bar{m}^d), \\ &\sigma = l_{a;b} m^a m^b, \quad \lambda = -n_{a;b}\bar{m}^a \bar{m}^b, \\ &\Phi_{11} = -\tfrac{1}{4} R_{ab}(l^a n^b + m^a \bar{m}^b), \quad \Lambda = R/24, \end{aligned} \tag{2.5}$$

where C_{abcd} is the Weyl tensor. $M(S)$ is interpreted as the total mass of the system in the limit when the two-sphere becomes infinitely large. The total mass is therefore

$$\tilde{M}(S) = \lim_{r\to\infty} M(S). \tag{2.6}$$

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In reality $\tilde{M}(S)$ is a time component of the total four-momentum of the system but the quantity gives mass because the three-momentum is zero in the asymptotic rest frame used. We may split $\tilde{M}(S)$ into two pieces $\tilde{M}_1$ and $\tilde{M}_2$ so that

$$\tilde{M}_1(S) = \lim_{r\to\infty}(4\pi)^{-3/2}\left(\int dS\right)^{1/2}\int(\Phi_{11}+\Lambda)dS,$$
$$\tilde{M}_2(S) = \lim_{r\to\infty}(4\pi)^{-3/2}\left(\int dS\right)^{1/2}\int(-\Psi_2-\sigma\lambda)dS. \tag{2.7}$$

In the next section we evaluate these quantities in the unperturbed Friedmann model. We shall find that the quantity $\tilde{M}_2$ is the interesting one as a candidate for mass. We call $\tilde{M}_2$ the Hawking mass. In Sec. V, we calculate the Hawking mass in a Tolman–Bondi model that asymptotically approaches the open Friedmann universe.

III. THE UNDISTURBED FRIEDMANN MODEL

The metric of an open Friedmann model can be written[9]

$$ds^2 = \Omega^2(\eta)[d\eta^2 - dR^2 - \sinh^2 R \times(d\theta^2+\sin^2\theta\, d\varphi^2)], \tag{3.1}$$

where the scale factor $\Omega(\eta)$ as a function of the conformal time η is

$$\Omega(\eta) = A(\cosh\eta - 1), \quad A>0. \tag{3.2}$$

We shall assume a universe filled with dustlike matter of zero pressure. The stress-energy tensor is that of a perfect fluid at rest relative to the above coordinates. It is given by

$$T_{ab} = \rho u_a u_b, \tag{3.3}$$

where ρ is the mass-energy density of the matter and u_a its velocity. The four-velocity is normalized by $u_a u^a = 1$ and, in the comoving coordinate system,

$$u_a = \Omega\eta_{;a}. \tag{3.4}$$

The evolution of the universe is determined by the Einstein equations

$$R_{ab} - \tfrac{1}{2}g_{ab}R = -8\pi T_{ab}, \tag{3.5}$$

from which we find that $4\pi\rho = 3A\Omega^{-3}$. We also have $R = 8\pi\rho$, which yields

$$\Lambda = \tfrac{1}{4}A\Omega^{-3} \tag{3.6}$$

in the undisturbed Friedmann metric. Since the metric is isotropic, the Ricci tensor has only two independent components. These are taken to be Λ and Φ_{00}, where

$$\Phi_{00} = -\tfrac{1}{2}R_{ab}l^a l^b. \tag{3.7}$$

It is readily obtained that $\Phi_{00} = 3A\Omega^{-5}$. We shall assume here and in the rest of this paper that the null tetrad is introduced along spherically symmetric null cones. With this choice it follows that $\Phi_{11} = 3\Lambda$.

We introduce a null coordinate $u = \eta - R$ and stereographic coordinates x_3, x_4 such that the metric may be expressed as

$$ds^2 = \Omega^2(\eta)[-du^2 + 2\,du\,d\eta - \sinh^2(\eta-u)Q^{-2}(dx_3^2+dx_4^2)], \tag{3.8}$$

where

$$Q = (1+\tfrac{1}{4}(x_3^2+x_4^2)). \tag{3.9}$$

The affine parameter r can be calculated from Eq. (2.3), which gives

$$r = A^2[\tfrac{1}{4}\sinh 2\eta - 2\sinh\eta + \tfrac{3}{2}\eta] \tag{3.10}$$

in a coordinate system where the origin of the affine parameter is at $\eta = 0$. In these coordinates surfaces of constant r are surfaces of constant η.

We now calculate the quantities given by Eq. (2.7) in the undisturbed Friedmann metric. Because $dS \sim \Omega^4(\eta)$, we find that

$$\tilde{M}_1(S) \sim \lim_{r\to\infty}\Omega^3(\eta) = \infty. \tag{3.11}$$

The metric (3.1) is conformally flat and therefore Ψ_2 is zero. The complex shear σ vanishes because of spherical symmetry and we find

$$\tilde{M}_2(S) = 0. \tag{3.12}$$

So the piece $\tilde{M}_1$ of the total mass diverges while the piece $\tilde{M}_2$ vanishes in the unperturbed Friedmann model. We may "renormalize" this mass by discarding the infinite contribution from $\tilde{M}_1$. As Hawking suggested, the piece $\tilde{M}_2$ may then be a candidate for mass in a model that asymptotically approaches the open Friedmann model. We shall test this conjecture for a dust-filled Friedmann universe with a nonhomogeneous distribution of matter.

IV. SPHERICALLY SYMMETRIC EXPANDING UNIVERSE

We consider a spherically symmetric universe filled with dustlike matter of mass density ρ (see Ref. 10). The matter distribution is not necessarily homogeneous but the pressure is assumed to be zero. The spherical symmetry allows us to write the metric as

$$ds^2 = dt^2 - e^{2\alpha}dR^2 - r^2(d\theta^2+\sin^2\theta\, d\varphi^2), \tag{4.1}$$

where α and r are arbitrary functions of R and t. We use a comoving coordinate system where the four-velocity u^a has components (1,0,0,0). From the Einstein equations we obtain the following equations:

$$e^{2\alpha} = r'^2/[1+2E(R)], \tag{4.2}$$
$$\tfrac{1}{2}\dot{r}^2 - m(R)/r = E(R), \tag{4.3}$$
$$4\pi\rho = m'/r'r^2, \tag{4.4}$$

where $E(R)$ and $m(R)$ are arbitrary functions of integration. The prime denotes the partial derivative with respect to R, and the dot denotes the partial derivative with respect to t. The function $m(R)$ plays the role of an effective gravitational mass in Eq. (4.3), which has the same form as the Newtonian energy equation. From Eq. (4.4) we find that

$$m(R) = 4\pi\int_0^R \rho r^2 r'\,dR, \tag{4.5}$$

which can be interpreted as the total amount of mass-energy interior to a shell of matter with comoving radius R (see Ref. 11). The function $E(R)$ represents the total energy per unit mass of a shell of matter at radial coordinate R. Taking the initial conditions to be such that $\dot{r}>0$, we notice that the universe will expand indefinitely if $E(R)$ is positive for all R.

If $E(R)$ is negative for some values of R, the radial velocity $\dot{r}$ will become zero for $r=-m/E$, and the corresponding shells of matter will start to recollapse. We shall in the following assume that $E(R)>0$, for all values of R. In parametric form the solution to Eq. (4.3) may then be written

$$t=(m/(2E)^{3/2})(\sinh\eta-\eta),$$
$$r=(m/2E)(\cosh\eta-1). \tag{4.6}$$

If we take

$$\tilde{m}(R)=A\sinh^3 R,\quad \tilde{E}(R)=\tfrac{1}{2}\sinh^2 R, \tag{4.7}$$

we obtain the familiar open Friedmann model. In that case the parameter η simply denotes the conformal time coordinate.

We now let

$$m(R)=\tilde{m}(R)(1+f(R)),$$
$$E(R)=\tilde{E}(R)(1+g(R)), \tag{4.8}$$

where the functions $f(R), g(R)\to 0$ as $R\to\infty$. This yields a spherically symmetric model that asymptotically approaches the open Friedmann model at large radial distances R. The crucial point is how fast it approaches the undisturbed Friedmann model. We determine the asymptotic fall-off behavior by requiring that

$$m(R)\to\tilde{m}(R)+m_0,\quad \text{as } R\to\infty, \tag{4.9}$$

where m_0 is a constant. This leads us to a class of functions $f(R)$ with an asymptotic behavior as $R\to\infty$:

$$f(R)\sim C_1 e^{-3R}, \tag{4.10}$$

where C_1 is a positive constant. This yields

$$m_0=\tfrac{1}{8}C_1 A. \tag{4.11}$$

Similarly, we let $g(R)$ represent a class of functions with an asymptotic behavior at large radial distances:

$$g(R)\sim C_2 e^{-3R}, \tag{4.12}$$

where C_2 is positive. This choice gives

$$E(R)\to\tilde{E}(R),\quad \text{as } R\to\infty. \tag{4.13}$$

In order to have a constant mass density near the origin we also require that $f\sim$const and $g\sim$const as $R\to 0$. The solution (4.6) becomes

$$t=(1+f-\tfrac{3}{2}g)A(\sinh\eta-\eta),$$
$$r=\sinh R(1+f-g)\Omega(\eta), \tag{4.14}$$

in the asymptotic limit $R\to\infty$. To first order in f and g the metric then takes the form

$$\begin{aligned} ds^2=\Omega^2(\eta)[&(1+2h)d\eta^2-6hA(\sinh\eta-\eta)\Omega^{-1}\,d\eta\,dR\\ &-(1-4h-3g+6hA^2\sinh\eta\\ &\times(\sinh\eta-\eta)\Omega^{-2})dR^2\\ &-\sinh^2 R(1+2h+g)(d\theta^2+\sin^2\theta\,d\varphi^2)], \end{aligned} \tag{4.15}$$

where

$$h\equiv f-\tfrac{3}{2}g. \tag{4.16}$$

The mass density is given by

$$\begin{aligned} 4\pi\rho=3A\Omega^{-3}[&1-3hA^2\sinh\eta(\sinh\eta-\eta)\Omega^{-2}\\ &+6e^{-2R}h(A^2\sinh\eta(\sinh\eta-\eta)\Omega^{-2}-\tfrac{2}{3})] \end{aligned} \tag{4.17}$$

at large radial distances.

We now realize that there is a difficulty with the physical interpretation of this expression. If for a moment we let $C_2=0$, the leading-order term of the mass density perturbation yields a negative contribution to ρ. However, physically we have added mass to the model since $m(R)$ is greater than the background value $\tilde{m}(R)$ ($C_1>0$). We also notice from Eq. (4.14) that we have an ambiguity in the choice of time slicing of the space-time since surfaces of constant η no longer are the same as surfaces of constant t, the proper time. The difficulty arises because the value of the mass density perturbation changes with different time slicings of space-time. Since ρ is nonzero and time dependent in the background space-time, the mass density perturbation is not invariant under infinitesimal coordinate transformations of the form

$$\eta\to\eta^*=\eta+\xi^\eta, \tag{4.18}$$

where $|\xi^\eta|\ll 1$. By transforming back to a physically more sensible time coordinate, then, we may cure this difficulty with the interpretation of the density perturbation.

A coordinate transformation of the sort (4.18) induces a gauge change in the metric perturbation γ_{ab} given by

$$\gamma_{ab}\to\gamma^*_{ab}=\gamma_{ab}-2\xi_{(a;b)}, \tag{4.19}$$

where ξ^a means the four-vector field with components $(\xi^\eta,0,0,0)$. We write the metric coefficients in the form

$$g_{ab}=\tilde{g}_{ab}+\gamma_{ab}, \tag{4.20}$$

where $\tilde{g}_{ab}$ is the background metric. Indices of γ_{ab} are raised and lowered with $\tilde{g}_{ab}$ and the semicolon means the covariant derivative relative to $\tilde{g}_{ab}$. We now require that the new metric coefficient $\gamma^*_{\eta R}$ vanishes under the coordinate transformation (4.18). This condition implies that the metric will not have any off-diagonal terms, corresponding to a time-orthogonal coordinate system. We obtain

$$\xi^\eta=hA(\sinh\eta-\eta)\Omega^{-1}, \tag{4.21}$$

which by means of the gauge transformation (4.19) gives the new metric (dropping the asterisks)

$$\begin{aligned} ds_2=\Omega^2(\eta)[&d\eta^2-(1-4h-3g+4hA^2\sinh\eta\\ &\times(\sinh\eta-\eta)\Omega^{-2})dR^2\\ &-\sinh^2 R(1+2h+g-2hA^2\sinh\eta\\ &\times(\sinh\eta-\eta)\Omega^{-2})(d\theta^2+\sin^2\theta\,d\varphi^2)]. \end{aligned} \tag{4.22}$$

Since the time–time component of the metric perturbation is zero, this choice of gauge is also the same as the synchronous gauge.[12] It should be pointed out that surfaces of constant η now coincide with surfaces of constant proper time t.

The coordinate transformation (4.18) implies a gauge change of the mass density,

$$\rho\to\rho^*=\rho-\tilde{\rho}_{;\eta}\xi^\eta, \tag{4.23}$$

which by means of Eq. (4.21) gives the new mass density (again dropping the asterisk)

$$\begin{aligned} 4\pi\rho=3A\Omega^{-3}&\\ &\times[1+6e^{-2R}h(A^2\sinh\eta(\sinh\eta-\eta)\Omega^{-2}-\tfrac{2}{3})]. \end{aligned} \tag{4.24}$$

In the new gauge the mass density perturbation is positive if

$h > 0$, in particular it is positive for $C_2 = 0$. Thus we may take the point of view that the new time coordinate is a more reasonable one, in the sense that the interpretation of the density perturbation becomes more physical.

Bardeen has solved the problem of gauge ambiguity of energy density perturbations in a different framework.[13] Bardeen's approach is based on constructing gauge-invariant quantities which have inherent physical meaning and eliminate any gauge choice. Applied to our case of zero pressure and comoving coordinates the gauge-invariant density perturbation amplitude may be written

$$\epsilon = \frac{\delta\rho}{\tilde{\rho}} - 3\Omega^{-1}\frac{d\Omega}{d\eta}\gamma_{\eta R}. \tag{4.25}$$

Computed in either of the coordinate systems given by Eqs. (4.15) or (4.22) this gives

$$\epsilon = 6e^{-2R}h(A^2 \sinh\eta(\sinh\eta - \eta)\Omega^{-2} - \tfrac{2}{3}), \tag{4.26}$$

which is in agreement with the expression (4.24). In other words, in the comoving time-orthogonal gauge the mass density perturbation $\delta\rho$ can be exactly identified with the gauge-invariant quantity ϵ; i.e., $\delta\rho = \epsilon\tilde{\rho}$.

We finally introduce a null coordinate u given by

$$u = \eta - R + p(\eta)g(R) + q(\eta)h(R), \tag{4.27}$$

where the functions $p(\eta)$ and $q(\eta)$ are determined by demanding that $\gamma_{\eta\eta} = 0$ in the (u,η,θ,φ) coordinate system. Now taking the asymptotic limit $u = \text{const}$, $\eta \to \infty$, we get

$$\begin{aligned} p(\eta) &= -\tfrac{1}{2}, \\ q(\eta) &= -\tfrac{1}{2}A\Omega^{-1}\log\Omega + \tfrac{1}{2}(\log A/2 + \tfrac{7}{4})A\Omega^{-1}, \end{aligned} \tag{4.28}$$

where $q(\eta)$ is expanded as a power series in Ω with terms of the form $\Omega^{-m}\log^n\Omega (m \geqslant 1,\ n = 0,1)$. This yields a perturbed metric

$$\begin{aligned} ds^2 = \Omega^2(\eta)\big[&-(1 - hA\Omega^{-1}\log\Omega + hA\Omega^{-1}(\log A/2 + \tfrac{11}{4}))du^2 \\ &+ 2(1 - \tfrac{1}{2}hA\Omega^{-1}\log\Omega + \tfrac{1}{2}hA\Omega^{-1}(\log A/2 + \tfrac{11}{4}))du\,d\eta \\ &- \sinh^2(\eta - u)Q^{-2}(1 + hA\Omega^{-1}\log\Omega - hA\Omega^{-1}(\log A/2 + \tfrac{9}{4}))(dx_3^2 + dx_4^2)\big], \end{aligned} \tag{4.29}$$

where x_3, x_4 are stereographic coordinates and Q is given by Eq. (3.9).

The task is now a purely computational one using this metric to find the perturbation in the Weyl tensor that will give us the mass of the density perturbation. We carry out this calculation in the next section. It should be added that the gauge ambiguity problem of the density perturbation discussed in this section is not relevant to the evaluation of the Hawking mass. $\tilde{M}_2$ is a gauge-invariant quantity since it vanishes in the background space-time. The Hawking mass therefore does not change under a coordinate transformation and is unambiguously defined for the class of space-times given by Eq. (4.29).

V. CALCULATION

We compute the quantity $\tilde{M}_2$ given from Eq. (2.7) by

$$\tilde{M}_2(S) = \lim_{r\to\infty}(4\pi)^{-3/2}\left(\int dS\right)^{1/2}\int(-\Psi_2)dS. \tag{5.1}$$

The complex shear σ vanishes because of spherical symmetry. The Weyl tensor vanishes in the unperturbed Friedmann metric so from Eq. (2.5) we have

$$\Psi_2 = -\tfrac{1}{2}\delta C_{abcd}(l^a n^b l^c n^d - l^a n^b m^c \bar{m}^d), \tag{5.2}$$

where δC_{abcd} is the perturbed Weyl tensor. It may be written

$$\begin{aligned} \delta C_{abcd} = \delta R_{abcd} &- (\tilde{g}_{a[c}\delta R_{d]b} + \tilde{g}_{b[d}\delta R_{c]a}) \\ &- (\gamma_{a[c}\tilde{R}_{d]b} + \gamma_{b[d}\tilde{R}_{c]a}) \\ &+ \tfrac{1}{3}\delta R\tilde{g}_{a[c}\tilde{g}_{d]b} + \tfrac{1}{3}\tilde{R}(\tilde{g}_{a[c}\gamma_{d]b} + \tilde{g}_{b[d}\gamma_{c]a}). \end{aligned} \tag{5.3}$$

For our purposes it is sufficient to calculate the perturbation of the Riemann tensor δR_{abcd} because one can show that all the terms involving the Ricci tensor or the scalar curvature fall off faster at null infinity. Generally, if γ_{ab} is the metric perturbation on a curved space-time, the perturbed Riemann tensor is given by

$$\delta R_{abcd} = \delta R_{abc}{}^e\tilde{g}_{ed} + \tilde{R}_{abc}{}^e\gamma_{ed}, \tag{5.4}$$

where

$$\delta R_{abc}{}^e = \nabla_{[a}(\nabla^e\gamma_{b]c} - \nabla_{|c|}\gamma_{b]}{}^e - \nabla_{b]}\gamma_c{}^e). \tag{5.5}$$

The contribution to Ψ_2 from the second term in Eq. (5.4) falls off faster at $\mathscr{I}^+$ than the contribution from the first term and may be neglected. Similarly, the last term in Eq. (5.5) can be written

$$\nabla_{[a}\nabla_{b]}\gamma_c{}^e = -\tfrac{1}{2}\tilde{R}_{abc}{}^d\gamma_d{}^e + \tfrac{1}{2}\tilde{R}_{abd}{}^e\gamma_c{}^d \tag{5.6}$$

and gives terms with a faster falloff behavior. Therefore, to leading order in the asymptotic expansion we have

$$\delta C_{abcd} = \nabla_{[a}(\nabla_{|d|}\gamma_{b]c} - \nabla_{|c|}\gamma_{b]d}). \tag{5.7}$$

In our coordinates the tetrad vectors may be expressed as[5]

$$\begin{aligned} l^a &= \frac{dx^a}{dr} = \Omega^{-2}\delta^a_\eta, \\ n^a &= \delta^a_u + U\Omega^{-2}\delta^a_\eta + X^i\delta^a{}_i, \quad i = 3,4, \\ m^a &= \xi^i\delta^a{}_i, \end{aligned} \tag{5.8}$$

where

$$\begin{aligned} &U = \tfrac{1}{2}\Omega^2 + O(1), \quad X^i = O(\Omega^{-4}), \\ &\xi^i = \xi^{i0}\Omega^{-2} + O(\Omega^{-3}). \end{aligned} \tag{5.9}$$

This yields a leading-order contribution to Ψ_2 given by

$$\Psi_2 = -\tfrac{1}{2}\Omega^{-4}\delta C_{\eta u\eta u}. \tag{5.10}$$

From Eq. (5.7) we obtain

$$\delta C_{\eta u\eta u} = \nabla_{[\eta}(\nabla_{|u|}\gamma_{u]\eta} - \nabla_{|\eta|}\gamma_{u]u}) = 2A\Omega h, \tag{5.11}$$

which yields

$$\Psi_2 = -A\Omega^{-3}h. \tag{5.12}$$

The function h is defined by Eq. (4.16) and may be expressed as

$$h = Ce^{-3R} \simeq Ce^{-3\eta}e^{3u}, \tag{5.13}$$

where

$$C \equiv C_1 - \tfrac{3}{2}C_2. \tag{5.14}$$

We have here used the approximation $u \simeq \eta - R$ of Eq. (4.27). Using that $e^{-\eta} \simeq \frac{1}{2}A\Omega^{-1}$ we find

$$\Psi_2 = -\tfrac{1}{8}CA^4 e^{3u}\Omega^{-6}, \tag{5.15}$$

in the asymptotic limit $u = \text{const}$, $\eta \to \infty$.

The coordinates x_3 and x_4 are chosen so that the leading term in g^{ij} is a conformally flat metric. From Eq. (2.2) we have

$$\begin{aligned} g^{ij} &= -(\xi^{i0}\bar{\xi}^{j0} + \bar{\xi}^{i0}\xi^{j0})\Omega^{-4} + O(\Omega^{-5}) \\ &= -2P\bar{P}\delta^{ij}\Omega^{-4} + O(\Omega^{-5}), \end{aligned} \tag{5.16}$$

where $P(u,x_i) = \xi^{30} = -i\xi^{40}$. To obtain agreement with the unperturbed metric (3.8) we take

$$P = (1/\sqrt{2})AQ(x_i)e^u, \tag{5.17}$$

where Q is given by Eq. (3.9). The surface area element dS is then

$$dS = \tfrac{1}{2}P^{-2}\Omega^4\, dx_3\, dx_4. \tag{5.18}$$

Inserted into Eq. (5.1) this yields

$$\begin{aligned} \tilde{M}_2(S) &= \lim_{r\to\infty} (8\pi A)^{-1}e^{-u}\Omega^6 \int (-\Psi_2)P^{-2}\, dx_3\, dx_4 \\ &= \tfrac{1}{8}CA. \end{aligned} \tag{5.19}$$

Thus we obtain a finite and nonzero value of the Hawking mass in the Tolman–Bondi model. We notice that the result is of similar form as Eq. (4.11) and that $\tilde{M}_2$ agrees with m_0 if we let the constant C_2 vanish. The discovery that the Hawking mass is sensitive not only to changes in the effective gravitational mass $m(R)$ but also to changes in the total energy of a shell of matter $E(R)$ is connected to the fact that $m(R)$ and $E(R)$ diverge in the open Friedmann model and that the infinite contributions have beeen "renormalized" away.

VI. CONCLUSION

In this paper we have computed the Hawking mass $\tilde{M}_2$ in a Tolman–Bondi model that asymptotically approaches the open Friedmann universe. In the unperturbed Friedmann model, $\tilde{M}_2$ vanishes and represents the "renormalized" mass of the infinite total mass $\tilde{M}$. Since $\tilde{M}_2$ is finite and nonzero in the perturbed model, it seems reasonable to regard the Hawking mass as representing the total mass of the disturbance. It can be shown that there is no contribution to $\tilde{M}_1$ due to the perturbation.

We note that the expression (5.19) is independent of u, i.e., $\tilde{M}_2$ is a constant and has the same value on any null hypersurface $u = \text{const}$. This is not surprising since there is no gravitational radiation in our model of spherical symmetry. As discovered by Hawking,[5] in a system with gravitational radiation $\tilde{M}_2$ depends on u and obeys a conservation law similar to that of the Bondi mass in asymptotically flat space-time.

It is interesting to notice that the function $h(R)$ given by Eq. (4.16) is the gauge-invariant perturbation amplitude of the functions $m(R)$ and $E(R)$. We may write

$$h = \delta m/\tilde{m} - \tfrac{1}{2}\delta E/\tilde{E}, \tag{6.1}$$

which is gauge invariant under the coordinate transformation

$$R \to R' = R + \xi^R. \tag{6.2}$$

where $|\xi^R| \ll 1$. By Eqs. (5.1) and (5.12), the Hawking mass is proportional to this gauge-invariant quantity. Therefore, if the falloff behavior is such as given by Eqs. (4.10) and (4.12), $\tilde{M}_2$ is proportional to both the change in the effective gravitational mass $m(R)$ and the change in the total energy of a shell of matter $E(R)$.

From Eq. (4.26) the perturbation amplitude of the mass density is $\epsilon \sim e^{-2R}h$ at large radial distances. In the asymptotic limit $u = \text{const}$, $\eta \to \infty$ this yields a perturbation in the mass density given by $\delta\rho \sim \Omega^{-8}$. The boundary conditions are therefore such that

$$\Lambda = \tfrac{1}{4}A\Omega^{-3} + O(\Omega^{-8}). \tag{6.3}$$

These boundary conditions are of one power higher in Ω^{-1} than the ones that allow a general radiation field in the system.[5] This reflects the asymptotic behavior of a scalar perturbation as discussed in this paper, as opposed to a tensor perturbation due to gravitational waves.[14]

Finally, it should be pointed out that our calculation of the Hawking mass may also serve as a test for the definition of mass proposed by Penrose.[15] While the Penrose mass is a candidate for a quasilocal mass, it can also be considered as a definition of mass at null infinity. For a spherically symmetric space-time it can be shown that the Penrose mass agrees with the quantity $\tilde{M}$ given by Hawking.[16] We may therefore "renormalize" the Penrose mass in a similar fashion to what we did to the total mass $\tilde{M}$. If we discard the diverging terms involving Φ_{11} and Λ, the "renormalized" Penrose mass at null infinity is given by

$$M_P^{(\text{ren.})} = \lim_{r\to\infty} (1/4\pi)(-\Psi_2)(\Delta^3/4\pi)^{1/2}, \tag{6.4}$$

where $\Delta = \int dS$ is the surface area. This expression vanishes in the unperturbed open Friedmann universe. In the nonhomogeneous Tolman–Bondi model all we must compute is the asymptotic behavior of Ψ_2, which we already have done. Using the expression (5.15) and the area element (5.18), the "renormalized" Penrose mass completely agrees with the result (5.19) for the Hawking mass.

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