On the commutant of an irreducible set of operators in real Hilbert space

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The relation between irreducibility and the structure of the commutant is studied for a set of linear bounded operators on a real Hilbert space of arbitrary dimension. The results are applied to the investigation of irreducible sets of semilinear operators on a complex or quaternionic Hilbert space.

I. INTRODUCTION

For an irreducible set $\mathscr{A}$ of linear mappings from a linear space V over a field K into itself the *commutant* $\mathscr{A}'$ (i.e., the set of all linear mappings commuting with all mappings of $\mathscr{A}$) is a division algebra over K (see, e.g., Ref. 1, Sec. II, p. 118). Here, irreducibility means the nonexistence of a nontrivial $\mathscr{A}$-invariant linear subset. In the more general situation, where K is a skew field and where $\mathscr{A}$ consists of semilinear mappings, $\mathscr{A}'$ is still a division algebra, but over a smaller field $K_{\mathscr{A}}$ consisting of all central elements of K being invariant under all automorphisms of K generated by the semilinear mappings in $\mathscr{A}$ (Ref. 2, Proposition 3). Furthermore, if $X \in \mathscr{A}'$ has an eigenvalue $\lambda \in K_{\mathscr{A}}$, then $X = \lambda 1$, where 1 is the identity mapping of V (Ref. 2, Proposition 2). These results are based on Schur's lemma. A more detailed description of $\mathscr{A}'$ can be achieved restricting the dimension of V and specifying the nature of K. So, for instance, if $\dim V < \infty$ and if K is an algebraically closed field, one gets in the linear case $\mathscr{A}' = K1$, i.e., Burside's theorem. Particularly interesting for applications is the special case that K is the field $\mathbb{R}$ of real numbers, or the field $\mathbb{C}$ of complex numbers, or the skew field $\mathbb{H}$ of quaternionic numbers. Assuming $\dim V < \infty$, in each of these three cases it turns out that $\mathscr{A}'$ is isomorphic either to $\mathbb{R}$ or to $\mathbb{C}$ or to $\mathbb{H}$ [Ref. 2, Theorem 1; cf. (3)–(5) for examples]. The crucial inputs for this result are Frobenius' theorem telling us that the only finite-dimensional division algebras over $\mathbb{R}$ are $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$ (Ref. 1, Sec. I, p. 430), and the fact that every finite-dimensional division algebra over an algebraically closed field is isomorphic to the field itself (Ref. 1, Sec. I, p. 429) (actually, this is applied in the case of the complex field only). For $\mathbb{K} = \mathbb{R}$ the above statement $\mathscr{A}' \simeq \mathbb{R}, \mathbb{C}$, or $\mathbb{H}$ is proven in Ref. 3 (p. 119, Theorem 2) even in the case where $\dim V$ is countable. The main step of the proof consists in showing that any finite subset of $\mathscr{A}'$ generates a finite-dimensional division subalgebra of $\mathscr{A}'$. Then Frobenius' theorem is applied.

The aim of the present paper is to free these results from any dimensional restrictions in the case that V is a Hilbert space and that the notions used so far are adapted to this case in a natural way. The most commonly used Hilbert spaces are the real and the complex ones. Their importance for analysis and physics need not be stressed. We will deal with the less popular quaternionic Hilbert spaces, too, for two reasons. First, considering an irreducible set of linear operators in a real Hilbert space, we may find the commutant being isomorphic to $\mathbb{H}$. This is most naturally interpreted in terms of a quaternionic Hilbert space. Second, Hilbert spaces over $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$ arise as possibilities of equal weight from the lattice theoretical foundation of quantum theory, see, e.g., Ref. 4. In this framework symmetry transformations of a physical system are represented by semilinear unitary operators and an irreducible set of symmetries characterizes an elementary system. This is the physical reason for being interested in irreducibility as studied in this paper. For an elaboration of quantum theory in quaternionic Hilbert space see, e.g., Refs. 5 and 6.

Modifying the purely algebraic situation reported at the beginning let now $\mathscr{A}$ consist of *bounded semilinear* operators on a Hilbert space H over $\mathbb{K} = \mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$. Correspondingly, the *commutant* $\mathscr{A}'$ consists of *bounded* linear operators and *irreducibility* refers to *closed* linear subsets. In the present paper we shall concern ourselves with the structure of $\mathscr{A}'$ for an irreducible $\mathscr{A}$.

Our considerations center on the case $\mathbb{K} = \mathbb{R}$ since the other cases are reduced to the real one by realification (Sec. III). Here semilinearity and linearity coincide. Obviously $\mathscr{A}' = [\mathscr{A}]'$ and $\mathscr{A}$ is irreducible iff $[\mathscr{A}]$ is, where $[\mathscr{A}]$ denotes the strongly closed algebra generated by $\mathscr{A} \cup \{1\}$. $[\mathscr{A}]$ is even weakly closed (Ref. 7, p. 64, Theorem 3.12). The analysis of $\mathscr{A}'$ in Sec. II is decisively based on the $*$ condition that $[\mathscr{A}]$ is a $*$ algebra, i.e., that $A \in [\mathscr{A}] \to A^* \in [\mathscr{A}]$. In other words, $\mathscr{A} \cup \{1\}$ is supposed to generate a real von Neumann algebra $\mathscr{N}$. As in the complex case the latter is equivalently characterized by $\mathscr{N} = \mathscr{N}^*$ and $\mathscr{N} = \mathscr{N}''$. [The proof (Ref. 8, p. 5, Theorem 1.2.1) of the double commutant theorem applies literally to the real case.] The $*$ condition on $\mathscr{A}$ may be sharpened to the more practicable condition that $\mathscr{A}$ generates a $*$ algebra (without topological closure) or that even

$$\text{for any } A \in \mathscr{A} \text{ there are } b \in \mathbb{R} \text{ and } B \in \mathscr{A} \text{ such that } A^* = bB. \tag{1}$$

Important examples of (1) are, first, that $\mathscr{A}$ consists of self-adjoint or skew-adjoint operators and, second, that $\mathscr{A}$ is the range of a unitary (projective) representation of a group.

The main result of Sec. II is that a real von Neumann algebra is irreducible if and only if its commutant is isomorphic to $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$ (Theorem 2). We think that the given proof may be of some interest. It does not recur to complexification (cf. Remark 3) but consists mainly in an analysis of what we

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call a *real skew-adjoint algebra*. [See (2) following.] This notion takes account of the characteristic properties of the commutant algebras under consideration. Skew-adjoint algebras are, in particular, *normed division algebras*. So one could base the proof on the real version of the Gelfand–Mazur theorem (Ref. 9, p. 73, Theorem 7) and care separately for the * compatibility of the isomorphism (Remark 1).

Pleasurably, a short elementary analysis of skew-adjoint algebras is possible, and we take this direct way (Theorem 1). Let us emphasize that, anyway, the * condition cannot be dropped. It ensures that the commutant is self-adjoint and that reducibility and decomposability are equivalent for $\mathscr{A}$. So, for instance, the algebra of all real triangular matrices of dimension $\geqslant 2$ is ruled out, which is reducible although its commutant is isomorphic to $\mathbb{R}$. Moreover, in general, a nontrivial commutant $\mathscr{A}'$ does not imply the decomposability of $\mathscr{A}$. As an example in complex Hilbert space take for $\mathscr{A}$ the set of all multiplication operators on Hardy space H^2 by functions in H^∞, which is its own commutant and which is not decomposable. Of course, answering the question of whether any irreducible set of bounded linear operators in a complex Hilbert space has a trivial commutant would decide either the invariant subspace problem or the transitive operator algebra problem (see, e.g., Ref. 10).

An interesting variation of our analysis follows replacing the * condition by the weaker *normality condition*, i.e., that $[\mathscr{A}]$ is generated by normal operators. (If $\dim H < \infty$, actually it is not weaker; this follows from Ref. 10 (p. 175, Corollary 9.12) since a normal matrix is completely normal and, hence, $[\mathscr{A}]$ is reductive. The proofs are easily transferred to the real case.) By the Theorem of Fuglede–Putman–Rosenblum (its proof, in Ref. 7, p. 300, Theorem 12.16, applies literally to the real case) it then follows that $\mathscr{A}' = (\mathscr{A} \cup \mathscr{A}^*)'$ such that $\mathscr{A}'$ is a real skew-adjoint algebra if $\mathscr{A}$ is irreducible. The analysis then proceeds to Theorem 1. However, the normality condition, unlike the * condition, does not ensure the irreducibility of $\mathscr{A}$ in the case of a trivial commutant $\mathscr{A}'$. As an example, in complex Hilbert space let $\mathscr{A} = \{U, Q\}$, where U is the bilateral shift and Q is the orthogonal projection onto Hardy space H^2. Then H^2 is invariant under $\mathscr{A}$. Because of Ref. 7, p. 300, Theorem 12.16, $\mathscr{A}'$ is a von Neumann algebra and, hence, would contain a nontrivial orthogonal projection if $\mathscr{A}' \neq \mathbb{C}1$ were assumed. This, however, would contradict Ref. 10, p. 39, Theorem 3.6 and p. 41, Corollary 3.10.

II. THE COMMUTANT OF AN IRREDUCIBLE SET OF REAL OPERATORS

Throughout this section let $\mathscr{A}$ denote a set of bounded linear operators on a real Hilbert space H such that $\mathscr{A} \cup \{1\}$ generates a real von Neumann algebra. The latter is the case if (1) is valid.

Lemma 1: $\mathscr{A}$ is irreducible if and only if $\mathscr{A}'$ contains no self-adjoint elements except the real multiples of the identity operator.

Proof: Without loss of generality $\mathscr{A}$ is a * algebra. Let M be a subspace of H and let P be the self-adjoint projection operator with range M. Then M is invariant under $A \in \mathscr{A}$ iff $PAP = AP$. Therefore M is invariant under A and A^* iff P commutes with A. Now the assertion follows from the fact that a self-adjoint operator belongs to $\mathscr{A}'$ iff all its spectral projections do so. ■

Therefore, if $\mathscr{A}$ is irreducible, the real * algebra $\mathscr{A}'$ enjoys the further property:

> For any self-adjoint element A of the algebra there is a real number $\varphi(A)$ such that $A = \varphi(A)E$, $E \equiv$ unit element. For every nonzero element A of the algebra it is $\varphi(A^*A) > 0$. (2)

Any element of a * algebra can be written as $A = A_s + A_a$, where $A_s := \frac{1}{2}(A + A^*)$ is self-adjoint and $A_a := \frac{1}{2}(A - A^*)$ is skew-adjoint. Therefore, the content of (2) is essentially that only the skew-adjoint part of any element is nontrivial. Let us call a real * algebra with unit satisfying (2) a *real skew-adjoint algebra*. [The positivity condition in (2) is independent as simple examples show.] There are three well-known examples of such algebras: $\mathbf{R}$, $\mathbf{C}$, and $\mathbf{H}$ with $h^* := \bar{h}$ and $\varphi(h^*h) = |h|^2$. We are going to show that actually they are the only ones.

Theorem 1: Let $\mathscr{S}$ be a real skew-adjoint algebra. Then $\mathscr{S}$ is isomorphic (as a real * algebra) to $\mathbf{R}$ or $\mathbf{C}$ or $\mathbf{H}$.

Proof: If all elements of $\mathscr{S}$ are self-adjoint, then $\mathscr{S} \to \mathbf{R}$, $A \to \varphi(A)$ is an isomorphism. Otherwise choose $X \in \mathscr{S}$ with $X \neq X^*$. Then $I := \varphi(X_a^* X_a)^{-1/2} X_a$ satisfies $I^* = -I$, $I^2 = -E$. If $\mathscr{S}$ is commutative, IA_a is always self-adjoint and hence $A = A_s + I(-IA_a) = \varphi(A_s)E + \varphi(-IA_a)I$ so that $\mathscr{S} \to \mathbf{C}$, $aE + bI \to a + ib$, is a * isomorphism. If $\mathscr{S}$ is not commutative, choose $Y \in \mathscr{S}$ not commuting with I. Then Y_a is skew-adjoint and linearly independent of E and I. Indeed, $Y_a = aE + bI$ implies $Y = Y_s + Y_a = [\varphi(Y_s) + a]E + bI$ and hence $YI = IY$. Now, $Z := Y_a + \frac{1}{2}(IY_a + Y_aI)I$ satisfies $ZI = -IZ$, $Z^* = -Z$, $Z \neq 0$. Putting $J := \varphi(Z^*Z)^{-1/2} Z$ we get $JI = -IJ$, $J^* = -J$, $J^2 = -E$. Here J is linearly independent of E and I, since Y_a is. Trivial algebra shows that $K := IJ$ satisfies $K^* = -K$, $K^2 = -E$, $JK = I = -KJ$, $KI = J = -IK$. Furthermore, $(aE + bI + cJ + d)(aE - bI - cJ - dK) = (a^2 + b^2 + c^2 + c^2)E$ proves the linear independence of E, I, J, and K. Therefore, $\mathbf{H} \to \mathscr{S}$, $a + ib + jc + kd \to aE + bI + cJ + dK$ is an injective * homomorphism. Now, the following identity holds:

$$\begin{aligned} A &= A_s - \tfrac{1}{2}(A_aI + IA_a)I - \tfrac{1}{4}(A_aJ + JA_a - KA_aI + IA_aK)J \\ &\quad - \tfrac{1}{4}(A_aK + KA_a - IA_aJ + JA_aI)K \\ &=: H_0 + H_1I + H_2J + H_3K, \end{aligned}$$

where the H_n are self-adjoint. Hence $A = \varphi(H_0)E + \varphi(H_1)I + \varphi(H_2)J + \varphi(H_3)K$, implying the surjectivity of the above homomorphism. ■

Remark 1: Obviously $\langle A | B \rangle := \varphi(\frac{1}{2}[A^*B + B^*A])$ is a scalar product on the real skew-adjoint algebra $\mathscr{S}$. Therefore, in particular, $\mathscr{S}$ is a normed algebra with $\|A\| := [\varphi(A^*A)]^{1/2}$. Moreover, because of $A^*A = \varphi(A^*A)E$, each nonzero element $A \in \mathscr{S}$ has the unique inverse $A^{-1} = \|A\|^{-2} A^*$. Thus $\mathscr{S}$ is a real normed division algebra. According to the real version of the Gelfand–Mazur theorem (Ref. 9, p. 73, Theorem 7) there is a real normed algebra isomorphism from $\mathscr{S}$ onto $\mathbb{K} = \mathbf{R}, \mathbf{C}$, or $\mathbf{H}$. Let us see that it

is even a * isomorphism. Denote by $\hat{}$ the involution on $\mathbb{K}$ being the image of the * operation on $\mathscr{S}$. Since $\mathscr{S}$ is skew adjoint it follows that the only self-adjoint elements $h = \hat{h}$ of $\mathbb{K}$ are the reals. However, this property is characteristic of the (ordinary) complex conjugation on $\mathbb{K}$. Indeed, this is obvious in the case $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$. In the quaternionic case there is a nonzero $q \in \mathbb{H}$ with $q^2 \in \mathbb{R}$ such that $h = q\bar{h}q^{-1}$. This is because any two involutions are connected by an automorphism, which is inner since all automorphisms of $\mathbb{H}$ are inner, and because the center of $\mathbb{H}$ consists of the reals only. Here, $q^2 \in \mathbb{R}$ implies the alternative $\bar{q} = q$ or $\bar{q} = -q$, i.e., q real or q a linear combination of i, j, and k. In the case of the latter there is an $h \in \mathbb{H}$ with $\bar{h} = -h$ anticommuting with q. For example, take for h the image of j under an inner automorphism mapping $|q|i$ on q. Then, indeed, $\hat{h} = h$ although h is not real, contradicting $(\mathbb{H}, \hat{})$ being skew adjoint. Therefore q is real, and $\hat{}$ coincides with complex conjugation. Thus we have an alternative proof of Theorem 1. ∎

We remember that $\mathscr{A}'$ is a skew-adjoint algebra if $\mathscr{A}$ is irreducible and that the only self-adjoint elements of $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$ are the real multiples of the unit. So we infer from Theorem 1 and Lemma 1 the following theorem.

Theorem 2: $\mathscr{A}$ is irreducible if and only if $\mathscr{A}'$ is * isomorphic to $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$.

In particular, this means that $\mathscr{A}'$ is the range of a * representation in H of one of these fields. From this the explicit structure of $\mathscr{A}'$ follows.

Lemma 2: Up to a real Hilbert space isomorphism there is only one irreducible real * representation of $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$, namely,

$$a \to a \quad \text{for the real numbers,}$$

$$a + ib \to \begin{pmatrix} a & -b \\ b & a \end{pmatrix} \quad \text{for the complex numbers,}$$

$$a + ib + jc + kd \to \begin{pmatrix} a & -b & -c & -d \\ b & a & -d & c \\ c & d & a & -b \\ d & -c & b & a \end{pmatrix}$$

for the quaternionic numbers.

Every real * representation of $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$ is an orthogonal sum of (possibly noncountably many) copies of the irreducible one.

Proof: We give the proof for the quaternionic case. Let π be any real * representation of $\mathbb{H}$. For any unit vector x consider the π-invariant four-dimensional subspace $V_x := \{\pi(q)x | q \in \mathbb{H}\}$. With respect to its orthonormal basis $\{x, \pi(i)x, \pi(j)x, \pi(k)x\}$ the restriction of π to V_x is the representation indicated above. It is irreducible since $V_y = V_x$ for any unit vector $y \in V_x$. But if $y \perp V_x$ then $V_y \perp V_x$ easily follows. So a simple application of Zorn's lemma completes the proof. ∎

It is now easy to get a survey of the irreducible real von Neumann algebras.

Theorem 3: Any irreducible real von Neuman algebra is isomorphic (as a real * algebra) to $L(H)$, the set of all bounded *linear* operators on a real, complex, or quaternionic Hilbert space H, taken as a *real* * algebra. The isomorphism is implied by a Hilbert space isomorphism. Explicitly, we get the following representation of the real, complex, and quaternionic type (left side) with its respective commutant (right side):

$$\begin{array}{l} L(H) \\ \left\{\begin{pmatrix} A & -B \\ B & A \end{pmatrix} \middle| A,B \in L(H)\right\} \\ \left\{\begin{pmatrix} A & B & C & D \\ -B & A & -D & C \\ -C & D & A & -B \\ -D & -C & B & A \end{pmatrix} \middle| A,B,C,D, \in L(H)\right\} \end{array} \qquad \begin{array}{l} \mathbb{R}1, \\ \left\{\begin{pmatrix} a1 & -b1 \\ b1 & a1 \end{pmatrix} \middle| a,b \in \mathbb{R}\right\} \simeq \mathbb{C}, \\ \left\{\begin{pmatrix} a1 & -b1 & -c1 & -d1 \\ b1 & a1 & -d1 & c1 \\ c1 & d1 & a1 & -b1 \\ d1 & -c1 & b1 & a1 \end{pmatrix} \middle| a,b,c,d, \in \mathbb{R}\right\} \simeq \mathbb{H}, \end{array} \tag{3}$$

where H in (3) is a *real* Hilbert space.

Proof: Taking into account the relation between real, complex, and quaternionic Hilbert space discussed at the beginning of Sec. III, the proof follows combining Theorem 2, the double commutant theorem, and Lemma 2. ∎

Remark 2: If $\mathscr{A}'$ is isomorphic to $\mathbb{C}$ or $\mathbb{H}$, any skew-adjoint element $I \in \mathscr{A}'$, $I^2 = -1$, endows H with a complex linear structure $(a + ib)x := ax + bIx$ and a complex valued scalar product $\langle x|y\rangle_I := \langle x|y\rangle - i\langle x|Iy\rangle$, which turn H into a complex Hilbert space H_I (different from the complexification of H). Any $A \in \mathscr{A}$ is also a linear operator on H_I, and we use the notation A_I to stress this. Note that $(A^*)_I = (A_I)^*$. Now, in these terms the alternative for $\mathscr{A}'$ may be described as follows: the complex case occurs iff $(\mathscr{A}_I)' = \mathbb{C}1_I$, the quaternionic case occurs iff there is a Hilbert space isomorphism $\iota: H_I \to H_{-I}$ such that $\iota A_I \iota^{-1} = A_{-I}$ for all $A \in \mathscr{A}$ (ι gives rise to the quaternionic element J).

Remark 3: $\mathscr{A}'$ may be analyzed alternatively by means of the complexification $H_{\mathbb{C}}$ of H. Let $\mathscr{A}_{\mathbb{C}} = \{A \oplus A | A \in A\}$ refer to the identification $H_{\mathbb{C}} = H \oplus H$, and let $\mathscr{L}$ be the antilinear canonical conjugation satisfying $\mathscr{L}^2 = 1$, $\mathscr{L}^* = \mathscr{L}$. Then $\mathscr{A}$ is irreducible iff $\mathscr{A}_{\mathbb{C}} \cup \{\mathscr{L}\}$ is irreducible. In these terms the three possibilities in Theorem 2 manifest themselves as follows: in the real case $\mathscr{A}_{\mathbb{C}}$ is irreducible, in the complex case $\mathscr{A}_{\mathbb{C}}$ is the orthogonal sum of two inequivalent irreducible operator systems, and in the quaternionic case $\mathscr{A}_{\mathbb{C}}$ is the orthogonal sum of two equivalent irreducible operator systems. A nonstraightforward point in this analysis is to see that $\mathscr{A}_{\mathbb{C}}$ consists of irreducible components and the number of them cannot exceed 2. This may be proved as Theorem 1 in Ref. 11 with the operator $(1/p)\Sigma_{i=1}^{p} U(r_i) A U(r_i)^{-1}$ replaced by $\frac{1}{2}(A + \mathscr{L}A\mathscr{L})$.

III. THE COMMUTANT OF AN IRREDUCIBLE SET OF SEMILINEAR OPERATORS

In quaternionic Hilbert space (see Ref. 5, Secs. 1A and 1B for a brief exposition) left-multiplication L_q by a quaternion q acts as semilinear operator on H: $L_q(hx) = h^q L_q(x)$, where $h^q := qhq^{-1}$ for all $h \in \mathbb{H}$. In particular let $I := L_i$,

$J := L_j$, and $K := L_k$, where i, j, k are the imaginary units. The real Hilbert space $H_{\mathbb{R}}$ underlying H is the same set as H with the same real-linear structure, equipped with the real scalar product $\langle\ |\ \rangle_{\mathbb{R}} := \mathrm{Re}\langle\ |\ \rangle$ being the real part of the original one. Moreover, it is endowed with the (real-) linear operators L_q constituting a real * representation of $\mathbb{H}$ (cf. Lemma 2). With its aid the quaternionic structure can be regained. In particular, it is $\langle x|y\rangle = \langle x|y\rangle_{\mathbb{R}} - i\langle x|Iy\rangle_{\mathbb{R}} - j\langle x|Jy\rangle - k\langle x|Ky\rangle_{\mathbb{R}}$. Conversely, given a real Hilbert space carrying a real * representation π of the quaternions the analogous formula endows it with a quaternionic linear structure such that $\pi(q) = L_q$. Then the $\mathbb{H}$-linear operators are just the $\mathbb{R}$-linear ones commuting with L_q or $\pi(q)$, respectively.

In particular, the commutant of a set $\mathscr{A}$ of bounded semilinear operators on a quaternionic Hilbert space does not change if $\mathscr{A}$ is enlarged by the operators L_q. Therefore without loss of generality let them already be in $\mathscr{A}$. Then $\mathscr{A}$ is irreducible if and only if $\mathscr{A}_{\mathbb{R}}$, the set of the operators in $\mathscr{A}$ acting on $H_{\mathbb{R}}$, is irreducible. Thus, imposing the * condition on $\mathscr{A}_{\mathbb{R}}$, which is ensured if, for instance, $\mathscr{A}$ satisfies (1) with $b \in \mathbb{H}$, the reduction to the real case succeeds. (See Ref. 4, p. 160, Theorem 11 for a partial result.) The complex case yields the same result by the same method. So we have the following.

Corollary: Let $\mathscr{A}$ be a set of bounded semilinear operators on a Hilbert space over $\mathbb{K}$ with $\{L_h\,|h \in \mathbb{K}\} \subset A$ and $\mathscr{A}_{\mathbb{R}}$ satisfying the * condition. Then $\mathscr{A}$ is irreducible if and only if $\mathscr{A}'$ is isomorphic to $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$ in the sense of real * algebras.

Let us now account for the realization of the predicted cases. We observe that $\mathscr{A}'$ is the range of a * representation of $\mathbb{K}$ by linear operators. So the following lemma (continuing Lemma 2) determines its possible structure. For the sake of brevity we omit the proof though it is not completely straightforward.

Lemma 3: Up to a Hilbert space isomorphism the irreducible * representations of $\mathbb{K}$ (as a real * algebra) by linear bounded operators on complex or quaternionic Hilbert space are

$$\left.\begin{array}{l} a \to a \\ z \to z \text{ and } z \to \bar{z} \\ z \to R_{\bar{z}} \end{array}\right\} \text{ for the complex numbers,}$$

$$\left.\begin{array}{l} a + ib + jc + kd \to \begin{pmatrix} a - ib & c - id \\ -c - id & a + ib \end{pmatrix} \\ q \to R_{\bar{q}} \end{array}\right\}$$

for the quaternionic numbers,

where, for any $q \in \mathbb{H}$, $R_q h := hq$ is a linear operator on the left Hilbert space $\mathbb{H}$. Every * representation of $\mathbb{K}$ is an orthogonal sum of (possibly noncountably many) irreducible ones.

It remains to complete the list initiated in Theorem 3. The right side of the list is the commutant of the left side, while the left side consists of all *semilinear* bounded operators which commute with all operators of the right side. In (5) each side is the commutant of the other side if on the left side the sets are replaced by their subsets of *linear* operators:

$$\begin{array}{ll}
\{\text{all semilinear bounded operators on H}\} & \mathbb{R}1, \\
L(H) & \mathbb{C}1, \\
\left\{\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \middle| A \in L(H), B \in L(H')\right\} \cup & \left\{\begin{pmatrix} z1 & 0 \\ 0 & \bar{z}1' \end{pmatrix} \middle| z \in \mathbb{C}\right\} \simeq \mathbb{C}, \\
\left\{\begin{pmatrix} 0 & B\mathscr{L}' \\ C\mathscr{L} & 0 \end{pmatrix} \middle| B \in L(H', H), C \in L(H, H')\right\} & \\
\left\{\begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix} \middle| A \in L(H)\right\} U \left\{\begin{pmatrix} 0 & -B\mathscr{L} \\ B\mathscr{L} & 0 \end{pmatrix} \middle| B \in L(H)\right\} & \left\{\begin{pmatrix} \bar{w}1 & \bar{z}1 \\ -z1 & w1 \end{pmatrix} \middle| w, z \in \mathbb{C}\right\} \simeq \mathbb{H}, \qquad (4)
\end{array}$$

where $\mathscr{L}$ is a conjugation on the complex Hilbert space H;

$$\begin{array}{ll}
\{\text{all semilinear bounded operators on } H\} & \mathbb{R}1 \\
\{(L_q R_{w_\iota\kappa})_{\iota\kappa} | q \in \mathbb{H},\ w_{\iota\kappa} \in \mathbb{C} \text{ defining a bounded operator}\} & \{(R_z \delta_{\iota\kappa})_{\iota\kappa} | z \in \mathbb{C}\} \simeq \mathbb{C}, \\
\{(L_q a_{\iota\kappa})_{\iota\kappa} | q \in \mathbb{H},\ a_{\iota\kappa} \in \mathbb{R} \text{ defining a bounded operator}\} & \{(R_q \delta_{\iota\kappa})_{\iota\kappa} | q \in \mathbb{H}\} \simeq \mathbb{H}, \\
 & (5)
\end{array}$$

where the matrix elements refer to an orthonormal basis (e_ι) of the quaternionic Hilbert space H and $R_q h e_\iota = hqe_\iota$ for all $q, h \in \mathbb{H}$.

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Internal structure of fermions

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We investigate the equations $P\psi = k\psi + h$ with the range of ψ contained in an appropriate Clifford algebra. Next we define, on the bundle ΨM of the minimal left ideals of the Clifford algebra, the unique connection $\tilde{\nabla}$ which produces the Christoffel connection ∇ on M. To unify the whole picture we have to introduce an additional degree of freedom α which numerates the set of global fields of mutually annihilating primitive idempotents on M. Now the geometrical "duality" of the spinor fields given by the primary as well as by the composed character of the sections of ΨM implies the existence of some internal gauge interaction B_μ which changes α. The generators of the holonomy group of ∇ that do not belong to the Crumeyrolle algebra are responsible for this internal interaction.

I. INTRODUCTION

Let V be a $(n = s + t)$-dimensional real vector space and Q a nonsingular quadratic form on V of signature (s,t). The universal Clifford algebra $\mathscr{C}(Q)$ of the quadratic form Q is an $\mathbb{R}$-algebra with the following properties.

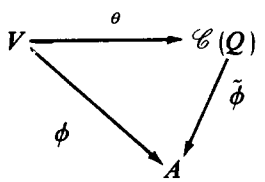
(a) $\exists$ a linear function

$$\theta: V \to \mathscr{C}(Q),$$

such that

$$\theta(v)^2 = Q(v)\cdot 1, \quad \forall v \in V. \tag{1.1}$$

(b) For all linear function ϕ: $V \to A$, where A is an $\mathbb{R}$ algebra with a unity such that $\phi(v)^2 = Q(v)\cdot 1$, $\exists$ a unique morphism $\tilde{\phi}$: $\mathscr{C}(Q) \to A$ such that the diagram



(1.2)

commutes. The property (b) tells us that $\mathscr{C}(Q)$ is generated by the image $\theta(V)$ or when we identify $\theta(V)$ with V that $\mathscr{C}(Q)$ is generated by V.

Let $\{v_\mu\}$ be an orthonormal base of V and B be the bilinear form associated with the quadratic form Q. We can see that $\mathscr{C}(Q)$ is spanned by elements

$$\{1, v_\mu, v_\mu, v_\nu, \cdots v_1 \vee v_2 \vee v_3 \vee \cdots \vee v_{s+t}\} \tag{1.3}$$

and equipped with the associative and distributive product $\vee$, which we shall call the Clifford product. It is induced by

$$v_\mu \vee v_\nu = v_\mu \wedge v_\nu + B(v_\mu, v_\nu)\cdot 1. \tag{1.4}$$

Thus the underlying vector space of the Clifford algebra $\mathscr{C}(Q)$ can be seen as the direct sum of p-vector spaces $\mathscr{C}^p$, i.e.,

$$\mathscr{C}(Q) = \bigoplus_{p/0}^{n} \mathscr{C}^p. \tag{1.5}$$

The canonical basis for $\mathscr{C}^p$ consists of the products

$$v_s = v_{i_1} \vee v_{i_2} \cdots v_{i_p} = v_{i_1} \wedge v_{i_2} \cdots \wedge v_{i_p},$$
$$1 \leqslant i_1 < i_2 < \cdots < i_p \leqslant n. \tag{1.6}$$

Thus the dimension of $\mathscr{C}(Q)$ is equal to 2^n. There exists also another decomposition of $\mathscr{C}(Q)$. Namely, it can be written as

$$\mathscr{C}(Q) = \mathscr{C}^+(Q) \oplus C^-(Q), \tag{1.7}$$

where $C^+(Q) = \oplus_{p\,\text{even}} \mathscr{C}^p$ is the so-called even subalgebra of $\mathscr{C}(Q)$ and $\mathscr{C}^-(Q) = \oplus_{p\,\text{odd}} \mathscr{C}^p$ is only the subspace of $\mathscr{C}(Q)$.

Let ω be a general element of $\mathscr{C}(Q)$. From (1.4) we see that the Clifford multiplication $v_\mu \vee \omega$ contains two parts. We shall write then in the form

$$v_\mu \vee \omega = v_\mu \wedge \omega + v_\mu \cdot \omega. \tag{1.8}$$

In this approach the Clifford algebra $\mathscr{C}(Q)$ is given quite abstractly.

Now let $V = R^{s,t}$. In this realization $\mathscr{C}(Q)$ will be denoted by $R_{s,t}$ and will be spanned by

$$\{1, e_\mu, e_\mu \wedge e_\nu, \ldots, e_1 \wedge e_2 \wedge e_3 \wedge \cdots \wedge e_n\}, \tag{1.9}$$

where $\{e_\mu\}$ is an orthogonal basis of $R^{s,t}$ and

$$e_\mu \vee e_\nu = e_\mu \wedge e_\nu + g_{\mu\nu}\cdot 1. \tag{1.10}$$

Here $g_{\mu\nu} = \text{diag}(\underbrace{+\cdots+}_{s}\ \underbrace{-\cdots-}_{t})$ is the metric tensor associated with Q. The general element of the considered realization of the Clifford algebra has the form

$$\psi = \psi^0 + \psi^\mu e_\mu + \psi^{\mu\nu} e_\mu \wedge e_\nu + \cdots + \psi^{12\cdots n} e_1 \wedge \cdots \wedge e_n. \tag{1.11}$$

However, we can also realize (V,Q) as the dual vector space, i.e., $(R^{s,t})^*$. in other words, we can consider the differential forms dx^μ of the vector space $R^{s,t}$. In this realization the universal Clifford algebra $\mathscr{C}(Q)$ is spanned by

$$\{1, dx^\mu, dx^\mu \wedge dx^\nu, \ldots, dx^1 \wedge dx^2 \wedge \cdots \wedge dx^n\}, \tag{1.12}$$

and similarly as above the distributive and associative Clifford product is induced by that of the generating elements dx^μ, i.e.,

$$1 \vee 1 = 1, \quad 1 \vee dx^\mu = dx^\mu \vee 1 = dx^\mu,$$
$$dx^\mu \vee dx^\nu = dx^\mu \wedge dx^\nu + g^{\mu\nu}\cdot 1. \tag{1.13}$$

Now the general element of the considered realization of $\mathscr{C}(Q)$ can be written as

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$$\psi = \psi_0 + \psi_\mu\, dx^\mu + \psi_{\mu\nu}\, dx^\mu \wedge dx^\nu + \cdots \psi_{12\cdots n}\, dx^1 \wedge \cdots \wedge dx^n \tag{1.14}$$

and (1.13) gives us[2]

$$dx^\mu \vee \psi = dx^\mu \wedge \psi + dx^\mu \lrcorner \psi. \tag{1.15}$$

II. OPERATOR P

Let us consider a vector space (V,Q) and its Clifford algebra $\mathscr{C}(Q)$. It is known[3] that we can define an inner product $(\cdot)_Q$ on the underlying vector space of $\mathscr{C}(Q)$. This product is induced by a quadratic form Q over V as follows.

(i) If $\phi \in \mathscr{C}^p$ and $\phi' \in \mathscr{C}^{p'}$ with $p \neq p'$ then $(\phi,\phi')_Q := 0$.

(ii) If $\phi = v_{i_1} \vee v_{i_2} \vee \cdots \vee v_{i_p}$, $\phi' = v_{i'_1} \vee v_{i'_2} \vee \cdots\ v_{i'_{p'}}$,

where $\{v_i\}$ is an orthonormal basis of (V,Q), then

$$(\phi,\phi')_Q := \det(B(v_i,v_{j'})).$$

(iii) The general case $\phi,\phi' \in \mathscr{C}(Q)$ can be reduced by linearity to (i) and (ii). Thus we can treat (V,Q) and $\mathscr{C}(Q)$ as two Banach spaces and introduce differentiable mappings

$$\psi: V \to \mathscr{C}(Q). \tag{2.1}$$

Definition 1: Let ψ be a differentiable function from the orthogonal vector space (V,Q) to the Clifford algebra $\mathscr{C}(Q)$ or to some of its subspace W. The P operator will be given as[4]

$$P = v_1 \frac{\partial}{\partial x_1} + v_2 \frac{\partial}{\partial x_2} + \cdots + v_n \frac{\partial}{\partial x_n},$$

i.e.,

$$P\psi = v_\mu \vee \partial^\mu \psi. \tag{2.2}$$

Of course, we can use the relation (1.8) and write (2.2) as

$$P\psi = v_\mu \wedge \partial^\mu \psi + v_\mu \cdot \partial^\mu \psi. \tag{2.3}$$

So we obtain easily the following properties of P:

$$\begin{aligned} &\text{(i)} \quad P: \mathscr{C}^p \to \mathscr{C}^{p-1} \oplus \mathscr{C}^{p+1}, \\ &\text{(ii)} \quad P(\psi_1 + \psi_2) = P\psi_1 + P\psi_2, \\ &\text{(iii)} \quad P(P\psi) = P^2\psi, \\ &\text{(iv)} \quad P^2 = \Box, \quad \forall \psi_1,\psi_2,\psi: V \to \mathscr{C}(Q). \end{aligned} \tag{2.4}$$

From now we shall focus our attention on the respective differential maps $\psi: V \to \mathscr{C}(Q)$ satisfying the equation

$$P\psi = k\psi + h, \quad \text{with } k,h \in \mathscr{C}(Q). \tag{2.5}$$

We shall see that depending on the value of k and h, as well as depending on the range of ψ, we obtain different equations which are very important in physics.

Let us consider the realization of V and $\mathscr{C}(Q)$ by the space $R^{s,t}$ and algebra $R_{s,t}$, respectively. Then

$$\psi: R^{s,t} \to R_{s,t}$$

and Eq. (2.5) will have the form

$$e_\mu \vee \frac{\partial \psi}{\partial x_\mu} = k\psi + h, \quad k,h \in R_{s,t}. \tag{2.6}$$

Let us consider the following examples.

I. $k = h = 0$, i.e., Eq. (2.5) or equivalently (2.6) has the form

$$P\psi = 0. \tag{2.7}$$

A. The signature of Q is equal to $(s,t) = (2,0)$. (See Ref. 5.) In Clifford algebra $R_{2,0}$ is the direct sum of p vectors, i.e.,

$$R_{2,0} = R^0_{2,0} \oplus R^1_{2,0} \oplus R^2_{2,0} \tag{2.8}$$

and

$$R^+_{2,0} = R^0_{2,0} \oplus R^2_{2,0}. \tag{2.9}$$

(a) The range of ψ is contained in $R^1_{2,0}$, i.e.,

$$\psi: x_1e_1 + x_2e_2 \rightsquigarrow ue_1 + ve_2 \tag{2.10}$$

or

$$\psi(x_1,x_2) = ue_1 + ve_2.$$

Equation (2.7)

$$\left(e_1 \frac{\partial}{\partial x_1} + e_2 \frac{\partial}{\partial x_2}\right)(ue_1 + ve_2) = 0 \tag{2.11}$$

gives us

$$\frac{\partial u}{\partial x_1} = -\frac{\partial v}{\partial x_2}, \quad \frac{\partial v}{\partial x_1} = \frac{\partial u}{\partial x_2}. \tag{2.12}$$

However, we know that for a complex-valued function $u + iv = f(x_1 + ix_2)$ of the complex variable $x_1 + ix_2$ the Cauchy–Riemann equations have the form

$$\frac{\partial u}{\partial x_1} = \frac{\partial v}{\partial x_2}, \quad \frac{\partial u}{\partial x_2} = -\frac{\partial v}{\partial x_1}. \tag{2.13}$$

Thus we see that Eq. (2.7) gives us in this case (indirectly) the Cauchy–Riemann equations (it will be a matter of orientation of $R^{2,0}$ to obtain the Cauchy–Riemann equations directly).

(b) The range of ψ is contained in the even subalgebra $R^+_{2,0}$. In other words, we examine now the even fields

$$\psi: x_1e_1 + x_2e_2 \rightsquigarrow u + ve_1e_2. \tag{2.14}$$

Now Eq. (2.7) has the form[6]

$$\left(e_1 \frac{\partial}{\partial x_1} + e_2 \frac{\partial}{\partial x_2}\right)(u + ve_{12}) = 0 \tag{2.15}$$

and gives us also the Cauchy–Riemann equations.

(c) Let $S(2,0)$ to the space of algebraic spinors for the just considered quadratic form. Then $S(2,0)$ can be obtained as a minimal left ideal of $R_{2,0}$ determined by the primitive idempotent f of the form

$$f = \tfrac{1}{2}(1 + e_1), \tag{2.16}$$

i.e.,

$$S(2,0) = R_{2,0} f. \tag{2.17}$$

If can be seen that this spinor space is a two-dimensional real linear subspace of $R_{2,0}$ spanned by the elements

$$\begin{aligned} s_1 &= f = \tfrac{1}{2}(1 + e_1), \\ s_2 &= e_2 f = \tfrac{1}{2}(e_2 - e_{12}). \end{aligned} \tag{2.18}$$

Let us consider the map ψ whose range is contained in $S(2,0)$:

$$\psi: R^{2,0} \to S(2,0), \quad x_1e_1 + x_2e_2 \rightsquigarrow us_1 + vs_2. \tag{2.19}$$

In this case Eq. (2.7) has the form

$$\left(e_1 \frac{\partial}{\partial x_1} + e_2 \frac{\partial}{\partial x_2}\right)(us_1 + vs_1) = 0 \tag{2.20}$$

and also yields the Cauchy–Riemann (CR) equations (2.13). It means that $(u, -v)$ is the gradient of some harmonic function κ, i.e.,

$$u=\frac{\partial\kappa}{\partial x_1},\quad -v=\frac{\partial\kappa}{\partial x_2},\quad \frac{\partial^2\kappa}{\partial x_1^2}+\frac{\partial^2\kappa}{\partial x_2^2}=0. \tag{2.21}$$

Again, when κ is a harmonic function, then u,v given by (2.21) satisfy the CR equations.

B. The signature of Q is equal to $(s,t)=(3,0)$. Let us consider maps $\psi: R^{3,0}\to R_{3,0}$ whose ranges are contained in $R^1_{3,0}$, i.e., ψ are vector fields. We can write

$$\psi(x_1,x_2,x_3)=y_1e_1+y_2e_2+y_3e_3. \tag{2.22}$$

Equation (2.7) has the form

$$\left(e_1\frac{\partial}{\partial x_1}+e_2\frac{\partial}{\partial x_2}+e_3\frac{\partial}{\partial x_3}\right)(y_1e_1+y_2e_2+y_3e_3)=0. \tag{2.23}$$

It means that

$$\frac{\partial y_1}{\partial x_1}+\frac{\partial y_2}{\partial x_2}+\frac{\partial y_3}{\partial x_3}=0 \tag{2.24}$$

and

$$e_{23}\left(\frac{\partial u_3}{\partial x_2}-\frac{\partial u_2}{\partial x_3}\right)+e_{31}\left(\frac{\partial u_1}{\partial x_3}-\frac{\partial u_3}{\partial x_1}\right)+e_{12}\left(\frac{\partial u_2}{\partial x_1}-\frac{\partial u_1}{\partial x_2}\right)=0. \tag{2.25}$$

The last equation implies that the vector field ψ can be written as the gradient of some function κ: $R^{3,0}\to\mathbb{R}\cong\mathbb{R}^0_{3,0}$, i.e.,

$$\psi=P\kappa. \tag{2.26}$$

Now from (1.23) we have

$$P^2\kappa=0, \tag{2.27}$$

i.e., κ is a harmonic function. Conversely, when κ is a harmonic function then $\psi=P\kappa$ satisfies (2.23).

C. The signature of Q is given as $(s,t)=(n,0)$ and the map ψ is a vector field

$$\psi: R^{n,0}\to R^1_{n,0}\hookrightarrow R_{n,0}. \tag{2.28}$$

It can represent, for example, the velocity of the flow of an uncompressible fluid in hydrodynamics in n-dimensional Euclidean space. Equation (2.7) implies (similarly to case B) that the flow is irrotational (i.e., that the velocity ψ is the gradient of its scalar potential κ: $R^{n,0}\to\mathbb{R}\cong R^0_{n,0}$) as well as that there are no sources. Thus we obtain again that the scalar potential κ is harmonic.

D. The signature of Q is equal to $(s,t)=(3,1)$.

(a) A map ψ is a vector field, i.e., ψ: $R^{3,1}\to R^1_{3,1}$. When we identify ψ with the electromagnetic potential, Eq. (2.7) is equivalent to the Lorentz gauge condition plus the differential equations expressing a zero electromagnetic field in terms of the potential.[7]

(b) The map ψ has a range contained in the bivector subspace $R^2_{3,1}$ of $R_{3,1}$:

$$\psi(x_1,x_2,x_3,x_4)=\psi_{14}e_{14}+\psi_{24}e_{24}+\psi_{34}e_{34}+\psi_{23}e_{23}+\psi_{31}e_{31}+\psi_{12}e_{12}. \tag{2.29}$$

Now, when we identify ψ with the electromagnetic field, the equation $P\psi=0$ is equivalent to the Maxwell equations in vacuum.[8]

III. $k=0$, $h\neq 0$, i.e., our general equation (2.6) has the form

$$P\psi=h. \tag{2.30}$$

Let us consider the Minkowski space-time $R^{3,1}$ again and let ψ have its range in the bivector subspace $R^2_{3,1}$ of $R_{3,1}$ as before. By the property (i) of the P operator we see that h can have a range contained only in $R^1_{3,1}\oplus R^3_{3,1}$. We shall assume that h is some vector field, i.e.,

$$h: R^{3,1}\to R^1_{3,1}. \tag{2.31}$$

Now Eq. (2.30) describes the Maxwell equation with the current vector h. It expresses the fact that the one-vector part of $P\psi$ is equal to the given electric source h and that the three-vector part of $P\psi$ vanishes, i.e., there are no magnetic sources. In other words it means that the bivector-valued electromagnetic field ψ has a vector potential A. It may be required that A is related to ψ by the equation

$$PA=\psi \tag{2.32}$$

(similarly to in the cases B and C).

But

$$PA=e_\mu\wedge\partial^\mu A+e_\mu\cdot\partial^\mu A \tag{2.33}$$

is contained in $R^0_{3,1}\oplus R^2_{3,1}$. The vanishing of the scalar part of PA described by Eq. (2.32) gives us a supplementary condition on the vector potential A which is called the Lorentz condition. From (2.30) we have that

$$P^2\psi=Ph. \tag{2.34}$$

Since the operator P^2 does not change the multivector character of any ψ, $P^2\psi$ is again a bivector. However, $Ph\subset R^0_{3,1}\oplus R^2_{3,1}$. Hence, we see that the scalar part of Ph has to be equal to zero. This is just the continuity equation for sources h.

III. $k\neq 0$, $h=0$, i.e., our general equation (2.5) [or $\equiv$ (2.6)] has the form

$$P\psi=k\psi. \tag{2.35}$$

When k is a constant scalar, i.e., $k\in R^0_{s,t}$, we shall call Eq. (2.35) the generalized Dirac equation. As we shall see, it will be exactly the Dirac equation when ψ: $R^{s,t}\to\Psi(s,t)$, where $\Psi(x,t)$ is the Dirac spinor space determined by some minimal left ideal of the corresponding Clifford algebra.

III. KÄHLER–DIRAC OPERATOR K

Let us consider the space $(R^{s,t})^*$ of differential forms on space $R^{s,t}$. Let $\phi: R^{s,t}\to\Lambda(R^{s,t})^*$ be a general differential form, i.e.,

$$\phi(x)=\phi^0(x)+\phi^\mu(x)dx_\mu+\phi^{\mu\nu}dx^\mu\wedge dx^\nu+\cdots+\phi^{12\cdots n}dx_1\wedge\cdots\wedge dx_n. \tag{3.1}$$

Let d be the exterior derivative $d:\Lambda^p\to\Lambda^{p+1}$. We can write it as

$$d\phi=dx_\mu\wedge\partial^\mu\phi. \tag{3.2}$$

The Hodge map $*:\Lambda^p\to\Lambda^{n-p}$, given by

$$\varphi\wedge *\varphi'=(\varphi,\varphi')_Q\omega,\quad \forall p\text{ forms }\varphi,\varphi', \tag{3.3}$$

where ω is a orienting n form with $(\omega,\omega)_Q=1$, allows us to introduce the operator δ which is formally Q adjoint to the d operator

$$\delta=-*d*. \tag{3.4}$$

Definition 2: We shall call the first-order operator $d-\delta$ operating on differential forms the Kähler–Dirac operator and we shall denote it by K.

It is known that $d-\delta$ is a "square root" of the Laplacian operator $\Box = -(d\delta + \delta d)$. Moreover, it can be checked[9] that

$$\delta\phi = -\,dx_\mu \lrcorner \partial^\mu \phi, \tag{3.5}$$

i.e., the operator K operating on differential forms can be written

$$K\phi = (d-\delta)\phi$$

or

$$K\phi = dx_\mu \wedge \partial^\mu \phi + dx_\mu \lrcorner \partial^\mu \phi. \tag{3.6}$$

Now let us recall that the underlying vector spaces for the Grassman algebra of differential forms and the Clifford algebra associated with $(R^{s,t})^*$ are exactly the same. Of course on $\wedge(R^{s,t})^*$ we can introduce the structure of the Clifford algebra, i.e., we can introduce the Clifford multiplication on $\wedge(R^{s,t})^*$. In this way we obtain the so-called Kähler–Atiyah algebra which carries both the exterior algebra and Clifford algebra structures. Because (3.1) has exactly the same form as (1.14), as well as that (3.6) is equal to the right side of (1.15), we obtain that in the realization of the Clifford algebra by differential forms operator P is equal to the Kähler–Dirac operator K.

IV. DIRAC OPERATOR D

It is known that for any Clifford algebra $\mathscr{C}(V,Q)$ we can find its faithful matrix representation. For the Clifford algebras which are simple (it is always when the dimension of the generating vector space n is even) the entries of this matrix repesentation will belong to one of the $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{H}$ division algebras. For the rest of the cases the entries belong to one of the ${}^2\mathbb{R}$ or ${}^2\mathbb{G}$ double fields. However, in any case the Clifford algebra of the complexified vector space $V^{\mathbb{C}}$ has its faithful matrix representation given by the algebra $\mathbb{C}(2^r)$ of $2^r \times 2^r$ complex matrixes. (r is the integral part of $n/2$, i.e., $r = [n/2]$.)

In this way we have that any element of $\mathscr{C}^{\mathbb{C}}(Q) = \mathscr{C}(Q^{\mathbb{C}})$ has its matrix realization. Hence the function ψ, introduced by (2.1), i.e., $\psi: V^{\mathbb{C}} \to \mathscr{C}^{\mathbb{C}}(Q)$, will be given by the matrices depending on $v \in V^{\mathbb{C}}$. Let us take $\psi: V \to {}^{\mathbb{C}}(Q)$, i.e., let us restrict ourselves to the functions with the target given by $V \subset V^{\mathbb{C}}$. Let us denote the matrix representation of the elements v_μ forming an orthonormal basis of V by γ_μ. Of course $\partial_\mu \psi$ will be given also by matrices which have the form

$$((\partial_\mu \psi)_{ab}) = (\partial_\mu \psi_{ab}), \tag{4.1}$$

where ψ_{ab} is an appropriate matrix element of the matrix ψ. Now we can take the realization of $\mathscr{C}^{\mathbb{C}}(Q)$ by the complexification $R^{\mathbb{C}}_{s,t}$ of the Clifford algebra of the pseudo-Riemannian vector space $R^{s,t}$ or by the complex differential forms on $R^{s,t}$. We have already seen that in the first case the operator P can be written as

$$P = e_\mu \vee \partial^\mu,$$

whereas in the second realization of $\mathscr{C}^{\mathbb{C}}(Q)$,

$$P = dx_\mu \vee \partial^\mu,$$

and is exactly equal to the Kähler–Dirac operator $K = d - \delta$.

Now, when we consider the matrix representation of the Clifford algebra, the above two realizations give the same. In other words, the operator P as well as K operating on the matrix-valued functions ψ have the form $\gamma_\mu \partial^\mu$. This is just the famous form of the operator D,

$$D = \gamma_\mu \partial^\mu, \tag{4.2}$$

introduced by Dirac in 1928. Thus we can say that the Dirac operator D is the matrix realization of the operators P and K. It follows from the fact that as e_μ and dx_μ are realized by the same matrix γ_μ, then the general elements (1.11) and (1.14) with the same coefficients are also given by the same matrix ψ. Moreover, it can be checked that the matrix elements of the differential form $(d-\delta)\psi$ are equal to the appropriate matrix elements of the differential form $dx_\mu \vee \partial^\mu \psi$, i.e.,

$$((d-\delta)\psi)_{ab} = (dx_\mu)_{ac}(\partial^\mu \psi)_{cb} = (\gamma_\mu \partial^\mu \psi)_{ab}. \tag{4.3}$$

Taking the matrix representation of the Clifford algebra $\mathscr{C}^{\mathbb{C}}(Q)$ as well as of a map ψ we can construct all kinds of equations introduced in Example I of Sec. III. In this way we obtain the matrix realizations of, for example, Cauchy–Riemann or Maxwell equations. However we shall be interested mainly in the equations (2.35) with ψ having the range in the minimal left ideal $\Psi(s,t)$ of $R^{\mathbb{C}}_{s,t}$. Because we can always fix the basic matrixes γ_μ (generating $R^{\mathbb{C}}_{s,t}$) in such a way that the spinor space $\Psi(s,t)$ is represented by matrices of the form

$$\Psi(s,t) = \left\{ \begin{pmatrix} \psi_1 & 0 & 0 & \cdots & 0 \\ \psi_2 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & ! \\ \psi_N & 0 & 0 & \cdots & 0 \end{pmatrix} \begin{matrix} \psi_\alpha \in \mathbb{C} \\ N = 2^r \end{matrix} \right\}, \tag{4.4}$$

Eq. (2.35) (in its matrix realization) is exactly equal to the Dirac equation $\gamma_\mu \partial^\mu \psi = m\psi$.

V. MANIFOLDS

Let M be a pseudo-Riemannian manifold and TM its tangent bundle. The matrix tensor $g_{\mu\nu}$ on M allows us to construct the Clifford albegra $\mathscr{C}(T_xM, g(x))$ at each point $x \in M$. In this way we obtain the so-called Clifford bundle $\mathscr{C}(TM) = \cup_{x \in M} \mathscr{C}(T_xM, g(x))$. However, similarly as before, we can realize the Clifford algebras of the quadratic forms determined by g starting from the cotangent bundle. In other words, we can construct a vector bundle $\mathscr{C}(T^*M) = \cup_{x \in M} \mathscr{C}(T^*_xM, g(x))$. This realization is sometimes called the cotangential Clifford bundle.

Let X be a vector field over M, i.e., X is a cross section of the tangent bundle TM. Similarly as for vector spaces we can introduce an operator P acting on the sections of a given realization of the Clifford bundle. Hence we obtain that for the tangentian Clifford bundle $\mathscr{C}(TM)$,

$$P = X \vee \nabla_X, \tag{5.1}$$

where ∇_X is the covariant derivative on M. For the cotangential realization of the Clifford bundle $\mathscr{C}(T^*M)$

$$P = X^* \vee \nabla_X, \tag{5.2}$$

where X^* is an appropriate section of T^*M determined by X.

In any local neighborhood $U \subset M$ with a coordinate basis $\{x^\mu\}$ the local cotangent-space is spanned by the differentials dx^μ. Now the P operator can be written as

$$P = dx^\mu \vee \nabla_{\partial/\partial x^\mu}, \tag{5.3}$$

i.e.,

$$P = dx^\mu \wedge \nabla_\mu + dx^\mu \lrcorner \nabla_\mu = d - \delta = K. \tag{5.4}$$

The relations (5.4) are a generalization of the formulas (3.6) for vector spaces to the case of the manifold and can be easily checked.[10]

Similarly as before we can consider Eq. (2.5) for ψ given by the sections of the Clifford bundle $\mathscr{C}^{\mathbb{C}}(T^*M)$ itself or by the sections of some of its vector subbundles. However, if ψ is a section of the even Clifford subbundle or two-forms subbundle or one-forms subbundle we have essentially the same situation as in the previous subsections. It is caused by the fact that the covariant derivative ∇_μ is also the covariant derivative of the just-mentioned vector bundles. But the situation will change when we consider cross sections of the spinor bundle ΨM. The vector bundle ΨM is defined by the global field of primitive idempotents $f(x)$ which at each point $x \in M$ determines a left minimal ideal of $\mathscr{C}^{\mathbb{C}}(T_x^*M,g)$. In a general case ∇_μ is not a linear endomorphism of the bundle of left minimal ideals generated by f.

This situation is caused by the fact that f is not parallel translated along any curve on M. Thus in a general case ∇_x maps a section of ΨM onto a section of $\mathscr{C}^{\mathbb{C}}(T^*M)$. In these cases the Kähler–Dirac equation $P\psi \equiv K\psi = \kappa\psi$ has no solution in ΨM.

If we want ∇_x to be a linear endomorphism of ΨM we have to impose strong restrictions on the metric tensor g (or rather on its holonomy group). These restrictions seem to be unphysical ones and, for example, for the Schwarzschild metric cannot be fulfilled. (Obviously they hold in a pseudo-Riemannian flat space-time V.) For these reasons some physicists reject the realization of the Dirac spinor bundle by the minimal left ideals of the complexified (tangential or cotangential) Clifford bundle. However, according to us just these difficulties could help us to understand more deeply the geometrical nature of spinor fields and their internal interactions.

VI. INTERNAL STRUCTURE OF FERMIONS

Let us assume that we have some fixed global field of primitive idempotents f on M. Let ΨM denote the vector bundle of minimal left ideals of $\mathscr{C}^{\mathbb{C}}(T^*M)$ determined by f. Using the anti-involutions of $\mathscr{C}^{\mathbb{C}}(T^*M)$ induced by the identity or reversal transformation of the cotangent bundle T^*M we can construct[11] the bijection

$$\chi_\delta : \Psi M \otimes \Psi M \to \mathscr{C}^{\mathbb{C}}(T^*M), \tag{6.1}$$

which satisfies the property

$$\chi_\delta(s\varphi(x), s\psi(x)) = s\chi_\delta(\varphi(x), \psi(x))\beta_\delta(s), \tag{6.2}$$

for any invertible element $s \in \mathscr{C}^{\mathbb{C}}(T_x^*M)$ and for any cross sections $\varphi(x)$, $\psi(x)$ of the bundle ΨM.

Let us denote by $K_\delta \subset \Psi M \otimes \Psi M$ the coimage of T^*M by the bijection χ_δ. The formula (6.2) tells us that if $s \in \mathrm{Spin}_+(s,t)$ then $\chi_\delta(K_\delta) = T^*M$ will be transformed by an appropriate proper orthogonal transformation. Any section ψ of the bundle ΨM can be treated as a Ψ-valued 0-form on M. However to define the exterior differential of a vector-bundle-valued p form on M we have to use a connection on this vector bundle. In case of a general manifold M it cannot be the Christoffel connection ∇ generated by the metric tensor g. However it has to be a connection which produces ∇ by an isomorphism χ_δ.

Let us denote by $\Gamma(\cdot)$ the spaces of smooth sections of a considered vector bundle. The connection $\tilde{\nabla}$ on ΨM is a bilinear map

$$\tilde{\nabla} : \Gamma(TM) \times \Gamma(\Psi M) \to \Gamma(\Psi M) \tag{6.3}$$

written

$$(X,\psi) \rightsquigarrow \tilde{\nabla}_X \psi,$$

and such that

$$\begin{aligned} &\text{(i)}\ \tilde{\nabla}_{tX}\psi = t\tilde{\nabla}_X\psi, \\ &\text{(ii)}\ \tilde{\nabla}_X t\psi = (X\cdot t)\psi + t\tilde{\nabla}\psi, \end{aligned} \tag{6.4}$$

for any function t on M, for any vector field $X \in \Gamma(TM)$ and for any spinor field $\psi' \in \Gamma(\Psi M)$. Here $\tilde{\nabla}_X\psi$ is called the covariant derivative of ψ in the direction of X. In a local neighborhood $U \subset M$ with a coordinate basis $\{x^\mu\}$ and spinor basis $\{\rho_i\}, i = 1,\ldots,N$,

$$\tilde{\nabla} s_i = \tilde{\Theta}_i^j s_j, \tag{6.5}$$

where $\tilde{\Theta} = (\tilde{\Theta}_i^j)$ is a matrix of complex one-forms.

For $\psi = \psi^i s_i$ over U we have

$$\tilde{\nabla}\psi = d\psi^i s_i + \psi^j \tilde{\nabla}_{s_j} = (d\psi^i + \psi^j \tilde{\Theta}_j^i) s_i. \tag{6.6}$$

Let us introduce $\tilde{\Gamma}_{\mu j}^i = \tilde{\Theta}_j^i(\partial/\partial x\mu)$, i.e.,

$$\tilde{\Theta}_j^i = \tilde{\Gamma}_{\mu j}^i \, dx^\mu. \tag{6.7}$$

Now

$$\tilde{\nabla}\psi = (\partial_\mu \psi^i + \tilde{\Gamma}_{\mu j}^i \psi^j)\, dx^\mu \otimes s_i, \tag{6.8}$$

or, equivalently,

$$\tilde{\nabla}_\mu \psi = (\partial_\mu \psi^i + \tilde{\Gamma}_{\mu j}^i \psi^j) s_i. \tag{6.8'}$$

As usual, we can introduce the curvature $\tilde{R}$ of the connection $\tilde{\nabla}$ by

$$\begin{aligned} &\tilde{R}(x,y)\psi = \tilde{\nabla}_X \tilde{\nabla}_Y \psi - \tilde{\nabla}_Y \tilde{\nabla}_X \psi + \tilde{\nabla}_{[X,Y]}\psi, \\ &\quad \forall\, X,Y \in \Gamma(TM), \quad \forall\, \psi \in \Gamma(\Psi M). \end{aligned} \tag{6.9}$$

Let us denote the ΨM-valued p forms on M by $\Lambda^p(\Psi M)$. Now, the exterior differential

$$\tilde{d} : \Lambda^p(\Psi M) \to \Lambda^{p+1}(\Psi M) \tag{6.10}$$

is defined in the following way:

$$\begin{aligned} &\tilde{d}\omega(X_1,\ldots,X_{p+1}) \\ &= \sum_{j1}^{p+1} (-1)^{j-1} \tilde{\nabla}_{X_j} \omega(X_1,\ldots,\hat{X}_j,x_{p+1}) \\ &\quad + \sum_{j<k} (-1)^{j+k} \omega([X_j,X_k],X_1,\ldots,\hat{X}_j,\ldots,\hat{X}_k,\ldots,X_{p+1}), \end{aligned} \tag{6.11}$$

for any $\omega \in \Lambda^p(\Psi M)$ and $X_1,\ldots,X_{p+1} \in \Gamma(TM)$.

Thus we can easily see that the square of the exterior

differential $\tilde{d}$ of the ΨM valued 0-form $\psi \in \Gamma(\Psi M)$ is equal to

$$\tilde{d}^2\psi(X,Y) = \tilde{R}(X,Y)\psi, \tag{6.12}$$

and for the p form $\omega \in \Lambda^p(\Psi M)$ we have

$$\tilde{d}\omega = \tilde{R} \wedge \omega. \tag{6.13}$$

Now let us take the tensor product $\Psi M \otimes \Psi M$. The connection $\tilde{\nabla}$ on ΨM defines the connection on this tensor bundle. Namely, we have

$$\tilde{\nabla}(\psi \otimes \varphi) = \tilde{\nabla}\psi \otimes \varphi + \psi \otimes \tilde{\nabla}\varphi, \quad \forall \psi,\varphi \in \Gamma(\Psi M). \tag{6.14}$$

Let the basis one-forms $dx^\mu = e^\mu$ be given by

$$e^\mu = \chi_\delta\Big(\sum a^{\mu ij}(x) s_i \otimes s_j\Big), \tag{6.15}$$

over $U \subset M$.

Here, the $a^{\mu ij}$ are some appropriate functions over U uniquely determined by χ_δ. Because

$$e^\mu e^\nu = e^\mu \wedge e^\nu + g^{\mu\nu}\cdot 1, \tag{6.16}$$

the functions $a^{\mu ij}$ have to satisfy some additional properties. The covariant derivative of e^ν is given by the Christoffel connection ∇ on T^*M, i.e.,

$$\nabla_\mu e^\nu = \Gamma^\nu_{\mu\rho} e^\rho. \tag{6.17}$$

However, we want to obtain the same result using the relation (6.15) and the formulas (6.14) and (6.8'). For this the coefficients $\tilde{\Gamma}^i_{\mu j}$ have to be given by

$$\tilde{\Gamma}^i_{\mu k} a^{\nu kj} + \tilde{\Gamma}^j_{\mu k} a^{\nu ik} = -\partial_\mu a^{\nu ij} + \Gamma^\nu_{\mu\rho} a^{\rho ij}. \tag{6.18}$$

We shall give the concrete form of $\tilde{\Gamma}^i_{\mu k}$ for a fixed dimension n and signature (s,t) and for a concrete relation (6.15).

Thus we come to the following picture: the pseudo-Riemanian structure on M determines the Christoffel connection ∇ which passes to the Clifford bundles $\mathscr{C}^{\mathbb{C}}(TM)$ or $\mathscr{C}^{\mathbb{C}}(T^*M)$, respectively. However, in a general case this connection cannot pass to the spinor bundle ΨM of the left minimal ideals. Nevertheless, owing to the bijection χ_δ we can determine the unique connection $\tilde{\nabla}$ on ΨM which produces ∇ on M. Let ψ be a spinor field over M, i.e., $\psi \in \Gamma(\Psi M)$. Because $\Psi M \hookrightarrow \mathscr{C}^{\mathbb{C}}(T^*M)$ the field ψ can be treated in two different ways: as a ΨM valued 0-form on M or as a section of $\mathscr{C}^{\mathbb{C}}(T^*M)$. In the first case the action of any vector field X on ψ will be determined by the connection $\tilde{\nabla}$ and will define another spinor field $\tilde{\nabla}_X\psi \in \Gamma(\Psi M)$. However, in the second case the action of the vector field X will produce a section $\nabla_X\psi$ of the Clifford bundle which does not belong to $\Gamma(\Psi M)$.

Have we any contradictions here? Where is the origin of the above situation?

We see from the above considerations that we can give to ΨM the primary nature. Namely, we can start with the bundle ΨM over M equipped with the connection $\tilde{\nabla}$ and produce the rest as vector bundles, among others the Clifford bundle $\mathscr{C}^{\mathbb{C}}(T^*M)$ as well as the connection ∇. Thus for any element, say $s \in \mathrm{Spin}_+(x,t)$, we have to do with two kinds of transformations

$$s: \Psi_X \to \Psi_X; \quad \psi \rightsquigarrow s\psi \tag{6.19}$$

and

$$s: \Psi_X \hookrightarrow \chi_\delta(\Psi_X \otimes \Psi_X) \to s\Psi_X s^{-1}. \tag{6.20}$$

Hence, if we treat ψ as a primary object, i.e., as a ΨM valued 0-form then we transform $\psi(x)$ by an element s according to (6.19). But if we look on the spinor $\psi(x)$ as on the composed object using the bijection χ_δ, i.e., $\Psi_X \hookrightarrow \chi_\delta(\Psi_X \otimes \Psi_X) = \mathscr{C}^{\mathbb{C}}(T^*_X M)$ then the transformation by any elements $s \in \mathrm{Spin}_+(s,t)$ is given by (6.20).

Of course, we have the same situation for the flat spacetime V. However, in this case the holonomy group related with the metric tensor g contains only the trivial element $e \in \mathrm{SO}_+(s,t)$. It implies that then both kinds of transformations (6.19) and (6.20) are equivalent and give the same result. We can also express this fact writing

$$\nabla_\mu = \tilde{\nabla}_\mu = \partial_\mu, \tag{6.21}$$

for any vector space V.

The situation will change when we consider the gravitation. Then the holonomy group is not trivial and we have to do with those two kinds of transformations (6.19) and (6.20) which provide different results. This is just the reason of the two unequivalent ways of the action of a given vector field X on ψ.

Thus although in the general case of a manifold M the operators P and K are equal to each other, they cannot have their domain and target contained in the bundle ΨM. In another way we can say that the exterior deviation $\tilde{d}$ operating on ΨM valued p forms is not equal to the ordinary exterior derivative d. However, we have that

$$\tilde{\nabla}_\mu\psi = \nabla_\mu\psi + B_\mu\psi \tag{6.22}$$

and we shall try to give the physical interpretation of the additional part B_μ.

As we have told the spinor bundle ΨM is determined by the global field of primitive idempotents f. It is known[12] that f can be written (at least locally over U) as

$$f = (1/2^r)(1+\omega_{s_1})\cdots(1+\omega_{s_2}), \tag{6.23}$$

where the ω_{s_i} are appropriate, square one, mutually commuting elements of $\Gamma(\mathscr{C}^{\mathbb{C}}(T^*M))$.

Let us denote f by f^1 and ΨM by $\Psi^1 M$, respectively. We can define the set $\{f^\alpha\}$, $\alpha = 1,\ldots,N = 2^r$ of mutually anihilating primitive idempotents by

$$f^\alpha = (1/2^r)(1+\epsilon^\alpha_1\omega_{s_1})\cdots(1+\epsilon^\alpha_r\omega_{s_2}), \tag{6.24}$$

with $\epsilon^\alpha_i = \pm 1$. Thus when we fix a global field of primitive idempotents $f = f^1$, simultaneously we have fixed all fields f^α, $\alpha = 1,\ldots,N$. But each f^α determines the vector bundle $\Psi^\alpha M = \mathscr{C}^{\mathbb{C}}(T^*M)f^\alpha$. In this manner we have obtained the decomposition of the Clifford bundle onto N mutally supplementing spinor bundles:

$$\mathscr{C}^{\mathbb{C}}(T^*M) = \bigoplus_{\alpha=1}^{N} \Psi^\alpha M. \tag{6.25}$$

It means that if we treat $\Psi M = \Psi^1 M$ as a primary given object then we have to introduce N internal degrees of freedom, i.e., N different kinds of spinor fields ψ^α, $\alpha = 1,\ldots,N$. We see that an element $s \in \mathrm{Spin}_+(s,t)$ operating according to (6.19) does not change the decomposition (6.25), but the action given by (6.20) mixes different spinor fields ψ^α between themselves.

Let us look at this situation when we realize Clifford

algebras by the matrix algebras. The decomposition (6.25) is equivalent to the decomposition of the matrices onto their columns.

It is obvious that whereas the left multiplication of a given matrix, say A, by another matrix, say B, does not transform the columns of A between themselves, the right multiplication of A by B will transform them.

The Christoffel connection which passes to the Clifford bundle determines the transformation of all elements of T^*M (under parallel translations) by appropriate elements of the holonomy group. It corresponds to the transformation (6.20) of the Clifford bundle. Thus we see that only in the cases of the flat space-time or when the holonomy group preserves f under the (6.20) transformation we will not change the internal degree of freedom α of the spinor fields $\psi \in \Gamma(\Psi^1 M)$.

The isotropy groups of f under the action (6.20) were investigated and (in many cases) calculated by Crumeyrolle.[13] For this reason we shall call them Crumeyrolle groups.

Thus we have obtained that only those generators of the holonomy group which do not belong to the Crumeyrolle albegra are responsible for the part B_μ of the connection $\tilde{\nabla}_\mu$.

Let us summarize the above situation. We have seen that if we want to understand a Dirac spinor field as a section of the bundle $\Psi^1 M$, then first of all we have to introduce internal degrees of freedom $\alpha = 1,...,N$. Moreover, we have to agree that the gravitational interaction implies the existence of some internal interaction given by the fields B_μ. This interaction changes the just introduced inertial coordinate α. Besides, the number of fields B_μ depends on the concrete holonomy group of a given gravitational field.

Thus only in the case of the experimental justification of this hypothesis it is reasonable to speak about the realization of the Dirac spinor bundle by the bundle of left minimal ideals of the Clifford bundle. In the opposite case we have to consider the Dirac spinors only as the abstractly given elements of the vector bundle associated to the principal spinor bundle.

VII. DIRAC EQUATION

It is natural, according to the Dirac intention, to define the Dirac operator D as operating on the sections of the $\Psi' M$ bundle. Hence we shall assume that

$$D = \gamma^\mu \tilde{\nabla}_\mu. \tag{7.1}$$

We can check that for any spinor fields $\psi, \varphi \in \Gamma(\Psi^1 M)$ we have

$$\chi_\delta[(D\psi \otimes \varphi) + \psi \otimes D(\varphi)] = (d - \delta)\chi_\delta(\psi \otimes \varphi). \tag{7.2}$$

Hence, if ψ and φ are the solutions of the Dirac equation, i.e., if they satisfy the relations

$$D\psi = \kappa_1 \psi, \quad D\varphi = \kappa_2 \varphi, \tag{7.3}$$

then the field $F \in \Gamma(\mathscr{C}^{\mathbb{C}}(T^*M))$ equal to $F = \chi_\delta(\psi \otimes \varphi)$ satisfies the equation

$$PF = (\kappa_1 + \kappa_2)F. \tag{7.4}$$

Let F be some spinor field, i.e., $F = \psi \in \Gamma(\Psi^1 M)$. Using the bijection χ_δ we can treat it as the composed object. Now, Eq. (7.2) means that it can be obtained as the image of the solutions of the Dirac equation only when the Christoffel connection is flat or its holonomy group is equal to the Crumeyrolle group. In other words, only when

$$\nabla_\mu = \tilde{\nabla}_\mu$$

can any solutions $\psi, \varphi \in \Gamma(\Psi^1 M)$ of the Dirac equation produce (by χ_δ) a section of a bundle of minimal left ideals over M.

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[1]Here, $\wedge$ denotes the exterior product of vectors.
[2]dx^μ is Q adjoint to dx^μ, i.e., $dx^\mu \lrcorner dx\Psi = B(dx^\mu, dx^\nu)$.
[3]P. Becher and H. Joos, Z. Phys. C **15**, 343 (1982); W. Graf, Ann. Inst. H. Poincaré, **29**, 85 (1978); I. Benn and R. Tucker, Commun. Math. Phys. **89**, 341 (1983).
[4]Here, $\partial/\partial x^\mu$ denotes the partial differentiation of the coefficients.
[5]P. Lounesto, "Spinor values regular functions in hypercomplex analysis," Rep. No HTKK-MAT-A154 (1979).
[6]If there is no danger of confusion, instead of ee we shall also write ee or shorter e.
[7]See Graf, Ref. 3.
[8]I. Salingaros, J. Math. Phys. **22**, 1918 (1981); **22**, 226 (1981).
[9]See Ref. 3.
[10]See Ref. 3.
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Topological properties of unbounded bicommutants

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We consider different possible definitions of unbounded commutants and unbounded bicommutants of a set or an algebra of unbounded operators. We investigate their behavior with respect to various topologies. In particular we give sufficient conditions in order that bicommutants be the closure of the original set of operators with respect to some of those topologies. We investigate some special classes of algebras (symmetric, self-adjoint, regular, V^* algebras) for which several or all of the bicommutants coincide and are the closure of the algebra with respect to some or all of the considered topologies.

I. INTRODUCTION

In recent years, many authors have been interested in the study of unbounded operator algebras from a mathematical point of view and also for their applications to quantum field theories. It appeared very quickly that if one tries to build a theory analogous to the theory of von Neumann algebras, but this time for unbounded operators, many difficulties and pathologies occur. That is the reason why several authors have considered special classes of algebras like symmetric, self-adjoint algebras[1–3] and more recently V^* algebras.[4] In those particular classes, several results of the bounded case may be extended.

One of the important ingredients in the theory of von Neumann algebras is the notion of the commutant of a set of operators. When we deal with unbounded operators many different notions of a commutant may be introduced. The commutant may be taken among bounded operators[3,5] and it can be "weak" or "strong." On the other hand, we may allow unbounded operators in the commutant so that we shall have unbounded (weak or strong) commutants.[1,4,6]

In this paper we consider mainly unbounded commutants and unbounded bicommutants of a $*$-invariant set of unbounded operators. We have two different unbounded commutants and four different unbounded bicommutants and we investigate their topological properties. Indeed we can define several topologies on our set of unbounded operators. We consider here three topologies: the weak, the strong, and the strong* topology (see Sec. III). This last topology is a particular case of quasiuniform topologies introduced in Ref. 7 and which have already been useful for problems involving unbounded operators.[8,9] The strong* topology appears to play a natural role in the sense that all the commutants and the bicommutants we consider are closed in this topology, although they are not necessarily strongly or weakly closed. Nevertheless, one of them, the strong unbounded bicommutant, is weakly closed, so that it seems that weak commutants behave well in the strong* topology and strong commutants behave well in the weak topology.

In Sec. IV we answer the question: When is the weak unbounded bicommutant the closure of the algebra with respect to the strong* topology and when is the strong bicommutant the weak closure of the algebra? We give several criteria in order that those two results hold separately or simultaneously.

In this section we also introduce a fourth topology, the so-called commutant topology, which plays a role similar to the strong* topology, in the sense that commutants are also closed with respect to it. This topology seems thus also natural and it is quite intrinsic because it is defined directly from the algebra and its weak commutant rather than from the Hilbert space structure. We give some criteria in order that the weak unbounded bicommutant be the closure of the algebra with respect to that topology.

After a few remarks about strongly*-continuous linear functionals we end Sec. IV with the study of self-adjoint algebras: those algebras have only two different unbounded bicommutants, both weakly closed.

Finally in Sec. V we particularize to regular op* algebras, V^* algebras, and SV^* algebras. Those last have been introduced[4] in order to extend to unbounded operators properties of von Neumann algebras. We show that a V^* algebra is always closed with respect to the strong* topology and to the commutant topology. Moreover, for a self-adjoint V^* algebra, the four unbounded bicommutants coincide with the algebra, which is, in this case, closed with respect to the four topologies introduced above.

II. DEFINITIONS AND ELEMENTARY PROPERTIES

A. Definitions

Let $\mathscr{H}$ be a Hilbert space and $\mathscr{D}$ a dense linear subset of it. Following Ref. 4 we denote by $C(\mathscr{D},\mathscr{H})$ the set of all closable operators A in $\mathscr{H}$ such that $\mathscr{D}\subseteq D(A)\cap D(A^*)$.

As remarkable subsets of $C(\mathscr{D},\mathscr{H})$ we have first $B(\mathscr{H})$, the set of bounded operators in $\mathscr{H}$, and on the other hand the $*$ algebra $L^+(\mathscr{D})$ (or $C_{\mathscr{D}}$) of elements $A\in C(\mathscr{D},\mathscr{H})$ such that $A\mathscr{D}\subseteq\mathscr{D}$ and $A^*\mathscr{D}\subseteq\mathscr{D}$ (see Ref. 10). These operators are continuous with respect to the weak topology $\sigma(\mathscr{D},\mathscr{D})$.

Let $\mathfrak{A}$ be a subset of $C(\mathscr{D},\mathscr{H})$. We denote by $\mathfrak{A}_b$ its bounded part

$$\mathfrak{A}_b=\{A\in\mathfrak{A}\cap B(\mathscr{H})\}\,.$$

If $\mathfrak{A}$ is an involutive subalgebra of $L^+(\mathscr{D})$ with identity, $\mathfrak{A}$ is called an op* algebra.[10]

An op* algebra is called *symmetric* if for every $A\in\mathfrak{A}$, $(1+A^*A)^{-1}$ exists and lies in $\mathfrak{A}_b$.

An op* algebra is called *self-adjoint* if

$$\mathscr{D}=\mathscr{D}^*\equiv\bigcap_{A\in\mathfrak{A}}D(A^*)\,.$$

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B. Topologies

Several topologies may be defined on $C(\mathscr{D},\mathscr{H})$.

(a) The weak topology is defined by the set of seminorms

$$A\in C(\mathscr{D},\mathscr{H})\mapsto|(Af,g)|\,,\quad f,g\in\mathscr{D}\,.$$

(b) The strong topology is defined by the set of seminorms

$$A\in C(\mathscr{D},\mathscr{H})\mapsto\|Af\|\,,\quad f\in\mathscr{D}\,.$$

(c) The strong* topology[11] is defined by the set of seminorms

$$A\in C(\mathscr{D},\mathscr{H})\mapsto\max\{\|Af\|,\|A^*f\|\}$$

or

$$\|Af\|+\|A^*f\|\,,\quad f\in\mathscr{D}\,.$$

Notice that one advantage of this third topology is that the involution $A\to A^*$ is continuous with respect to it, as it is also for the weak topology but not for the strong.

A second advantage to consider is that $C(\mathscr{D},\mathscr{H})$ is complete with respect to this topology. Indeed if A^α is a Cauchy net in $C(\mathscr{D},\mathscr{H})$ with respect to the strong* topology, then for every $f\in\mathscr{D}$, $A^\alpha f$ and $A^{\alpha*}f$ are Cauchy nets in $\mathscr{H}$. Let $g=\text{s-lim}\,A^\alpha f$ and $g^*=\text{s-lim}\,A^{\alpha*}f$; then putting $g=Af$ we get a well-defined linear operator on $\mathscr{D}$. For every $f,h\in\mathscr{D}$ we have

$$(Ah,f)=\lim_\alpha(A^\alpha h,f)=\lim_\alpha(h,A^{\alpha*}f)=(h,g^*)\,.$$

This shows that $f\in D(A^*)$ and $g^*=A^*f$ for every $f\in\mathscr{D}$ so that $A\in C(\mathscr{D},\mathscr{H})$.

C. Commutants

Since we are dealing with unbounded operators, several notions of commutants can be considered and we begin by recalling them.

Let $\mathfrak{A}$ be a $*$-invariant subset of $C(\mathscr{D},\mathscr{H})$.

The "weak unbounded commutant"[4]

$$\mathfrak{A}'_\sigma=\{X\in C(\mathscr{D},\mathscr{H})|(X^*f,Ag)=(A^*f,Xg)\,,\quad\forall f,g\in\mathscr{D}\,,\quad\forall A\in\mathfrak{A}\}$$

is a $*$-invariant linear subset of $C(\mathscr{D},\mathscr{H})$.

Its bounded part $\mathfrak{A}'_w=\mathfrak{A}'_\sigma\cap B(\mathscr{H})$ is the weak commutant which has been considered in Refs. 3 and 5.

It is a $*$-invariant linear subset of $B(\mathscr{H})$ and it is closed in $B(\mathscr{H})$ for the usual weak topology. Here $\mathfrak{A}'_w$ will be called the "weak bounded commutant."

It is also interesting to consider strong commutants: the "strong unbounded commutant" is defined as

$$\mathfrak{A}'_c\equiv\mathfrak{A}'_\sigma\cap L^+(\mathscr{D})=\{X\in L^+(\mathscr{D})|(A^*X^*f,g)=(f,AXg)\,,\quad\forall f,g\in\mathscr{D}\,,\quad\forall A\in\mathfrak{A}\}\,.$$

It is easy to see that it is an op* algebra even if $\mathfrak{A}$ is not one. We can reformulate this definition as follows:

$$\mathfrak{A}'_c=\{X\in L^+(\mathscr{D})|AXf=(X^*\restriction_{\mathscr{D}})^*Af,\quad\forall f\in\mathscr{D},\ \forall A\in\mathfrak{A}\}\,.$$

In particular, if $\mathfrak{A}$ is itself contained in $L^+(\mathscr{D})$ then we get back the definition of Ref. 6

$$\mathfrak{A}\subseteq L^+(\mathscr{D})\Rightarrow\mathfrak{A}'_c=\{X\in L^+(\mathscr{D})|AXf=XAf,\quad\forall f\in\mathscr{D}\,,\quad\forall A\in\mathfrak{A}\}\,.$$

Finally we can also consider the "strong bounded commutant", $\mathfrak{A}'_s\equiv\mathfrak{A}'_c\cap B(\mathscr{H})$, which is also an op* algebra. We also have $\mathfrak{A}'_s=\mathfrak{A}'_w\cap L^+(\mathscr{D})$. The inclusions between those four commutants are thus

$$\begin{array}{ccc}\mathfrak{A}'_w&\subseteq&\mathfrak{A}'_\sigma\\ \cup&&\cup\\ \mathfrak{A}'_s&\subseteq&\mathfrak{A}'_c\,.\end{array}$$

In this paper the main role will be played by the unbounded commutants $\mathfrak{A}'_\sigma$ and $\mathfrak{A}'_c$; the two others appear only for technical reasons. So when we say weak or strong commutant we always mean the unbounded one unless we state "bounded" explicitly.

Remark: Several authors have introduced commutants for unbounded operator algebras. The similarities or the differences between those commutants and ours are the following: $\mathfrak{A}'_\sigma$ is the part of $\Pi(\mathfrak{A})^c$ in Ref. 1 which is stable with respect to the operation of taking the adjoint. The same relation exists between $\mathfrak{A}'_c$ above and $\Pi(\mathfrak{A})^c_s$ of Ref. 1, and between $\mathfrak{A}'_s$ above and $\mathfrak{A}'_s$ of Ref. 5.

D. Bicommutants

We may define four "unbounded bicommutants."

(a) $\mathfrak{A}''_{\sigma\sigma}=\{Y\in C(\mathscr{D},\mathscr{H})|(Y^*f,Xg)=(X^*f,Yg)\,,\quad\forall f,g\in\mathscr{D}\,,\quad\forall Y\in\mathfrak{A}'_\sigma\}$

is a $*$-invariant subset of $C(\mathscr{D},\mathscr{H})$ containing $\mathfrak{A}$. As a consequence of this $\mathfrak{A}'''_{\sigma\sigma\sigma}=\mathfrak{A}'_\sigma$ and $\mathfrak{A}'''''_{\sigma\sigma\sigma\sigma\sigma}=\mathfrak{A}''_{\sigma\sigma}$.

(b) $\mathfrak{A}''_{cc}=\{Y\in L^+(\mathscr{D})|YXf=XYf,\quad\forall f\in\mathscr{D}\,,\quad\forall X\in\mathfrak{A}'_c\}$.

Here $\mathfrak{A}''_{cc}$ is an op* algebra and is equal to $\mathfrak{A}'''''_{ccccc}$. If, moreover, $\mathfrak{A}\subseteq L^+(\mathscr{D})$, then $\mathfrak{A}\subseteq\mathfrak{A}''_{cc}$ and $\mathfrak{A}'_c=\mathfrak{A}'''_{ccc}$.

(c) $\mathfrak{A}''_{c\sigma}=\{Y\in C(\mathscr{D},\mathscr{H})|(Y^*f,Xg)=(X^*f,Yg),\quad\forall f,g\in\mathscr{D}\,,\quad\forall X\in\mathfrak{A}'_c\}$.

It is a $*$-invariant subset of $C(\mathscr{D},\mathscr{H})$ containing both $\mathfrak{A}''_{\sigma\sigma}$ and $\mathfrak{A}''_{cc}$.

(d) $\mathfrak{A}''_{\sigma c}=\mathfrak{A}''_{\sigma\sigma}\cap L^+(\mathscr{D})$

is an op* algebra.

Between those four commutants, we have the following inclusions:

$$\begin{array}{ccccc}\mathfrak{A}''_{\sigma\sigma}&\subseteq&\mathfrak{A}''_{c\sigma}&\subseteq&C(\mathscr{D},\mathscr{H})\\ \cup&&\cup&&\cup\\ \mathfrak{A}''_{\sigma c}&\subseteq&\mathfrak{A}''_{cc}&\subseteq&L^+(\mathscr{D})\,.\end{array}$$

If $\mathfrak{A}\subseteq L^+(\mathscr{D})$ then $\mathfrak{A}$ is contained in the four bicommutants, but if $\mathfrak{A}\not\subseteq L^+(\mathscr{D})$ then $\mathfrak{A}$ is only contained in $\mathfrak{A}''_{\sigma\sigma}$ and $\mathfrak{A}''_{c\sigma}$.

III. TOPOLOGICAL PROPERTIES OF THE COMMUTANTS

For algebras of bounded operators in $\mathscr{H}$ we know that the usual commutants are weakly closed and *a fortiori*

strongly closed subalgebras of $B(\mathscr{H})$ (see Ref. 12). For unbounded operators and unbounded commutants this result is no longer true and the question is: Under which topology is each commutant closed?

A. The weak unbounded commutant

As mentioned in Ref. 4, $\mathfrak{A}'_\sigma$ is not in general closed for the weak or the strong topology. However (Ref. 4, Proposition 4) if $\mathfrak{A}\mathscr{D}\subseteq\mathscr{D}$ then $\mathfrak{A}'_\sigma$ is a weakly closed subspace of $C(\mathscr{D},\mathscr{H})$. Similarly, a sufficient condition in order that $\mathfrak{A}''_{\sigma\sigma}$ be weakly closed is that $\mathfrak{A}'_\sigma\mathscr{D}\subseteq\mathscr{D}$. This condition is not automatically satisfied so that *a priori* a weak unbounded bicommutant need not be weakly or strongly closed.

Proposition 1: The $\mathfrak{A}'_\sigma$ is closed in $C(\mathscr{D},\mathscr{H})$ with respect to the strong* topology.

Proof: Let $X\in C(\mathscr{D},\mathscr{H})$ be the limit of a strong* converging net $X^\alpha\in\mathfrak{A}'_\sigma$. That means in particular that for every $f\in\mathscr{D}$, $\|(X^\alpha-X)f\|$ and $\|(X^{\alpha*}-X^*)f\|$ tend to zero and thus also the scalar products $(k,(X^\alpha-X)f)$ and $(k,(X^{\alpha*}-X^*)f)$, for every $f\in\mathscr{D}$ and for every $k\in\mathscr{H}$. So we have for every $f,g\in\mathscr{D}$ and for every $A\in\mathfrak{A}$

$$(X^*f,Ag)=\lim_\alpha(X^{\alpha*}f,Ag)=\lim_\alpha(A^*f,X^\alpha g)$$
$$=(A^*f,Xg),$$

i.e., $X\in\mathfrak{A}'_\sigma$ □

Corollary 2: (i) $\mathfrak{A}''_{\sigma\sigma}$ and $\mathfrak{A}''_{c\sigma}$ are closed in $C(\mathscr{D},\mathscr{H})$ for the strong* topology; (ii) $\mathfrak{A}''_{c\sigma}$ is strongly and weakly closed in $C(\mathscr{D},\mathscr{H})$ (because $\mathfrak{A}'_c\mathscr{D}\subseteq\mathscr{D}$).

Remark: In the proof of Proposition 1 we have used the fact that X^α tends to X in the topology defined by the seminorms $X\to(k,Xf)$ and $X\to(k,X^*f)$ where $f\in\mathscr{D}$ and $k\in\mathscr{H}$. This topology is weaker than the s^* topology and so we showed that $\mathfrak{A}'_\sigma$ is closed with respect to that topology, too. This will be useful later in Sec. IV.

B. The strong unbounded commutant

Proposition 3: $\mathfrak{A}'_c$ is closed in $L^+(\mathscr{D})$ with respect to the strong* topology.

Proof: Let $X\in L^+(\mathscr{D})$ such that there exists a net X^α in $\mathfrak{A}'_c$ converging in the strong* topology. As in the proof of Proposition 1, we show $X\in\mathfrak{A}'_\sigma$. Since we assume that $X\in L^+(\mathscr{D})$ this implies $X\in\mathfrak{A}'_c$. □

Remark: This also shows that $\mathfrak{A}'_c$ is not necessarily closed in $C(\mathscr{D},\mathscr{H})$.

Proposition 4: If $\mathfrak{A}\mathscr{D}\subseteq\mathscr{D}$, then $\mathfrak{A}'_c$ is closed in $L^+(\mathscr{D})$ with respect to the weak topology (and the strong *a fortiori*).

Proof: In the proof of Proposition 1, Ag and A^*f now belong to $\mathscr{D}$ and the limit can be taken in the weak sense. □

Remark: For op* algebras this was already proved in Ref. 6, and similarly for the next corollary.

Corollary 5: $\mathfrak{A}''_{cc}$ is weakly closed in $L^+(\mathscr{D})$.

Corollary 6: $\mathfrak{A}''_{\sigma c}$ is closed in $L^+(\mathscr{D})$ for the strong* topology.

C. The role of the strong* topology

As we can see from the last two paragraphs all the unbounded commutants and bicommutants are closed for the strong* topology, some of them in $C(\mathscr{D},\mathscr{H})$ (the weak ones $\mathfrak{A}'_\sigma$, $\mathfrak{A}''_{\sigma\sigma}$, and $\mathfrak{A}''_{c\sigma}$) and others in $L^+(\mathscr{D})$ (the strong ones $\mathfrak{A}'_c$, $\mathfrak{A}''_{cc}$, and $\mathfrak{A}''_{\sigma c}$). This topology thus seems to be quite natural when we are dealing with unbounded operators and we can conjecture that it will play the role of the weak topology for bounded operators.

However, if we consider an op* algebra we may also consider the weak topology if we use only strong commutants and bicommutants [those are weakly closed in $L^+(\mathscr{D})$]. But if we want to use weak commutants, the strong* topology occurs immediately. The fact that this topology is natural may also be seen from the next proposition.

Proposition 7: Let $\mathfrak{A}_0\subseteq\mathfrak{A}\subseteq C(\mathscr{D},\mathscr{H})$ and assume that $\mathfrak{A}_0$ is a *-invariant set dense in $\mathfrak{A}$ for the strong* topology. Then

$$(\mathfrak{A}_0)'_\sigma=\mathfrak{A}'_\sigma,\quad(\mathfrak{A}_0)'_c=\mathfrak{A}'_c,\quad(\mathfrak{A}_0)'_w=\mathfrak{A}'_w,\quad(\mathfrak{A}_0)'_s=\mathfrak{A}'_s.$$

Proof: Let $X\in(\mathfrak{A}_0)'_\sigma$ and $A\in\mathfrak{A}$. By assumption, there exists a net A^α in $\mathfrak{A}_0$ such that $A^\alpha\to A$ in the strong* topology, and in particular $(k,(A^\alpha-A)f)\to0$ and $(k,(A^{\alpha*}-A^*)f)\to0$ for every $f\in\mathscr{D}$ and every $k\in\mathscr{H}$. Then for every $f,g\in\mathscr{D}$,

$$(X^*f,Ag)=\lim_\alpha(X^*f,A^\alpha g)=\lim_\alpha(A^{\alpha*}f,Xg)=(A^*f,Xg).$$

Hence $X\in\mathfrak{A}'_\sigma$ and $(\mathfrak{A}_0)'_\sigma\subseteq\mathfrak{A}'_\sigma$. The opposite inclusion is obvious.

The equalities for the strong, the weak bounded, and the strong bounded commutant follow immediately by their definitions as intersections of the weak unbounded commutant with $L^+(\mathscr{D})$ and/or $B(\mathscr{H})$. □

Remarks: For the bounded commutants this fact was already noticed in Ref. 9, Lemma 2.2.2.

If we assume $\mathfrak{A}_0$ dense in $\mathfrak{A}$ for a weaker topology such as the strong or the weak, only a part of those results remains true, namely, the statement about strong commutants.

Proposition 8: Let $\mathfrak{A}_0$ be a *-invariant subset of $C(\mathscr{D},\mathscr{H})$, dense in $\mathfrak{A}$ for the weak topology. Then

$$(\mathfrak{A}_0)'_c=\mathfrak{A}'_c\quad\text{and}\quad(\mathfrak{A}_0)'_s=\mathfrak{A}'_s.$$

Proof: Let A^α be a net in $\mathfrak{A}_0$ converging weakly to $A\in\mathfrak{A}$ and let $X\in(\mathfrak{A}_0)'_c$. By definition we have

$$(A^{\alpha*}X^*f,g)=(f,A^\alpha Xg),\quad\forall f,g\in\mathscr{D},$$

and since $X^*f\in\mathscr{D}$ and $Xg\in\mathscr{D}$ we can take the limit of both sides of this equality and get $X\in\mathfrak{A}'_c$. □

Remark: This argument does not work if X is in the weak commutant, for in that case X^*f and Xg do not belong to $\mathscr{D}$ and a weak limit cannot be taken.

IV. BICOMMUTANTS AND THE CLOSURE OF $\mathfrak{A}$

Since we have seen in the previous section that the four bicommutants are closed in the strong* topology and that some of them are also closed in the weak topology, the natural question to ask is: Do they coincide with the closure of $\mathfrak{A}$ in one or some of those topologies?

We give some criteria in order that the weak unbounded bicommutant coincide with the closure of $\mathfrak{A}$ in the strong* topology and that the strong unbounded bicommutant coincide with the closure in $L^+(\mathscr{D})$ of $\mathfrak{A}$ in any of those topolo-

gies. The ideas of the proofs are similar to some proofs of Ref. 4, although we consider here other topologies and some other commutants.

A. The weak unbounded bicommutant and the strong* topology

Proposition 9: Let $\mathfrak{M}\subset C(\mathscr{D},\mathscr{H})$ be a * algebra of bounded operators, containing 1. Then $\mathfrak{M}''_{\sigma\sigma}$ is the closure of $\mathfrak{M}$ in $C(\mathscr{D},\mathscr{H})$ with respect to the strong* topology (notation: $\mathfrak{M}''_{\sigma\sigma}=\overline{\mathfrak{M}}^{s^*}$).

Proof: Since by Corollary 2 we know that $\mathfrak{M}'_{\sigma\sigma}$ is closed in the strong* topology we have $\overline{\mathfrak{M}}^{s^*}\subseteq\mathfrak{M}'_{\sigma\sigma}$ and it remains to show the opposite inclusion.

(a) Let $f\in\mathscr{D}$ and consider the closed subspace of $\mathscr{H}$ generated by $\mathfrak{M}f$. Let P be the projection on this subspace $\overline{\mathfrak{M}f}$. Since every $M\in\mathfrak{M}$ is bounded, M leaves this subspace invariant and thus $PM=MP$. This implies that $P\in\mathfrak{M}'_w\subseteq\mathfrak{M}'_\sigma$.

Now take $Y\in\mathfrak{M}''_{\sigma\sigma}$ and any $g\in\mathscr{D}$. Then

$$((1-P)Yf,g)=(Yf,(1-P)g)=((1-P)f,Y^*g)=0\,.$$

Hence $Yf=PYf$, i.e., $Yf\in\mathfrak{M}f$.

We then conclude that given $Y\in\mathfrak{M}''_{\sigma\sigma}$, for every $\epsilon>0$, $f\in\mathscr{D}$ there exists $M\in\mathfrak{M}$ such that $\|(Y-M)f\|<\epsilon$.

(b) As the second step of the proof we show that $\mathfrak{M}''_{\sigma\sigma}\subseteq\overline{\mathfrak{M}}^{s}$. Recalling that the zero neighborhoods in the strong topology are of the form

$$\mathscr{V}_{f_1,f_2,\ldots,f_n,\epsilon}(0)=\{A\in C(\mathscr{D},\mathscr{H})\,|\,\|Af_1\|<\epsilon\,,\ \|Af_2\|<\epsilon,\ldots,\|Af_n\|<\epsilon\}\,,$$

for any *finite* sequence $f_1,f_2,\ldots,f_n$ of elements of $\mathscr{D}$ and any $\epsilon>0$, it suffices to prove that given $Y\in\mathfrak{M}''_{\sigma\sigma}$, $f_1,f_2\in\mathscr{D}$, and $\epsilon>0$, there exists $M\in\mathfrak{M}$ such that $Y-M$ belongs to $\mathscr{V}_{f_1,f_2,\epsilon}(0)$.

For this, consider the Hilbert space $\mathscr{H}\oplus\mathscr{H}$ and the set of unbounded operators $C(\mathscr{D}\oplus\mathscr{D},\mathscr{H}\oplus\mathscr{H})$. Every $M\in\mathfrak{M}$ defines a bounded operator

$$\tilde{M}=\begin{pmatrix}M&0\\0&M\end{pmatrix}$$

in $\mathscr{H}\oplus\mathscr{H}$ and let us denote by $\tilde{\mathfrak{M}}$ the set of such operators. Then $\tilde{\mathfrak{M}}$ is an op* algebra on $\mathscr{D}\oplus\mathscr{D}$ consisting of bounded operators only. We can compute explicitly the unbounded commutant and bicommutant of $\tilde{\mathfrak{M}}$ and we get, respectively,

$$\tilde{\mathfrak{M}}'_\sigma=\left\{\begin{pmatrix}X_{11}&X_{12}\\X_{21}&X_{22}\end{pmatrix}\middle|\,Xij\in\mathfrak{M}'_\sigma\,,\quad\text{for } i,j=1,2\right\}$$

and

$$\tilde{\mathfrak{M}}''_{\sigma\sigma}=\left\{\tilde{Y}=\begin{pmatrix}Y&0\\0&Y\end{pmatrix}\middle|\,Y\in\mathfrak{M}''_{\sigma\sigma}\right\}=\widetilde{\mathfrak{M}''_{\sigma\sigma}}\,.$$

Now, applying the result of part (a) of this proof to $\tilde{\mathfrak{M}}''_{\sigma\sigma}$, we get that $\forall\tilde{Y}\in\tilde{\mathfrak{M}}''_{\sigma\sigma}$, $\forall\tilde{f}\in\mathscr{D}\oplus\mathscr{D}$, and $\forall\epsilon>0$ there exists $\tilde{M}\in\tilde{\mathfrak{M}}$ such that $\|(\tilde{Y}-\tilde{M})\tilde{f}\|<\epsilon$. That is, if $\tilde{f}=(f_1,f_2)$: $\|(Y-M)f_1\|<\epsilon/2$ and $\|(Y-M)f_2\|<\epsilon/2$; hence, $Y-M\in\mathscr{V}_{f_1,f_2,\epsilon/2}(0)$. Since that is true for any neighborhood, we have that $Y\in\overline{\mathfrak{M}}^{s}$.

(c) The last thing we need to show in order to have $\mathfrak{M}''_{\sigma\sigma}\subseteq\overline{\mathfrak{M}}^{s^*}$ is that if $Y-M$ belongs to some neighborhood of zero of the form above, then Y^*-M^* belongs to this neighborhood as well. The proof is similar to (b) except for two differences: First we consider the direct sum $\mathscr{H}\oplus\overline{\mathscr{H}}$, where $\overline{\mathscr{H}}$ denotes the Hilbert space conjugate to $\mathscr{H}$ (i.e., the same set considered with the conjugate scalar multiplication $\lambda\circ f\equiv\bar{\lambda}f$ and endowed with the complex conjugate scalar product). (Remark: the norms in $\mathscr{H}\oplus\mathscr{H}$ and $\mathscr{H}\oplus\overline{\mathscr{H}}$ are identical.)

Second, we shall consider the set

$$\hat{\mathfrak{M}}=\left\{\hat{M}=\begin{pmatrix}M&0\\0&M^*\end{pmatrix}\middle|\,M\in\mathfrak{M}\right\}.$$

Endowed with the (mixed) product

$$\begin{pmatrix}M&0\\0&M^*\end{pmatrix}\circ\begin{pmatrix}N&0\\0&N^*\end{pmatrix}=\begin{pmatrix}MN&0\\0&N^*M^*\end{pmatrix}$$

and with the conjugate scalar multiplication

$$\lambda\circ\begin{pmatrix}M&0\\0&M^*\end{pmatrix}=\begin{pmatrix}\lambda M&0\\0&\bar{\lambda}M^*\end{pmatrix},$$

$\hat{\mathfrak{M}}$ becomes an op* algebra on $\mathscr{D}\oplus\overline{\mathscr{D}}$ of bounded operators in $\mathscr{H}\oplus\overline{\mathscr{H}}$.

If we compute the commutant and bicommutant of this algebra we get

$$\hat{\mathfrak{M}}'_\sigma=\left\{\begin{pmatrix}X_1&0\\0&X_2\end{pmatrix}\middle|\,X_1,X_2\in\mathfrak{M}'_\sigma\right\}$$

and

$$\hat{\mathfrak{M}}''_{\sigma\sigma}=\left\{\begin{pmatrix}Y_1&0\\0&Y_2\end{pmatrix}\middle|\,Y_1,Y_2\in\mathfrak{M}''_{\sigma\sigma}\right\}.$$

In particular, for every $Y\in\mathfrak{M}''_{\sigma\sigma}$ the element

$$\hat{Y}=\begin{pmatrix}Y&0\\0&Y^*\end{pmatrix}$$

belongs to $\hat{\mathfrak{M}}''_{\sigma\sigma}$. Applying point (a) of the proof to this particular element we have that for every $\hat{f}\in\mathscr{D}\oplus\overline{\mathscr{D}}$, $\forall\epsilon>0$ there exists $\hat{M}\in\hat{\mathfrak{M}}$ such that $\|(\hat{Y}-\hat{M})\hat{f}\|<\epsilon$.

If we take $\hat{f}=(f,f)$ for any $f\in\mathscr{D}$, this implies $\|(Y-M)f\|<\epsilon/2$ and $\|(Y^*-M^*)f\|<\epsilon/2$. Hence $Y\in\overline{\mathfrak{M}}^{s^*}$. □

Corollary 10: If $\mathfrak{M}\subseteq L^+(\mathscr{D})$, $\mathfrak{M}''_{\sigma c}$ is the closure of $\mathfrak{M}$ in $L^+(\mathscr{D})$ with respect to the strong* topology $\mathfrak{M}''_{\sigma c}=\overline{\mathfrak{M}}^{s^*}\cap L^+(\mathscr{D})$.

Proposition 11: Let $\mathfrak{A}$ be a *-invariant subset of $C(\mathscr{D},\mathscr{H})$. Assume that there exists a * algebra $\mathfrak{M}$ with identity, in the bounded part $\mathfrak{A}_b$ of $\mathfrak{A}$ such that $\mathfrak{M}'_\sigma=\mathfrak{A}'_\sigma$. Then $\mathfrak{A}''_{\sigma\sigma}=\overline{\mathfrak{A}}^{s^*}$.

Proof: That $\mathfrak{M}'_\sigma=\mathfrak{A}'_\sigma$, implies $\mathfrak{A}''_{\sigma\sigma}=\mathfrak{M}''_{\sigma\sigma}=\overline{\mathfrak{M}}^{s^*}$ by Proposition 9 and $\overline{\mathfrak{M}}^{s^*}\subseteq\overline{\mathfrak{A}}^{s^*}$. On the other hand, $\mathfrak{A}''_{\sigma\sigma}$ is strongly* closed so that $\overline{\mathfrak{A}}^{s^*}\subseteq\mathfrak{A}''_{\sigma\sigma}$. □

Corollary 12: If there exists a * algebra $\mathfrak{M}\subseteq\mathfrak{A}_b$, containing 1 and dense in $\mathfrak{A}$ for the strong* topology, then $\mathfrak{A}''_{\sigma\sigma}=\overline{\mathfrak{A}}^{s^*}$.

Proof: By Proposition 7 we have $\mathfrak{M}'_\sigma=\mathfrak{A}'_\sigma$. □

Corollary 13: If $\mathfrak{A}\subseteq L^+(\mathscr{D})$ is such that there exists a * algebra $\mathfrak{M}\subseteq\mathfrak{A}_b$, with identity, which is dense in $\mathfrak{A}$ for the strong* topology, then $\mathfrak{A}''_{\sigma c}=\overline{\mathfrak{A}}^{s^*}\cap L^+(\mathscr{D})$. □

Let us consider in particular the case of symmetric op* algebras. They indeed fit in the situation of Proposition 11 with $\mathfrak{M}=\mathfrak{A}_b$.

Proposition 14: Let $\mathfrak{A}$ be a symmetric op* algebra. Then

$\mathfrak{A}''_{\sigma\sigma} = \overline{\mathfrak{A}}^{s^*}$ and $\mathfrak{A}''_{\sigma c} = \overline{\mathfrak{A}}^{s^*} \cap L^+(\mathscr{D})$.

Proof: We show that $(\mathfrak{A}_b)'_\sigma = \mathfrak{A}'_\sigma$. Let $A = A^* \in \mathfrak{A}$; we know that $(1+A^2)^{-1}$ and $A(1+A^2)^{-1}$ belong to $\mathfrak{A}_b$. Consider $C \in (\mathfrak{A}_b)'_\sigma$. We have $(A(1+A^2)^{-1}f, Cg) = (C^*f, A(1+A^2)^{-1}g) = (C^*f, (1+A^2)^{-1}Ag) = ((1+A^2)^{-1}f, CAg)$ [because C commutes weakly with $(1+A^2)^{-1}$]. Because $\mathfrak{A}$ is symmetric we have $(1+A^2)^{-1}\mathscr{D} = \mathscr{D}$ so that the first and the last term of the equality show that $C \in \mathfrak{A}'_\sigma$ (see Ref. 13). □

Remark: A similar proof in Ref. 6 shows that $\mathfrak{A}'_w = (\mathfrak{A}_b)'_w$ so that finally for symmetric algebras each commutant is equal to the analogous commutant of the bounded part.

To end this paragraph concerning the strong* topology let us say a few words about strongly* continuous linear functionals.

Proposition 15: Every s^*-continuous (let s^* stand for strong*) linear functional ω on $\mathfrak{A} \subseteq C(\mathscr{D}, \mathscr{H})$ is a limit of weakly continuous linear functionals.

Proof: As in the proof of Proposition 9 we consider the extension

$$\hat{\mathfrak{A}} = \left\{ \hat{A} = \begin{pmatrix} A & 0 \\ 0 & A^* \end{pmatrix} \middle| A \in \mathfrak{A} \right\},$$

which becomes a *-invariant subset of $C(\mathscr{D} \oplus \overline{\mathscr{D}}, \mathscr{H} \oplus \overline{\mathscr{H}})$ with the mixed product when the product of two elements is defined.

For a fixed $f \in \mathscr{D}$ consider the following subspace of $\mathscr{H} \oplus \overline{\mathscr{H}}$:

$$\mathscr{K}_f = \overline{\left\{ \begin{pmatrix} A & 0 \\ 0 & A^* \end{pmatrix} \begin{pmatrix} f \\ f \end{pmatrix} \middle| \forall A \in \mathfrak{A} \right\}}.$$

Now for every $g = (g_1, g_2) \in \mathscr{D} \oplus \overline{\mathscr{D}}$, define a linear functional $\tilde{\omega}_g$ on $\mathscr{K}_f$ by

$$\tilde{\omega}_g \begin{pmatrix} Af \\ A^* f \end{pmatrix} = (g_1, Af) + (A^* f, g_2).$$

This functional is weakly and strongly continuous on $\mathscr{K}_f$. Putting

$$\omega_{g,f}(A) \equiv \tilde{\omega}_g \begin{pmatrix} Af \\ A^* f \end{pmatrix},$$

we define a linear functional on $\mathfrak{A}$, and moreover

$$|\omega_{g,f}(A)| \leqslant \kappa(\|Af\| + \|A^* f\|).$$

Hence this functional is s^* continuous.

Conversely, let ω be an s^*-continuous functional on $\mathfrak{A}$. There exists $f \in \mathscr{D}$ such that $|\omega(A)| \leqslant \kappa(\|Af\| + \|A^* f\|)$. Putting

$$\tilde{\omega} \begin{pmatrix} Af \\ A^* f \end{pmatrix} \equiv \omega(A),$$

we define in this way a linear functional on $\mathscr{K}_f$, which is strongly continuous. Then, by Riesz's theorem there exists a vector $h \in \mathscr{K}_f$, $h = (h_1, h_2)$, such that

$$\omega(A) = \tilde{\omega} \begin{pmatrix} Af \\ A^* f \end{pmatrix} = (h_1, Af) + (A^* f, h_2).$$

But $h \in \mathscr{K}_f$ means that there exists a Cauchy net A^α in $\mathfrak{A}$ such that $h_1 = \lim_\alpha A^\alpha f$ and $h_2 = \lim_\alpha A^{\alpha *} f$ so that, finally,

$$\omega(A) = \lim_\alpha (A^\alpha f, Af) + \lim_\alpha (A^* f, A^\alpha f). \qquad \square$$

B. A natural topology for the weak unbounded bicommutant

As we pointed out in the remark following Corollary 2, the s^* topology is not the only one for which a weak commutant or bicommutant is closed. Indeed, they are also closed for the topology defined by the seminorms $A \in C(\mathscr{D}, \mathscr{H}) \to (k, Af)$ and $A \in C(\mathscr{D}, \mathscr{H}) \to (k, A^* f)$ when f runs in $\mathscr{D}$ and k in $\mathscr{H}$.

Given a *-invariant subset $\mathfrak{A}$ of $C(\mathscr{D}, \mathscr{H})$ we can particularize the seminorms above by taking k of the form Xg, where $g \in \mathscr{D}$ and $X \in \mathfrak{A}'_\sigma$. We get in this way a topology on $C(\mathscr{D}, \mathscr{H})$ depending on $\mathfrak{A}'_\sigma$ and given explicitly by the seminorms

$$\begin{cases} p_{X,g}(A) = |(Xf, Ag)|, \\ q_{X,g}(A) = |(Xf, A^+ g)|, \end{cases}$$

for any $f, g \in \mathscr{D}$ and $X \in \mathfrak{A}'_\sigma$. Let us call this topology "c," the "commutant topology." This topology is weaker than the s^* topology and finer than the weak topology but not comparable to the strong one.

Proposition 16: Let $\mathfrak{A}$ be a *-invariant subset of $C(\mathscr{D}, \mathscr{H})$. Then $\mathfrak{A}''_{\sigma\sigma}$ is closed with respect to the commutant topology. That is, $\mathfrak{A}''_{\sigma\sigma} \supseteq \overline{\mathfrak{A}}^c \supseteq \overline{\mathfrak{A}}^{s^*}$.

Proof: It is obvious by the definition of $\mathfrak{A}''_{\sigma\sigma}$, the latter being an intersection of kernels of linear functionals continuous with respect to c

$$\omega_{X,f,g}(A) = (X^* f, Ag) - (A^* f, Xg),$$

with $f, g \in \mathscr{D}$ and $X \in \mathfrak{A}'_\sigma$. □

Proposition 17: Let $\mathfrak{A}$ be a *-invariant subset of $C(\mathscr{D}, \mathscr{H})$. Then we have

$$\overline{\mathfrak{A}}^s \cap \mathfrak{A}''_{\sigma\sigma} \subseteq \overline{\mathfrak{A}}^c.$$

Proof: Let $Y \in \overline{\mathfrak{A}}^s$. There exists $\{A^\alpha\} \subseteq \mathfrak{A}$ such that $Yf = \text{s-lim}\, A^\alpha f$ for every $f \in \mathscr{D}$, and moreover $\forall g \in \mathscr{D}$ and $X \in \mathfrak{A}'_\sigma$, we have

$$|(X^+ g, (Y - A^\alpha) f)| = p_{X^+ g, f}(Y - A^\alpha) \to 0.$$

On the other hand, if $Y \in \mathfrak{A}''_{\sigma\sigma}$ we have

$$\begin{aligned} q_{Xf,g}(Y - A^\alpha) &= |(Xf, (Y^* - A^{\alpha *}) g)| \\ &= |((Y - A^\alpha) f, X^+ g)| \to 0. \end{aligned}$$

We may conclude that $Y \in \overline{\mathfrak{A}}^c$. □

Corollary 18: If a *-invariant subset $\mathfrak{A}$ of $C(\mathscr{D}, \mathscr{H})$ is such that $\mathfrak{A}''_{\sigma\sigma} \subset \overline{\mathfrak{A}}^s$, then $\mathfrak{A}''_{\sigma\sigma} = \overline{\mathfrak{A}}^c$. □

Corollary 19: If $\mathfrak{A} \subseteq C(\mathscr{D}, \mathscr{H})$ satisfies one of the following conditions, then $\mathfrak{A}''_{\sigma\sigma} = \overline{\mathfrak{A}}^{s^*} = \overline{\mathfrak{A}}^c$.

(i) $\mathfrak{A}$ is an op* algebra of bounded operators.

(ii) $\mathfrak{A}$ contains an op* algebra $\mathfrak{M}$ of bounded operators such that $\mathfrak{M}'_\sigma = \mathfrak{A}'_\sigma$.

(iii) $\mathfrak{A}$ contains an op* algebra $\mathfrak{M}$ of bounded operators dense in $\mathfrak{A}$ for the s^* topology or for the commutant topology coming from $\mathfrak{M}'_\sigma$.

(iv) $\mathfrak{A}$ is a symmetric op* algebra.

C. Bicommutants and weak topology

Following Ref. 14, we call a subspace $\mathscr{K}$ of $\mathscr{H}''$ orthocomplemented with respect to $\mathscr{D}''$ iff we have the following.

(i) $\mathscr{K}$ is a closed subspace of $\mathscr{H}$ [i.e., corresponds to a bounded projection $P = P^* = P^2 \in B(\mathscr{H})$].

(ii) $P \in L^+(\mathscr{D})$ [which implies that $\mathscr{K} \cap \mathscr{D}$ is a $\sigma(\mathscr{D}, \mathscr{D})$-closed subspace of $\mathscr{D}$].

(iii) $\mathscr{K} \cap \mathscr{D}$ is norm dense in $\mathscr{K}$.

Proposition 20: Let $\mathfrak{A}$ be an op* algebra and assume that for every $f \in \mathscr{D}$ the closure $\overline{\mathfrak{A}f}^{\sigma}$ of $\mathfrak{A}f$ in the topology $\sigma(\mathscr{D}, \mathscr{D})$ is the intersection with $\mathscr{D}$ of a subspace $\mathscr{K}$ of $\mathscr{H}$, orthocomplemented with respect to $\mathscr{D}$. Then

$$\mathfrak{A}''_{cc} = \overline{\mathfrak{A}}^{w} \cap L^+(\mathscr{D}) \quad \text{and} \quad \mathfrak{A}''_{c\sigma} = \overline{\mathfrak{A}}^{w}.$$

Proof: Let P be the projection operator of $\overline{\mathfrak{A}f}^{\sigma}$. Since every $A \in \mathfrak{A}$ is $\sigma(\mathscr{D}, \mathscr{D})$ continuous, it leaves the subspace $\overline{\mathfrak{A}f}^{\sigma}$ invariant and thus $P \in \mathfrak{A}'_w$. By assumption $P \in L^+(\mathscr{D})$ so that finally P belongs to the four commutants $\mathfrak{A}'_s, \mathfrak{A}'_w, \mathfrak{A}'_c, \mathfrak{A}'_\sigma$. Now take $Y \in \mathfrak{A}''_{cc}$: $Yf = YPf = PYf$ and thus $Yf \in \overline{\mathfrak{A}f}^{\sigma}$, which implies that $Y \in \overline{\mathfrak{A}}^{w}$. Since $\mathfrak{A}''_{cc}$ lies in $L^+(\mathscr{D})$ we have $\mathfrak{A}''_{cc} \subseteq \overline{\mathfrak{A}}^{w} \cap L^+(\mathscr{D})$ and since we know (Corollary 5) that $\mathfrak{A}''_{cc}$ is weakly closed in $L^+(\mathscr{D})$ we have the equality.

Similarly, take $Y \in \mathfrak{A}''_{c\sigma}$. By the same calculation as in the proof of Proposition 9 we have $Yf = PYf \in \mathscr{K}$ and since by assumption $\overline{\mathfrak{A}f}^{\sigma}$ is norm dense in $\mathscr{K}$ it follows that Yf is a weak limit of elements of $\mathfrak{A}f$ and $\mathfrak{A}''_{c\sigma} \subseteq \overline{\mathfrak{A}}^{w}$. The equality follows from Corollary 2. □

We now have independent criteria in order that $\mathfrak{A}''_{\sigma\sigma} = \overline{\mathfrak{A}}^{s^*}$ and $\mathfrak{A}''_{cc} = \overline{\mathfrak{A}}^{w} \cap L^+(\mathscr{D})$. We shall now examine some situations where the two results hold at the same time.

Proposition 21: Let $\mathfrak{A}$ be an op* algebra. Assume that for every $f \in \mathscr{D}$, the projection P on the norm-closed subspace $\overline{\mathfrak{A}f}$ of $\mathscr{H}$ belongs to $L^+(\mathscr{D})$. Then

$$\mathfrak{A}''_{\sigma\sigma} = \mathfrak{A}''_{c\sigma} = \overline{\mathfrak{A}}^{s^*} = \overline{\mathfrak{A}}^{s} = \overline{\mathfrak{A}}^{w} = \overline{\mathfrak{A}}^{c}$$

and

$$\mathfrak{A}''_{\sigma c} = \mathfrak{A}''_{cc} = \overline{\mathfrak{A}}^{s^*} \cap L^+(\mathscr{D}) = \overline{\mathfrak{A}}^{s} \cap L^+(\mathscr{D}) = \overline{\mathfrak{A}}^{w} \cap L^+(\mathscr{D}) = \overline{\mathfrak{A}}^{c} \cap L^+(\mathscr{D}).$$

Proof: The assumption of this proposition is stronger than the hypothesis of Proposition 20. Indeed $\overline{\mathfrak{A}f} \cap \mathscr{D}$ is now $\sigma(\mathscr{D}, \mathscr{D})$ closed and coincides with $\overline{\mathfrak{A}f}^{\sigma}$. So the results of Proposition 20 hold and P belongs to $\mathfrak{A}'_s, \mathfrak{A}'_w, \mathfrak{A}'_c$, and $\mathfrak{A}'_\sigma$.

Now consider $Y \in \mathfrak{A}''_{\sigma\sigma}$ or $Y \in \mathfrak{A}''_{c\sigma}$. The same calculation then in the proof of Proposition 9 shows that $Yf \in \overline{\mathfrak{A}f}$ and $Y^*f \in \overline{\mathfrak{A}f}$. Hence $Y \in \overline{\mathfrak{A}}^{s^*}$. We thus have $\mathfrak{A}''_{\sigma\sigma} \subseteq \mathfrak{A}''_{c\sigma} \subseteq \overline{\mathfrak{A}}^{s^*} \subseteq \overline{\mathfrak{A}}^{s} \subseteq \overline{\mathfrak{A}}^{w}$, and since $\mathfrak{A}''_{\sigma\sigma}$ and $\mathfrak{A}''_{c\sigma}$ are strongly* closed we also have $\overline{\mathfrak{A}}^{s^*} \subseteq \mathfrak{A}''_{\sigma\sigma} \subseteq \mathfrak{A}''_{c\sigma}$ and $\mathfrak{A}''_{c\sigma} = \overline{\mathfrak{A}}^{w}$ by Proposition 20. Finally they are all equal.

Intersecting all members of this equality with $L^+(\mathscr{D})$ we get immediately the second line of the thesis. □

The conclusion of this proposition is that under those hypotheses there are only two bicommutants to consider. One is the closure of $\mathfrak{A}$ in $C(\mathscr{D}, \mathscr{H})$ for any of the four topologies we have introduced, and the other one is the closure of $\mathfrak{A}$ in $L^+(\mathscr{D})$ with respect to those four topologies.

Remark: In this proposition it is sufficient to ask that there exists a * subalgebra $\mathfrak{A}_0$ dense in $\mathfrak{A}$ for the strong* topology such that for every $f \in \mathscr{D}$ the projection on $\mathfrak{A}_0 f$ belongs to $L^+(\mathscr{D})$. The results of Proposition 21 then hold for $\mathfrak{A}$ because $\mathfrak{A}$ and $\mathfrak{A}_0$ have the same commutants and bicommutants. The result still remains true if we ask $\mathfrak{A}_0$ to be only weakly dense in $\mathfrak{A}$, although in this case only strong commutants are equal.

Proposition 22: Let $\mathfrak{A}$ be an op* algebra and $\mathfrak{A}_0$ a weakly dense sub*-algebra of it. If for every $f \in \mathscr{D}$ the subspaces $\overline{\mathfrak{A}_0 f}$ are orthocomplemented with respect to $\mathscr{D}$, then

$$\mathfrak{A}''_{\sigma\sigma} = \mathfrak{A}''_{c\sigma} = \overline{\mathfrak{A}}^{s^*} = \overline{\mathfrak{A}}^{s} = \overline{\mathfrak{A}}^{w} = \overline{\mathfrak{A}}^{c}$$

and

$$\mathfrak{A}''_{\sigma c} = \mathfrak{A}''_{cc} = \overline{\mathfrak{A}}^{s^*} \cap L^+(\mathscr{D}) = \overline{\mathfrak{A}}^{s} \cap L^+(\mathscr{D}) = \overline{\mathfrak{A}}^{w} \cap L^+(\mathscr{D}) = \overline{\mathfrak{A}}^{c} \cap L^+(\mathscr{D}).$$

Proof: The $\mathfrak{A}_0$ weakly dense in $\mathfrak{A}$ implies $\mathfrak{A}'_c = (\mathfrak{A}_0)'_c$. Hence $\mathfrak{A}''_{c\sigma} = (\mathfrak{A}_0)''_{c\sigma}$. Since $\mathfrak{A}_0$ satisfies the assumption of Proposition 21 we have $(\mathfrak{A}_0)''_{\sigma\sigma} = (\mathfrak{A}_0)''_{c\sigma}$ and so $\mathfrak{A}''_{c\sigma} = (\mathfrak{A}_0)''_{c\sigma} = (\mathfrak{A}_0)''_{\sigma\sigma} \subseteq \mathfrak{A}''_{\sigma\sigma} \subseteq \mathfrak{A}''_{c\sigma}$. Thus $\mathfrak{A}''_{\sigma\sigma} = (\mathfrak{A}_0)''_{\sigma\sigma}$.

Although weak commutants of $\mathfrak{A}_0$ and $\mathfrak{A}$ might be different, the bicommutants will be equal and the result then follows easily. □

This last proposition could be applied, for instance, to symmetric op* algebras because in this case the bounded part $\mathfrak{A}_b$ is weakly dense in $\mathfrak{A}$. It then suffices to ask that the subspaces $\overline{\mathfrak{A}_b f}$ be orthocomplemented.

Let us now describe some situations where the assumptions of Proposition 21 are satisfied.

Proposition 23: Let $\mathfrak{A}$ be an op* algebra such that $(\mathfrak{A}_b)'_s = (\mathfrak{A}_b)'_w$. Then for every $f \in \mathscr{D}$, the projection operator on $\overline{\mathfrak{A}f}$ belongs to $L^+(\mathscr{D})$.

Proof: Let P be the projection operator on the norm-closed subspace $\overline{\mathfrak{A}f}$. Every $A \in \mathfrak{A}_b$ leaves this subspace invariant so that $P \in (\mathfrak{A}_b)'_w$. Since by assumption $(\mathfrak{A}_b)'_w = (\mathfrak{A}_b)'_s$ and by definition $(\mathfrak{A}_b)'_s = (\mathfrak{A}_b)'_w \cap L^+(\mathscr{D})$, it follows that $P \in L^+(\mathscr{D})$. □

In the particular case of a symmetric op* algebra, we have[6] that $(\mathfrak{A}_b)'_w = \mathfrak{A}'_w$ and thus also $(\mathfrak{A}_b)'_s = \mathfrak{A}'_s$. The hypothesis of Proposition 23 thus becomes $\mathfrak{A}'_s = \mathfrak{A}'_w$ so that we have the next proposition.

Proposition 24: Let $\mathfrak{A}$ be a symmetric op* algebra such that $\mathfrak{A}'_s = \mathfrak{A}'_w$. Then for every $f \in \mathscr{D}$, the projection operator on $\overline{\mathfrak{A}f}$ belongs to $L^+(\mathscr{D})$. Hence

$$\mathfrak{A}''_{\sigma\sigma} = \mathfrak{A}''_{c\sigma} = \overline{\mathfrak{A}}^{s^*} = \overline{\mathfrak{A}}^{s} = \overline{\mathfrak{A}}^{w} = \overline{\mathfrak{A}}^{c}$$

and

$$\mathfrak{A}''_{\sigma c} = \mathfrak{A}''_{cc} = \overline{\mathfrak{A}}^{s^*} \cap L^+(\mathscr{D}) = \overline{\mathfrak{A}}^{s} \cap L^+(D) = \overline{\mathfrak{A}}^{w} \cap L^+(\mathscr{D}) = \overline{\mathfrak{A}}^{c} \cap L^+(\mathscr{D}).$$ □

This proposition applies to closed symmetric op* algebras because they are self-adjoint and hence satisfy $\mathfrak{A}'_s = \mathfrak{A}'_w$.

To end this section let us see what can be said about self-adjoint algebras in general. Some of them satisfy the hypothesis of Proposition 21: they are the closed symmetric ones as we have just seen and also the Abelian algebra generated by one single self-adjoint operator $T = T^+$ on its domain $D^\infty(T)$ (see Ref. 4). For other self-adjoint algebras we do not know in general if the projections on $\overline{\mathfrak{A}f}$ are in $L^+(\mathscr{D})$ and we have to check it in every particular case. Nevertheless,

because for self-adjoint algebras we have $\mathfrak{A}'_\sigma = \mathfrak{A}'_c$, they also have only two different unbounded bicommutants.

Proposition 25: Let $\mathfrak{A}$ be a self-adjoint op* algebra. Then

(i) $\mathfrak{A}''_{\sigma\sigma} = \mathfrak{A}''_{c\sigma}$ is weakly closed in $C(\mathscr{D}, \mathscr{H})$;

(ii) $\mathfrak{A}''_{\sigma c} = \mathfrak{A}''_{cc}$ is weakly closed in $L^+(\mathscr{D})$.

Proof: This is the immediate consequence of Corollaries 2 and 5.

Remark: We do not know, in that case, if the bicommutants are the closure of $\mathfrak{A}$ for the weak topology unless we are in the two cases mentioned above.

V. REGULAR op* ALGEBRAS AND V^* ALGEBRAS

In this last section we shall consider special classes of op* algebras which have been introduced in Ref. 4. The aim of introducing such classes was to find algebras of unbounded operators with properties similar to those of von Neumann algebras. This has motivated the introduction in Ref. 4 of regular op* algebras, V^* algebras, and SV^* algebras (to which some theorems of von Neumann algebras may be extended). It thus seems interesting to see what are the topological properties of the bicommutants of such algebras.

We first recall some definitions of Ref. 4.

An op* algebra is called *regular* iff $\mathfrak{A}''_{\sigma\sigma}$ maps $\mathscr{D}$ into itself.

A V^* *algebra* is an op* algebra which is equal to its weak unbounded bicommutant $\mathfrak{A} = \mathfrak{A}''_{\sigma\sigma}$.

If, moreover, $\mathfrak{A}$ is weakly closed then it is called $\overline{V}^*$ algebra.

An SV^* *algebra* is an op* algebra which is equal to a larger bicommutant (that we have not considered here so far) $\mathfrak{A} = \mathfrak{A}''_{w\sigma}$, and if it weakly closed then it is an $S\overline{V}^*$ algebra.

Obviously this third class is contained in the second one, which is contained in the first.

From the definition of a regular op* algebra, it follows immediately that they have only three unbounded bicommutants with the following relations: $\mathfrak{A}''_{\sigma\sigma} = \mathfrak{A}''_{\sigma c} \subseteq \mathfrak{A}''_{cc} \subseteq \mathfrak{A}''_{c\sigma}$.

An interesting situation occurs if a regular op* algebra satisfies the assumptions of one of Propositions 21–24, or if $\mathfrak{A}$ is self adjoint. Indeed, in that case the four bicommutants will coincide and we have the following proposition.

Proposition 26: Let $\mathfrak{A}$ be a regular op* algebra, either self-adjoint or such that $\forall f \in \mathscr{D}$ the projection operator P on $\overline{\mathfrak{A}f}$ belongs to $L^+(\mathscr{D})$. Then

$$\mathfrak{A}''_{\sigma c} = \mathfrak{A}''_{cc} = \mathfrak{A}''_{\sigma\sigma} = \mathfrak{A}''_{c\sigma}$$
$$= \overline{\mathfrak{A}}^{s^*} = \overline{\mathfrak{A}}^{s} = \overline{\mathfrak{A}}^{w} = \overline{\mathfrak{A}}^{c} \subseteq L^+(\mathscr{D}). \quad \square$$

Proposition 27: Let $\mathfrak{A}$ be a V^* algebra or an SV^* algebra. Then $\mathfrak{A} = \overline{\mathfrak{A}}^{s^*} = \overline{\mathfrak{A}}^{c}$.

That is, a V^* algebra is closed with respect to the strong* topology and with respect to the commutant topology.)

Proof: This follows from the fact that $\mathfrak{A} = \mathfrak{A}''_{\sigma\sigma}$, and from Corollaries 2 and 18. $\square$

Of course, if a V^* algebra is self adjoint we are in the situation of Proposition 26.

Proposition 28: Let $\mathfrak{A}$ be a self-adjoint V^* algebra. Then $\mathfrak{A}$ is equal to its four unbounded bicommutants and $\mathfrak{A}$ is weakly closed and closed with respect to the commutant topology. $\square$

Corollary 29: (i) A self-adjoint V^* algebra is a $\overline{V}^*$ algebra; (ii) A self-adjoint SV^* algebra is a $S\overline{V}^*$ algebra. $\square$

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Nontrivial zeros of the Racah quadrupole invariant

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It is shown that a class of nontrivial zeros of the Racah quadrupole invariant operator is given by two orbits of the group action of an infinite discrete subgroup of the proper two-dimensional Lorentz group SO(1,1) on the hyperbola $4x^2 - 3y^2 = \frac{11}{4}$.

I. INTRODUCTION

It has been known since Racah's[1] classical series of papers on spectroscopy that certain 6*j* symbols (Racah coefficients) may be zero even when all the triangle conditions for a tetrahedron are fulfilled (nontrivial zero). (A similar result is true for the 3*jm* symbols [Wigner–Clebsch–Gordan coefficients for SU(2)].) Judd[2] extended Racah's result, using a similar Lie algebraic treatment, while Koozekanani and Biedenharn[3] listed over a thousand nontrivial zeros of the Racah coefficient obtained from computer calculation (see also Bowick[4]). These results are presented and discussed in Vol. 9 of Ref. 5. More recently, Vanden Berghe *et al.*[6] have given further examples of nontrivial zeros of 6*j* symbols originating from Lie algebras.

The possibility for "explaining" zeros of the 6*j* symbol in consequence of Lie algebraic structures may be understood in the following way: Let l denote a Lie algebra that contains the Lie algebra su_2 as a subalgebra; that is, $l \supset su_2$. Then there always exists a basis of l such that each basis element is a unit irreducible tensor operator with respect to the subalgebra su_2. The structure constants in this basis are related to 6*j* symbols. Thus, the vanishing of a 6*j* symbol may imply the existence of a Lie subalgebra a with $a \subset l$ and $a \supset su_2$. Conversely, the existence of a Lie subalgebra a such that $l \supset a \supset su_2$ may imply the existence of a zero of a 6*j* symbol.

The zeros discovered by Racah, Judd, and Vanden Berghe *et al.* are all associated with Lie algebras as described above.

A different approach to the classification of the zeros of 3*jm* and 6*j* symbols has been used in Ref. 7. In this approach, it is observed that the explicit expression for each of these coefficients is an *alternating sum*. By restricting the domain of the angular momenta, it is possible to limit the number of terms in this sum to one term ("stretched" angular momentum), two terms, three terms,... . Thus, in the case of two or more terms, there is the possibility of obtaining zeros by equating the resulting two or more terms to zero. While there is no *a priori* reason for the zeros of such expressions to correspond to nontrivial zeros, it is a fact (see Ref. 7) that one obtains already a denumerably infinite family of nontrivial zeros for both the 3*jm* and 6*j* coefficients in the simplest two-term case. We henceforth use the term "zero of a 6*j* coefficient" (resp. of a 3*jm* coefficient) to mean a nontrivial zero in the sense that the entries in the symbol for the coefficient satisfy all domain constraints (triangle and projection quantum number rules).

The procedure described in the preceding paragraph is entirely equivalent to finding the zeros of the *polynomial part* of a Racah coefficient [resp. 3*jm* coefficient], when written in canonical pattern calculus form as given explicitly by Eqs. (4.98) and (A.18) of Appendix A, Chap. 4 in Ref. 5, Vol. 9 [resp. Eqs. (3.32) and (3.39)]. Accordingly, the Brudno classification scheme is by weights of the corresponding Racah (resp. Wigner) operator.

The purpose of the present paper is to present the zeros of a special class of 6*j* symbols corresponding to three-term cancellations in the sense described above, but which are restricted to the quadrupole invariant operator

$$\begin{Bmatrix} & 2 & \\ 4 & & 0 \\ & 2 & \end{Bmatrix}, \tag{1a}$$

which is defined by the following action on the so-called coupled basis vectors of the tensor product space $\mathscr{H}_{j_1} \otimes \mathscr{H}_{j_2}$, where $\mathscr{H}_{j_i}$ denotes any inner product vector space of dimension $2j_i + 1$ $(i = 1,2)$ that carries the irreducible representation D^{j_i} of SU(2):

$$\begin{Bmatrix} & 2 & \\ 4 & & 0 \\ & 2 & \end{Bmatrix} |(j_1 j_2) j m\rangle = [(2j_1+1)(2j_2+1)]^{1/2} \times W(j, j_1, j_2, 2; j_2, j_1) |(j_1 j_2) j m\rangle . \tag{1b}$$

Moreover, we restrict the present discussion to basis vectors in $\mathscr{H}_{j_1} \otimes \mathscr{H}_{j_2}$ having $j = j_2$. In standard 6*j*-symbol notation, the present paper is concerned with the zeros of 6*j* coefficients of the form

$$\begin{Bmatrix} j_2 & j_1 & j_2 \\ 2 & j_2 & j_1 \end{Bmatrix} = (-1)^{j_1 + 2j_2} W(j_2, j_1, j_2, 2; j_2, j_1) = 0 . \tag{2}$$

[See Eq. (4.35) in Ref. 5, Vol. 9.] While we could have started with Eq. (2) and developed the results given in the present paper, it is significant for future work on this subject to point out that each zero of the 6*j* coefficient (2) determines a corresponding vector $|(j_1 j_2) j_2 m\rangle$ in the null space of the Racah invariant operator given by Eq. (1a). [This is a general result for all zeros of 6*j* coefficients—see Eq. (4.35), Ref. 5, Vol. 9.] The domains of definition of j_1 and j_2 in the 6*j* coefficient in the left-hand side of Eq. (2) are, respectively,

$$2j_2 = \text{positive integer}, \quad j_1 \in \{1,2,\ldots,2j_2\} . \tag{3}$$

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While the determination of the zeros of the $6j$ symbol given by Eq. (2) is a highly specialized case, we believe the results are sufficiently interesting and important to justify this presentation. Let us turn now to the explicit formulation of the problem, developing first the necessary notations and concepts for stating its solution.

II. DETERMINATION OF ZEROS

Using the explicit expression for the Racah coefficient in Eq. (2), one easily finds that the necessary and sufficient condition for a zero is that the equation

$$3x^2 - 4y^2 = \tfrac{11}{4} \tag{4a}$$

be satisfied, where we have defined

$$x = j_1 + \tfrac{1}{2}, \quad y = j_2 + \tfrac{1}{2}. \tag{4b}$$

Accordingly, the domains of x and y for which we seek solutions of Eq. (4a) are, respectively,

$$2y = \text{positive integer} \geqslant 2, \quad x \in \{\tfrac{3}{2}, \tfrac{5}{2}, \ldots, 2y - \tfrac{1}{2}\}. \tag{4c}$$

Let us first consider the graph of relation (4a) for all $(x, y) \in \mathbf{R}^2$. For this it is useful to define the hyperbolic sets $\mathbf{H}_+ \subset \mathbf{R}^2$ and $\mathbf{H}_- \subset \mathbf{R}^2$ by

$$\mathbf{H}_+ = \{(x, y) \in \mathbf{R}^2 | 3x^2 - 4y^2 = \tfrac{11}{4}, x > 0\}, \tag{5a}$$

$$\mathbf{H}_- = \{(x, y) \in \mathbf{R}^2 | 3x^2 - 4y^2 = \tfrac{11}{4}, x < 0\}. \tag{5b}$$

Thus, the graph of relation (4a) is the set of points $\mathbf{H}_+ \cup \mathbf{H}_-$. Since the points in $\mathbf{H}_-$ are obtained from those in $\mathbf{H}_+$ by reflection through the y axis, it is sufficient for the present treatment to consider the hyperbolic set $\mathbf{H}_+$ alone.

We next introduce the matrix group G with elements defined by

$$G = \{g(\theta) | -\infty < \theta < \infty\}, \tag{6a}$$

where $g(\theta)$ is the 2×2 matrix given by

$$g(\theta) = \begin{pmatrix} \cosh\theta & (2\sqrt{3}/3)\sinh\theta \\ (\sqrt{3}/2)\sinh\theta & \cosh\theta \end{pmatrix} = A h(\theta) A^{-1}, \tag{6b}$$

where A is the fixed numerical matrix defined by

$$A = \begin{pmatrix} \frac{5}{2} & 4\sqrt{3}/3 \\ 2 & 5\sqrt{3}/4 \end{pmatrix} \tag{6c}$$

and $h(\theta)$ is the hyperbolic "rotation" matrix

$$h(\theta) = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix}. \tag{6d}$$

Thus, the group G is isomorphic to the Lorentz group $SO(1,1)/Z$ where Z denotes the two-element invariant subgroup $\{I, -I\}$. (The matrix A transforms the hyperbola $\mathbf{H} = \mathbf{H}_+ \cup \mathbf{H}_-$ to standard form $u^2 - v^2 = 1$.)

We now define the action of the matrix group G on the set $\mathbf{H}_+$ in the standard way: For each $g(\theta) \in G$, the map $g(\theta)$: $H_+ \to H_+$ is given by

$$g(\theta): (x, y) \mapsto (x(\theta), y(\theta)), \tag{7a}$$

where the image point $(x(\theta), y(\theta))$ of point (x, y) is obtained by matrix multiplication as

$$\begin{pmatrix} x(\theta) \\ y(\theta) \end{pmatrix} = g(\theta) \begin{pmatrix} x \\ y \end{pmatrix}. \tag{7b}$$

Finally, we introduce the infinite order discrete subgroup $G_\alpha \subset G$ defined by

$$G_\alpha = \{g_n = (g(\alpha))^n = g(n\alpha) | n = 0, \pm 1, \pm 2, \ldots\}, \tag{8a}$$

where α is the fixed numerical value of θ given by

$$\cosh\alpha = 7, \quad \sinh\alpha = 4\sqrt{3}. \tag{8b}$$

The matrix g_1 is given explicitly by

$$g_1 = \begin{pmatrix} 7 & 8 \\ 6 & 7 \end{pmatrix} \tag{9a}$$

with inverse

$$g_{-1} = (g_1)^{-1} = g(-\alpha) = \begin{pmatrix} 7 & -8 \\ -6 & 7 \end{pmatrix}. \tag{9b}$$

Using the preceding definitions and notations, we can now state our main mathematical result.

Theorem 1: The set of all points $\mathbf{K}_+$ in $\mathbf{H}_+$, such that the x coordinate is half an odd positive integer, is given by

$$\mathbf{K}_+ = \mathbf{K}_1 \cup \mathbf{K}_2, \tag{10a}$$

where the sets $\mathbf{K}_1$ and $\mathbf{K}_2$ are defined by

$$\mathbf{K}_1 = \left\{(x_n, y_n) \middle| \begin{pmatrix} x_n \\ y_n \end{pmatrix} = g_n \begin{pmatrix} \frac{3}{2} \\ 1 \end{pmatrix}, \quad n = 0, \pm 1, \pm 2, \ldots\right\}, \tag{10b}$$

$$\mathbf{K}_2 = \left\{(x'_n, y'_n) \middle| \begin{pmatrix} x'_n \\ y'_n \end{pmatrix} = g_n \begin{pmatrix} \frac{5}{2} \\ 2 \end{pmatrix}, \quad n = 0, \pm 1, \pm 2, \ldots\right\}. \tag{10c}$$

Proof: We first note that for each $(x, y) \in \mathbf{H}_+$ the coordinate x is half an odd integer (necessarily positive) if and only if $2y$ is an integer (including negative integers).

It is easily verified that either of the matrices g_1 or g_1^{-1} maps each point in $\mathbf{H}_+$ having an x coordinate of the form $(2k + 1)/2$ with k a positive integer and a y coordinate of the form $2y$ = integer into a new point in $\mathbf{H}_+$ of this same form. Thus, each point in $\mathbf{K}_+$ has an x coordinate that is half an odd positive integer.

Let us next prove the converse, namely, that each point in $\mathbf{H}_+$, with an x coordinate that is half an odd integer (necessarily positive), is contained in $\mathbf{K}_+$. We begin by noting that each point $(x, y) \in \mathbf{H}_+$ satisfies $6x > 6y - 1$ and $6x \leqslant 8y + 1$ for all $y \geqslant 1$; $6x < 7y$ for $y \geqslant 6$. These relations follow from $3x^2 - 4y^2 = \frac{11}{4}$, which implies $(6x)^2 = 48y^2 + 33$, so that $(6x)^2 > (6y - 1)^2$ and $(6x)^2 \leqslant (8y + 1)^2$ for $y \geqslant 1$; $(6x)^2 < (7y)^2$ for $y \geqslant 6$. Using these results, we now find that each point $(x, y) \in \mathbf{H}_+$ having $y \geqslant 1$ has an image (x', y') under the transformation g_1^{-1} in which $x' \leqslant x + 1$ and $y' \leqslant y + 1$. Moreover, if $y \geqslant 6$, then $y' > 0$. Suppose now that there exists a (finite) point $(x_0, y_0) \in \mathbf{H}_+$, which is not in $\mathbf{K}_+$, but which has an x_0 coordinate of the form $(2k + 1)/2$ with k a positive integer (necessarily, $2y_0$ = integer) and a y_0 coordinate with $y_0 \geqslant 6$. Since each application of the transformation g_1^{-1} to (x_0, y_0) reduces each coordinate by at least 1, there exists a unique nonnegative integer r such that $(g_1^{-1})^r$ transforms (x_0, y_0) to a point $(x_r, y_r) \in \mathbf{H}_+$ with $y_r \geqslant 6$, and such that one more transformation by g_1^{-1} yields a point (x_{r+1}, y_{r+1}) with $y_{r+1} < 6$. But then, since $6x_r < 7y_r$, it follows that $y_{r+1} > 0$. Thus, the

point (x_0, y_0) is transformed by $(g_1^{-1})^{r+1}$ to a point $(x_{r+1}, y_{r+1}) \in \mathbf{H}_+$ in which x_{r+1} is half an odd positive integer and $2y_{r+1}$ is an integer with $0 < y_{r+1} < 6$. But it is easily verified that among the points (x, y) with y coordinates $y = 1,2,...,5$ only the points $(\frac{3}{2},1)$ and $(\frac{5}{2},2)$ belong to $\mathbf{H}_+$ and have x coordinates that are half an odd integer; hence, $(x_0, y_0) \in \mathbf{K}_+$, which is a contradiction. ■

Using Theorem 1, we can now state the complete solution to the determination of all zeros of the Racah coefficient (2) with domain given by Eqs. (3).

Theorem 2: The set of all zeros of the equation

$$\begin{Bmatrix} j_2 & j_1 & j_2 \\ 2 & j_2 & j_1 \end{Bmatrix} = 0, \tag{11a}$$

such that all SU(2) conditions on the angular momenta are satisfied, namely, $2j_2 =$ positive integer and $j_1 \in \{1,2,...,2j_2\}$, is given by

$$j_1 = x_n - \tfrac{1}{2}, \quad j_2 = y_n - \tfrac{1}{2}, \tag{11b}$$

where $(x_n, y_n) \in \mathbf{K}_+$ with $n = 0,1,...$.

Proof: This is a trivial deduction from Theorem 1, it only being necessary to verify that $j_1 \leqslant 2j_2$; that is, $x_n \leqslant 2y_n - \frac{1}{2}$ for each $n = 0,1,...$. ■

III. CONCLUSIONS

We conclude with a number of remarks.

(a) The sets $\mathbf{K}_1$ and $\mathbf{K}_2$ are distinct orbits of the group action of G_α in $\mathbf{H}_+$.

(b) The discrete group with elements

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{12}$$

which is generated by reflection through the x and y axes, may be adjoined to G_α thereby obtaining a group $\tilde{G}_\alpha$ whose action transforms solutions $(x_n, y_n) \in \mathbf{K}_+$ having both $x_n > 0$ and $y_n > 0$ to the other branches of the hyperbola $\mathbf{H}$. The transformation of the angular momentum pair (j_1, j_2) corresponding to the group (12) are those generated by the substitutions $j_1 \to -j_1 - 1$, $j_2 \to j_2$ and $j_1 \to j_1$, $j_2 \to -j_2 - 1$. This type of substitution (generically, $j \to -j - 1$) is a well-known symmetry of $3jm$ and $6j$ coefficients; it is particularly obvious in the pattern calculus forms of these coefficients and corresponds to the extension of these coefficients to the group SU(1,1).

(c) Since

$$\begin{pmatrix} \frac{3}{2} \\ -1 \end{pmatrix} = g_1^{-1} \begin{pmatrix} \frac{5}{2} \\ 2 \end{pmatrix},$$

the two orbits $\mathbf{K}_1$ and $\mathbf{K}_2$ with respect to the action of G_α become a single orbit under the action of $\tilde{G}_\alpha$.

(d) There are other families of zeros of the type discussed in this paper obtained by applying the Regge symmetries of the $6j$ coefficient.

(e) The Racah coefficient occurring in Eq. (1b) also has zeros for $j \neq j_2$. The enumeration of these zeros is more difficult than those considered here; this will be reported on in another paper.

(f) Equation (4a), when multiplied by 4, has integer solutions and is a Diophantine equation known as Pell's equation. There is, of course, a general theory of such equations (see, for example, Chrystal[8]). As we have shown above, the special problem at hand can be treated by elementary means. This offers, perhaps, some hope that the Diophantine equations of higher order (quartic,...) that will occur for more general zeros of $6j$ coefficients can be treated.

(g) Zeros of $3jm$ and $6j$ coefficients imply zeros of the associated ${}_3F_2$ and ${}_4F_3$ hypergeometric series.

(h) Zeros of $6j$ coefficients may imply algebraic substructures for the general Racah–Wigner algebra in addition to the Lie algebraic structure mentioned earlier.

(i) For the physicist, it is the Racah invariant operators that provide a basis for all SU(2) invariants of the group SU(2)×SU(2) (and the $3nj$ symbols for higher products). Mathematicians have a quite different view of this subject (see Kung and Rota[9]). Zeros of $6j$ coefficients may have some implication for this latter view.

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Symmetry chains and adaptation coefficients

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Given a symmetry chain of physical significance it becomes necessary to obtain states which transform properly with respect to the symmetries of the chain. In this article we describe a method which permits us to calculate symmetry-adapted quantum states with relative ease. The coefficients for the symmetry-adapted linear combinations are obtained, in numerical form, in terms of the original states of the system and can thus be represented in the form of numerical tables. In addition, one also obtains automatically the matrix elements for the operators of the symmetry groups which are involved, and thus for any physical operator which can be expressed either as an element of the algebra or of the enveloping algebra. The method is well suited for computers once the physically relevant symmetry chain, or chains, have been defined. While the method to be described is generally applicable to any physical system for which semisimple Lie algebras play a role we choose here a familiar example in order to illustrate the method and to illuminate its simplicity. We choose the nuclear shell model for the case of two nucleons with orbital angular momentum $l = 1$. While the states of the entire shell transform like the smallest spin representation of SO(25) we restrict our attention to its subgroup $SU(6) \times SU(2)_T$. We determine the symmetry chains which lead to total angular momentum $SU(2)_J$ and obtain the symmetry-adapted states for these chains.

I. INTRODUCTION

In this article we describe a method for an explicit construction of symmetry-adapted bases for chains of symmetries. Given a symmetry chain, symmetry adaptation of quantum mechanical states according to a symmetry chain is an extremely important step if one indeed wants to make full use of symmetry properties. The first, and relatively easy step, consists in the determination of the symmetry properties of the states of a physical system. That is to assign to each state, if possible, unique labels which characterize its transformation properties with respect to the various symmetry groups of the symmetry chain.

Tables which contain such symmetry characterizations of states of quantum systems are found quite commonly in the literature. Familiar examples are the symmetry classification of states for the atomic[1-3] and nuclear[4,5] shell models.

The second, and much more difficult step, consists in the *explicit construction* of the symmetry-adapted physical states. That is, the coefficients need to be determined, for each symmetry group of the chain, which define the symmetry-adapted state in terms of the original states of the physical system. While a symmetry classification of the transformation properties of the states alone permits us to draw important information regarding selection rules, the symmetry-adapted states need to be known in explicit form if matrix elements are to be calculated. It is quite apparent from the literature that this second step is much more difficult. This is demonstrated by the lack of extensive tables and by the many methods which have been developed to solve this difficult task. Isoscalar factors and coefficients of fractional parentage represent some of the methods employed.[1,6]

In this article we want to describe a method for the determination of the coefficients for symmetry-adapted states which is both relatively easy and valid for a large class of symmetry chains; namely for all symmetry chains which involve semisimple Lie algebras.

The method is based upon Dykin's theory for the embedding of semisimple Lie algebras in semisimple Lie algebras.[7-9] The method yields the actual coefficients for the symmetry-adapted states. That is, it is a numerical method and thus well suited for computer use. Apart from the coefficients of the symmetry-adapted states this method also yields the matrix representations of all symmetries which are involved in a symmetry chain. That is, the method automatically gives the matrix elements of any physical operator which can be expressed in terms of the generators of the symmetry groups of the chain.

In order to illustrate the method we choose a familiar example. We take the example from the nuclear shell model.[4,6] The nucleons have spin and isospin $\frac{1}{2}$ and, for orbital angular momentum $l = 1$ for the individual nucleons, there are 4096 states in the nuclear shell. These states transform irreducibly with respect to the special orthogonal group SO(25) (see Refs. 1 and 3). In fact they transform like the spin representation of SO(25) with highest weight $\frac{1}{2}(1,1,...,1)$ (12 components). The special unitary group SU(12) forms a subgroup of SO(25). With respect to this subgroup the shell breaks up into a direct sum of irreducible representations, each of which forms a configuration of states. The two-particle states then transform irreducibly with respect to SU(12) and the representation is characterized by the highest weight $\frac{1}{2}(1,1,-1,...,-1)$ (12 components). This representation contains $15 \times 3 + 21 \times 1 = 66$ states. Since we merely want to give in this article an outline which describes our method we calculate the symmetry-adapted states for the 15 isotopic

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spin-1 states only. This is done via the three possible symmetry chains which correspond to j–j coupling, L–S coupling, and seniority-dependent coupling. Moreover, the matrix elements are obtained for the generators of all the symmetry groups involved (at least implicitly, for reasons of space; they can be read off easily).

The coefficients for the symmetry-adapted states will be given in the form of tables which are analogous to the familiar tables for Clebsch–Gordan coefficients. These tables then permit to switch easily from one kind of symmetry adaptation to another one by simply reading off the coefficients for the desired symmetry adaptation of the states.

II. STATE LABELING FOR SYMMETRY CHAINS

In this section we define the symmetry chains and determine the transformation properties of the two-particle states according to the three chains. The symmetry chains are defined through a set of embedding matrices.[9]

Using the technique of creation and annihilation operators for fermions[1,3] it is easily shown that for nucleons having orbital angular momentum $l = 1$ the states of the complete shell transform like the (smallest) spin representation of SO(25). Then, employing the methods of Refs. 7–9, the symmetry chains of Fig. 1 are found. Note that in between the symmetry group $SU(6)\times SU(2)_T$ and $SU(2)_J \times SU(2)_T$ there exist no additional symmetry chains.

In Fig. 1 the symbols T,S,L,J stand for total isotopic spin, total spin, total orbital angular momentum, and total angular momentum. The symbol v denotes the seniority quantum number. The suffix $\uparrow$ stands for $l+\frac{1}{2}$ and the suffix $\downarrow$ for $l-\frac{1}{2}$.

In Fig. 1, the highest weights are given for those representations which we consider in this article. Note that the 15 states which we actually discuss form a subset of the 4096 states of SO(25) which transforms irreducibly with respect to SU(6). These 15 states are two nucleon states with $l = 1$. In Fig. 1 we also give the dimension of the representations involved.

The three symmetry chains which are given in Fig. 1 correspond to L–S coupling, j–j coupling, and a seniority-v-dependent coupling. Which of these couplings dominates the physical process will depend on the nature of the nucleons considered.

The defining matrices for the embeddings through the chains of Fig. 1 are[3,9] (I_n denotes the $n\times n$ unit matrix)

$$f(\mathrm{SO}(25)\to\mathrm{SU}(12)) = I_{12}, \tag{2.1}$$

$$f(\mathrm{SU}(12)\to\mathrm{SU}(6)\times\mathrm{SU}(2)_T) = \begin{bmatrix} I_6 & I_6 \\ \frac{1}{2}(1\,1\,1\,1\,1\,1 & -1\,-1\,-1\,-1\,-1\,-1) \end{bmatrix}, \tag{2.2}$$

$$f(\mathrm{SU}(6)\to\mathrm{SU}(3)\times\mathrm{SU}(2)_S) = \begin{bmatrix} I_3 & I_3 \\ \frac{1}{2}(1\,1\,1 & -1\,-1\,-1) \end{bmatrix}, \tag{2.3}$$

$$f(\mathrm{SU}(3)\to\mathrm{SO}(3)_L) = (1,0,-1), \tag{2.4}$$

$$f(\mathrm{SO}(3)_L\times\mathrm{SU}(2)_S\to\mathrm{SU}(2)_J) = (1,1), \tag{2.5}$$

$$f(\mathrm{SU}(6)\to\mathrm{Sp}(6)_v) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \end{bmatrix}, \tag{2.6}$$

$$f(\mathrm{Sp}(6)_v\to\mathrm{SO}(3)_L\times\mathrm{SU}(2)_S) = \begin{bmatrix} 1\,0\,-1 \\ \frac{1}{2}(1\,1\,1) \end{bmatrix}, \tag{2.7}$$

$$f(\mathrm{SU}(6)\to\mathrm{SU}(4)_\uparrow\times\mathrm{SU}(2)_\downarrow) = \left[\begin{array}{c|cccccc} \frac{1}{4} & 3 & -1 & 0 & 0 & -1 & -1 \\ & -1 & 3 & 0 & 0 & -1 & -1 \\ & -1 & -1 & 0 & 0 & 3 & -1 \\ & -1 & -1 & 0 & 0 & -1 & 3 \\ \hline \frac{1}{2} & 0 & 0 & -1 & 1 & 0 & 0 \\ & 0 & 0 & 1 & -1 & 0 & 0 \end{array}\right], \tag{2.8}$$

$$f(\mathrm{SU}(4)_\uparrow\to\mathrm{Sp}(4)_\uparrow) = \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \end{bmatrix}, \tag{2.9}$$

$$f(\mathrm{Sp}(4)_\uparrow\to\mathrm{SU}(2)_\uparrow) = \tfrac{1}{2}(3,1), \tag{2.10}$$

$$f(\mathrm{SU}(2)_\uparrow\times\mathrm{SU}(2)_\downarrow\to\mathrm{SU}(2)_J) = (1,1), \tag{2.11}$$

$$f(\mathrm{Sp})(6)_v\to\mathrm{Sp}(4)_\uparrow\times\mathrm{SU}(2)_\downarrow) = \begin{bmatrix} 1\,0\,0 \\ 0\,1\,0 \\ \frac{1}{2}(0\,0\,-1) \end{bmatrix}, \tag{2.12}$$

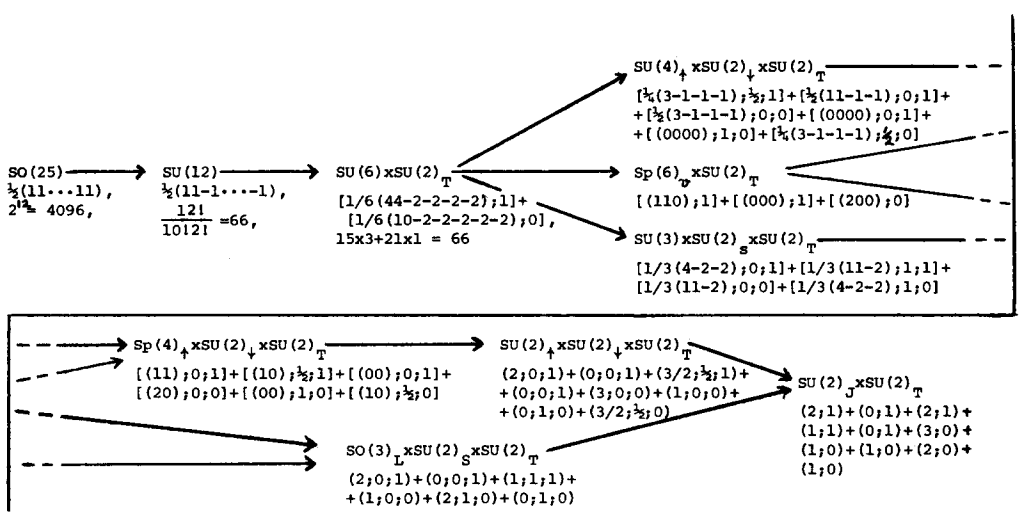

FIG. 1. The $l = 1$ symmetry chain and the two-particle representations.

$$f(\mathrm{SU})(6)\to\mathrm{SO}(3)_L\times\mathrm{SU}(2)_S)$$
$$=\left[\begin{array}{cccccc} 1 & 0 & -1 & 1 & 0 & -1 \\ \hline \tfrac{1}{2}(1 & 1 & 1 & -1 & -1 & -1) \end{array}\right], \tag{2.13}$$
$$f(\mathrm{SU}(6)\to\mathrm{SU}(2)_\uparrow\times\mathrm{SU}(2)_\downarrow)$$
$$=\frac{1}{2}\left[\begin{array}{cccccc} 3 & 1 & 0 & 0 & -1 & -3 \\ \hline 0 & 0 & -1 & 1 & 0 & 0 \end{array}\right], \tag{2.14}$$
$$f(\mathrm{SU}(6)\to\mathrm{SU}(2)_J)=\tfrac{1}{2}(3,1,-1,1,-1,-3). \tag{2.15}$$

III. SUBALGEBRAS AND THEIR EMBEDDINGS

In this section we want to give the embedding of the various algebras as subalgebras in the larger algebras. That is, given two Lie algebras $\tilde{L}$ and L we ask the question whether there exists an embedding f of $\tilde{L}$ in L such that $f(\tilde{L})$ satisfies in L the Lie products of $\tilde{L}$.

We denote the shift operators by E_α and the elements of the Cartan subalgebra by H_i. The symbol α stands for the roots, i.e., for the shift which is affected by E_α if acting upon a state. The index $i=1,2,\ldots,l,l$ the rank of the algebra [$i=1,2,\ldots,l+1$ for SU($l+1$)]. The e_i stands for the ith Cartesian unit vector, i.e., $(e_i)_j=\delta_{ij}$.

We obtain the following.

SO(25)→SU(12): The embedding of SU(12) in SO(25) is trivial as it is signified by the unit matrix I_{12}. That is, rejecting all shift operators of SO(25) whose α is not a root of SU(12) we obtain the subalgebra SU(12).

SU(12)→SU(6)×SU(2)$_T$: In this case we obtain, for the diagonal elements of SU(6) in SU(12),

$$f(\tilde{H}_i)=\sum_{k=1}^{12} f_{ik}H_k,\ i=1,2,\ldots,6.$$

Thus,

$$f(\tilde{H}_1)=H_1+H_7,\ f(\tilde{H}_2)=H_2+H_8,\ f(\tilde{H}_3)=H_3+H_9,$$
$$f(\tilde{H}_4)=H_4+H_{10},\ f(\tilde{H}_5)=H_5+H_{11},\ f(\tilde{H}_6)=H_6+H_{12} \tag{3.1}$$

are the six elements of the Cartan subalgebra of SU(6) embedded in SU(12). It is clear that

$$\tilde{m}_i=\sum_{k=1}^{12} f_{ik}m_k,\ i=1,2,\ldots,6 \tag{3.2}$$

defines weights $\tilde{m}=(\tilde{m}_1,\ldots,\tilde{m}_6)$ of SU(6); that is, the defining matrix f also yields the projection of the SU(12) weights upon the weights of its subalgebra SU(6).

One obtains similarly for the diagonal element T_3 of SU(2)$_T$ in SU(12)

$$T_3=\frac{1}{2}\sum_{i=1}^{6}H_i-\frac{1}{2}\sum_{i=7}^{12}H_i, \tag{3.3}$$

and the third component of isotopic spin is obtained through the projection

$$m_3^T=\tfrac{1}{2}(m_1+m_2+\cdots+m_6)$$
$$-\tfrac{1}{2}(m_7+m_8+\cdots+m_{12}), \tag{3.4}$$

where the m_i, $i=1,2,\ldots,12$, are the components of an SU(12) weight [as well as of an SO(25) weight, since the group SU(12) is trivially embedded in SO(25)]. Knowing this it is easy to understand why the representation of SU(12) with highest weight

$$\tfrac{1}{2}(1,1,-1,\ldots,-1)\quad(12\text{ components})$$

decomposes into the direct sum of representations of SU(6)×SU$_T$(2) with highest weights

$$(\tfrac{1}{6}(4,4,-2,-2,-2,-2);1)$$
$$+(\tfrac{1}{6}(10,-2,-2,-2,-2,-2);0).$$

Note that for the case of these particular representations all other weights are obtained through permutations of components only, except for the representation 1 of SU(2)$_T$ which has the three weights 1,0, −1.

We do not give here the embedding of the shift operators E_α since we will not need them in the following.

SU(6)→SU(3)×SU(2)$_S$: Since SU(2)$_T$ shows up in the form of a direct product on both sides we need not consider it. Thus, we are left with the embedding of SU(3)×SU(2)$_S$ in SU(6). This is obtained for SU(3) as

$$f(\tilde{H}_1)=H_1+H_4,\ f(\tilde{H}_2)=H_2+H_5,\ f(\tilde{H}_3)=H_3+H_6,$$
$$\begin{aligned} f(\tilde{E}_{(1\,-1\,0)})&=E_{e_1-e_2}+E_{e_4-e_5},\\ f(\tilde{E}_{(0\,1\,-1)})&=E_{e_2-e_3}+E_{e_5-e_6},\\ f(\tilde{E}_{(1\,0\,-1)})&=E_{e_1-e_3}+E_{e_4-e_6}, \end{aligned} \tag{3.5}$$

and for SU(2)$_S$ as

$$\begin{aligned} f(S_3)&=\tfrac{1}{2}(H_1+H_2+H_3-H_4-H_5-H_6),\\ f(S_+)&=(1/\sqrt{2})(E_{e_1-e_4}+E_{e_2-e_5}+E_{e_3-e_6}),\\ f(S_-)&=(1/\sqrt{2})(E_{-e_1+e_4}+E_{-e_2+e_5}+E_{-e_3+e_6}). \end{aligned} \tag{3.6}$$

The e_i on the right sides of the equations are six component vectors since the operators on the right sides belong to SU(6).

It always holds that

$$f(\tilde{E}_{-\alpha})=\sum_\alpha c_\alpha^* E_{-\alpha}, \tag{3.7}$$

with the star denoting complex conjugation.

SU(6)→SU(3)→SO(3)$_L$: Since SU(2)$_S$ shows up in the form of a direct product we can ignore it. We get for the embedding SU(6)→SU(3)→SO(3)$_L$,

$$\begin{aligned} f(L_3)&=\tilde{H}_1-\tilde{H}_3=H_1+H_4-H_3-H_6,\\ f(L_+)&=\tilde{E}_{(1\,-1\,0)}+\tilde{E}_{(0\,1\,-1)}\\ &=E_{e_1-e_2}+E_{e_4-e_5}+E_{e_2-e_3}+E_{e_5-e_6},\\ f(L_-)&=\tilde{E}_{(-1\,1\,0)}+\tilde{E}_{(0\,-1\,1)}\\ &=E_{-e_1+e_2}+E_{-e_4+e_5}+E_{-e_2+e_3}+E_{-e_5+e_6}. \end{aligned} \tag{3.8}$$

This is SO(3)$_L$ first embedded in SU(3) and then in SU(6).

SU(6)→SU(3)×SU(2)$_S$→SO(3)$_L$×SU(2)$_S$→SU(2)$_J$: The combined defining matrix of SU(2)$_J$ in SU(6) is given as

$$f=\tfrac{1}{2}(3,1,-1,1,-1,-3), \tag{3.9}$$

and we obtain, for the embedding of SU(2)$_J$ in SU(6),

$$\begin{aligned} f(J_3)&=\tfrac{1}{2}(3H_1+H_2-H_3+H_4-H_5-3H_6),\\ f(J_+)&=E_{e_1-e_2}+E_{e_2-e_3}+E_{e_4-e_5}+E_{e_5-e_6}\\ &\quad+(1/\sqrt{2})(E_{e_1-e_4}+E_{e_2-e_5}+E_{e_3-e_6}),\\ f(J_-)&=E_{-e_1+e_2}+E_{-e_2+e_3}+E_{-e_4+e_5}+E_{-e_5+e_6}\\ &\quad+(1/\sqrt{2})(E_{-e_1+e_4}+E_{-e_2+e_5}+E_{-e_3+e_6}). \end{aligned} \tag{3.10}$$

SU(6)→Sp(6)$_v$: The embedding of Sp(6)$_v$ in SU(6) is given as

$$
\begin{aligned}
&f(\tilde{H}_1) = H_1 - H_6,\ f(\tilde{H}_2) = H_2 - H_5,\ f(\tilde{H}_3) = H_3 - H_4,\\
&f(\tilde{E}_{e_1-e_2}) = E_{e_1-e_2} + E_{e_5-e_6},\\
&f(\tilde{E}_{e_2-e_3}) = E_{e_2-e_3} + E_{e_4-e_5},\\
&f(\tilde{E}_{2e_3}) = \sqrt{2}E_{e_3-e_4}.
\end{aligned}
\tag{3.11}
$$

As before, the shift operators which correspond to the negative roots are given by the same expressions in terms of the negative roots of SU(6). The remaining shift operators are defined through Lie products.

Sp(6)$_v$→SO(3)$_L$×SU(2)$_s$: SO(3)$_L$ is embedded in Sp(6)$_v$ as

$$
\begin{aligned}
&f(L_3) = f(\tilde{H}_1) - f(\tilde{H}_3) = H_1 - H_3 + H_4 - H_6, \text{ in SU(6)},\\
&f(L_+) = f(\tilde{E}_{(1\,-1\,0)}) + f(\tilde{E}_{(01\,-1)})\\
&\quad = E_{e_1-e_2} + E_{e_5-e_6}\\
&\quad\quad + E_{e_2-e_3} + E_{e_4-e_5}, \text{ in SU(6)}.
\end{aligned}
\tag{3.12}
$$

SU(2)$_s$ is embedded in Sp(6)$_v$ as

$$
\begin{aligned}
&f(S_3) = \tfrac{1}{2}(f(\tilde{H}_1) + f(\tilde{H}_2) + f(\tilde{H}_3))\\
&\quad = \tfrac{1}{2}(H_1 - H_6 + H_2 - H_5 + H_3 - H_4), \text{ in SU(6)},\\
&f(S_+) = \tfrac{1}{2}f(\tilde{E}_{(020)}) + (1/\sqrt{2})f(\tilde{E}_{(101)})\\
&\quad = (1/\sqrt{2})E_{e_2-e_5} + (1/\sqrt{2})(E_{e_1-e_4} + E_{e_3-e_6}), \text{ in SU(6)}.
\end{aligned}
\tag{3.13}
$$

SU(6)→SU(4)$_\uparrow$×SU(2)$_\downarrow$:

$$
\begin{aligned}
&f(\tilde{H}_1) = \tfrac{1}{4}(3H_1 - H_2 - H_5 - H_6),\\
&f(\tilde{H}_2) = \tfrac{1}{4}(-H_1 + 3H_2 - H_5 - H_6),\\
&f(\tilde{H}_3) = \tfrac{1}{4}(-H_1 - H_2 + 3H_5 - H_6),\\
&f(\tilde{H}_4) = \tfrac{1}{4}(-H_1 - H_2 - H_5 + 3H_6),\\
&f(\tilde{E}_{e_1-e_2}) = E_{e_1-e_2},\ f(\tilde{E}_{e_2-e_3}) = E_{e_2-e_5},\\
&f(\tilde{E}_{e_3-e_4}) = E_{e_5-e_6},
\end{aligned}
$$

for SU(4)$_\uparrow$ in SU(6). Here we have subtracted $\frac{1}{4}(H_1 + H_2 + H_5 + H_6)$ in order to have the property

$$\sum_{i=1}^{4} f(\tilde{H}_i) = 0.$$

And for SU(2)$_\downarrow$ in SU(6),

$$
\begin{aligned}
&f(M_3) = \tfrac{1}{2}(H_4 - H_3),\\
&f(M_+) = (1/\sqrt{2})E_{e_4-e_3},\\
&f(M_-) = (1/\sqrt{2})E_{-e_4+e_3}.
\end{aligned}
\tag{3.14}
$$

SU(4)$_\uparrow$→Sp(4)$_\uparrow$:

$$
\begin{aligned}
&f(\tilde{H}_1) = H_1 - H_4,\ f(\tilde{H}_2) = H_2 - H_3,\\
&f(\tilde{E}_{e_1-e_2}) = E_{e_1-e_2} + E_{e_3-e_4},\\
&f(\tilde{E}_{2e_2}) = \sqrt{2}E_{e_2-e_3}.
\end{aligned}
\tag{3.15}
$$

Sp(4)$_\uparrow$→SU(2)$_\uparrow$:

$$
\begin{aligned}
&f(N_3) = \tfrac{1}{2}(3H_1 + H_2),\\
&f(N_+) = \sqrt{(3/2)}E_{e_1-e_2} + E_{2e_2}.
\end{aligned}
\tag{3.16}
$$

Sp(6)$_v$→Sp(4)$_\uparrow$×SU(2)$_\downarrow$:

$$
\begin{aligned}
&f(\tilde{H}_1) = H_1,\ f(\tilde{H}_2) = H_2,\\
&f(\tilde{E}_{e_1-e_2}) = E_{e_1-e_2},\ f(\tilde{E}_{2e_2}) = E_{2e_2},\\
&f(M_3) = -\tfrac{1}{2}H_3,\ f(M_+) = \tfrac{1}{2}E_{-2e_3}.
\end{aligned}
\tag{3.17}
$$

SU(6)→SU(4)$_\uparrow$×SU(2)$_\downarrow$→Sp(4)$_\uparrow$×SU(2)$_\downarrow$→SU(2)$_I$×SU(2)$_\downarrow$→SU(2)$_J$:

$$
\begin{aligned}
&f(J_3) = f(M_3) + f(N_3)\\
&\quad = \tfrac{1}{2}(3H_1 + H_2 - H_3 + H_4 - H_5 - 3H_6),\\
&f(J_+) = f(M_+) + f(N_+)\\
&\quad = \sqrt{(3/2)}(E_{e_1-e_2} + E_{e_5-e_6})\\
&\quad\quad + \sqrt{2}E_{e_2-e_5} + (1/\sqrt{2})E_{e_4-e_3}.
\end{aligned}
\tag{3.18}
$$

IV. SYMMETRY ADAPTATION COEFFICIENTS AND MATRIX ELEMENTS

A. Symmetry adaptation coefficients

The embedding of SU(6)×SU(2)$_T$ in SO(25) yields the symmetry-adapted states with respect to SU(6)×SU(2)$_T$. It is seen from the defining matrices for this embedding that the two-particle states transform like the states of the representations $(\frac{1}{6}(4,4,-2,-2,-2,-2);1) + (\frac{1}{6}(10,-2,-2,-2,-2,-2);0)$ of SU(6)×SU(2)$_T$. That is, the totality of two nucleon states transforms according to two irreducible representations of SU(6), the first of which has isotopic spin 1, the second has isotopic spin zero. Thus for a realization of these representations in terms of products of one-particle wave functions appropriately symmetrized expressions have to be used [see Eq. (4.4)].

We consider now the representation $\frac{1}{6}(4,4,-2,-2,-2,-2)$ of SU(6). We could obtain the symmetry-adapted states through the embedding of the shift operators of SU(6) in SO(25). However, the situation is here quite simple if one realizes that the states of this representation can be chosen as Slater determinants for two nucleons. Let

$$\varphi_i(m_l, m_s) \tag{4.1}$$

denote a single nucleon wave function for the ith nucleon with third component of orbital angular momentum m_l and third component of spin m_s. The possible values $(m_l,m_s),J_z$ are

$$
\begin{array}{lcccccc}
 & (1,\frac{1}{2}),\frac{3}{2} & (0,\frac{1}{2}),\frac{1}{2} & (-1,\frac{1}{2}),-\frac{1}{2} & (1,-\frac{1}{2}),\frac{1}{2} & (0,-\frac{1}{2}),-\frac{1}{2} & (-1,-\frac{1}{2}),-\frac{3}{2}\\
i= & 1 & 2 & 3 & 4 & 5 & 6
\end{array}
\tag{4.2}
$$

Note that J itself is in general not a good quantum number with respect to this basis of SU(6). The values $i = 1,2,...,6$ label the six possible values (m_l,m_s) in the order indicated. We introduce the symbol

$$\{1--1--\}. \tag{4.3}$$

The two 1's in the symbol { } represent the occupation of the corresponding (m_l,m_s) states by nucleons. This symbol thus represents two nucleon wave functions. That is

$$\{1--1--\}$$

$$\equiv \frac{1}{\sqrt{2}}(\varphi_1(1,\tfrac{1}{2})\varphi_2(1,-\tfrac{1}{2}) - \varphi_1(1,-\tfrac{1}{2})\varphi_2(1,\tfrac{1}{2})). \tag{4.4}$$

These wave functions are seen to be antisymmetric. There are 15 wave functions of this type which form a basis for the representation $\frac{1}{6}(4,4,-2,-2,-2,-2)$ of SU(6), while the 21 symmetric combinations form a basis for the representation $\frac{1}{6}(10,-2,-2,-2,-2,-2)$ of SU(6).

The relationship of the states $\{1\,1----\}$ with the states $|\frac{1}{6}(4,4,-2,-2,-2,-2)\rangle$ of SU(6) is made as follows. The index i of Eqs. (4.2) and (4.3) corresponds to the index i of the elements H_i of SU(6). It holds

$$H_i|m\rangle = m_i|m\rangle,\quad m=(m_1,m_2,\ldots,m_6),$$

and the H_i "measures" whether the ith nucleon is contained in the state or not. If $m_i>0$, then the nucleon with the quantum numbers (m_l,m_s), which correspond to the value i by Eqs. (4.2) and (4.3), is present. If $m_i<0$, this particular nucleon is not contained in the state. Thus

$$|\tfrac{1}{6}(4,4,-2,-2,-2,-2)\rangle \leftrightarrow \{1\,1----\},$$

$$|\tfrac{1}{6}(4,-2,-2,4,-2,-2)\rangle \leftrightarrow \{1--1--\},$$

and so forth. One could add a multiple of the identity matrix I_6 to each of the H_i without changing the commutation relations. For example the new H_i' could be chosen as

$$H_i' = H_i + \tfrac{2}{6}I_6.$$

The eigenvalues of H_i are now 1 or 0 and the weights of SU(6) take on the form (1 1 0 0 0 0) (and all permutations). Then the 1's characterize the presence of a nucleon with the quantum numbers given by the position of the 1's.

In order to illustrate the method of calculation of symmetry-adapted states we carry out the symmetry adaptation $SU(6)\to SU(3)\times SU(2)_S$ in detail.

There are 15 states of the type (4.4). The defining matrix, Eq. (2.3), yields the weights of $SU(3)\times SU(2)_S$ which correspond to the states $\{\ \}$. For example,

$$f(\tilde{H}_1)\{1\,1----\} = (H_1+H_4)|\tfrac{1}{6}(4,4,-2,-2,-2,-2)\rangle = \tfrac{1}{3}\{1\,1----\},$$

$$f(\tilde{H}_2)\{1\,1----\} = (H_2+H_5)|\tfrac{1}{6}(4,4,-2,-2,-2,-2)\rangle = \tfrac{1}{3}\{1\,1----\},$$

$$f(\tilde{H}_3)\{1\,1----\} = (H_3+H_6)|\tfrac{1}{6}(4,4,-2,-2,-2,-2)\rangle = -\tfrac{2}{3}\{1\,1----\},$$

$$f(S_3)\{1\,1----\} = \tfrac{1}{2}(H_1+H_2+H_3-H_4-H_5-H_6) \times |\tfrac{1}{6}(4,4,-2,-2,-2,-2)\rangle = 1\cdot\{1\,1----\},$$

and thus the vector $\{11----\}$ of SU(6) corresponds, under restriction of SU(6) to the subgroup $SU(3)\times SU(2)_S$, to the weight $(\frac{1}{3}(1,1,-2);1)$. Then, making use of the property that the highest weight of irreducible representations of simple compact Lie algebras is unique, and of the embedding of the shift operators of $SU(3)\times SU(2)_S$ in SU(6), Eqs. (3.5) and (3.6), the symmetry-adapted states can be calculated. Some care needs to be taken for weight subspaces whose dimension exceeds 1.

TABLE I. $SU(6)\to SU(3)\times SU(2)_S$.

SU(3) x SU(2)$_S$ \ SU(6)	{11----}	{1-1---}	{1--1--}	{1---1-}	{1----1}	{-11---}	{-1-1--}	{-1--1-}	{-1---1}	{--11--}	{--1-1-}	{--1--1}	{---11-}	{---1-1}	{----11}
[1/3(4-2-2);0]		1													
[1/3(1 1-2);0]		1/√2				1/√2									
[1/3(-24-2);0]								1							
[1/3(1-2 1);0]				1/√2						1/√2					
[1/3(-2-24);0]											1				
[1/3(-211);0]									1/√2		1/√2				
[1/3(11-2);1]	1														
[1/3(11-2);0]		-1√2				1√2									
[1/3(11-2);-1]													1		
[1/3(1-21);1]		1													
[1/3(1-21);0]				-1/√2						1/√2					
[1/3(1-21);-1]														1	
[1/3(-211);1]						1									
[1/3(-211);0]									-1/√2		1/√2				
[1/3(-211);-1]															1

TABLE II. $SU(6) \to [SU(3) \times SU(2)_S] \to SO(3)_L \times SU(2)_S$.

$SU(6)$ / $[SU(3) \times SU(2)_S]$ / $SO(3)_L \times SU(2)_S$	{11----}	{1-1---}	{1--1--}	{1---1-}	{1----1}	{-11---}	{-1-1--}	{-1--1-}	{-1---1}	{--11--}	{--1-1-}	{--1--1}	{---11-}	{---1-1}	{----11}
{11----} [1/3(4-2-2);0] (2;0)			1												
(1;0)			$1/\sqrt{2}$			$1/\sqrt{2}$									
(0;0)				$1/\sqrt{6}$			$2/\sqrt{6}$		$1/\sqrt{6}$						
(-1;0)								$1/\sqrt{2}$		$1/\sqrt{2}$					
(-2;0)											1				
(0;0)				$1/\sqrt{3}$			$-1\sqrt{3}$		$1/\sqrt{3}$						
{11----} [1/3(2-1-1);1] (1;1)		1													
(1;0)			$1/\sqrt{2}$			$-1/\sqrt{2}$									
(1;-1)												1			
(0;1)		1													
(0;0)				$1/\sqrt{2}$					$-1/\sqrt{2}$						
(0;-1)													1		
(-1;1)						1									
(-1;0)								$1/\sqrt{2}$		$-1/\sqrt{2}$					
(-1;-1)															1

TABLE III. $SU(6) \to [SU(3) \times SU(2)_S] \to [SO(3)_L \times SU(2)_S] \to SU(2)_J$.

$SU(6)$ / $[SU(3) \times SU(2)_S]$ / $[SO(3)_L \times SU(2)_S]$ / $SU(2)_J$	{11----}	{1-1---}	{1--1--}	{1---1-}	{1----1}	{-11---}	{-1-1--}	{-1--1-}	{-1---1}	{--11--}	{--1-1-}	{--1--1}	{---11-}	{---1-1}	{----11}
{11----} [1/3(4-2-2);0] (2;0) 2			1												
1			$1/\sqrt{2}$			$1/\sqrt{2}$									
0				$1/\sqrt{6}$			$2/\sqrt{6}$		$1/\sqrt{6}$						
-1								$1/\sqrt{2}$		$1/\sqrt{2}$					
-2											1				
(0;0) 0				$1/\sqrt{3}$			$-1/\sqrt{3}$		$1/\sqrt{3}$						
{11----} [1/3(2-1-1);1] (1;1) 2	1														
1		$1/\sqrt{2}$		$1/2$		$-1/2$									
0				$1/\sqrt{3}$	$1/\sqrt{6}$				$-1/\sqrt{3}$			$1/\sqrt{6}$			
-1							$1/2$		$-1/2$				$1/\sqrt{2}$		
-2															1
1		$1/\sqrt{2}$		$-1/2$		$1/2$									
0					$1/\sqrt{2}$							$-1/\sqrt{2}$			
-1							$1/2$		$-1/2$				$-1/\sqrt{2}$		
0				$-1/\sqrt{6}$	$1/\sqrt{3}$				$1/\sqrt{6}$			$1/\sqrt{3}$			

TABLE IV. $SU(6) \to Sp(6)_v$.

$Sp(6)_v$ \ SU(6)	{11----}	{1-1---}	{1--1--}	{1---1-}	{1----1}	{-11---}	{-1-1--}	{-1--1-}	{-1---1}	{--11--}	{--1-1-}	{--1--1}	{---11-}	{---1-1}	{----11}
{11----}															
(110)	1														
(101)		1													
(10-1)			1												
(1-10)				1											
$(000)_1$				$1/\sqrt{2}$			$1/\sqrt{2}$								
$(000)_2$				$-1/\sqrt{6}$			$1/\sqrt{6}$		$\sqrt{2/3}$						
(011)					1										
(01-1)						1									
(-110)								1							
(0-11)										1					
(-101)											1				
(0-1-1)												1			
(-10-1)													1		
(-1-10)															1
{11----}															
(000)				$-1/\sqrt{3}$			$1/\sqrt{3}$		$-1/\sqrt{3}$						

TABLE V. $SU(6) \to SU(4)_\uparrow \times SU(2)_\downarrow$.

$SU(4)_\uparrow \times SU(2)_\downarrow$ \ SU(6)	{11----}	{1-1---}	{1--1--}	{1---1-}	{1----1}	{-11---}	{-1-1--}	{-1--1-}	{-1---1}	{--11--}	{--1-1-}	{--1--1}	{---11-}	{---1-1}	{----11}
[1/2(11-1-1);0]	1														
[1/2(1-11-1);0]				1											
[1/2(-111-1);0]								1							
[1/2(1-1-11);0]					1										
[1/2(-11-11);0]									1						
[1/2(-1-111);0]															1
[1/4(3-1-1-1);1/2]			1												
[1/4(-13-1-1);1/2]							1								
[1/4(-1-13-1);1/2]													-1		
[1/4(-1-1-13);1/2]														-1	
[1/4(3-1-1-1);-1/2]		1													
[1/4(-13-1-1);-1/2]						1									
[1/4(-1-13-1);-1/2]											-1				
[1/4(-1-1-13);-1/2]												-1			
[(0000);0]										1					

TABLE VI. $SU(6) \to [SU(4) \times SU(2)] \to Sp(4)_{\uparrow} \times SU(1)_{\downarrow}$.

$[SU(4) \times SU(2)]$ / $Sp(4)_{\uparrow} \times SU(2)_{\downarrow}$ \ SU(6)	{11----}	{1-1---}	{1--1--}	{1---1-}	{1----1}	{-11---}	{-1-1--}	{-1--1-}	{-1---1}	{--11--}	{--1-1-}	{--1--1}	{---11-}	{---1-1}	{----11}
{11----}															
[1/2(11-1-1);0]															
[(11);0]	1														
[(1-1);0]				1											
[(00);0]					$1/\sqrt{2}$				$1/\sqrt{2}$						
[(-11);0]										1					
[(-1-1);0]															1
[(00);0]					$1/\sqrt{2}$				$-1/\sqrt{2}$						
{11----}															
[1/4(3-1-1-1);1/2]															
[(10);1/2]		1													
[(01);1/2]						1									
[(0-1);1/2]											1				
[(-10);1/2]												1			
[(10);-1/2]			1												
[(01);-1/2]							1								
[(0-1);-1/2]													1		
[(-10);-1/2]														1	
{11----}															
[(0000);0]															
[(00);0]										1					

TABLE VII. $SU(6) \to [Sp(6)] \to SO(3)_L \times SU(2)_S$.

$[Sp(6)]$ / $SO(3)_L \times SU(2)_S$ \ SU(6)	{11----}	{1-1---}	{1--1--}	{1---1-}	{1----1}	{-11---}	{-1-1--}	{-1--1-}	{-1---1}	{--11--}	{--1-1-}	{--1--1}	{---11-}	{---1-1}	{----11}
{11----}															
(110)															
(2;0)			1												
(1;0)				$1/\sqrt{2}$			$1/\sqrt{2}$								
(0;0)					$1/\sqrt{6}$			$2/\sqrt{6}$		$1/\sqrt{6}$					
(-1;0)									$1/\sqrt{2}$		$1/\sqrt{2}$				
(-2;0)												1			
{11----}															
(110)															
(1;1)	1														
(1;0)				$1/\sqrt{2}$			$-1/\sqrt{2}$								
(1;-1)													1		
(0;1)		1													
(0;0)					$1/\sqrt{2}$					$-1/\sqrt{2}$					
(0;-1)														1	
(-1;1)						1									
(-1;0)									$1/\sqrt{2}$		$-1/\sqrt{2}$				
(-1;-1)															1
{11----}															
(000)															
(0;0)					$1/\sqrt{3}$			$-1/\sqrt{3}$		$1/\sqrt{3}$					

TABLE VIII. $SU(6)\to[SU(4)\times SU(2)]\to[Sp(4)\times SU(2)]\to[SU(2)\times SU(2)]\to SU(2)_J$.

[SU(4) x SU(2)] / [Sp(4) x SU(2)] / [SU(2) x SU(2)] / $SU(2)_J$ \ SU(6)	{11----}	{1-1---}	{1--1--}	{1---1-}	{1----1}	{-11---}	{-1-1--}	{-1--1-}	{-1---1}	{--11--}	{--1-1-}	{--1--1}	{---11-}	{---1-1}	{----11}
[1/4(3-1-1-1);1/2]															
[(10);1/2]															
(3/2;1/2)															
2			1												
1		1/2					$\sqrt{3}/2$								
0						$1/\sqrt{2}$							$-1/\sqrt{2}$		
-1											$-\sqrt{3}/2$			$-1/2$	
-2												-1			
1	$\sqrt{3}/2$						$-1/2$								
0						$1/\sqrt{2}$							$1/\sqrt{2}$		
-1											$-1/2$			$\sqrt{3}/2$	
[1/2(11-1-1);0]															
[(11);0]															
(2;0)															
2	1														
1				1											
0					$1/\sqrt{2}$				$1/\sqrt{2}$						
-1										1					
-2															1
(0;0)															
0					$1/\sqrt{2}$				$-1/\sqrt{2}$						
[(0000);0]															
[(00);0]															
(0;0)															
0										-1					

TABLE IX. $Sp(6)_v\to(L,S)$.

(L,S) \ $Sp(6)_v$	(110)	(101)	(10-1)	(1-10)	$(000)_1$	$(000)_2$	(011)	(01-1)	(-110)	(0-11)	(-101)	(0-1-1)	(-10-1)	(-1-10)	(000)
(110)															
(2;0)			1												
(1;0)				$1/\sqrt{2}$				$1/\sqrt{2}$							
(0;0)					$\sqrt{3}/2$	$1/2$									
(-1;0)									$1/\sqrt{2}$	$1/\sqrt{2}$					
(-2;0)											1				
(110)															
(1;1)	1														
(1;0)		1													
(1;-1)							1								
(0;1)				$-1/\sqrt{2}$				$1/\sqrt{2}$							
(0;0)					$-1/2$	$\sqrt{3}/2$									
(0;-1)									$-1/\sqrt{2}$	$1/\sqrt{2}$					
(-1;1)												1			
(-1;0)													1		
(-1;-1)														1	
(000)															
(0;0)															1

TABLE X. $Sp(6)_v \to Sp(4)_\uparrow \times SU(2)_\downarrow$.

$Sp(4)_\uparrow \times SU(2)_\downarrow$ \ $Sp(6)_v$	(110)	(101)	(10-1)	(1-10)	$(000)_1$	$(000)_2$	(011)	(01-1)	(-110)	(0-11)	(-101)	(0-1-1)	(-10-1)	(-1-10)	(000)
{11----}															
(110)															
(11;0)	1														
(1-1;0)				1											
(00;0)					1										
(-11;0)									1						
(-1-1;0)														1	
{11----}															
(110)															
(10;1/2)			1												
(01;1/2)								1							
(-10;1/2)													1		
(0-1;1/2)												1			
(10;-1/2)		1													
(01;-1/2)							1								
(-10;-1/2)										-1					
(0-1;-1/2)											-1				
{11----}															
(110)															
(00;0)						1									
{11----}															
(000)															
(00;0)															1

An example will illustrate the above. The highest SU(3) weight that one obtains is $(\frac{1}{3}(4,-2,-2);0)$ and corresponds to $\{1--1--\}$. Thus, $\{1--1--\}$ is a unique SU(3) vector and we can construct the SU(3) representation to which it belongs by acting upon this vector with the SU(3) shift operators. The shift operators do what their subscript indicates. For example, the operator

$$f(E_{(-110)}) = E_{-e_1+e_2} + E_{-e_4+e_5}$$

yields (in general) a linear combination of two states. In the first state the first component is decreased by 1 and the second component increased by 1, while in the second state the fourth component is decreased by 1 and the fifth increased by 1. That is

$$f(E_{(-110)})\{1--1--\} = \{-1-1--\} + \{1---1-\}.$$

This then is another (unnormalized) SU(3) state, which belongs to weight $(\frac{1}{3}(1,1,-2);0)$. Acting in turn upon this state one obtains

$$f(E_{(-110)})(\{-1-1--\} + \{1---1-\}) = 2\{-1--1-\}.$$

The state $\{-1--1-\}$ is again an SU(3) state and its weight is $(\frac{1}{3}(-2,4,-2);0)$. This state is mapped to zero:

$$f(E_{(-110)})\{-1--1-\} = 0.$$

It is easily checked that $f(S_\pm)$ maps all these states to zero, i.e., they correspond to a spin singlet.

The labeling of the one-particle states of SU(6), Eq. (4.1), as given by Eq. (4.2), is based upon their transformation properties according to the symmetry chain given by Eq. (3.10). The *same* states of SU(6) transform *differently* if instead the symmetry chain given by Eq. (3.18) is chosen. The labels of the SU(6) states according to this symmetry chain are given as

$\lvert J,J_3\rangle$	=	$\lvert\frac{3}{2},\frac{3}{2}\rangle$,	$\lvert\frac{3}{2},\frac{1}{2}\rangle$,	$\lvert\frac{1}{2},-\frac{1}{2}\rangle$,	$\lvert\frac{1}{2},\frac{1}{2}\rangle$,	$\lvert\frac{3}{2},-\frac{1}{2}\rangle$,	$\lvert\frac{3}{2},-\frac{3}{2}\rangle$
i	=	1	2	3	4	5	6

Thus it follows that the two symmetry chains, Eq. (3.10) and Eq. (3.18), determine two *distinct* bases for the *same* representations of $SU(2)_J$, namely $J = \frac{3}{2},\frac{1}{2}$. The two bases are obtained as two distinct sets of linear combinations of the basis elements Eq. (4.2) of the six-dimensional irreducible representation of SU(6). The symmetry chain Eq. (3.10) corresponds to L–S coupling, while the symmetry chain Eq. (3.18) describes j–j coupling.

For the two-particle states ($l = 1$, $s = 1/2$)^2 one obtains in L–S coupling (a = antisymmetric, s = symmetric)

$$(1;\tfrac{1}{2})\times(1;\tfrac{1}{2}) = \underset{ss}{(2;1)} + \underset{sa}{(2;0)} + \underset{as}{(1;1)} + \underset{aa}{(1;0)} + \underset{ss}{(0;1)} + \underset{sa}{(0;0)},$$

where only the antisymmetric total angular momentum states

$$2+(2+1+0)+0$$

survive, while in j–j coupling one obtains

$$(1;\tfrac{1}{2})\times(1;\tfrac{1}{2})=(\tfrac{3}{2};\tfrac{3}{2})+(\tfrac{3}{2};\tfrac{1}{2})+(\tfrac{1}{2};\tfrac{3}{2})+(\tfrac{1}{2};\tfrac{1}{2}),$$

where again the antisymmetric total angular momentum states

$$(2+0)+(2+1)+0$$

survive. While the $SU(2)_J$ representation content consists of the same representations for both symmetry chains, it is clear that the form of the $SU(2)_J$ states, expressed in terms of the same two-particle SU(6) states [the same SU(6) representation], depends on the symmetry chain (coupling) which is chosen. The embedding of the two symmetry chains in the same group SU(6) thus establishes a relationship among the two types of couplings which is equivalent to finding the transformation brackets which relate the two distinct $SU(2)_J$ bases.

B. Matrix elements

In this section we give the matrix elements for some of the subalgebras of the symmetry chain Fig. 1. Only the less obvious cases of matrix representations will be considered. The matrix elements are arrived at in a natural manner if one calculates the symmetry-adapted states given in Tables I–X.

The raising and lowering operators of SU(n) can be represented as $n\times n$ matrices[10]

$$E_{e_j-e_i}\leftrightarrow(C^j_i)_{st}\equiv\delta_{js}\delta_{it}, \tag{4.5}$$

where the δ are Kronecker symbols. The diagonal elements H_i are then given as

$$H_i\leftrightarrow(C^i_i)_{st}\equiv\delta_{is}\delta_{it}. \tag{4.6}$$

The Lie products are given by the commutators

$$[C^j_i,C^l_k]=\delta_{il}C^j_k-\delta_{kj}C^l_i. \tag{4.7}$$

In these equations $i,j,s,t=1,2,\ldots,n$. We choose in the following the phases in such a manner that relation (4.7) is satisfied. That is, we give the matrix elements for the simple negative roots and the diagonal elements H_i only. Equation (4.7) then determines the remaining matrix elements. A useful property to remember is

$$f(\tilde{E}_{-\alpha})=f(\tilde{E}_\alpha)^+, \tag{4.8}$$

where the symbol $+$ denotes Hermitian conjugation. The ordering of the states is so chosen as to correspond to the ordering of the states in the tables.

SU(3)×SU(2)$_s$:

$(\frac{1}{3}(4-2-2);0)$,

$$f(E_{(-110)})=\begin{bmatrix}0&0&0&0&0&0\\ \sqrt{2}&0&0&0&0&0\\ 0&\sqrt{2}&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&0&0\end{bmatrix},$$

$$f(E_{(0-11)})=\begin{bmatrix}0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&\sqrt{2}&0&0&0\\ 0&0&0&\sqrt{2}&0&0\end{bmatrix},$$

$$f(H_1)=\mathrm{diag}\tfrac{1}{3}(4,1,-2,1,-2,-2),$$

$$f(H_2)=\mathrm{diag}\tfrac{1}{3}(-2,1,4,-2,-2,1),$$

$$f(H_3)=\mathrm{diag}\tfrac{1}{3}(-2,-2,-2,1,4,1);$$

$(\frac{1}{3}(1,1,-2);1)$,

$$f(S_-)=\begin{bmatrix}-\begin{bmatrix}0&0&0\\1&0&0\\0&1&0\end{bmatrix}&&&\\ &-\begin{bmatrix}0&0&0\\1&0&0\\0&1&0\end{bmatrix}&&\\ &&\begin{bmatrix}0&0&0\\1&0&0\\0&1&0\end{bmatrix}&\end{bmatrix},$$

$$f(S_+)=\begin{bmatrix}-\begin{bmatrix}0&1&0\\0&0&1\\0&0&0\end{bmatrix}&&&\\ &-\begin{bmatrix}0&1&0\\0&0&1\\0&0&0\end{bmatrix}&&\\ &&-\begin{bmatrix}0&1&0\\0&0&1\\0&0&0\end{bmatrix}&\end{bmatrix},$$

$$f(\tilde{E}_{(-110)})=\begin{bmatrix}[\,0\,]&&&\\ &[\,0\,]&&\\ &&\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}[\,0\,]&\end{bmatrix},$$

$$f(\tilde{E}_{(0-11)})=\begin{bmatrix}[\,0\,]&&&\\ \begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}&[\,0\,]&&\\ &&[\,0\,]&\end{bmatrix},$$

$$f(S_3)=\mathrm{diag}(1,0,-1,1,0,-1,1,0,-1),$$

$$f(\tilde{H}_1)=\mathrm{diag}\tfrac{1}{3}(1,1,1,1,1,1,-2,-2,-2),$$

$$f(\tilde{H}_2)=\mathrm{diag}\tfrac{1}{3}(1,1,1,-2,-2,-2,1,1,1),$$

$$f(\tilde{H}_3)=\mathrm{diag}\tfrac{1}{3}(-2,-2,-2,1,1,1,1,1,1).$$

Sp(6)$_v$:

(110) The nonzero matrix elements are

$$f(\tilde{E}_{(-1\,1\,0)}): a_{54}=\sqrt{2},\ a_{72}=1,\ a_{83}=1,\ a_{95}=\sqrt{2},\ a_{11,10}=1,\ a_{13,12}=1.$$

$$f(\tilde{E}_{(0\,-1\,1)}): a_{21}=1,\ a_{43}=1,\ a_{58}=1/\sqrt{2},\ a_{68}=\sqrt{3/2},\ a_{95}=1/\sqrt{2},\ a_{96}=\sqrt{3/2},\ a_{11,9}=1,\ a_{14,13}=1.$$

$$f(\tilde{E}_{(0\,0\,-2)}): a_{32}=\sqrt{2},\ a_{87}=\sqrt{2},\ a_{12,10}=\sqrt{2},\ a_{13,11}=\sqrt{2}.$$

$$f(\tilde{H}_1)=\mathrm{diag}(1,1,1,1,0,0,0,0,-1,0,-1,0,-1,-1),$$

$$f(\tilde{H}_2)=\mathrm{diag}(1,0,0,-1,0,0,1,1,1,-1,0,-1,0,-1,-1),$$

$$f(\tilde{H}_3)=\mathrm{diag}(0,1,-1,0,0,0,1,-1,0,1,1,-1,-1,-1,0).$$

Sp(4):

(11),

$$f(\tilde{E}_{(-110)})=\begin{vmatrix}0&0&0&0&0\\0&0&0&0&0\\0&\sqrt{2}&0&0&0\\0&0&\sqrt{2}&0&0\\0&0&0&0&0\end{vmatrix},$$

$$f(\tilde{E}_{(00-2)})=\begin{vmatrix}0&0&0&0&0\\\sqrt{2}&0&0&0&0\\0&0&0&0&0\\0&0&0&0&0\\0&0&0&\sqrt{2}&0\end{vmatrix},$$

$$f(\tilde{H}_1)=\mathrm{diag}(1,1,0,-1,-1),$$

$$f(\tilde{H}_2)=\mathrm{diag}(1,-1,0,1,-1,).$$

(10),

$$f(\tilde{E}_{-110)})=\begin{vmatrix}0&0&0&0\\1&0&0&0\\0&0&0&0\\0&0&1&0\end{vmatrix},$$

$$f(\tilde{E}_{(00-2)})=\begin{vmatrix}0&0&0&0\\0&0&0&0\\0&\sqrt{2}&0&0\\0&0&0&0\end{vmatrix},$$

$$f(\tilde{H}_1)=\mathrm{diag}(1,0,0,-1),$$

$$f(\tilde{H}_2)=\mathrm{diag}(0,1,-1,0).$$

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Spinor group and its restrictions

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A realization of the spinor algebra of the rotation group SO(N), $N = 2n$ or $2n + 1$, in the covering algebra of U(2^n) is exploited to obtain explicit representation matrices for the SO(N) generators in the basis adapted to the subgroup chain SO(N)⊃U(n)⊃U($n-1$)⊃···⊃U(1). As a special case the computation of matrices of U(n) representations characterized by a k-column Young tableau is reduced to the evaluation of at most k-box totally symmetric representations of U(2^n).

I. INTRODUCTION

The spinor algebra of the rotation groups SO(N), $N = 2n$ or $2n + 1$, were recently realized by Nikam and Sarma[1] (NS) by an embedding in the covering algebra of U(2^n). This led to a simple realization of the multispinor basis of SO(N) in terms of the canonical basis spanning the representations of U(2^n). One of the major problems encountered by NS was that multiply occurring states of a given representation of SO(N), having the same weight, could not be satisfactorily labeled. As an illustration of this problem note that the weight $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$ of the representation $\langle \frac{3}{2}\,\frac{1}{2}\,\frac{1}{2}\,-\frac{1}{2}\rangle$ of SO(8) occurs three times. An obvious solution to this state labeling problem is to adapt the multispinor basis to the Gelfand–Tsetlin canonical chain[2] SO(N)⊃SO($N-1$)⊃···SO(3)⊃SO(2). However, this mathematically ideal chain of subgroups suffers from two drawbacks. First, while SO($2n$) is a regular subgroup[3] of SO($2n+1$), the group SO($2n-1$) is not a regular subgroup of SO($2n$). Second, in many physical applications we may not need all the subgroups of SO(N) but rather a special class of subgroup chains such as

$$\mathrm{SO}(N)\supset \mathrm{U}(n)\supset \mathrm{U}(n-1)\supset\cdots\supset \mathrm{U}(1), \tag{1}$$

or

$$\mathrm{SO}(N)\supset \mathrm{U}(n)\supset \mathrm{SO}(n)\supset\cdots\supset \mathrm{SO}(3)\supset \mathrm{SO}(2). \tag{2}$$

Thus, most chains which are encountered in physical applications will start with the embedding of U(n) in SO(N). Since U(n) is a regular subgroup of SO(N), this fact makes the symmetry adaptation SO(N)↓U(n) a relatively simple task.

We shall consider the subgroup chain (1) in some detail in Sec. II. Starting with a brief summary of an earlier work by NS we indicate a simple procedure for the restriction SO(N)↓U(n), using the SO(8)↓U(4) case as an example. In Sec. III we present a brief discussion of this scheme and consider the nature of a class of operators of SO(N) which can be used to characterize rearrangement processes in systems described by specific symmetry under U(n). In particular we indicate how general k-column U(n) representation matrices can be simply obtained by considering at most k-box totally symmetric representations of U(2^n).

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II. THE RESTRICTION SO(N)↓U(n) ($N = 2n, 2n+1$)

Consider the fundamental representation space V_{2^n} of U(2^n) spanned by an ordered orthonormal set of spinors

$$V_{2^n} = \mathrm{Span}\{|k\rangle \equiv |(m_{1k} m_{2k}\cdots m_{nk})\rangle \quad |k = 1,2,\ldots,2^n;\ |m_{ik}| = \tfrac{1}{2},\ \forall i\}. \tag{3}$$

The 2^{2n} unitary shift operators on V_{2^n},

$$E_{ij} \equiv |(m_{1i} m_{2i}\cdots m_{ni})\rangle\langle(m_{1j} m_{2j}\cdots m_{nj})|, \tag{4}$$

induce the transformations

$$E_{ij}|k\rangle = \delta_{jk}|i\rangle, \tag{5}$$

where

$$\delta_{jk} = \prod_{p=1}^{n} \delta(m_{pj}, m_{pk}). \tag{6}$$

Using a subset of these shift operators we define a set of n linear operators $\{X_a | a = 1,\ldots,n\}$ as [cf. Eq. (29) of NS]

$$X_a = \sum_{k=1}^{2^n}{}' (-)^{p_a} E_{(m_{1k}\cdots m_{ak} = (1/2)\cdots m_{nk})(m_{1k}\cdots m_{ak} = -(1/2)\cdots m_{nk})}, \tag{7}$$

where

$$p_a = \sum_{l=a+1}^{n} \left(m_{lk} + \frac{1}{2}\right),$$

and the prime on the summation symbol indicates that the m_{ak} values are fixed as explicitly indicated. Since also

$$E_{ij}^{\dagger} = E_{ji}, \tag{8}$$

we can define an additional set of n operators $\bar{X}_a$ as

$$\bar{X}_a = X_a^{\dagger}. \tag{9}$$

The set of $2n$ operators, $\{X_a, \bar{X}_a | a = 1,\ldots,n\}$, which satisfy the fermion-type anticommutation relations on V_{2^n}, can now be used to define a set of commutators[4,5]

$$\Lambda_{aa} = [X_a, \bar{X}_a], \quad a = 1,\ldots,n; \tag{10a}$$

$$\Lambda_{ab} = [X_a, \bar{X}_b], \tag{10b}$$

$$\Lambda_{a\bar{b}} = [X_b, X_a], \tag{10c}$$

$$\Lambda_{\bar{a}\bar{b}} = [\bar{X}_a, X_b], \tag{10d}$$

$$\Lambda_{\bar{a}b} = [\bar{X}_b, \bar{X}_a], \quad a \neq b = 1,\ldots,n. \tag{10e}$$

Using the commutator algebra for E_{ij} of U(2^n), it readily follows that Eqs. (10) lead to the forms defined by Eqs. (11),

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(16), (21), (15), and (20) of NS, respectively. They can be conveniently expressed in the following compact form, e.g.,

$$\Lambda_{ab} = (-)^{b-a+1} \sum_{i,j,k} (-)^{r_2(j)} E_{\epsilon + 2^{n-b}, \epsilon + 2^{n-a}} \quad (a \neq b)$$

and (11a)

$$\Lambda_{a\bar{b}} = (-)^{b-a+1} \sum_{i,j,k} (-)^{r_2(j)} E_{\epsilon, \epsilon + 2^{n-a} + 2^{n-b}}, \quad (11b)$$

where

$$\epsilon \equiv \epsilon_{ab}(i,j,k) = i + 2^{n+1-b}(j + 2^{b-a}k),$$

with the summations extending over

$$i = 1,2,\ldots,2^{n-b},$$
$$j = 0,1,\ldots,(2^{b-a-1} - 1),$$
$$k = 0,1,\ldots,(2^{a-1} - 1),$$

and $r_2(j)$ designates the digital sum of $(j)_2$, the latter representing the binary form of j. The remaining generators follow from relations $\Lambda_{ab} = -\Lambda_{\bar{b}\bar{a}}$ and $\Lambda_{a\bar{b}} = \Lambda^{\dagger}_{\bar{b}a}$. These operators define the Lie algebra of SO($2n$). The generators of SO($2n+1$) are then obtained by adjoining to the above operators (10) the $2n$ operators $\Lambda_{0a} \equiv X_a$ and $\Lambda_{0\bar{a}} \equiv \bar{X}_a$ defined by Eqs. (7) and (9). Their explicit form is

$$\Lambda_{a0} = (-)^{n-a+1} \sum_{i,k} (-)^{r_2(i)} E_{\tilde{\epsilon}, \tilde{\epsilon} + 2^{n-a}}, \quad (12)$$

where

$$\tilde{\epsilon} \equiv \tilde{\epsilon}_a(i,k) = \epsilon_{aa}(i,0,k) = i + 2^{n+1-a}k,$$

with i and k given as in Eqs. (11). The multispinor basis spanning any representation $\langle \lambda_1 \lambda_2 \cdots \lambda_n \rangle$ $(\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant |\lambda_n|$ for all integer or all half-integer $\lambda_i)$ can now be obtained following NS.

The set of n^2 generators Λ_{ab} $(a,b, = 1,\ldots,n)$, Eqs. (10a) and (10b), define the Lie algebra of U(n) satisfying

$$[\Lambda_{ab}, \Lambda_{cd}] = \Lambda_{ad}\delta_{bc} - \Lambda_{cb}\delta_{ad}, \quad (13)$$

and

$$\Lambda^{\dagger}_{ab} = \Lambda_{ba}. \quad (14)$$

Thus, U(n) defines a regular subalgebra of SO(N). Since U(n) admits only non-negative integer representations, we introduce a constant shift for the diagonal generators and define

$$H_a = \Lambda_{aa} + \tfrac{1}{2}N', \quad (15)$$

where N' is the rank of the U(2^n) representation from which the given representation of SO(N) is subduced. The weight space basis of U(n) is then characterized by the ordered eigenvalue set $(\omega_1 \omega_2 \cdots \omega_n)$ of the operators H_a, $a = 1,\ldots,n$.

As an illustration of the restriction SO(N)$\downarrow$U(n) we consider the representation $\langle \frac{3}{2}\frac{1}{2}\frac{1}{2} -\frac{1}{2}\rangle$ of SO(8). This representation requires for its definition at least a rank 3 spinor space $[V_{2^4}]$[8] of U(16). Since it is immaterial what representation of U(16) we choose, we select the simplest one, namely $[1^3\,\dot{0}]$, which yields the highest weight state (HWS) $(\frac{3}{2}\frac{1}{2}\frac{1}{2} -\frac{1}{2})$ of SO(8). Using the ordered set of fundamental spinor basis states [cf. Eq. (24) of NS] we find the HWS of this representation of SO(8) to be

$$|\langle \tfrac{3}{2}\tfrac{1}{2}\tfrac{1}{2} -\tfrac{1}{2}\rangle(\tfrac{3}{2}\tfrac{1}{2}\tfrac{1}{2} -\tfrac{1}{2})\rangle = \begin{array}{|c|}\hline 1 \\ \hline 4 \\ \hline 6 \\ \hline \end{array}, \quad (16)$$

where the Weyl tableau notation[6,7] has been used on the right-hand side to label the canonical basis states of U(16). The fact that Eq. (16) represents the HWS can be readily verified by noting that all elementary weight raising generators [cf. Eqs. (11)],

$$\begin{aligned} \Lambda_{12} &= E_{5,9} + E_{6,10} + E_{7,11} + E_{8,12}, \\ \Lambda_{23} &= E_{3,5} + E_{4,6} + E_{11,13} + E_{12,14}, \\ \Lambda_{34} &= E_{2,3} + E_{6,7} + E_{10,11} + E_{14,15}, \\ \Lambda_{3\bar{4}} &= E_{1,4} + E_{5,8} + E_{9,12} + E_{13,16}, \end{aligned} \quad (17)$$

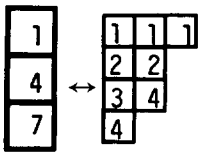
of SO(8) annihilate it. Since the subset $\{\Lambda_{a,a+1} | a = 1,2,3\}$ also annihilates the HWS(16), it is also a HWS of U(4) characterized by the weight (3,2,2,1) as follows from Eq. (15). Thus, we can write

$$|\langle \tfrac{3}{2}\tfrac{1}{2}\tfrac{1}{2} -\tfrac{1}{2}\rangle(\tfrac{3}{2}\tfrac{1}{2}\tfrac{1}{2} -\tfrac{1}{2})\rangle = \begin{array}{|c|}\hline 1 \\ \hline 4 \\ \hline 6 \\ \hline \end{array} \leftrightarrow \begin{array}{|c|c|c|}\hline 1 & 1 & 1 \\ \hline 2 & 2 \\ \cline{1-2} 3 & 3 \\ \cline{1-2} 4 \\ \cline{1-1} \end{array}. \quad (16')$$

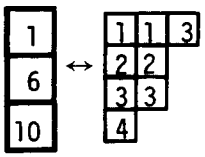
Before proceeding to the HWS of other representations of U(4), it is useful to consider the correspondence between the spinor basis indices m_{ik} and the orbital indices defining the fundamental representation V_n of U(n). Applying the weight generators, Eq. (15), to any fundamental spinor of U(2^n), we obtain an eigenvalue $+1$ for each $m_{ik} = \frac{1}{2}$ (or $+$ sign) occurring in the spinor, and 0 for each $m_{ik} = -\frac{1}{2}$ (or $-$ sign) occurring in it. The nonzero eigenvalues of H_a $(a = 1,\ldots,n)$ on any spinor of V_{2^n} may be interpreted as indicating the occupancy of that orbital in the set $\{\phi_a | a = 1,\ldots,n\}$ spanning V_n of U(n)$\subset$SO(N). The validity of this identification follows from the fact that the weight-raising(-lowering) generators $\Lambda_{ab}; a < b$ $(\Lambda_{ab}; a > b)$ of SO(N) acting on V_{2^n} induce the shifts $(\cdots - \cdots + \cdots) \overset{\Lambda_{ab}}{\leftrightarrow} (\cdots + \cdots - \cdots)$, which in turn induce the shifts $(H_a, H_b) = (1,0) \leftrightarrow (0,1)$ implying that Λ_{ab} are shift operators on V_n of U(n). Thus for a multispinor state, such as that given by Eq. (16'), this correspondence and Eq. (15) yield the configuration $\phi_1^3 \phi_2^2 \phi_3^2 \phi_4$ of $[V_4]$[8]. Since the state (16') is a HWS of U(4), the Weyl tableau representation follows.

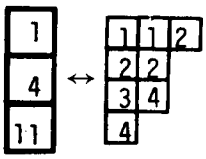
The realization of the lower weight states of [3221] of U(4), and the highest weights of other representations belonging to $\langle \frac{3}{2}\frac{1}{2}\frac{1}{2} -\frac{1}{2}\rangle$ of SO(8), can be obtained by exploiting this identification and the harmonic level excitation procedure[8,9] for SO(8). This procedure is based on the successive application of elementary lowering generators $\Lambda_{a+1,a}$ $(a = 1,2,3)$ and $\Lambda_{\bar{4}3}$ of SO(8) to the HWS of Eq. (16'). Applying these generators [given by Hermitian adjoints of the raising ones, Eq. (17)] to Eq. (16') we obtain (after normalization) the distinct nonzero basis states for the first level states of the harmonic level excitation diagram[8,9] (HLED), namely

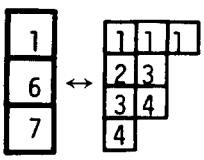
$$\Lambda_{21}(16'): (\tfrac{1}{2}\tfrac{3}{2}\tfrac{1}{2} -\tfrac{1}{2}) = \begin{array}{|c|}\hline 1 \\ \hline 4 \\ \hline 10 \\ \hline \end{array} \leftrightarrow \begin{array}{|c|c|c|}\hline 1 & 1 & 2 \\ \hline 2 & 2 \\ \cline{1-2} 3 & 3 \\ \cline{1-2} 4 \\ \cline{1-1} \end{array}, \quad (18)$$

$\Lambda_{43}(16')$: $(\frac{3}{2}\,\frac{1}{2}\,-\frac{1}{2}\,\frac{1}{2})=$  (19)

Proceeding to the next level of HLED we obtain

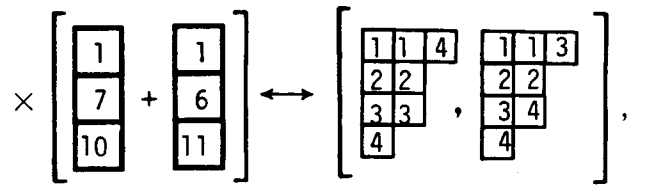
$\Lambda_{32}(18)$: $(\frac{1}{2}\,\frac{1}{2}\,\frac{3}{2}\,-\frac{1}{2})=$  , (20)

$\left.\begin{matrix}\Lambda_{43}(18)\\ \Lambda_{21}(19)\end{matrix}\right\}$: $(\frac{1}{2}\,\frac{3}{2}\,-\frac{1}{2}\,\frac{1}{2})=$  , (21)

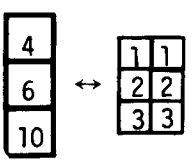
$\Lambda_{32}(19)$: $(\frac{3}{2}\,-\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})=$  . (22)

At the third level of HLED we obtain several states having the same weight, namely,

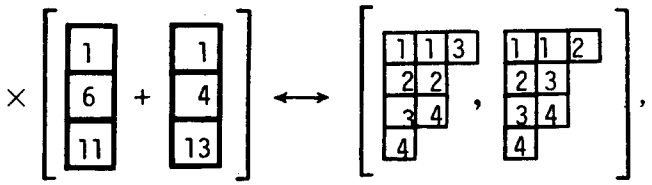
$\Lambda_{43}(20)$: $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})'_1=\dfrac{1}{\sqrt{2}}$



(23)

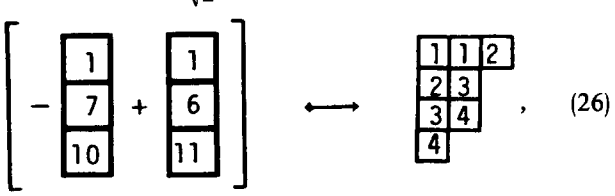
$\Lambda_{\overline{43}}(20)$: $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,-\frac{3}{2})=$  , (24)

$\Lambda_{32}(21)$: $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})'_2=\dfrac{1}{\sqrt{2}}$

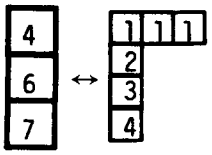


(25)

$\Lambda_{21}(22)$: $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})'_3=\dfrac{1}{\sqrt{2}}$

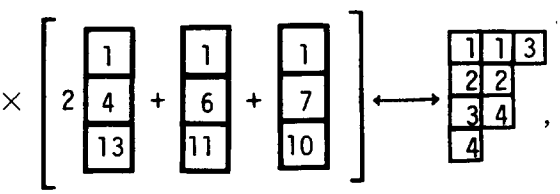


(26)

$\Lambda_{\overline{43}}(22)$: $(\frac{3}{2}\,-\frac{1}{2}\,-\frac{1}{2}\,-\frac{1}{2})=$  . (27)

In the same way we proceed to the subsequent levels of HLED until the lowest weight state is reached. The states defined by Eqs. (23)–(27) need some explanation for the way they are characterized at the U(4) level. The states defined by Eqs. (24) and (27) are readily verified to be the HWS of U(4) characterized by the weights (2220) and (3111) using Eq. (15). Hence the Weyl tableaux representations used. The state given by Eq. (26) defines uniquely the first of the lexically ordered Weyl tableau for the configuration $\phi_1^2\,\phi_2^2\,\phi_3^2\,\phi_4^2$ of [3221] of U(4), $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})_1=(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})'_3$. (Equivalently, it corresponds to the highest Yamanouchi symbol.) The other two states of this weight are then obtained by Schmidt orthogonalization procedure yielding

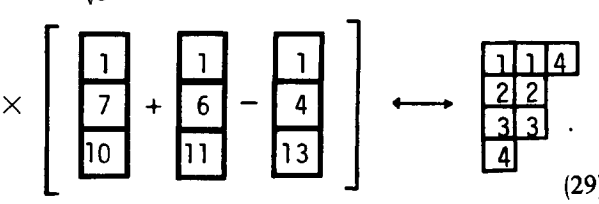
$(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})_2=\dfrac{1}{\sqrt{6}}$



(28)

and

$(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})_3=\dfrac{1}{\sqrt{3}}$

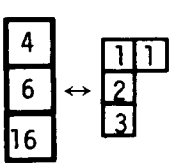


(29)

The other multispinor basis states spanning $\langle\frac{3}{2}\,\frac{1}{2}\,\frac{1}{2}\,-\frac{1}{2}\rangle$ of SO(8) may be obtained analogously using the SO(8)↓U(4) subduction. From the tables of Patera *et al.*,[10,11] we find that

$$\langle\tfrac{3}{2}\,\tfrac{1}{2}\,\tfrac{1}{2}\,-\tfrac{1}{2}\rangle=2[211]+[222]+[200]+[110] \quad (30)$$

for SO(8)↓SU(4). The twofold multiplicity at the SU(4) level was resolved by Patera *et al.*[10,11] using the intermediate subgroup SO(7). In our approach we find the HWS for one of these representations to be given by Eq. (16). Proceeding similarly we get another HWS

$|\langle\frac{3}{2}\,\frac{1}{2}\,\frac{1}{2}\,-\frac{1}{2}\rangle(\frac{1}{2}\,-\frac{1}{2}\,-\frac{1}{2}\,-\frac{3}{2})\rangle=$  (31)

belonging to [2110] of U(4). Consequently, the use of U(4) rather than SU(4) obviates the need to use the chain SO(8) ⊃SO(7)⊃SU(4). This type of multiplicity appears frequently in the tables of Patera *et al.*[10,11]

III. DISCUSSION

The analysis of Sec. II indicates that the multiplicity problem for the SO(N) multispinor states is resolved to a large extent by exploiting the chain (1). The reason for choosing the chain (1) rather than the canonical chain SO(N) $\supset$SO($N-1$)$\supset\cdots\supset$SO(2) is twofold. First, the fact that U(n) is a regular subgroup of SO(N) leads to a considerable simplification of the basis states determination. Second, U(n) is a very useful group in the many-body correlation problem.[12–15] Explicit algebraic expressions are available for U(n) generator matrix elements in the canonical basis[12–16] and these have been successfully implemented in large-scale computations.[17–21] In spite of this success it is interesting to examine the nature of the U(n) basis obtained by a subduction from a covering group such as SO(N). As indicated in Sec. II, every basis state of the carrier space for the representation $[\lambda_1\lambda_2\cdots\lambda_n]$ of U(n) can be realized as a multispinor basis state of SO(N). For this realization we need a spinor of rank $2\lambda_1$. However, in each such state there are $\lambda_1+\lambda_n$ spinors $1\equiv(+\ +\cdots+)$ with all $m_{i1}=\frac{1}{2}$. These spinors are not at all affected by the generators Λ_{ab} ($a,b=1,\ldots,n$) of U(n) for reasons given in Sec.II. Consequently, these spinors can be ignored when considering the weight space basis of SO(N) induced by the representation $[\lambda_1\lambda_2\cdots\lambda_n]$ of U(n), so that only spinors of rank $2\lambda_1-(\lambda_1+\lambda_n)=\lambda_1-\lambda_n$ need be considered as long as we are not concerned with the specific representation of SO(N) in which $[\lambda_1\lambda_2\cdots\lambda_n]$ is embedded. The SO(N) basis thus generated is characterized by the ordered set of weights $(\omega_1\omega_2\cdots\omega_n)$ with

$$\omega_i=\lambda_i-\tfrac{1}{2}(\lambda_1-\lambda_n),\quad i=1,\ldots,n. \tag{32}$$

For example, the representation [332000] of U(6) is characterized by rank 3 spinors of weight $(\frac{3}{2}\frac{3}{2}\frac{1}{2}\ -\frac{3}{2}\ -\frac{3}{2}\ -\frac{3}{2})$ of SO(12) which are stable under $\Lambda_{ab}(a,b=1,\ldots,6)$. The HWS of $[\lambda_1\lambda_2\cdots\lambda_n]$ of U(n) follows if we choose a set of spinors satisfying the above weight structure and ordered in such a way that in each spinor all the $+$'s precede all the $-$'s when read from left to right. This ensures, as outlined in Sec. II, that all weight-raising generators of U(n) annihilate this multispinor state thus yielding the HWS. Thus, for example, the HWS for [332000] of U(6) with the weight $(\frac{3}{2}\frac{3}{2}\frac{1}{2}\ -\frac{3}{2}\ -\frac{3}{2}\ -\frac{3}{2})$ is the third rank product $\boxed{8}\times\boxed{8}\times\boxed{16}$ where $\boxed{8}\equiv(+\ +\ +\ -\ -\ -)$ and $\boxed{16}\equiv(+\ +\ -\ -\ -\ -)$. Since odd and even spinors of SO($2n$) cannot be mixed, we note that the highest representation of SO(12) in which $(\frac{3}{2}\frac{3}{2}\frac{1}{2}\ -\frac{3}{2}\ -\frac{3}{2}\ -\frac{3}{2})$ can be contained is $\langle\frac{3}{2}\frac{3}{2}\frac{3}{2}\frac{3}{2}\frac{3}{2}\frac{3}{2}\ -\frac{1}{2}\rangle$, whose HWS can be chosen as $\boxed{1}\boxed{2}\boxed{2}$. Thus, the covering representation of [332000] of U(6) is this representation of SO(12). Since each spinor of V_{2^n} can be regarded as an antisymmetric state at the U(n) level, it follows that all representations of this group expressed in terms of the totally symmetric representation of SO(N) are symmetrized direct products of single column Young diagrams. Thus, for the HWS considered above, we have

$$\boxed{8}\boxed{8}\boxed{16}=\left[\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}\times\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}\times\begin{array}{c}\boxed{1}\\\boxed{2}\end{array}\right]_{\rm sym}$$

$$=\frac{1}{\sqrt{3}}\left\{\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}\times\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}\times\begin{array}{c}\boxed{1}\\\boxed{2}\end{array}+\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}\times\begin{array}{c}\boxed{1}\\\boxed{2}\end{array}\times\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}+\begin{array}{c}\boxed{1}\\\boxed{2}\end{array}\times\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}\times\begin{array}{c}\boxed{1}\\\boxed{2}\\\boxed{3}\end{array}\right\}. \tag{33}$$

In order to better illustrate the simplifications achieved in computing the U(n) representation matrices, we consider the 27-dimensional irreducible representation [420] of U(3). [Explicit representation matrices for U(3) generators Λ_{ab} ($a,b=1,2,3$) can be found in Ref. 12.] The HWS is easily found in this case to be

$$|1\rangle\equiv\boxed{2}\boxed{2}\boxed{4}\boxed{4}\ . \tag{34}$$

Applying U(3) elementary lowering generators,

$$\Lambda_{21}=E_{53}+E_{64},\qquad \Lambda_{32}=E_{32}+E_{76}, \tag{35}$$

we obtain at the first level of HLED the states

$$\Lambda_{21}|1\rangle=\sqrt{2}\ \boxed{2}\boxed{2}\boxed{4}\boxed{6}=\sqrt{2}|2\rangle,\qquad \Lambda_{32}|1\rangle=\sqrt{2}\ \boxed{2}\boxed{3}\boxed{4}\boxed{4}=\sqrt{2}|4\rangle, \tag{36}$$

where the ket symbols are labeled by the sequential numbers of the corresponding lexically ordered Gelfand–Tsetlin basis. The next level yields

$$\Lambda_{21}|4\rangle=\boxed{2}\boxed{4}\boxed{4}\boxed{5}+\sqrt{2}\ \boxed{2}\boxed{3}\boxed{4}\boxed{6}=\sqrt{3}|5\rangle,\qquad \Lambda_{32}|4\rangle=\sqrt{2}\ \boxed{3}\boxed{3}\boxed{4}\boxed{4}=\sqrt{2}|8\rangle, \tag{37}$$

and

$$\Lambda_{21}|2\rangle=\sqrt{3}\ \boxed{2}\boxed{2}\boxed{6}\boxed{6}=\sqrt{2}|3\rangle,\qquad \Lambda_{32}|2\rangle=\sqrt{2}\ \boxed{2}\boxed{3}\boxed{4}\boxed{6}+\boxed{2}\boxed{2}\boxed{4}\boxed{7}\ . \tag{38}$$

The last state has the same weight (210) as the state $|5\rangle$. Schmidt orthonormalization to $|5\rangle$ gives

$$|13\rangle=(3\ \boxed{2}\boxed{2}\boxed{4}\boxed{7}+\sqrt{2}\ \boxed{2}\boxed{3}\boxed{4}\boxed{6}-2\ \boxed{2}\boxed{4}\boxed{4}\boxed{5}\ )/\sqrt{15}, \tag{39}$$

so that

TABLE. I. The list of weights and corresponding Gelfand–Tsetlin states of the [420] irreducible representation of U(3) represented by the U(8) Weyl tableaux.

(3 1 -1) $|1\rangle =$ 2 2 4 4 (2 2 -1) $|2\rangle =$ 2 2 4 6

(1 3 -1) $|3\rangle =$ 2 2 6 6 (3 0 0) $|4\rangle =$ 2 3 4 4

(2 1 0) $|5\rangle = (\sqrt{2}$ 2 3 4 6 $+$ 2 4 4 5 $)/\sqrt{3}$

$|13\rangle = (\sqrt{2}$ 2 3 4 6 $- 2$ 2 4 4 5 $+ 3$ 2 2 4 7 $)/\sqrt{15}$

(1 2 0) $|6\rangle = (\sqrt{2}$ 2 4 5 6 $+$ 2 3 6 6 $)/\sqrt{3}$

$|14\rangle = (-\sqrt{2}$ 2 4 5 6 $+2$ 2 3 6 6 $+3$ 2 2 6 7 $)/\sqrt{15}$

(0 3 0) $|7\rangle =$ 2 5 6 6 (3 -1 1) $|8\rangle =$ 3 3 4 4

(2 0 1) $|9\rangle = ($ 3 3 4 6 $+$ 3 4 4 5 $)/\sqrt{2}$

$|15\rangle = ($ 3 3 4 6 $-$ 3 4 4 5 $+2\sqrt{2}$ 2 3 4 7 $)/\sqrt{10}$

(1 1 1) $|10\rangle = ($ 3 3 6 6 $+$ 4 4 5 5 $+ 2$ 3 4 5 6 $)/\sqrt{6}$

$|16\rangle = ($ 3 3 6 6 $-$ 4 4 5 5 $+ 2$ 2 3 6 7 $+ 2$ 2 4 5 7 $)/\sqrt{10}$

$|22\rangle = ($ 3 3 6 6 $+$ 4 4 5 5 $-$ 3 4 5 6 $+$

$+3$ 2 2 7 7 $+3$ 2 3 6 7 $- 3$ 2 4 5 7 $)/\sqrt{30}$

(0 2 1) $|11\rangle = ($ 3 5 6 6 $+$ 4 5 5 6 $)/\sqrt{2}$

$|17\rangle = ($ 3 5 6 6 $-$ 4 5 5 6 $+2\sqrt{2}$ 2 5 6 7 $)/\sqrt{10}$

(-1 3 1) $|12\rangle =$ 5 5 6 6 (2 -1 2) $|18\rangle =$ 3 3 4 7

(1 0 2) $|19\rangle = ($ 3 3 6 7 $+\sqrt{2}$ 3 4 5 7 $)/\sqrt{3}$

$|23\rangle = (2$ 3 3 6 7 $-\sqrt{2}$ 3 4 5 7 $+ 3$ 2 3 7 7 $)/\sqrt{15}$

(0 1 2) $|20\rangle = (\sqrt{2}$ 3 5 6 7 $+$ 4 5 5 7 $)/\sqrt{3}$

$|24\rangle = (\sqrt{2}$ 3 5 6 7 $- 2$ 4 5 5 7 $+ 3$ 2 5 7 7 $)/\sqrt{15}$

(-1 2 2) $|21\rangle =$ 5 5 6 7 (1 -1 3) $|25\rangle =$ 3 3 7 7

(0 0 3) $|26\rangle =$ 3 5 7 7 (-1 1 3) $|27\rangle =$ 5 5 7 7

$$\Lambda_{32}|2\rangle = (2/\sqrt{3})|5\rangle + \sqrt{\tfrac{5}{3}}|13\rangle. \tag{40}$$

Continuing this process we easily generate the complete Gelfand–Tsetlin basis, given in Table I, and evaluate at the same time all the nonvanishing generator matrix elements exploiting only a simple rule for action of Λ_{ab} on totally symmetric states. We stress that any other k-column irreducible representation of U(n) can be treated with the same ease and that the nonelementary generator matrices are just as easily calculated, e.g.,

$$\Lambda_{31}|1\rangle = (E_{74} - E_{52})\ \boxed{2}\boxed{2}\boxed{4}\boxed{4}$$

$$= \sqrt{2}(\ \boxed{2}\boxed{2}\boxed{4}\boxed{7}\ -\ \boxed{2}\boxed{4}\boxed{4}\boxed{5}\ )$$

$$= -\sqrt{\tfrac{2}{3}}\,|5\rangle + \sqrt{\tfrac{10}{3}}\,|13\rangle. \tag{41}$$

Thus, we can easily realize the Lie algebra of SO(N) using the embedding U(2^n) $\supset$ SO(N) and since only totally symmetric representations of U(2^n) are required to obtain any U(n) irreducible representation, simple algorithms for generation of explicit representation matrices of generators can be given.

Let us, finally, indicate other possible advantages of the U(2^n) $\supset$ SO(N) $\supset$ U(n) chain for the many-fermion correlation problem. Invoking a higher than U(n) symmetry for many-body systems, we can first of all consider also particle number nonconserving operators. However, even for systems with well-defined particle number a subdivision into the subsystems with variable particle number can be advantageous.[22] As an illustration, consider the operator

$$\Theta = \sum_{a<b} \Lambda_{\bar{b}a}\Lambda_{a\bar{b}}, \tag{42}$$

which belongs to the center of the SO(N) and hence conserves not only the rank but also the weight of each basis state of U(n). [In fact, Θ is similar to an SO(N) Casimir operator $\Sigma_{a,b}\Lambda_{ba}\Lambda_{ab}$.] Unlike the generators of U(n), however, the generators $\Lambda_{a\bar{b}}$ and $\Lambda_{\bar{b}a}$ can affect the vacuum state spinors $1\equiv(+\ +\ +\cdots+)$ and $2^n\equiv(-\ -\ -\cdots-)$. Inclusion of these [SU(n)-invariant vacuum] spinors in defining the HWS of a representation of U(n) will lead to an interesting result under the action of Θ, since this operator redistributes the $+$'s and $-$'s among the defining spinors. Since the number and location of $+$'s in each spinor indicates the occupancy of the corresponding $\phi_i \in V_n$, it follows that Θ transfers these ϕ_i's from one antisymmetric subsystem to another. This is best illustrated on a simple example. Consider the HWS $\psi_1 \equiv$ [1 8] of the representation of [2111] of U(4)$\subset$SO(8). Applying Θ to ψ_1 we obtain (after normalization)

$$\Theta\psi_1 = (\sqrt{3}/2)\psi_1 + \tfrac{1}{2}\psi_2, \tag{43}$$

where

$$\psi_2 = (1/\sqrt{3})(\ \boxed{2}\boxed{7} - \boxed{3}\boxed{6} + \boxed{4}\boxed{5}\ ). \tag{44}$$

Note that while both ψ_1 and ψ_2 are HWS of [2111], ψ_1 consists of symmetrized products

$$\left\{ \begin{array}{|c|}\hline\ \\ \hline\ \\ \hline\ \\ \hline\ \end{array} \times \boxed{\ } \right\}_{\text{sym}} \tag{45}$$

and ψ_2 belongs to

$$\left\{ \begin{array}{|c|}\hline\ \\ \hline\ \\ \hline\ \end{array} \times \begin{array}{|c|}\hline\ \\ \hline\ \end{array} \right\}_{\text{sym}}. \tag{46}$$

Thus, Θ induces a subsystem rearrangement and its nonvanishing matrix elements between states of the types (45) and (46) give the weightage with which each rearrangement takes place. Other possible interesting operator combinations of SO(N) generators are worth examining.

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Grassmann analogs of classical matrix groups

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In general, if the parameters of a real or complex algebraic matrix group are replaced by Grassmann parameters, without changing the algebraic constraints, the resulting set fails to form a group. It is shown how to remedy this defect of naive Grassmannification by generalizing the constraint relations. In particular, it is shown how to define Grassmann analogs of the orthogonal, unitary, and symplectic groups.

I. INTRODUCTION

In a recent paper,[1] Ebner initiated the study of Grassmann analogs of classical matrix groups. Ebner's idea was that a group, whose elements are real or complex matrices subject to algebraic constraints, should be Grassmannified by replacing the field of real or complex numbers by a Grassmann algebra, retaining the algebraic constraints without change. Grassmannification is deemed to be successful if the resulting set is actually a group. Ebner[1] showed that, although general linear groups could be Grassmannified successfully, the same was not true of orthogonal groups. Thus the concept of Grassmannification seemed to be of limited scope. In this paper we demonstrate that Grassmannification is, on the contrary, a natural and widely applicable process provided that we allow the defining relations of the classical matrix groups to be modified on replacing the parameter set by a Grassmann algebra. We construct Grassmann generalizations of the classical orthogonal, unitary, and symplectic groups.

Our paper and that of Ebner[1] are contributions to the development of matrix groups beyond the well-established theory of matrix supergroups.[2] We recall, for example, from Rittenberg,[3] that a matrix supergroup consists of invertible matrices of the form

$$\left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right), \tag{1}$$

where the entities in the square matrices A and D (respectively, the rectangular matrices B and C) are even (respectively, odd or uneven) elements from a Grassmann algebra. A number of these supergroups and the corresponding infinitesimal Lie superalgebras, also listed in Ref. 3, have received considerable attention in recent years both with respect to their interesting mathematical properties[2,4] and to the applications to supersymmetric theories of particle physics.[5] We remark that the groups we consider in this paper are Lie groups and, although not actually Lie supergroups, they are subgroups of the Lie supergroups of matrices of the form (1), having unit superdeterminant and for which $A = D$ and $B = C$.

The contents of the paper are as follows. In Sec. II we review the elementary theory of Grassmann algebras and introduce some terminology which we find useful in our development. Section III contains a review of the Grassmannified full matrix group of Ebner[1] together with some remarks relating to special subgroups and the observation that the group can be embedded in the supergroup mentioned above. In Sec. IV we give our definition of Grassmannified classical matrix groups and establish their structure as semidirect products. In the remaining sections, Secs. V, VI, and VII we consider in detail the Grassmannification of the classical orthogonal, unitary, and symplectic groups.

II. GRASSMANN ALGEBRAS

Denote by $B_p(F)$ the Grassmann algebra, over the field F, generated by the identity 1 and the p independent generators θ_i, $1 \leqslant i \leqslant p$. Then $B_p(F)$ has as basis the 2^p independent monomials

$$\begin{aligned} &1\,, \\ &\theta_i\,, \quad 1 \leqslant i \leqslant p\,, \\ &\theta_i\theta_j\,, \quad 1 \leqslant i < j \leqslant p\,, \\ &\vdots \\ &\theta_1\theta_2 \cdots \theta_p\,. \end{aligned} \tag{2}$$

The product in $B_p(F)$ is associative and is subject to the identity

$$\theta_i\theta_j + \theta_j\theta_i = 0\,, \tag{3}$$

for all i, j.

The general element of $B_p(F)$ can be written as

$$x = \alpha_0 1 + \sum_{i=1}^{p} \alpha_i\theta_i + \sum_{i<j} \alpha_{ij}\theta_i\theta_j + \cdots + \alpha_{12\ldots p}\theta_1\theta_2\cdots\theta_p\,, \tag{4}$$

where $\alpha_0, \alpha_i, \alpha_{ij}, \ldots$ belong to F.

The summand

$$x_k = \sum_{i_1 < i_2 \cdots i_k} \alpha_{i_1 i_2 \cdots i_k}\,\theta_{i_1}\theta_{i_2}\cdots\theta_{i_k}\,, \tag{5}$$

which is a homogeneous element of degree k, we call the k th part of x, for $k = 1,2,\ldots,p$. Then

$$x_{\text{nil}} = \sum_{k=1}^{p} x_k\,, \quad x_{\text{num}} = x - x_{\text{nil}}\,, \tag{6}$$

define the nilpotent and numeric parts of x, respectively.

Corresponding to expression (4) for a general element is the direct sum decomposition

$$B_p = \bigoplus_{k=0} B_{p,k}\,, \tag{7}$$

where $B_{p,k}$ contains the homogeneous elements of degree $k > 0$, and $B_{p,0}$ contains all numeric elements. We have for

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convenience suppressed mention of the field F. Then

$$B_{p,k}\cdot B_{p,k'} \subseteq \begin{cases} B_{p,k+k'}, & k+k' \leqslant p, \\ \{0\} & k+k' > p, \end{cases} \tag{8}$$

which implies that B_p is a Z-graded algebra. There is a secondary grading by Z_2

$$B_p = B_{p,e} \oplus B_{p,u}, \tag{9}$$

where $B_{p,e}$ (respectively, $B_{p,u}$) consists of linear combinations of elements of even (respectively, uneven; i.e., odd) degree. At the element level

$$x = x_e + x_u, \tag{10}$$

where $x_e \in B_{p,e}$ is the even part of x and $x_u \in B_{p,u}$ is the uneven part of x. Furthermore, as a consequence of (3)

$$\begin{aligned} x_e\, y_e &= y_e x_e, \\ x_e\, y_u &= y_u x_e, \\ x_u\, y_u &= -y_u x_u, \end{aligned} \tag{11}$$

for all x_e, $y_e \in B_{p,e}$ and x_u, $y_u \in B_{p,u}$. The members of the set $B_{p,e} \cup B_{p,u}$ are the even and uneven elements of B_p. Here, $B_{p,e}$, but not $B_{p,u}$, is a subalgebra of B_p.

With respect to multiplication, the inverse x^{-1} of $x \in B_p$ exists, and is unique, if and only if $x_{\text{num}} \neq 0$. The set of all invertible elements in B_p is a multiplicative group, which we call the Grassmann group and denote by B_p^*. There is a subgroup B_p^{**}, the unipotent Grassmann group, consisting of those elements x for which $x_{\text{num}} = 1$. Then B_p^{**} is a normal subgroup of B_p^* and appears in the semidirect product decomposition

$$B_p^* = F^* \circledS B_p^{**}, \tag{12}$$

where F^* is the multiplicative group of nonzero elements of the field F. Two other natural subgroups are the intersections of B_p^* and B_p^{**} with $B_{p,e}$. Finally, if $F = R$ or C, then B_p^* and B_p^{**} are Lie groups over F of dimensions 2^p and $2^p - 1$, respectively.

III. THE FULL MATRIX GROUP $G_n(p,F)$

The Grassmann group B_p^* is the analog in B_p of the group F^* of the field F. Noting that F^* can be considered as the group of invertible 1×1 matrices over F, we can ask if there is a Grassman analog of the general linear group of invertible $n\times n$ matrices over F. An affirmative answer to this question was given by Ebner,[1] who defined the Grassmannified full matrix group. In our notation let M be an $n\times n$ matrix with entries in $B_p(F)$. We denote the set of all such matrices by $M_n(p,F)$. Then we can write

$$M = M_{\text{num}} + M_{\text{nil}}, \tag{13}$$

where the matrix elements of M_{num} (respectively, M_{nil}) contain only the numeric (respectively, nilpotent) parts of the matrix elements of M. It is not difficult to see that M is invertible if and only if M_{num} is invertible, or equivalently, if and only if $\det M_{\text{num}} \neq 0$. This condition is also equivalent to $\det M_e \neq 0$, where M_e is the matrix whose entries are the even parts of those of M, and the determinant makes sense because $B_{p,e}$ is a commutative algebra. It is perhaps worthwhile interjecting here that the usual definition of the determinant of a matrix does not extend unambiguously, let alone multiplicatively, to general Grassmann matrices. Also, $\det M_e$ is not multiplicative. For supermatrices, however, there is a multiplicative function called the superdeterminant.[5,6]

It is straightforward to check that the set of all invertible $n\times n$ matrices over $B_p(F)$ forms a group. This group, which we denote by $G_n(p,F)$, has a number of easily defined subgroups:

$$\begin{aligned} SG_n(p,F) &= \{M{:}\det M_{\text{num}} = 1\}, \\ IG_n(p,F) &= \{M{:}M_{\text{num}} = 1\}, \\ EG_n(p,F) &= \{M{:}M_u = 0\}, \end{aligned} \tag{14}$$

and intersections of SG_n, IG_n with EG_n. Clearly,

$$IG_n \leqslant SG_n \leqslant G_n, \tag{15}$$

with strict inclusions for $n > 1$. For $n = 1$ we have

$$\begin{aligned} G_1(p,F) &= B_p^*(F), \\ IG_1(p,F) &= SG_1(p,F) = B_p^{**}(F). \end{aligned} \tag{16}$$

Of more interest, however, are the subgroups in which the nilpotent parts of matrix elements are subject to algebraic constraints. It is such subgroups which we consider in the next section.

To close this section we note that the full matrix group $G_n(p,F)$, although not a matrix supergroup in the usual sense, let alone a Lie supergroup, is isomorphic to a subgroup of the Lie supergroup Q_{2n} of $2n\times 2n$ invertible supermatrices of the form

$$\left(\begin{array}{c|c} A & B \\ \hline B & A \end{array}\right), \tag{17}$$

where A (respectively, B) is an $n\times n$ even (respectively, uneven) Grassmann matrix. To see this we merely check that

$$M = M_e + M_u \rightarrow \left(\begin{array}{c|c} M_e & M_u \\ \hline M_u & M_e \end{array}\right) \tag{18}$$

is multiplicative.

This isomorphism enables us to define subgroups of Q_{2n}. We note that the elements of Q_{2n} have supertrace zero and unit superdeterminant. It remains to be seen whether this isomorphism is a useful tool in Grassmann group theory, possibly taking advantage of the ω-superdeterminant on Q_{2n} (see Rittenberg[3]).

IV. SUBGROUPS OF $G_n(p,F)$

Ebner[1] has shown, as a counterexample to the general applicability of Grassmannification, that it is not possible to Grassmannify the real orthogonal group in the obvious way. Ebner observes that the set of members $G_n(p,R)$ which satisfy

$$MM^t = 1, \tag{19}$$

where t means the usual matrix transpose, does not form a group. The failure to form a group can be seen in the context of the following result.

Theorem 1: Let X be a fixed member of $G_n(p,F)$, and let $\omega{:}M \rightarrow M^\omega$ be an operation on $M_n(p,F)$ preserving the identity matrix. Define the set

$$\Lambda = \{M \in G_n(p,F){:}MXM^\omega = X\}. \tag{20}$$

Then Λ forms a group if and only if we have the following.

(i) $(M^\omega)^{-1} = (M^{-1})^\omega$, for all $M \in \Lambda$.

(ii) $(MN)^\omega = N^\omega M^\omega$, for all $M, N \in \Lambda$.

Proof: We are given that ω preserves the identity matrix, which ensures, from definition (20), that Λ contains the identity.

If $M \in \Lambda$, then, again from (20), both M and $M^\omega \in G_n(p,F)$. This in particular implies that both M and M^ω are invertible. The constraint relation (20) can therefore be rewritten

$$M^{-1} X (M^\omega)^{-1} = X . \tag{21}$$

It follows that Λ contains M^{-1} if and only if

$$(M^\omega)^{-1} = (M^{-1})^\omega . \tag{22}$$

If $M, N \in \Lambda$, then

$$\begin{aligned} MNX(MN)^\omega &= X(M^\omega)^{-1}(N^\omega)^{-1}(MN)^\omega \\ &= X(N^\omega M^\omega)^{-1}(MN)^\omega . \end{aligned} \tag{23}$$

Then $MN \in \Lambda$ if and only if

$$(MN)^\omega = N^\omega M^\omega . \tag{24}$$

The theorem is seen to be true when we recall that a set with a binary, associative product, and containing an identity, is a group if and only if it is closed under the taking of inverses and products. This concludes the proof.

Taking X to be the identity matrix and ω to be the ordinary matrix transpose, the set Λ defined by (20) fails to be a group because the transpose operation does not satisfy (24). We shall see, however, in Sec. V, that is is possible to extend the matrix transpose operation in a number of ways each of which gives rise to a group in accordance with Theorem 1. Now we consider the structural consequences of imposing some further conditions on the operation and the matrix X.

We say that the operation ω is Z linear if

$$(M_1 + M_2)^\omega = M_1^\omega + M_2^\omega , \tag{25}$$

for all Grassmann matrices M_1, M_2.

We say that ω is numeric if

$$(M^\omega)_{\text{num}} = (M_{\text{num}})^\omega , \tag{26}$$

for all M. Then, if ω is also Z linear, we have

$$(M^\omega)_{\text{nil}} = (M_{\text{nil}})^\omega . \tag{27}$$

We say that $M = 1 + P$ is unipotent if $P_{\text{num}} = 0$. Using these definitions we can state and prove Theorem 2.

Theorem 2: A group Λ defined by a condition of the form (20), where X is numeric and ω is a Z linear, numeric operation, has the semidirect product factorization,

$$\Lambda = \Lambda_{\text{num}} \circledS \Lambda_{\text{uni}} , \tag{28}$$

where Λ_{num} is the subgroup consisting of numeric matrices and Λ_{uni} is the normal subgroup consisting of unipotent matrices. Furthermore, Λ_{uni} is nilpotent in the usual group theoretic sense.

Proof: Λ_{num} and Λ_{uni} are subgroups of Λ because each contains the identity and is closed under the taking of inverses and products. Furthermore, if $M \in \Lambda$ and $1 + P \in \Lambda_{\text{uni}}$, then the identity

$$M(1+P)M^{-1} = 1 + MPM^{-1} , \tag{29}$$

establishes that Λ_{uni} is a normal subgroup of Λ.

If $M = M_{\text{num}} + M_{\text{nil}}$ is an arbitrary member of Λ then condition (20) can be written as

$$(M_{\text{num}} + M_{\text{nil}})X((M_{\text{num}})^\omega + (M_{\text{nil}})^\omega) = X , \tag{30}$$

using the Z linearity of ω. But both X and ω are numeric, so the numeric part of (30) gives

$$M_{\text{num}} X (M_{\text{num}})^\omega = X . \tag{31}$$

Thus $M_{\text{num}} \in \Lambda_{\text{num}}$. In particular, M_{num} is invertible so we write

$$M = M_{\text{num}} + M_{\text{nil}} = M_{\text{num}}(1 + P) , \tag{32}$$

where $P_{\text{num}} = 0$. Here, $1 + P$ is both unipotent and a member of Λ, so it belongs to Λ_{uni}. Furthermore, it is clear that $\Lambda_{\text{num}} \cap \Lambda_{\text{uni}} = \{1\}$, from which it follows that the factorization (32) is unique. This establishes that Λ has the semidirect product structure (28).

We must now show that Λ_{uni} is a nilpotent group.[7] First observe that any matrix P for which $P_{\text{num}} = 0$ can be decomposed as a sum of homogeneous components

$$P = P_1 + P_2 + \cdots + P_p , \tag{33}$$

where the matrix elements of P_k are homogeneous of degree k, $k = 1,2,\ldots,p$. Define the set

$$\begin{aligned} \Lambda_{\text{uni},k} = \{ 1 + P : 1 + P \in \Lambda_{\text{uni}} \text{ and } P_i = 0 , \\ \text{for all } i < k \} . \end{aligned} \tag{34}$$

Then $\Lambda_{\text{uni},k}$ is a subgroup of Λ_{uni} and there is a chain of subgroups

$$\Lambda_{\text{uni}} = \Lambda_{\text{uni},1} \geqslant \Lambda_{\text{uni},2} \geqslant \cdots \geqslant \Lambda_{\text{uni},p+1} = \{1\} . \tag{35}$$

If we form the lower central series of Λ_{uni},

$$\Lambda_{\text{uni}} = \Gamma_1 \geqslant \Gamma_2 \geqslant \cdots , \tag{36}$$

then we can check that $\Gamma_i \leqslant \Lambda_{\text{uni},i}$, for all i. In particular the lower central series (36) terminates, which implies that Λ_{uni} is nilpotent.

Corollary: The series (35) is a central series which is normalized by Λ.

Proof: If $1 + P \in \Lambda_{\text{uni}}$, then $(1+P)^{-1} = 1 + P'$ for P' with $P'_{\text{num}} = 0$. Also, if $1 + Q(k) \in \Lambda_{\text{uni},k}$ and $M \in \Lambda_{\text{num}}$, then

$$\begin{aligned} &M(1+P)(1+Q(k))(1+P)^{-1}M^{-1} \\ &\quad = 1 + MQ(k)M^{-1} + \text{terms of degree} > k . \end{aligned} \tag{37}$$

In (37), taking M to be the identity, we see that $\Lambda_{\text{uni},k}$ is normal in Λ_{uni}. But, *a fortiori*, the homogeneous component of lowest degree in $Q(k)$, namely of degree k, is fixed under conjugation. This means that $\Lambda_{\text{uni},k}/\Lambda_{\text{uni},k+1}$ lies in the center of $\Lambda_{\text{uni}}/\Lambda_{\text{uni},k+1}$ for all k. Thus (35) is a central series.[7]

Furthermore, if M is not necessarily the identity in (37), it is clear that $MQ(k)M^{-1}$ has no component of degree less than k, so the right-hand side of (37) lies in $\Lambda_{\text{uni},k}$. Thus $\Lambda_{\text{uni},k}$ is normal in the whole of Λ. This completes the proof.

Theorem 2 reduces the problem of determining Λ to the independent problems of finding Λ_{num} and Λ_{uni}. However, if we are trying to Grassmannify a classical matrix group, then Λ_{num} will be that group and can therefore be assumed known. To solve the second problem we seek the set of unipotent matrices $M = 1 + P$ which satisfy condition (20). This reduces to

$$PX + XP^{\omega} = -PXP^{\omega}. \tag{38}$$

In general this still leaves us with an unpleasant nonlinear equation to solve. For our purposes we can achieve a substantial computational simplification by further restricting the form of the operation ω. We now assume that ω is homogeneous of degree zero: That means if M is a matrix, homogeneous of degree k, then so is M^{ω}, for all k. This restriction is stronger than demanding ω to be numeric, and further implies that ω stabilizes the central series (35). To take advantage we write P in terms of its homogeneous components, as in (33). We substitute into (38) and equate terms of the same degree of homogeneity:

$$\begin{aligned}
&P_1X + XP_1^{\omega} = 0,\\
&P_2X + XP_2^{\omega} = -P_1XP_1^{\omega},\\
&P_3X + XP_3^{\omega} = -(P_2XP_1^{\omega} + P_1XP_2^{\omega}),\\
&P_4X + XP_4^{\omega} = -(P_3XP_1^{\omega} + P_2XP_2^{\omega} + P_1XP_3^{\omega}),\\
&\vdots\\
&P_pX + XP_p^{\omega}\\
&\quad = -(P_{p-1}XP_1^{\omega} + P_{p-2}XP_2^{\omega} + \cdots P_1XP_{p-1}^{\omega}).
\end{aligned} \tag{39}$$

Now the determination becomes a problem in linear rather than nonlinear algebra. To see this it is perhaps now time to curtail the general treatment and to look at the particular problems of Grassmannifying a selection of the classical matrix groups. We first consider the real orthogonal groups.

V. GRASSMANN ORTHOGONAL GROUPS

If Λ_{num} is the $n\times n$ real orthogonal group, the X of Theorem 1 is the identity matrix, and the operation ω must coincide with the transpose for numeric matrices. The simplest way of extending the transpose to non-numeric matrices is to combine it with a certain $B_p(R)$ action, $*$, on matrix elements, which is independent of and leaves invariant their positions. We impose the following conditions on $*$ in order to satisfy the requirements of Theorem 1.

(i) $*$ is an R-linear transformation which respects the Z grading of B_p.

(ii) $(xy)* = y*x*$, for all $x,y,\in B_p$.

(iii) $(x*)* = x$, for all $x\in B_p$.

Conditions (i) and (ii) together imply that $*$ is completely determined by its linear action on a set of generators and (iii) further implies that this action is invertible. Choosing x to be numeric in (ii), we see that $*$ leaves invariant the numeric elements of B_p. Let $\theta = (\theta_1,\theta_2,\theta_3,\ldots,\theta_p)^t$ be the column vector whose entries are members of a set of generators. Then

$$\theta* = A\theta, \tag{40}$$

where A is an invertible $p\times p$ numeric matrix. Evidently condition (iii) implies that $A^2 = 1$. There are of course many solutions of this equation, of which we only require the simplest class representatives with respect to some reasonable equivalence relation. In fact, if $\phi = R\theta$ is another set of generators, where R is an invertible matrix, then the $*$ matrix of ϕ is RAR^{-1}. It is sensible to seek solutions A under the usual matrix equivalence relation

$$A\sim RAR^{-1}. \tag{41}$$

We have Lemma 1.

Lemma 1:

$$A\sim \text{Diag}(\epsilon_1,\epsilon_2,\ldots,\epsilon_p),$$

where $\epsilon_i = \pm 1$ and $\epsilon_i \geqslant \epsilon_{i+1}$ for all i.

Proof: Here, A satisfies a polynomial equation with distinct real factors. By a standard result of linear algebra,[8] A is diagonalizable and has eigenvalues $\epsilon_i = \pm 1$, $1\leqslant i\leqslant p$. Allowing for permutations amongst the generators we can arrange for $\epsilon_i \geqslant \epsilon_{i+1}$ for $1\leqslant i\leqslant p-1$.

It follows from Lemma 1 that there are $p+1$ inequivalent operations $*$. For each such operation we can extend to the whole of $M_n(p,R)$ by application to matrix entries, and then define an adjoint ω by

$$M^{\omega} = (M^t)* = M(*)^t, \tag{42}$$

for all $M\in M_n(p,R)$.

The set of Grassmann orthogonal matrices defined by such an operation is

$$\Lambda = \{M\in G_n(p,R) : MM^{\omega} = 1\}. \tag{43}$$

Thus $M\in\Lambda$ if and only if $M^{\omega} = M^{-1}$. Condition (i) of Theorem 1 reduces to $M = (M^{\omega})^{\omega}$, which is easily seen to be satisfied. Indeed $M = (M^{\omega})^{\omega}$ is valid for all members of $M_n(p,R)$. We now show that condition (ii) is also valid for all members of $M_n(p,R)$ and therefore in particular valid for all members of Λ.

We first observe, as has been assumed in (18), that any Grassmann matrix can be decomposed as

$$M = M_e + M_u, \tag{44}$$

where the matrix elements of M_e (respectively, M_u) are even (respectively, uneven) members of $B_p(R)$. We say that M is even (respectively, uneven) if $M_u = 0$ (respectively, $M_e = 0$).

For such matrices we define

$$|M| = \begin{cases} 0, & \text{if } M \text{ is uneven},\\ 1, & \text{if } M \text{ is uneven}. \end{cases} \tag{45}$$

Then it is easy to show that

$$(MN)^t = (-1)^{|M||N|}N^tM^t, \tag{46}$$

and

$$(MN)* = (-1)^{|M||N|}M*N*, \tag{47}$$

and therefore

$$(MN)^{\omega} = N^{\omega}N^{\omega}, \tag{48}$$

for all even and uneven members of $M_n(p,R)$. Using the decomposition (44), the identity (48) extends to all members of $M_n(p,R)$.

Finally, noting that ω preserves the identity, Theorem 1 establishes that Λ is a group.

By construction, each possible ω is Z linear and homogeneous of degree zero. It follows that the structure Theorem 2 applies to each of the $p+1$ distinct Grassmannified orthogonal groups and that we may use the linear constructive theory, embodied in (39), to find the unipotent subgroups.

Let us now consider specific forms for the operation ω. Of the $p+1$ inequivalent forms we choose for illustration the two simplest. The first, which we refer to as positive, leaves invariant all first-degree parts, and the second, which we refer to as negative, reverses the signs of all first-degree parts. For notation we use $O_n^{(r)}(p,R)$ to mean that Grass-

mannified orthogonal group for which r of the numbers ϵ_i, $i = 1,2,\ldots,p$, defining the relevant ω, are $+1$.

A. Positive orthogonal group $O_n^{(p)}(p,R)$

If ω is the positive operation and P_k is homogeneous of degree k, then

$$P_k^{\omega} = (-1)^{(1/2)k(k-1)} P_k^t . \tag{49}$$

Then the system (39) becomes

$$\begin{aligned} &P_1 + P_1^t = 0 , \\ &P_2 - P_2^t = -P_1 P_1^t , \\ &P_3 - P_3^t = P_1 P_2^t - P_2 P_1^t , \\ &P_4 + P_4^t = P_1 P_3^t - P_2 P_2^t - P_3 P_1^t , \\ &\vdots . \end{aligned} \tag{50}$$

Each of these equations has the form

$$\begin{aligned} &A + A^t = S , \\ \text{or} \quad &\\ &B - B^t = T , \end{aligned} \tag{51}$$

where S,T are matrices of appropriate symmetry with respect to matrix transposition and of appropriate degree of homogeneity. The general solution for A (respectively, B) is $\frac{1}{2}S$ (respectively, $\frac{1}{2}T$) plus an arbitrary antisymmetric (respectively, symmetric) matrix. Thus P_1 contains $\frac{1}{2}n(n-1)\binom{p}{1}$ free real parameters, P_2 contains $\frac{1}{2}n(n+1)\binom{p}{2}$ parameters, etc. We can calculate the dimension of $O_n^{(p)}(p,R)$ as a real Lie group, to be

$$\begin{aligned} &\frac{1}{2}n(n-1)\binom{p}{0} + \frac{1}{2}n(n-1)\binom{p}{1} + \frac{1}{2}n(n+1)\binom{p}{2} + \cdots \\ &= \frac{1}{2}n^2 \sum_{r=0}^{p} \binom{p}{r} - \frac{1}{2}n\left\{\binom{p}{0} + \binom{p}{1} - \binom{p}{2} - \binom{p}{3} + \cdots\right\} = 2^{p-1}n^2 - \tfrac{1}{2}nf(p) . \end{aligned} \tag{52}$$

To compute $f(p)$ we observe that

$$(1+i)^p = \binom{p}{0} + i\binom{p}{1} - \binom{p}{2} - i\binom{p}{3} + \cdots , \tag{53}$$

so that

$$\begin{aligned} f(p) &= \mathrm{Re}(1+i)^p + \mathrm{Im}(1+i)^p \\ &= 2^{p/2}(\cos(\pi p/4) + \sin(\pi p/4)) . \end{aligned} \tag{54}$$

Therefore

$$\begin{aligned} \dim O_n^{(p)}(p,R) &= 2^{p-1}n^2 - (n/2)2^{p/2} \\ &\quad \times(\cos(\pi p/4) + \sin(\pi p/4)) . \end{aligned} \tag{55}$$

B. Negative orthogonal group $O_n^{(0)}(p,R)$

If ω is the negative operation and P_k is homogeneous of degree k, then

$$P_k^{\omega} = (-1)^{(1/2)k(k+1)} P_k^t . \tag{56}$$

The system (39) becomes

$$\begin{aligned} &P_1 - P_1^t = 0 , \\ &P_2 - P_2^t = P_1 P_1^t , \\ &P_3 + P_3^t = P_1 P_2^t + P_2 P_1^t , \\ &P_4 + P_4^t = -P_1 P_3^t + P_2 P_2^t + P_3 P_1^t . \end{aligned} \tag{57}$$

An analysis similar to that for $O_n^{(p)}(p,R)$ gives

$$\begin{aligned} \dim O_n^{(0)}(p,R) &= 2^{p-1}n^2 - (n/2)2^{p/2} \\ &\quad \times(\cos(\pi p/4) - \sin(\pi p/4)) . \end{aligned} \tag{58}$$

VI. GRASSMANN UNITARY GROUP

If A_{num} is the $n \times n$ complex unitary group, the X of Theorem 1 is the identity matrix, and the operation ω must coincide with the Hermitian conjugate for numeric matrices. For general Grassmann matrices we combine the transpose with an operation $*$ on $B_p(C)$ which satisfies the following.

(i) $*$ is a conjugate-linear transformation which respects the Z grading of B_p.

(ii) $(xy)^* = y^* x^*$, for all $x, y \in B_p$.

(iii) $(x^*)^* = x$, for all $x \in B_p$.

Here, $*$ is determined by its action on a set of generators:

$$\theta^* = B\theta , \tag{59}$$

where B is a complex invertible $p \times p$ numeric matrix. Condition (iii) implies

$$\overline{B}B = B\overline{B} = 1 , \tag{60}$$

where the bar means complex conjugation. We seek solutions of (60) up to the equivalence relation

$$B \simeq \overline{R} B R^{-1} , \tag{61}$$

where R is a complex invertible matrix.

Lemma 2: Every solution of (60) is equivalent to the identity.

Proof: Here, $\overline{B}$ has a finite number of eigenvalues. Hence we can find α such that $e^{i\alpha}$ is not an eigenvalue of $\overline{B}$. It follows that

$$Q = ie^{i\alpha/2} 1 - ie^{-i\alpha/2}\overline{B} \tag{62}$$

is invertible. Also we have

$$BQ = ie^{i\alpha/2} B - ie^{-i\alpha/2} 1 = \overline{Q} . \tag{63}$$

We deduce, putting $R^{-1} = Q$, that $B \sim 1$. The ω operation obtained from $*$ satisfies the conditions of Theorems 1 and 2. Thus a Grassmann unitary group $U_n(p,C)$ exists. To determine the structure of the unipotent subgroup we examine the action of $*$ on elements of fixed degree in $B_p(C)$. First we can check

$$(\theta_{i_1}\theta_{i_2}\cdots\theta_{i_k})^* = (-1)^{(1/2)k(k-1)} \theta_{i_1}\theta_{i_2}\cdots\theta_{i_k} . \tag{64}$$

Then, if $z_k = x_k + iy_k$ has degree k in $B_p(C)$,

$$z_k^* = (-1)^{(1/2)k(k-1)}(x_k - iy_k) , \tag{65}$$

where x_k, y_k, $B_p(R)$ are the real and imaginary parts of z_k. Extending this action to matrices, if

$$P_k = P_{k,\mathrm{re}} + iP_{k,\mathrm{im}} \tag{66}$$

is the decomposition of a complex Grassmann matrix of de-

gree k into real and imaginary parts, then

$$P_k^{\omega} = (-1)^{(1/2)k(k-1)}(P_{k,\mathrm{re}}^t - iP_{k,\mathrm{im}}^t) . \tag{67}$$

Hence the system (39) becomes

$$\begin{aligned} &P_{1,\mathrm{re}} + iP_{1,\mathrm{im}} + (P_{1,\mathrm{re}}^t - iP_{1,\mathrm{im}}^t) = 0 , \\ &P_{2,\mathrm{re}} + iP_{2,\mathrm{im}} - (P_{2,\mathrm{re}}^t - iP_{2,\mathrm{im}}^t) = -P_1 P_1^{\omega} , \\ &\vdots . \end{aligned} \tag{68}$$

The dimension of $U_n(p,c)$, as a real Lie group, is

$$\begin{aligned} n^2\binom{p}{0} &+ \left\{\frac{1}{2}n(n-1)+\frac{1}{2}n(n+1)\right\}\binom{p}{1} \\ &+ \left\{\frac{1}{2}n(n+1)+\frac{1}{2}n(n-1)\right\}\binom{p}{2} + \cdots \\ &= n^2 \sum_{r=0} \binom{p}{r} = n^2 2^p . \end{aligned} \tag{69}$$

VII. GRASSMANN SYMPLECTIC GROUP

If Λ_{num} is the $2n\times 2n$ real (or complex) symplectic group $\mathrm{Sp}(2n,R)$ [or $\mathrm{Sp}(2n,C)$], the matrix X of Theorem 1 is the skew-symmetric matrix

$$J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}, \tag{70}$$

and the operation ω must coincide with the ordinary transpose for numeric matrices. We note that $J^{-1} = -J$. In our development there is no essential difference between the real and complex group, and we assume for definiteness that we are dealing with the real case. The extension of the transpose to general Grassmann matrices is taken to be any of those used for the orthogonal groups. This ensures that the condition (ii) of Theorem 1 is satisfied for all members of $G_{2_n}(p,R)$ and therefore, in particular, for all members of

$$\Lambda = \{M \in G_{2n}(p,R) : MJM^{\omega} = J\} . \tag{71}$$

To deal with condition (i) of Theorem 1, we suppose $M\in\Lambda$ and first take the inverse of both sides of the defining relation, giving

$$(M^{\omega})^{-1} J M^{-1} = J . \tag{72}$$

This can be rewritten as

$$JM^{-1} = M^{\omega} J . \tag{73}$$

We apply ω to this relation, giving

$$(M^{-1})^{\omega} J = JM . \tag{74}$$

In this we have used $J^{\omega} = -J$, $M^{\omega\omega} = M$, and condition (ii) of Theorem 1, which we have observed above is satisfied. Finally, multiply (72) on the right by M and compare with (74). Thus

$$(M^{-1})^{\omega} = (M^{\omega})^{-1} , \tag{75}$$

for all $M\in\Lambda$. This is precisely condition (i) of Theorem 1.

It follows that Λ forms a group, which we shall call a Grassmann symplectic group. As in the case of Grassmann orthogonal groups there are $p+1$ different cases depending on the specific choice of ω. To exemplify the dimensionality analysis we only consider the positive operation.

A. Positive symplectic group $\mathrm{Sp}_{2n}^{(p)}(p,R)$

If ω is the positive operation, then combining (39) with (49) for the constraints on the homogeneous parts of P, we have

$$\begin{aligned} &P_1 J + J_1 P_1^t = 0 , \\ &P_2 J - JP_2^t = -P_1 JP_1^t , \\ &P_3 J - JP_3^t = P_1 JP_2^t - P_2 JP_1^t , \\ &\vdots . \end{aligned} \tag{76}$$

Each of these equations is of the form

$$\begin{aligned} &AJ + JA^t = S , \\ &\text{or} \\ &BJ - JB^t = T , \end{aligned} \tag{77}$$

where S, T are $2n\times n$ matrices of appropriate symmetry, with respect to matrix transposition, and of appropriate degree of homogeneity. Then the general solution for A (respectively, B) is $-\frac{1}{2}SJ$ (respectively, $-\frac{1}{2}TJ$) plus a general solution of (77) with zero right-hand side. Thus P contains $(2n^2+n)\binom{p}{1}$ real parameters, P_2 contains $(2n^2-n)\binom{p}{2}$ real paraemters, etc. The dimension of $\mathrm{Sp}_{2n}^{(p)}(p,R)$ is easily calculated to be

$$\begin{aligned} \dim \mathrm{Sp}_{2_n}^{(p)}(p,R) &= 2^{p+1}n^2 + n2^{p/2} \\ &\times(\cos(\pi p/4) + \sin(\pi p/4)) . \end{aligned} \tag{78}$$

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On the infrared singularity of the resolvent of some Yang–Mills-type operators

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For operators of Yang–Mills type $H = \Sigma_{j=1}^{4}[-i(\partial/\partial x_j)\otimes 1 + A_j(x)]^2 + W(x)$ in $L^2(\mathbb{R}^4)\otimes\mathscr{Y}$ the infrared singularity of the resolvent $(H-\zeta)^{-1}$ is described completely in terms of asymptotic expansions as $\zeta\to 0$. $A_j(x)$ and $W(x)$ are required to satisfy $A_j(x) = O(|x|^{-2-\delta})$, $W(x) = O(|x|^{-2-\delta})$, as $|x|\to\infty$, $\delta > 0$.

I. INTRODUCTION AND SUMMARY

The present paper is concerned with the structure of the infrared singularity of the resolvent of a Euclidean Yang–Mills operator in $\mathscr{H} = L^2(\mathbb{R}^4)\otimes\mathscr{Y}$ ($\mathscr{Y}$ a finite-dimensional Hilbert space). One is interested in the resolvent because it is the covariance of a Gaussian process.

The operators considered here have the form

$$H = H_A + W = \sum_{j=1}^{4}\left(-i\frac{\partial}{\partial x_j}\otimes 1 + A_j(x)\right)^2 + W(x), \tag{1.1}$$

where $W(x)$ and the Yang–Mills potentials $A_j(x)$ are functions on $\mathbb{R}^4$ with values in the Hermitian operators on $\mathscr{Y}$. The $A_j(x)$ are related to the internal symmetries of the system. The $W(x)$ can describe additional coupling to the Yang–Mills potentials via the field tensor and also coupling to other external fields.

The results on the resolvent $R(\zeta) = (H-\zeta)^{-1}$ are given in the form of asymptotic expansions as $\zeta\to 0$. In order to obtain results with only algebraic decay of $A_j(x)$ and $W(x)$ it is necessary to use a somewhat complicated topology for the expansion. The expansions are given in the operator norm of the bounded operators from $\mathbb{H}^{-1,s}$ to $\mathbb{H}^{1,-s'}$, where $\mathbb{H}^{1,s}$ denotes the weighted Sobolev space (see Sec. II). The $s, s' > 0$ are suitably chosen, depending on the order of the expansion.

Disregarding topology, we can briefly describe the results as follows. First consider $R_A(\zeta) = (H_A-\zeta)^{-1}$, H_A as in (1.1). For generic $A_j(x)$ (see Assumption 2.3) we have

$$R_A(\zeta) = F_0 + \zeta\log\zeta F_1^1 + \zeta F_1^0 + \zeta^2(\log\zeta)^2 F_2^2 + \zeta^2\log\zeta F_2^1 + \zeta^2 F_2^0 + o(\zeta^2),$$

as $\zeta\to 0$. The F_j^k are explicitly given.

Adding W we get expansions of four different types, depending on whether zero is an eigenvalue, a zero resonance, both, or neither, for $H = H_A + W$. Let us note that a zero resonance occurs when $Hu = 0$ has a solution of $u\neq 0$ in a space slightly larger than $\mathscr{H}$. The leading singularity can be described in each case as follows.

(i) If zero is neither an eigenvalue nor a zero resonance

$$R(\zeta) = B_0 + O(\zeta\log\zeta) \quad \text{as } \zeta\to 0.$$

(See Theorem 3.4.)

(ii) If zero is a zero resonance, but not an eigenvalue, let $\{\psi_j\}_{j=1}^{N_0}$ denote a maximal linearly independent set of zero resonance functions, suitably normalized;

$$R(\zeta) = -\frac{1}{\zeta\log\zeta}\sum_{j=1}^{N_0}\langle\cdot,\psi_j\rangle\psi_j + O((\zeta(\log\zeta)^2)^{-1}) \quad \text{as } \zeta\to 0.$$

(See Theorem 3.5 for a more precise result.)

(iii) If zero is an eigenvalue, but not a zero resonance, let P_0 be the orthogonal projection in $\mathscr{H}$ onto eigenspace for eigenvalue zero:

$$R(\zeta) = -(1/\zeta)P_0 + \log\zeta C_0 + O(1) \quad \text{as } \zeta\to 0.$$

Note that besides the expected ζ^{-1} singularity there is also a $\log\zeta$ singularity. C_0 is found explicitly. (See Theorem 3.6.)

(iv) If zero is both an eigenvalue and a zero resonance, a specific choice of zero resonance functions $\{\psi_j\}$ gives an expansion where the leading term is the sum of the leading terms in (ii) and (iii) above. (See Theorem 3.7 for a more precise statement.)

Several results on asymptotic expansion of the resolvent of Schrödinger operators in the low energy limit have been obtained recently.[1–4] Expansions are obtained by applying a perturbation argument to the expansion of the kernel of the resolvent of the Laplacian, which is given in terms of a Hankel function. The argument needed to obtain the results of the present paper are similar to those given by Jensen–Kato[1] and Jensen,[3] so some details will be omitted here. The perturbation arguments require a decay $A_j(x) = O(|x|^{-2-\delta})$ and $W(x) = O(|x|^{-2-\delta})$ as $|x|\to\infty$, $\delta > 0$. Topologically nontrivial Yang–Mills potentials have a slower decay or too-strong local singularities to satisfy our assumptions. Recent results[5] indicate that an expansion of $R(\zeta)$ with, e.g., $A_j(x)$ the instanton solution will have a form different from the expansions given here.

The results obtained here can be used to obtain asymptotic expansions of the regularized perturbation determinant in the infrared limit. These results will be given elsewhere.

It is possible to include an external metric in the operator H_A, provided it satisfies an assumption similar to Assumption 2.3. For several results on Yang–Mills operators with an external metric, see Cotta-Ramusino *et al.*[6]

Finally let us note that the results given here are specific to four dimensions. Results are known in any dimensions,[1–4]

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but we have restricted our attention to the physically interesting one.

II. NOTATION AND PRELIMINARY RESULTS

In this section we introduce our notation and give some preliminary results. Let $\mathscr{Y}$ be a finite-dimensional Hilbert space. Our basic Hilbert space is $\mathscr{H} = L^2(\mathbb{R}^4) \otimes \mathscr{Y}$. Let $\mathscr{S}'(\mathbb{R}^4)$ denote the tempered distributions and $\mathscr{F}$ the Fourier transform. The weighted Sobolev space is given by

$$H^{m,s}(\mathbb{R}^4) = \{f \in \mathscr{S}'(\mathbb{R}^4) \mid \|f\|_{m,s} = \|(1+x^2)^{s/2}(1-\Delta)^{m/2} f\|_{L^2} < \infty\},$$

for any $m, s \in \mathbb{R}$. The spaces used here are given by

$$\mathbb{H}^{m,s} = H^{m,s}(\mathbb{R}^4) \otimes \mathscr{Y}.$$

The inner product $\langle \cdot, \cdot \rangle$ on $\mathscr{H} = \mathbb{H}^{0,0} = L^2(\mathbb{R}^4) \otimes \mathscr{Y}$ extends to a natural duality between $\mathbb{H}^{m,s}$ and $\mathbb{H}^{-m,-s}$, $m, s \in \mathbb{R}$. We also note that the Fourier transform $\mathscr{F} \otimes 1$ extends to an isomorphism from $\mathbb{H}^{m,s}$ to $\mathbb{H}^{s,m}$ for any $m, s \in \mathbb{R}$.

We consider operators of the form

$$H = H_A + W = \sum_{j=1}^{4} \left(-i \frac{\partial}{\partial x_j} \otimes 1 + A_j(x) \right)^2 + W(x),$$

where $A_j(x)$ and $W(x)$, $x \in \mathbb{R}^4$, are Hermitian operators on $\mathscr{Y}$. In some computations it is convenient to decompose H_A as follows:

$$H_A = H_0 + V_A, \quad H_0 = -\Delta \otimes 1,$$

$$V_A = \sum_{j=1}^{4} \left(\left(-i \frac{\partial}{\partial x_j} \otimes 1 \right) A_j(x) + A_j(x) \left(-i \frac{\partial}{\partial x_j} \otimes 1 \right) + A_j(x)^2 \right).$$

In applications, $A_j(x)$ and $W(x)$ are multiplication by Hermitian matrices (in a given basis in $\mathscr{Y}$) for each $x \in \mathbb{R}^4$. We need some regularity and decay assumptions. The following general assumption is used for $U = V_A$ and $U = W$.

Assumption 2.1: Let U be a symmetric operator such that for some $\beta > 0$, U defines a compact operator from $\mathbb{H}^{1,s}$ to $\mathbb{H}^{-1,s+\beta}$ for all $s \in \mathbb{R}$.

If $A_j(x)$ is a multiplication operator and V_A is defined as above, V_A compact from $\mathbb{H}^{1,0}$ to $\mathbb{H}^{-1,\beta}$ implies that V_A is compact from $\mathbb{H}^{1,s}$ to $\mathbb{H}^{-1,s+\beta}$ for any $s \in \mathbb{R}$. This follows by computing the commutator between V_A and $(1+x^2)^{s/2}$. The same result holds for $W(x)$.

As an example consider $A_j(x)$ and $W(x)$ which are multiplication operators. Let $|||\cdot|||$ denote any norm on the bounded operators on $\mathscr{Y}$. Assume

$$|||A_j(x)||| \leqslant c(1+|x|)^{-\mu},$$

$$|||W(x)||| \leqslant c(1+|x|)^{-\mu},$$

for some $\mu > 0$, $c > 0$. Then V_A and W satisfy Assumption 2.1 for any $\beta < \mu$.

Let V_A and W satisfy Assumption 2.1. Then $H_A = (-\Delta \otimes 1) + V_A$ and $H = H_A + W$ are the self-adjoint operators obtained from the quadratic form sum.[7,8]

Let $B(m, s; m', s') = B(\mathbb{H}^{m,s}, \mathbb{H}^{m',s'})$ denote the bounded operators from $\mathbb{H}^{m,s}$ to $\mathbb{H}^{m',s'}$, with the operator norm. We also use the notation

$$\mathbb{H}^{m,s+0} = \bigcup_{t>s} \mathbb{H}^{m,t}, \quad \mathbb{H}^{m,s-0} = \bigcap_{t<s} \mathbb{H}^{m,t},$$

but we do not introduce any topology on these vector spaces.

Let $R_0(\zeta) = (H_0 - \zeta)^{-1}$. In Jensen[3] an asymptotic expansion for $(-\Delta - \zeta)^{-1}$ was obtained by expanding the integral kernel of this operator, which is given explicitly in terms of a Hankel function. Only the two finite expansions used in the sequel are given here. In the sequel we assume $\operatorname{Im} \zeta \geqslant 0$ and $\log \zeta$ denotes the principal branch of the natural logarithm. We have the following lemma.[3,4]

Lemma 2.2: (i) Let $s, s' > 2$. We have in $B(-1, s; 1, -s')$ the expansion

$$R_0(\zeta) = G_0 + \zeta \log \zeta G_1^1 + \zeta G_1^0 + o(\zeta) \quad \text{as } \zeta \to 0.$$

(ii) Let $s, s' > 4$. We have in $B(-1, s; 1, -s')$ the expansion

$$R_0(\zeta) = = G_0 + \zeta \log \zeta G_1^1 + \zeta G_1^0 + \zeta^2 \log \zeta G_2^1 + \zeta^2 G_2^0 + o(\zeta^2) \quad \text{as } \zeta \to 0.$$

(iii) The coefficients are given as follows. $G_j^k = \tilde{G}_j^k \otimes 1$, and $\tilde{G}_j^k$ are given by the following integral kernels:

$$\tilde{G}_0 : (4\pi^2)^{-1} |x-y|^{-2},$$

$$\tilde{G}_1^1 : -(4\pi^2)^{-1} 1,$$

$$\tilde{G}_1^0 (4\pi)^{-2} (\pi i - \gamma) \cdot 1 - (8\pi^2)^{-1} \log(|x-y|/2),$$

$$\tilde{G}_2^1 : (8\pi^2)^{-1} |x-y|^2,$$

$$\tilde{G}_2^0 : -(8\pi^2)^{-1} (\tfrac{3}{2} - 2\gamma + \pi i)|x-y|^2 + (4\pi)^{-2} \log(|x-y|/2)|x-y|^2.$$

Here γ is Euler's constant.

(iv) The coefficients have the following properties:

$$G_0 \in B(-1, s; 1, -s'), \quad \text{for } s, s' > 0, \quad s + s' \geqslant 2,$$

$$G_1^1, G_1^0 \in B(-1, s; 1, -s'), \quad \text{for } s, s' > 2,$$

$$G_2^1, G_2^0 \in B(-1, s; 1, -s'), \quad \text{for } s, s' > 4.$$

In discussing expansions of the resolvent $R(\zeta) = (H_A + W - \zeta)^{-1}$ we are interested in separating the contribution from $A_j(x)$. For this purpose we need the following assumption.

Assumption 2.3: Let V_A satisfy Assumption 2.1 for some $\beta > 2$. Assume that the operator $1 + G_0 V_A \in B(1, -s; 1, -s)$, $0 < s < \beta$, is invertible.

Note that Lemma 2.2 (iv) and Assumption 2.1 on V_A for $\beta > 2$ imply $G_0 V_A \in B(1, -s; 1, -s)$ for any s, $0 < s < \beta$. Assumption 2.3 means[9] that 0 is a regular point for H_A. Therefore[10] $H_A u = 0$ has only the trivial solution $u = 0$ in $\mathbb{H}^{1,-s}$, $0 < s \leqslant 2$. When $A_j(x)$ is multiplicative, 0 is not an eigenvalue.[6] Thus in this case the assumption excludes a zero resonance. Let us note that Assumption 2.3 is satisfied generically; i.e., consider a family

$$H_{\kappa A} = \sum_{j=1}^{4} \left(-i \frac{\partial}{\partial x_j} \otimes 1 + \kappa A_j(x) \right)^2.$$

Then the assumption is satisfied except for a discrete set of $\kappa \in \mathbb{R}$, as is easily seen using the analytic Fredholm theorem.[8]

We have the following expansion result for the resolvent $R_A(\zeta)=(H_A-\zeta)^{-1}=(H_0+V_A-\zeta)^{-1}$.

Theorem 2.4: Let V_A satisfy Assumption 2.3.

(i) Let V_A satisfy Assumption 2.1 for some $\beta=\beta(V_A)>2$. Let $s,s'>2$. We then have in $B(-1,s;1,-s')$ the expansion

$$R_A(\zeta)=F_0+\zeta\log\zeta F_1^1+\zeta F_1^0+o(\zeta),$$

as $\zeta\to 0$.

(ii) Let V_A satisfy Assumption 2.1 for some $\beta=\beta(V_A)>4$. Let $s,s'>4$. We then have in $B(-1,s;1,-s')$ the expansion

$$R_A(\zeta)=\sum_{j=1}^{2}\sum_{l=0}^{j}F_j^l\zeta^j(\log\zeta)^l+o(\zeta^2),$$

as $\zeta\to 0$.

(iii) The coefficients are given as follows. We write $X=(1+G_0V_A)^{-1}$ and $X^*=(1+V_AG_0)^{-1}$. Then

$$F_0=F_0^0=XG_0=G_0X^*,$$
$$F_1^1=XG_1^1X^*,$$
$$F_1^0=XG_1^0X^*,$$
$$F_2^2=-XG_1^1V_AXG_1^1X^*,$$
$$F_2^1=XG_2^1X^*-XG_1^1V_AXG_1^0X^*-XG_1^0V_AXG_1^1X^*,$$
$$F_2^0=XG_2^0X^*-XG_1^0V_AXG_1^0.$$

(iv) The coefficients satisfy

$F_0\in B(-1,s;1,-s')$ for $s,s'>0$, $s+s'\geq 2$, $\beta(V_A)>2$,

$F_1^1,F_1^0\in B(-1,s;1,-s')$ for $s,s'>2$, $\beta(V_A)>2$,

$F_2^2,F_2^1,F_2^0\in B(-1,s;1,-s')$ for $s,s'>4$, $\beta(V_A)>4$.

Proof: These results follow from Jensen,[3] except the improved conditions on s, s', β, which are due to Murata.[4]

III. INFRARED EXPANSIONS FOR THE EUCLIDEAN YANG–MILLS OPERATOR

We begin our discussion of $R(\zeta)=(H-\zeta)^{-1}$ by classifying the possibilities for the point zero in the spectrum of H, using the coefficients in the expansion of $R_A(\zeta)=(H_A-\zeta)^{-1}$. The proofs run along the line of Jensen,[3] except that here $\dim\mathscr{V}>1$. We shall sketch the changes necessary to accommodate this case. The idea of the proofs is to use the expansion for $(H_0+V_A+W-\zeta)^{-1}$, which can be obtained as in Jensen[3] and Murata,[4] and then to separate out the contribution from V_A, using assumption 2.3.

Let V_A,W satisfy Assumption 2.1 with $\beta=\beta(V_A)=\beta(W)>2$. Let V_A satisfy Assumption 2.1. Then

$$\tilde{\mathscr{M}}=\{u\in\mathbb{H}^{1,-s}|(1+G_0(V_A+W))u=0\},$$
$$\tilde{\mathscr{N}}=\{v\in\mathbb{H}^{-1,s}|(1+(V_A+W)G_0)v=0\},$$

$0<s<\beta$. These spaces are finite-dimensional and independent[3] of s. By assumption $(1+G_0V_A)$ is invertible. Thus one has

$$1+G_0(V_A+W)=(1+G_0V_A)(1+(1+G_0V_A)^{-1}G_0W)$$
$$=(1+G_0V_A)(1+F_0W),$$

and then $(0<s<\beta)$

$$\mathscr{M}=\{u\in\mathbb{H}^{1,-s}|(1+F_0W)u=0\}=\tilde{\mathscr{M}},$$
$$\mathscr{N}=\{v\in\mathbb{H}^{-1,s}|(1+WF_0)v=0\}=(1+V_AG_0)\tilde{\mathscr{N}}.$$

Let us note that generically $\mathscr{M}=\mathscr{N}=\{0\}$. More precisely, consider $H(\kappa)=H_A+\kappa W$. The compactness of F_0W implies that (with an obvious notation) $\mathscr{M}(\kappa)=\mathscr{N}(\kappa)=\{0\}$ except for a discrete set of $\kappa\in\mathbb{R}$.

Lemma 3.1: Under the above assumptions we have the following.

(i) $(H_A+W)\mathscr{M}=\{0\}$.

(ii) $\mathscr{M}=\{u\in\mathbb{H}^{1,-s}|(H_A+W)u=0\}$, $0<s\leq 2$.

Proof: See Jensen–Kato[1] and Jensen.[3]

Lemma 3.2: Let $u\in\mathscr{M}$. Then $u\in\mathscr{H}(=\mathbb{H}^{0,0}=L^2(\mathbb{R}^4)\otimes\mathscr{V})$ if and only if $F_1^1Wu=0$.

Proof: We use some results from Jensen.[3] Let $u\in\mathscr{M}$. Then $u\in\mathscr{H}$ if and only if $G_1^1(V_A+W)u=0$. This condition is rewritten as follows. By Lemma 3.1 $u\in\mathbb{H}^{1,0-0}$, and $(H_0+V_A+W)u=0$. $H_0u=-(V_A+W)u\in\mathbb{H}^{-1,2+0}$, so (see Ref. 3) $u=G_0H_0u$, and $(1+G_0(V_A+W))u=0$. Hence

$$(V_A+V_AG_0V_A+V_AG_0W)u=0$$

and

$$(V_A+W+V_AG_0V_A+V_AG_0W)u=Wu.$$

Thus one has

$$(1+G_0V_A)(V_A+W)u=Wu$$

or

$$(V_A+W)u=(1+G_0V_A)^{-1}Wu.$$

Then the condition $G_1^1(V_A+W)u=0$ can be written $G_1^1(1+V_AG_0)^{-1}Wu=0$ or, using Theorem 2.4 (iii), $F_1^1Wu=0$.

Let P_0 denote the orthogonal projection onto eigenspace for eigenvalue zero for H in $\mathscr{H}$. If zero is not an eigenvalue, $P_0=0$. Lemma 3.2 shows $\dim(\mathscr{M}/P_0\mathscr{H})=\operatorname{rank}(F_1^1W)\leq\dim\mathscr{V}$, and simple examples using spherical square well potentials show that $\dim(\mathscr{M}/P_0\mathscr{H})$ can have any value between 0 and $\dim\mathscr{V}$. If $\mathscr{M}/P_0\mathscr{H}\neq 0$, H is said to have a *zero resonance*.

Any function $\psi\in\mathscr{M}\setminus P_0\mathscr{H}$ can be called a zero resonance eigenfunction. There is a choice[1,3] of a maximal linearly independent set in $\mathscr{M}\setminus P_0\mathscr{H}$, which gives a particularly simple form of the expansions. Note that no such result is given by Murata.[4]

Let us briefly describe how this set is chosen. Let Q be the canonical projection onto the algebraic null space[11] for $1+G_0V_A(=\mathscr{M})$. Assume $\beta>4$ and write $V=V_A+W$ for simplicity. Define in $\mathbb{H}^{1,-s}$, $0<s<\beta-2$, the operators

$$Q_0=1-Q,\quad Q_1=(1-P_0VG_1^0V)Q,\quad Q_2=P_0VG_1^0VQ.$$

By definition $Q_0+Q_1+Q_2=1$, and one can show $Q_jQ_k=\delta_{jk}Q_k$, $j,k=0,1,2$. We use these operators to classify the point zero in the spectrum of H. Here 0 is said to be *a regular* point for H, if $Q_1=Q_2=0$. Here, 0 is said to be an *exceptional* point of the *first* (*second*; *third*) *kind*, if $Q_1\neq 0$, $Q_2=0$ ($Q_1=0$, $Q_2\neq 0$; $Q_1\neq 0$, $Q_2\neq 0$). In other words, if $\mathscr{M}=\{0\}$, 0 is a regular point. If $\mathscr{M}\neq\{0\}$, and contains only zero resonance functions, 0 is an exceptional point of the first

kind. If $\mathcal{M} \neq \{0\}$ and $\mathcal{M} \subset \mathcal{H}$, 0 is an exceptional point of the second kind.

The canonical zero resonance functions are chosen as follows. Assume $Q_1 \neq 0$. Choose a basis for $\mathcal{Y}$ such that we can assume $\mathcal{Y} = \mathbb{C}^N$. For $s > 2$, $\mathbb{H}^{1,-s}$ contains a copy of $\mathbb{C}^N$, viz, the constant functions. Thus we can consider $G_1^1 V$ as a map from $\mathcal{M}$ to $\mathbb{C}^N$. Call it Φ. By Lemma 3.2 the null space of Φ is $P_0\mathcal{H}$. Then $N_0 = \dim \operatorname{ran} \Phi = \dim \mathcal{M} - \dim P_0\mathcal{H}$. Let $\{e_j\}_{j=1,\ldots,N_0}$ denote an orthonormal basis for the range of Φ. There exist $\psi_j \in \mathcal{M}$, $j = 1,\ldots,N_0$, such that $\Phi\psi_j = 4\pi e_j$. Since the null space of Φ is $P_0\mathcal{H}$, we can assume $Q_1\psi_j = \psi_j$. This set $\{\psi_j\}_{j=1,\ldots,N_0}$ is the *normalized canonical zero resonance function*. Obviously, this choice is not unique, but two different sets are related by a unitary transformation.

Lemma 3.3: For small ζ the operator

$$Q_1^* V(\log \zeta G_1^1 + G_1^0) V Q_1$$

is invertible in $B(Q_1\mathbb{H}^{1,-s}, Q_1^*\mathbb{H}^{-1,s})$, $2 < s < \beta - 2$. The inverse is given by

$$Q_1(-\log \zeta Q_1^* Q_1 + Q_1^* V G_1^0 V Q_1)^{-1} Q_1^* = -\frac{1}{\log \zeta} \sum_{j=1}^{N_0} \langle \cdot, \psi_j \rangle \psi_j + O(|\log \zeta|^{-2}),$$

as $\zeta \to 0$. Here $V = V_A + W$ and $\{\psi_j\}_{j=1,\ldots,N_0}$ is a set of normalized canonical zero resonance functions.

Proof: See similar proofs in Jensen–Kato[1] and Jensen.[3]

A complete description of the possible singularities for $R(\zeta) = (H - \zeta)^{-1} = (H_A + W - \zeta)^{-1}$ is given in the following four theorems, corresponding to the four possible cases.

Theorem 3.4: Let 0 be a regular point for H. Assume $\beta = \beta(V_A) = \beta(W) > 2$, and $s, s' > 2$. We then have in $B(-1, s; 1, -s')$ the expansion

$$R(\zeta) = B_0 + \zeta \log \zeta B_1^1 + \zeta B_1^0 + o(\zeta)$$

as $\zeta \to 0$. The coefficients are given by

$$B_0 = (1 + F_0 W)^{-1} W,$$

$$B_1^1 = (1 + F_0 W)^{-1} F_1^1 (1 + W F_0)^{-1},$$

$$B_1^0 = (1 + F_0 W)^{-1} F_1^0 (1 + W F_0)^{-1}.$$

Proof: It follows as in Jensen[3,12] that we have

$$\begin{aligned} R(\zeta) = {} & (1 + G_0(V_A + W))^{-1} G_0 \\ & + \zeta \log \zeta (1 + G_0(V_A + W))^{-1} G_1^1 \\ & \times (1 + (V_A + W) G_0)^{-1} \\ & + \zeta (1 + G_0(V_A + W))^{-1} G_1^0 \\ & \times (1 + (V_A + W) G_0)^{-1} \\ & + o(\zeta). \end{aligned}$$

We now use

$$1 + G_0(V_A + W) = (1 + G_0 V_A)(1 + F_0 W)$$

and

$$1 + (V_A + W) G_0 = (1 + W F_0)(1 + V_A G_0),$$

together with Assumption 2.3 and Theorem 2.4.

Theorem 3.5: Let 0 be an exceptional point of the first kind for H. Assume $\beta = \beta(V_A) = \beta(W) > 4$ and $s, s' > 2$. We then have in $B(-1, s; 1, -s')$ the expansion

$$\begin{aligned} R(\zeta) = {} & -\zeta^{-1} Q_1 (\log \zeta Q_1^* Q_1 \\ & - Q_1^* W F_1^0 W Q_1)^{-1} Q_1^* + B + o(1) \end{aligned}$$

as $\zeta \to 0$. B is a bounded operator which can be found explicitly.

Proof: It follows as in Jensen.[3,12] We note that as in the proof of Lemma 3.2 we have

$$\begin{aligned} & Q_1^*(V_A + W) G_1^0 (V_A + W) Q_1 \\ & = Q_1^* W (1 + V_A G_0)^{-1} G_1^0 (1 + G_0 V_A)^{-1} W Q_1 \\ & = Q_1^* W F_1^0 W Q_1. \end{aligned}$$

Let us note that Lemma 3.3 and Theorem 3.5 show that the leading singularity in the case of an exceptional point of the first kind is given by

$$R(\zeta) = -\frac{1}{\zeta \log \zeta} \sum_{j=1}^{N_0} \langle \cdot, \psi_j \rangle \psi_j + O(|\zeta (\log \zeta)^2|^{-1}),$$

as $\zeta \to 0$.

Theorem 3.6: Let 0 be an exceptional point of the second kind for H. Assume $\beta(V_A) = \beta(W) > 4$, and $s, s' > 2$. In $B(-1, s; 1, -s')$ we then have

$$R(\zeta) = -\zeta^{-1} P_0 + \log \zeta P_0 W F_2^1 P_0 + C + o(1),$$

as $\zeta \to 0$. Here C is a bounded operator which can be found explicitly.

Proof: Existence of the expansion

$$\begin{aligned} R(\zeta) = {} & -\zeta^{-1} P_0 + \log \zeta P_0 (V_A + W) \\ & \times G_2^1 (V_A + W) P_0 + C + o(1) \end{aligned}$$

follows as in Jensen.[3,12]. As shown in the proof of Lemma 3.2 one has for $u \in \mathcal{M}$, $(V_A + W)u = (1 + V_A G_0)^{-1} W u$. Hence

$$\begin{aligned} & P_0(V_A + W) G_2^1 (V_A + W) P_0 \\ & = P_0 W (1 + G_0 V_A)^{-1} G_2^1 (1 + V_A G_0)^{-1} W P_0. \end{aligned}$$

Lemma 3.2 implies $G_1^1 (1 + V_A G_0)^{-1} W P_0 = 0$. Using Theorem 2.4 (iii), we then find

$$P_0 W (1 + G_0 V_A)^{-1} G_2^1 (1 + V_A G_0)^{-1} W P_0 = P_0 W F_2^1 W P_0.$$

Note that in case 0 is an exceptional point of the second kind for H, i.e., every function $\mathcal{M}$ is an eigenfunction for eigenvalue zero for H, we have besides the expected singularity $-\zeta^{-1} P_0$ also a logarithmic singularity. It follows from the explicit expression that

$$\operatorname{rank}(P_0 W F_2^1 W P_0) \leqslant \min(\dim P_0\mathcal{H}, 4 \cdot \dim \mathcal{Y}).$$

Using spherical square well potentials it is possible to give an example where $P_0 W F_2^1 W P_0 = 0$, and another where $\operatorname{rank} P_0 W F_2^1 W P_0 = 4 \cdot \dim \mathcal{Y}$. (In this example $4 \cdot \dim \mathcal{Y} = \dim P_0\mathcal{H}$). Details can be found in Jensen.[3]

Theorem 3.7: Let 0 be an exceptional point of the third kind for H. Assume $\beta(V_A) = \beta(W) > 4$ and $s, s' > 2$. We then have in $B(-1, s; 1, -s')$ the expansion

$$\begin{aligned} R(\zeta) = {} & -\zeta^{-1} P_0 + \zeta^{-1} Q_1 (\log \zeta Q_1^* Q_1 \\ & - Q_1^* W F_1^0 W Q_1)^{-1} Q_1^* \\ & + \log \zeta P_0 W F_2^1 W P_0 + D + o(1), \end{aligned}$$

as $\zeta \to 0$. Here D is a bounded operator which can be found explicitly.

Proof: The proof is similar to the ones given above, using results from Jensen[3] and Murata.[4]

Let us note that the simple form of the expansion above requires the specific choice of Q_1 made above.

Let us conclude this section with several remarks.

Remark 3.8: (i) Expansion to any order can be given, with explicit coefficients.[3,4] Murata[4] has given a general procedure for finding all coefficients explicitly. Higher-order coefficients are extremely complicated. Higher-order expansions require larger values of β and s, s'. Precise results can be obtained.[4]

(ii) If $\mathscr{Y}$ is one dimensional the above results are contained in Jensen.[3,12] In this case H is a Schrödinger operator with external electromagnetic field.[13]

(iii) Note that Assumption 2.3 is required only because we want to use the decomposition $H = H_A + W$. If we use $H = H_0 + (V_A + W)$ directly in the statement of Theorems 3.4–3.7, this assumption is unnecessary, but V_A may contribute zero resonances.

IV. SOME RESULTS ON YANG–MILLS POTENTIALS

In this section we give some results on Yang–Mills potentials, which satisfy our Assumption 2.1 and a mild regularity assumption. We refer to Jackiw[14] for some basic facts on non-Abelian four-dimensional gauge theories. Let us recall a few results here. The basic objects are the Yang–Mills potentials $A_j(x)$, $j = 1,2,3,4, x \in \mathbb{R}^4$. In general $A_j(x)$ takes values in the Lie algebra of the gauge group G. Here we take $G = SU(2)$ as an example, and introduce a factor i in various formulas in order to take $A_j(x)$ as Hermitian matrices. To $A_j(x)$ is associated the field strength tensor

$$F_{jk}(x) = \partial_j A_k(x) - \partial_k A_j(x) + i[A_j(x), A_k(x)], \tag{4.1}$$

where $\partial_j = \partial/\partial x_j$ for simplicity. The action is given by

$$S(A) = \frac{1}{4} \sum_{j,k=1}^{4} \int_{\mathbb{R}^4} \mathrm{tr}(F_{jk}(x)^2) dx. \tag{4.2}$$

The pure Yang–Mills equations are the Euler equations associated with $S(A)$, viz.

$$\sum_{j=1}^{4} (\partial_j F_{jk}(x) + i[A_j(x), A_k(x)]) = 0. \tag{4.3}$$

Several classes of solutions to (4.3) are known, and are associated with the vacuum. Besides the trivial classical vacuum solution $A_j(x) = 0$ there exist topologically nontrivial vacua, e.g., the instanton solution.[15]

Let $A_j^V(x)$ be a solution to (4.3). Consider a perturbation of this vacuum solution

$$A_j(x) = A_j^V(x) + A_j^P(x).$$

This set $\{A_j(x)\}$ trivially satisfies the equation

$$\sum_{j=1}^{4} (\partial_j F_{jk}(x) + i[A_j(x), A_k(x)]) = J_k(x)$$

in the sense that current is defined by the left-hand side.

In Yang–Mills field theory the topological charge $Q(A)$ is an important gauge-independent quantity. Let us briefly recall its definition. Let ϵ_{jklm} be the Levi–Civita symbol with $\epsilon_{1234} = 1$. The dual to $F_{jk}(x)$ is given by

$${}^*F_{jk}(x) = \frac{1}{2} \sum_{l,m=1}^{4} \epsilon_{jklm} F_{lm}(x).$$

$Q(A)$ is defined by

$$Q(A) = \frac{1}{4\pi^2} \sum_{j,k=1}^{4} \int_{\mathbb{R}^4} \mathrm{tr}(F_{jk}(x) {}^*F_{jk}(x)) dx.$$

Proposition 4.1: Let $\{A_j^V(x)\}$ be the trivial solution, or the instanton solution, to (4.3). Let $A_j^P(x)$ be continuously differentiable in x and satisfy

$$A_j^P(x) = O(|x|^{-2-\delta}), \quad \partial_k A_j^P(x) = O(|x|^{-2-\delta}),$$

$j, k = 1,2,3,4$, as $|x| \to \infty$, for some $\delta > 0$. Then $A_j(x) = A_j^V(x) + A_j^P(x)$ satisfy

$$S(A) < \infty \text{ and } Q(A) = Q(A^V).$$

Proof: With an obvious notation we have

$$F_{jk}(A) = F_{jk}(A^V) + F_{jk}(A^P) + i[A_j^V, A_k^P] + i[A_j^P, A_k^V]. \tag{4.4}$$

In a suitable gauge $A_j^V(x) = O(|x|^{-1})$ as $|x| \to \infty$, and is a smooth function of x. The assumptions on $A_j^P(x)$ imply that each term in (4.4) is square integrable, hence $S(A) < \infty$.

Let

$$J_n = 2 \sum_{j,k,l=1}^{4} \epsilon_{njkl} \,\mathrm{tr}\left(A_j \partial_k A_l + \frac{2}{3} i A_j A_k A_l\right).$$

Then

$$\sum_{n=1}^{4} \partial_n J_n = \frac{1}{2} \sum_{j,k,l,m} \mathrm{tr}(\epsilon_{jklm} F_{jk} F_{lm}).$$

Thus one has

$$Q(A) = Q(A^V) + Q(A^P) + (2\pi^2)^{-1} \times \sum_{j,k,l,m} \int dx\, \partial_j \{\epsilon_{jklm} \,\mathrm{tr}(A_j^V \partial_k A_l^P + A_j^P \partial_k A_l^V + \tfrac{2}{3} i(A_j^V A_k^V A_l^P + A_j^P A_k^P A_l^V))\}.$$

The above integral vanishes by the divergence theorem. Furthermore, the assumptions on $A_j^P(x)$ imply $Q(A^P) = 0$.

The Yang–Mills potentials $A_j(x)$ are used as the operators $A_j(x)$ in H_A and H discussed in Secs. II and III. Let $A_j(x)$ be a nontrivial vacuum solution. It is known[14] that a smooth $A_j(x)$ has decay rate $O(|x|^{-1})$ or slower. Hence the results in Secs. II and III are not applicable to these $A_j(x)$. Recent results[5] indicate that a result similar to Theorem 2.4 with, e.g., $A_j(x)$ the instanton solutions will have a different form.

The results in Sec. II and III are applicable to $A_j(x)$ which are perturbations of the classical vacuum solutions $A_j^V(x) \equiv 0$. If $A_j(x)$ satisfy both Assumption 2.3 and the assumptions in Proposition 4.1, they have finite action and zero topological charge, and we have very complete results on the infrared behavior of the resolvent.

There is an explicit example which satisfies all our assumptions.

Example 4.2: There is an explicit solution of a SU(2) Yang–Mills field, coupled to a massless Higgs doublet.[16,17] We shall not go into any details, but we note that for generic values of the coupling constants[16] λ, e, the Assumption 2.3 is satisfied. The constructed $A_j(x)$ are smooth and satisfy $A_j(x) = O(|x|^{-3})$, $\partial_k A_j(x) = O(|x|^{-4})$ as $|x| \to \infty$. The constructed W satisfies $W(x) = O(|x|^{-4})$ as $|x| \to \infty$. Hence our assumptions are verified, and Theorem 3.4 is applicable.

V. BEHAVIOR OF EXPANSIONS UNDER GAUGE TRANSFORMATIONS

Let $x \to g(x)$ be a map from $\mathbb{R}^4$ to the gauge group G. Since each $g(x)$ is a unitary map in $\mathscr{V}$, g defined by $(gu)(x) = g(x)u(x)$ is a unitary map in $\mathscr{H} = L^2(\mathbb{R}^4) \otimes \mathscr{V}$. Only a restricted class of gauge transformations g, with the property that g is bounded from $\mathbf{H}^{1,s}$ to $\mathbf{H}^{1,s}$, for each $s \in \mathbb{R}$, is considered here. A sufficient condition on g is that $g(x)$ is differentiable with bounded derivative.

Two Yang–Mills potentials related by

$$A_j^2(x) = g(x)A_j^1(x)g(x)^{-1} + ig(x)\left(\frac{\partial}{\partial x_j} g(x)^{-1}\right) \tag{5.1}$$

are said to be equivalent under the gauge transformation g. For the restricted class of g we have

$$H_{A^2} = gH_{A^1}g^{-1} \quad \text{and} \quad R_{A^2}(\zeta) = gR_{A^1}(\zeta)g^{-1}.$$

If $A_j^1(x)$ and $A_j^2(x)$ both satisfy the assumption in Theorem 2.4, and are related by (5.1) for some g uniqueness of the coefficients in an asymptotic expansion implies

$$F_j^k(A^2) = gF_j^k(A^1)g^{-1}$$

(with an obvious notation) and thus equivalence of the coefficients.

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Symmetries of the higher-order KP equations

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Symmetry generators $T_n^{(l)} = tI_n + L_n^{(l)}$ are constructed for the l th-order Kadomtsev–Petviashvili (KP) equation for all $n \geqslant l-2$. In the case of the ordinary KP equation ($l=2$) these symmetries are those found by Chen *et al.* [Physica D **9**, 439 (1983)].

I. INTRODUCTION

The Kadomtsev–Petviashvili (KP) equation[1] is of interest for at least two reasons.

(1) It is relevant to certain physical problems.

(2) It is an extension to one more space variable of the well-studied Korteweg–de Vries (KdV) equation. In this connection it is worth knowing which, if any, of the remarkable properties of the KdV equation it shares.[2,3]

Recently,[4] it has been shown that the KP equation has an additional set of symmetries not inherited from the KdV equation.

Another property of the KdV equation is that it is but one of a hierarchy of equations. Here we want to point out the following.

(a) The KP equation is also but one of a hierarchy. (This is not very surprising. It results from the fact that the infinite set of constants are in involution.)

(b) For each member of the hierarchy there is an infinite set of new symmetries. These sets are different but are closely related.

II. KP EQUATION

We take the KP equation in the form[5]

$$q_t = \partial_x^{-1} q_{yy} - \partial_x (3q^2 + q_{xx}). \tag{1}$$

It is seen that this is a Hamiltonian system, i.e., it is of the form

$$q_t = [q, H], \tag{2}$$

when we define the Poisson brackets by

$$[F, G] = \int\int dx\, dy \frac{\delta F}{\delta q} \partial_x \frac{\delta G}{\delta q} \tag{3}$$

and take as the Hamiltonian

$$H = \int \left\{ \frac{(\partial_x^{-1} \partial_y q)^2}{2} + \frac{q_x^2}{2} - q^3 \right\} dx\, dy. \tag{4}$$

As stated above[2,3] this is a completely integrable system. The first few constants are

$$I_0 = \int \frac{q^2}{6} dx\, dy, \quad I_1 = \frac{1}{3} \int (q\, \partial_x^{-1} \partial_y q) dx\, dy,$$

$$I_2 \equiv H,$$

$$I_3 = \int \left\{ 2q_x q_y + \frac{2}{3} q (\partial_x^{-1} \partial_y)^3 q - 4q^2\, \partial_x^{-1} \partial_y q \right\} dx\, dy,$$

$$I_4 = \int \left\{ \frac{3}{2} (q_{xx})^2 + \frac{5}{6} (\partial_x^{-2} \partial_y^2 q)^2 - 15 q_x^2 q + 5 q_y^2 + \frac{15}{2} q^4 - 5q^2\, \partial_x^{-2} \partial_y^2 q - 5q (\partial_x^{-1} \partial_y q)^2 \right\} dx\, dy.$$

We remark that there is another constant which is not always mentioned. It is

$$I = -\int \frac{q}{18} dx\, dy. \tag{5}$$

(It will be shown to have a useful role.)

III. THE NEW SYMMETRIES

If we write Eq. (1) in the form

$$q_t = K_2(q) \quad \left(K_2(q) = \partial_x \frac{\delta I_2}{\delta q} \right), \tag{6}$$

then a solution δq of the linearized equation

$$\delta q_t = K_2'(\delta q) \quad \left(K_2'(\delta q) = \lim_{\epsilon \to 0} \frac{d}{d\epsilon} K_2(q + \epsilon \delta q) \right) \tag{7}$$

is called a symmetry.

Chen *et al.*[4] have shown that in addition to the classical symmetries $\delta q = [q, I_n]$ there are new symmetries of the form

$$\delta q = [q, T_n], \tag{8}$$

where

$$T_n = tI_n + J_n. \tag{9}$$

The first few of the functionals J_n are

$$J_0 = -\int \frac{xq}{18} dx\, dy, \quad J_1 = \int \frac{yq^2}{6} dx\, dy,$$

$$J_2 = \int \left\{ \frac{q^2 x}{6} + \frac{qy\, \partial_x^{-1} \partial_y q}{3} \right\} dx\, dy,$$

$$J_3 = \int \left\{ y \left[\frac{(\partial_x^{-1} \partial_y q)^2}{2} + \frac{q_x^2}{2} - q^3 \right] + \frac{qx\, \partial_x^{-1} \partial_y q}{3} \right\} dx\, dy,$$

$$J_4 = \int \left\{ 2yq_x q_y + \frac{2}{3} yq (\partial_x^{-1} \partial_y)^3 q - 3q^2 y\, \partial_x^{-1} \partial_y q - q^2\, \partial_x^{-1} \partial_y (yq) + \frac{(\partial_x^{-1} \partial_y q)^2 x}{2} + x \left(\frac{q_x^2}{2} - q^3 \right) \right\} dx\, dy.$$

[The role of the constant of Eq. (5) is now seen. It is used to construct J_0.]

Chen *et al.*[4] have derived relations between the Poisson brackets of the functionals I_n, J_n. (More precisely, they have obtained relations between Lie products of $[q, J_n]$ and $[q, I_n]$. However, we have shown[6] that these can be written as the following Poisson bracket relations:

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$$[I_n, I_m] = 0, \tag{10}$$

$$J_{m+n-2} = [3/(m-n)][J_m, J_n], \tag{11}$$

$$I_{m+n-2} = [3/(m+1)][I_m, J_n].) \tag{12}$$

Remark: Given I_0, J_0, J_3, J_4 these relations determine all the remaining I's and J's.

For example, if we choose $n = 3$ in Eq. (12) we have

$$I_{m+1} = [3/(m+1)][I_m, J_3].$$

Therefore,

$$I_1 = 3[I_0, J_3], \quad I_2 = \tfrac{3}{2}[I_1, J_3], \ldots .$$

Thus all I_m are generated by I_0 and J_3. Consider Eq. (11) with $n = 3$. It becomes

$$J_{m+1} = [3/(m-3)][J_m, J_3]. \tag{13}$$

Thus, $J_1 = -[J_0, J_3]$, and $J_2 = -\tfrac{3}{2}[J_1, J_3]$. However, if in Eq. (13) we put $m = 3$ we get the trivial identity $[J_3, J_3] = 0$. We cannot obtain J_4 from Eq. (11). However, given J_4 (as in the previous section) all other J_m are determined by Eq. (13).

IV. THE HIGHER-ORDER KP EQUATIONS

Just as for the KdV equation we have, in virtue of the involution property of the I_n, Eq. (10), an infinite hierarchy of KP equations. These are

$$q_t = K_l(q), \quad \text{where } K_l = \partial_x \frac{\delta I_l}{\delta q}. \tag{14}$$

They are all completely integrable—having the common set of contants I_n, $n = 0, 1, 2, \ldots$. In particular, then, these equations all have the classical symmetries $\delta q = [q, I_n]$.

The main question we wish to answer here is as to whether there are "new symmetries" for Eq. (14) for arbitrary l, i.e., are there $T_n^{(l)}$ such that

$$\delta q = [q, T_n^{(l)}] \tag{15}$$

satisfies

$$\delta q_t = K_l'[\delta q]. \tag{16}$$

Consider

$$T_n^{(l)} = tI_n + L_n^{(l)} \tag{17}$$

and suppose

$$[I_l, L_n^{(l)}] = I_n. \tag{18}$$

If δq is chosen as in Eq. (15) we have

$$\frac{d}{dt}\delta q = [q, I_n] + [[q, tI_n + L_n^{(l)}], I_l]. \tag{19}$$

By the Jacobi identity

$$[[q, tI_n + L_n^{(l)}], I_l] = -[[tI_n + L_n^{(l)}, I_l], q] - [[I_l, q], tI_n + L_n^{(l)}].$$

But $[I_n, I_l] = 0$ and so in virtue of Eq. (18)

$$[[q, tI_n + L_n^{(l)}], I_l] = -[q, I_n] - [[I_l, q], tI_n + L_n^{(l)}].$$

Therefore, Eq. (19) becomes

$$\frac{d}{dt}\delta q = [[q, I_l], tI_n + L_n^{(l)}]. \tag{20}$$

The theorem proved in Ref. 6 tells us that

$$K_l'[q, tT_n + L_n^{(l)}] = [[q, I_l], tI_n + L_n^{(l)}]. \tag{21}$$

Comparing Eqs. (20) and (21) we see that Eq. (16) is indeed satisfied. Thus δq is a symmetry—if we can construct $L_n^{(l)}$.

The construction is as follows: Equation (12) is

$$I_{r+s-2} = (3/(r+1))[I_r, J_s]. \tag{22}$$

Let $r = l$, $s = n - l + 2$. Equation (22) becomes

$$I_n = [I_l, (3/(l+1))\ J_{n-l+2}]. \tag{23}$$

Thus, an $L_n^{(l)}$ satisfying Eq. (18) is

$$L_n^{(l)} = (3/(l+1))\ J_{n-l+2}. \tag{24}$$

Some examples are

$$l = 0, \quad L_n^{(0)} = 3J_{n+2},$$

$$l = 1, \quad L_n^{(1)} = \tfrac{3}{2}\ J_{n+1},$$

$$l = 2, \quad L_n^{(2)} = J_n.$$

(This is precisely the case of Ref. 4.) Other examples are

$$l = 3, \quad L_n^{(3)} = \tfrac{3}{4}\ J_{n-1},$$

$$l = 4, \quad L_n^{(4)} = \tfrac{3}{5}\ J_{n-2}.$$

In general we have thus found symmetry generators $T_n^{(l)}$ for fixed l for all $n \geqslant l - 2$.

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Connections on infinitesimal fiber bundles and unified theories[a)]

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We provide an intrinsic coordinate-free formalism of Jordan's version of five-dimensional Kaluza–Klein or projective theory of relativity in terms of the so-called infinitesimal fiber bundles, whose structures are slightly more general than principal fiber bundles with connections. Higher-dimensional generalizations are then suggested, thereby providing a more comprehensive unified theory.

I. INTRODUCTION

Mathematically, a gauge field is the curvature of a connection on a principal fiber bundle over space-time with a certain structure group. Historically, Weyl[1] was the first to suggest such a connection, with the multiplicative group of positive real numbers as the structure group, in his pioneering attempt at a unified field theory of gravitation and electromagnetism.

Shortly after Weyl, Kaluza and Klein and later Veblen, Jordan, and others[2] gave another version of the unified theory, which is known as the five-dimensional or projective theory of relativity. Recently[3] we tried to formulate Jordan's version of projective relativity in an intrinsic, coordinate-free manner and found that when one abstracts the geometric structure of the theory one is led to the concept of so-called infinitesimal fiber bundles and Riemannian infinitesimal bundles whose structures are slightly more general than principal fiber bundles with connections. The object of this paper is to suggest that these structures may provide a fruitful direction in the search for more comprehensive unified gauge theories.

II. INFINITESIMAL FIBER BUNDLES AND CONNECTIONS

An infinitesimal fiber bundle (of fiber dimension one) is a collection (M, ϕ, V, X), where (i) M, V are smooth manifolds with $\dim V = n$, $\dim M = n+1$; (ii) $\phi: M \to V$ is a *submersion* of M *onto* V; and (iii) X is a nowhere vanishing vector field on M, such that if x, y lie on an integral curve of X, then $\phi(x) = \phi(y)$.

A "connection" on (M, ϕ, V, X) is a one-form q on M such that (i) $q(X) = 1$, and (ii) $\mathcal{L}_X q + 0$. Here, (M, ϕ, V, X, q) will denote an infinitesimal fiber bundle with connection q.

A principal circle bundle (M, π, V, S^1) has a fundamental vector field X generated by the action of S^1 on M and it admits a connection one-form q such that (i) and (ii) above are satisfied. Similarly, a principal line bundle $(M, \pi, V, \mathbb{R})$ can be made into an infinitesimal bundle with connection.

However, in contrast to a principal bundle (of fiber dimension one) the fibers of an infinitesimal bundle are not necessarily homeomorphic to each other. In general, the fiber of an infinitesimal bundle is a circle over some points of V and a line over others.

The "connection form" q provides a (direct sum) decomposition of the tangent space $T_m(M)$ at any point $m \in M$, into a *horizontal* subspace $H_m(M) = \{\epsilon_m \in T_m(M) | q_m(\epsilon_m)| = 0\}$ and a *vertical* subspace $V_m(M) = \{\lambda X_m | \lambda \in \mathbb{R}\}$. Thus ϵ_m can be written as

$$\epsilon_m = \epsilon^{\perp} + q_m(\epsilon_m) X_m, \quad q_m(\epsilon_m^{\perp}) = 0,$$

so that

$$\text{horizontal part of } \epsilon_m = \epsilon_m - q_m(\epsilon_m) X_m,$$

$$\text{vertical part of } \epsilon_m = q_m(\epsilon_m) X_m.$$

Note that $X_m^{\perp} = 0$, i.e., X_m is vertical.

Definitions: (1) A function $f \in C^{\infty}(M)$ is said to be a *projective function* if $f = f' \circ \phi$ for some $f' \in C^{\infty}(V)$. Let $C_0^{\infty}(M)$ denote the set of projective functions on M.

(2) A vector field $\epsilon \in \mathscr{X}(M)$ is said to be a *projective vector field* if $q(\epsilon) \in C_0^{\infty}(M)$ and ϵ is ϕ related to some vector field $\epsilon' \in \mathscr{X}(V)$.

Let $\mathscr{X}_0(M)$ denote the $C_0^{\infty}(M)$ module of projective vector fields on M and $\mathscr{H}_0(M)$ the horizontal subspace of $\mathscr{X}_0(M)$.

(3) A one-form $\omega \in \mathscr{X}^*(M)$ is said to be a *projective one-form* if $\omega(\epsilon) \in C_0^{\infty}(M)$ for all $\epsilon \in \mathscr{X}_0(M)$. Let $\mathscr{X}_0^*(M)$ denote the set of projective one-forms on M.

(4) A tensor field θ of type (r,s) is a *projective tensor field* or a *projector if* $\theta(\omega_1, ..., \omega_r, \epsilon_1, ..., \epsilon_s) \in C_0^{\infty}(M)$ for all $\omega_i \in \mathscr{X}_0^*(M)$, $\epsilon_j \in \mathscr{X}_0(M)$. Let $\tau_0(M)$ denote the set of all projectors on M.

Propositions: (1) $\theta \in \tau_0(M) \Rightarrow \mathcal{L}_X \theta = 0$.

(2) $\phi_{*m|_{H_m(M)}}: H_m(M) \to T_{\phi(m)}(V)$ is an *isomorphism* and $\operatorname{Ker} \phi_{*m} = V_m(M)$.

(3) Given a vector field $\epsilon' \in \mathscr{X}(V)$, the condition $\epsilon_m \in H_m(M)$ and $\phi_{*m} \epsilon_m = \epsilon'_{\phi(m)}$, $\forall\ m \in M$ defines a unique vector field $\phi^* \epsilon' \in \mathscr{H}_0(M)$, called the lift of ϵ'.

(4) Every $\epsilon \in \mathscr{X}_0(M)$ is ϕ related to some $\epsilon' \in \mathscr{X}(V)$. We thus have a *projection* map $\phi_*: \mathscr{X}_0(M) \to \mathscr{X}(V)$ and a lift ϕ^*: $\mathscr{X}(V) \tilde{\to} \mathscr{H}_0(M)$.

These processes can be generalized to arbitrary projectors θ and we can define θ to be horizontal if $\theta(\omega_1, ..., \omega_r, \epsilon_1, ..., \epsilon_s) = 0$ for at least one $\omega_i = q$ or $\epsilon_j = X$, and given a horizontal projector θ we can solve $\phi^* \theta' = \theta$ for θ'.

Definition: A pseudo-Riemannian metric g on M is said to be a projective metric if g is a symmetric projector of type

[a)] This is an enlarged version of what appears as an abstract in "Geometrical and Topological Methods in Gauge Theories," in *Lecture Notes in Physics*, Vol. 129, edited by J. Harnad and S. Shnider (Springer, New York, 1979), p. 152.

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(0, 2) and $g(X,X) = J \neq 0$ on M. Note that $\mathcal{L}_X g = 0$, i.e., X is a Killing vector field for g.

A projective metric g on an infinitesimal fiber bundle (M, ϕ, V, X) gives rise to a canonical connection q by

$$q = J^{-1} X^{\#},$$

where $X^{\#}$ is the one-form dual to X under the isomorphism provided by g.

From now on we shall suppose that (M, ϕ, V, X) is endowed with a projective metric g and the canonical connection $q = J^{-1} X^{\#}$, and we denote by (M, ϕ, V, X, g) such a pseudo-Riemannian infinitesimal bundle (or a Rib space).

Proposition: Given a Rib space (M, ϕ, V, X, g), $g_V = \phi_* g$ is a pseudo-Riemannian metric on V and

$$\text{signature of } g = \text{signature of } g_V + \text{sign } J.$$

III. PROJECTIVE RELATIVITY

The projective theory of relativity can now be formulated in the framework of a Rib space (M, ϕ, V, X, g), where V is the four-dimensional space-time, and g a projective metric such that g_V is a Lorentz metric with the proper space-time signature.

Let ∇ be now the Levi-Civita connection relative to g. Jordan[2] introduced a so-called congruent connection K as follows

$$K_\eta \epsilon = \nabla_\eta \epsilon + J^{-1} g(\epsilon, \nabla_\eta X) X - J^{-1} g(\epsilon, X) \nabla_\eta X,$$

for $\eta, \epsilon \in \mathscr{X}(M)$, which is the unique projective connection [K is projective if $K_\eta \epsilon \in \mathscr{X}_0(M)$ for all $\eta, \epsilon \in \mathscr{X}_0(M)$] such that

$$K_\eta \epsilon^{\perp} = (\nabla_\eta \epsilon^{\perp})^{\perp},$$

$$\zeta\,(g(\epsilon,\eta)) = g(K_\zeta \epsilon, \eta) + g(\xi, K_\zeta \eta),$$

for all $\epsilon, \eta, \zeta \in \mathscr{X}_0(M)$. Let R be the Riemann curvature tensor relative to K.

Proposition: $\phi_* R = R_V$, the Riemann curvature tensor on V relative to the Levi–Civita connection relative to g_V.

The projective interpretation of the electromagnetic field is as follows. The "curvature" of the "connection" form q,

$$dq = d(J^{-1} X^{\#}),$$

is a two-form on M given by

$$dq(\epsilon, \eta) = 2 J^{-1} g(K_X \epsilon, \eta).$$

If $g(X,X) = J = \kappa = \text{const}$, then $dq(\xi,\eta) = 2\kappa^{-1} g(\nabla_X \epsilon, \eta)$.

The two-form dq on M gives rise to a two-form F on V on projection, such that

$$dq = \phi^* F.$$

Here, F is closed, but not necessarily exact and is to be identified with the electromagnetic field tensor. In the absence of electromagnetic field, i.e., $F = 0$ (and $J = \kappa$), it can be shown that Tor $K = 0$ and $K = \nabla$.

Finally, the projection of Ricc $K = 0$ or some similar equations (obtained, say from some variational principle) gives the combined Maxwell–Einstein equations on V.

IV. REMARKS AND GENERALIZATION

Thus, as far as nonquantum unified theory of gravitation and electromagnetic field is concerned a possible geometric setup seems to be a Riemannian infinitesimal bundle.

This formalism seems to have some connection with the formalisms of G foliations (or Riemannian foliations)[4] or that of fibered spaces introduced by Yano and Ishihara.[5]

In contrast to conventional prrincipal fiber bundles there is no (structure) group action on an infinitesimal fiber bundle. However, in a Rib space the fundamental vector field generates a local one-parameter group of local isometries.

It should be possible to generalize this formalism to $(M, \phi, V, \epsilon, \omega)$, where $\dim M = \dim V + r$, ϵ is a r-dimensional (integrable) distribution, and ω is a r-dimensional (integrable) codistribution on M, such that $\omega_i(\epsilon_i) = 1$, $\mathcal{L}_{\epsilon_i} \omega_i = 0$. (Here ϵ_i, ω_i span ϵ and ω.)

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Mapping of connections on bundles and gauge field theories

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The problem of solving the combined gravitational and Yang–Mills field systems is regarded as a purely geometrical problem of determining a linear connection on the principal frame bundle $L(M)$ from a connection on a SU(2) principal bundle over a space-time M. It is suggested that mapping theorems of connections on bundles may provide a means of actually solving "field equations."

I. INTRODUCTION

In classical gauge field theories, whereas the electromagnetic or the Yang–Mills field arises from connections on U(1) or SU(2) principal bundles $P(M)$ over the space-time manifold M, the gravitational field arises as a linear connection on the GL(4) principal frame bundle $L(M)$ over M [or in particular on the SO(3,1) principal bundle of Lorentz frames on M].[1,2] According to the general theory of relativity every nongravitational field, via its energy-momentum tensor, should generate a gravitational field. Thus from the gauge viewpoint a SU(2) connection, which describes a Yang–Mills field, should determine a GL(4) connection according to the Einstein–Yang–Mills equations.

We wish to regard the problem of "solving the field equations" for a combined gravitational and Yang–Mills field system as a purely geometrical problem of determining a linear connection on the principal frame bundle $L(M)$ from a connection on a SU(2) principal bundle on M. It should be emphasized that we are not assuming any particular field equations (e.g., Einstein–Yang–Mills equations). What is assumed here only is that one has a nongravitational field interacting with and somehow determining the gravitational field.

A geometrical link between the two fields is provided by the well-known 2–1 covering homomorphism of SU(2) into SO(3) and thus into GL(4). It suggests therefore that we consider homomorphisms of principal bundles. Then there exists a mapping theorem of connection on bundles whenever there is a diffeomorphism of the base manifolds. This paper considers a simple possible application[3] of such a mapping theorem and shows how, in principle, one can compute the linear connection components from a Yang–Mills connection, given a base diffeomorphism.

II. THE MAPPING THEOREM OF CONNECTIONS ON BUNDLES[4]

Recall that a bundle homomorphism of a principal bundle (P, M, π, G) into another principal bundle (P', M', π', G') is a triple of C^∞ maps (f_P, f_G, f_M), where $f_P: P \to P'$, $f_M: M \to M'$ and $f_G: G \to G'$ is also a group homomorphism and such that (i) the diagram

$$\begin{array}{ccc} P & \xrightarrow{f_P} & P' \\ \downarrow\pi & & \downarrow\pi' \\ M & \xrightarrow{f_M} & M' \end{array}$$

commutes, and (ii) $f_P \circ R_g = R_{f_G(g)} \circ f_P$ for all $g \in G$. Here R_g and $R_{f_G(g)}$ are the group actions on P and P', respectively. The mapping theorem of connections on bundles then states the following theorem.

Theorem: Let (f_P, f_G, f_M) be a bundle homomorphism from (P, M, π, G) into (P', M', π', G') such that $f_M: M \to M'$ is now a diffeomorphism. Let Γ be a connection in P. Then there is a unique connection Γ' in P' such that the horizontal subspaces of Γ are mapped into the horizontal subspaces of Γ'.

III. APPLICATION TO GAUGE FIELDS

First of all, to see the relationship between Γ and Γ', let w, w' be the corresponding connection forms and Ω, Ω' the corresponding curvature forms of Γ, Γ', respectively. If now $\bar{G}$ and $\bar{G}'$ are the Lie algebras of G and G', respectively, the homomorphism $f_G: G \to G'$ induces a Lie algebra homomorphism $\bar{f}_G: \bar{G} \to \bar{G}'$. Then according to the theorem

$$f_P^*(w') = \bar{f}_G \cdot w \tag{1}$$

and

$$f_P^*(\Omega') = \bar{f}_G \cdot \Omega. \tag{2}$$

Equation (1) is to be interpreted as follows. For every $X_p \in T_p(P)$, $w'_{p'}((f_P)_{*p}(X_p)) \in \bar{G}'$, where $p' \in f_P(p)$. On the other hand, $w_p(X_p) \in \bar{G}$. Hence (1) means

$$w'_{p'}((f_{p*p}(X_p)) = \bar{f}_G(w_p(X_p)),$$

for all p and X_p. Similarly for (2).

We shall now apply the mapping theorem to the following situation. We take the same base manifold: $M = M' = \mathbb{R}$ (for simplicity), and $P = P(M) = M \times \mathrm{SU}(2) = \mathbb{R}^4 \times \mathrm{SU}(2)$, i.e., the SU(2) bundle over $\mathbb{R}^4$, and $P' = L(M) = \mathbb{R}^4 \times \mathrm{GL}(4)$, the frame bundle of $\mathbb{R}^4$. Let now $f_M: \mathbb{R}^4 \to \mathbb{R}^4$ be any C^∞ map. There is a natural 2–1 covering homomorphism of SU(2) into $\mathrm{SO}(3) \subset \mathrm{GL}(4)$. This gives us a homomorphism $f_G: \mathrm{SU}(2) \to \mathrm{GL}(4)$. If we now define $f_P: P \to P'$ by $(x, g) \to (f_M(x), f_G(g))$, where $x \in \mathbb{R}^4$ and $g \in \mathrm{SU}(2)$, it is easy to see that (f_P, f_G, f_M) is a bundle homomorphism of $P(M)$ into $L(M)$. If furthermore, f_M is a diffeomorphism of $\mathbb{R}^4$ onto $\mathbb{R}^4$, then the mapping theorem on connections says that a connection Γ on SU(2) bundle $P(M)$ determines uniquely a linear connection Γ' on the frame bundle $L(M)$ via Eqs. (1) and (2), such that the horizontal subspaces of $P(M)$ are mapped into the horizontal subspaces of $L(M)$.

Since SU(2), as a manifold, is homeomorphic to S^3, we can parametrize it by means of three real parameters $u = (u_1, u_2, u_3)$, as follows.

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A typical element of SU(2) is

$$\begin{pmatrix} x+iy & z+iw \\ -z+iw & x-iy \end{pmatrix},$$

with x, y, z, w real and $x^2+y^2+z^2+w^2=1$. The three parameters are thus given by

$$x=\frac{1-\Sigma_i u_i^2}{1+\Sigma_i u_i^2},$$

$$y=\frac{2u_1}{1+\Sigma_i u_i^2},$$

$$z=\frac{2u_2}{1+\Sigma_i u_i^2},$$

$$w=\frac{2u_3}{1+\Sigma_i u_i^2}.$$

Now the 2–1 covering homomorphism SU(2)→SO(3) is given, in terms of x, y, z, w, by

$$\begin{pmatrix} x+iy & z+iw \\ -z+iw & x-iy \end{pmatrix} \mapsto \begin{pmatrix} x^2-y^2-z^2+w^2 & 2(xy+zw) & -2(xz-yw) \\ -2(xy-zw) & x^2-y^2+z^2-w^2 & 2(yz+xw) \\ 2(xz+yw) & -2(xw-yz) & x^2+y^2-z^2-w^2 \end{pmatrix}.$$

We thus have a map: $\mathrm{SU}(2)\ni(u_1,u_2,u_3)\mapsto(a_k^i(u))\in\mathrm{SO}(3)$, and SO(3) itself can be homomorphically imbedded into GL(4), for example, as

$$(a_k^i(u))\mapsto\begin{pmatrix} (a_k^i(u)) & 0 \\ & 0 \\ & 0 \\ 0\ 0\ 0 & 1 \end{pmatrix}.$$

We thus have a homomorphism f_G from SU(2) into GL(4).

Let f_G: SU(2)→GL(4) be given by $u\mapsto a_\beta^\alpha(u)\in\mathrm{GL}(4)$, so that f_P: $\mathbb{R}^4\times\mathrm{SU}(2)\to\mathbb{R}^4\times\mathrm{GL}(4)$ is given by $(x,u)\mapsto(f_\lambda(x),a_\beta^\alpha(u))$, where f_M: $\mathbb{R}^4\to\mathbb{R}^4$ is $(x_\lambda)\mapsto(f_\lambda(x))$. We shall write the map as f_P: $(X_a)\mapsto(Y_A)$, where $(X_a)=(x,u)$ and $(Y_A)=(f_\lambda(x),a_\beta^\alpha(u))$. A Yang–Mills form w on $P(M)$ is then $w(X)=w_a(X)dX_a$, whereas a linear connection form w' on $L(M)$ is $w'(Y)=w'_A(Y)dY_A$. Equation (1) is then simply

$$\frac{\partial Y_A}{\partial X_a}w'_A(Y)=\bar{f}_G(w_a(X)). \tag{3}$$

Now

$$\begin{aligned} w'(Y)&=W'_A(Y)dY_A \\ &=\{(a^{-1})_\nu^\beta(u)(da_\mu^\nu(u)+\Gamma^\nu_{\alpha\lambda}(y)a_\mu^\lambda(u)dy_\alpha)\}E_\beta^\mu, \end{aligned}$$

where the $\Gamma^\nu_{\alpha\lambda}(y)$ are the connection components on the base manifold $\mathbb{R}^4$ and the $\{E_\beta^\mu\}$ are the standard basis of $\overline{\mathrm{GL}(4)}$, and

$$\begin{aligned} w(X)&=w_a(X)dX_a=\{w_a^i(X)dX_a\}E_i \\ &=\{w_j^i(u)du_j+w_\alpha^i(x,u)dx_\alpha\}E_i, \end{aligned}$$

where the $w_\alpha^i(x,u)$ are related to the Yang–Mills potentials and the $\{E_i\}$ are the basis of $\overline{\mathrm{SU}(2)}$. Thus from (3), we get

$$\begin{aligned} &\{(a^{-1})_\nu^\beta(u)(da_\mu^\nu(u)+\Gamma^\nu_{\alpha\lambda}(u)dy_\alpha)\}E_\beta^\mu \\ &\quad=\bar{f}_G(\{w_j^i(u)du_j+w_\alpha^i(x,u)dx_\alpha\}E_i). \end{aligned} \tag{4}$$

Recall that $\bar{f}_G=(f_G)_{*e}:T_e(\mathrm{SU}(2))\to T_{f_G(e)}(\mathrm{GL}(4))$, $\mathrm{SU}(2)\ni e\leftrightarrow(u=0)$. So we put $u=0$ above and let $\bar{f}_G(E_i)=C_{i\mu}^\beta E_\beta^\mu$. Then (4) becomes

$$\begin{aligned} &(a^{-1})_\nu^\beta(0)\left(\frac{\partial a_\mu^\nu(u)}{\partial u_i}\bigg|_{u=0}du_i+\Gamma^\nu_{\alpha\lambda}(y(x))a_\mu^\lambda(0)dy_\alpha\right) \\ &\quad=\{w_j^i(0)du_j+w_\alpha^i(x,0)dx_\alpha\}C_{i\mu}^\beta. \end{aligned} \tag{5}$$

But $a_\mu^\lambda(0)=(a^{-1})_\mu^\lambda(0)=\delta_\mu^\lambda$ and $w_j^i(0)=\delta_j^i$ so

$$C_{i\mu}^\beta=\frac{\partial a_\mu^\beta(u)}{\partial u_i}\bigg|_{u=0},$$

$$\Gamma^\beta_{\lambda\mu}(y(x))\frac{\partial y_\lambda}{\partial x_\alpha}=C_{i\mu}^\beta w_\alpha^i(x,0). \tag{6}$$

Equations (6) thus determine the connection components $\Gamma^\beta_{\lambda\mu}$ in terms of the Yang–Mills potentials w_α^i and the functions $y_\lambda=f_\lambda(x)$.

IV. CONCLUDING REMARKS

(1) Every diffeomorphism $(x_\lambda)\mapsto(y_\lambda=f_\lambda(x))$ of space-time M determines a linear connection on M in terms of a Yang–Mills potential in view of the natural homomorphism of SU(2) into GL(4).

(2) If the linear connection is to come from a Lorentz metric then it will have to satisfy the usual metric compatibility conditions.

(3) SU(2) can be homomorphically imbedded into GL(4) or SO(3,1) in two different ways, e.g.,

$$\begin{pmatrix} & & 0 \\ a_j^i(u) & & 0 \\ & & 0 \\ 0\ 0\ 0 & & 1 \end{pmatrix},\quad \begin{pmatrix} 1 & 0\ 0\ 0 \\ 0 & a_j^i(u) \\ 0 & \\ 0 & \end{pmatrix}.$$

Each of these homomorphisms gives rise to different linear connections according to (6).

(4) Equations (6) also show that the contribution of the Yang–Mills potentials to the connection components is, in general, nonsymmetric and would thus give rise to *torsion* in the connection.

(5) Similar conclusions apply to the case of the electromagnetic field which arises out of connections on a U(1) bundle over M, because there exist also natural homomorphisms of U(1) into GL(4) (cf. Appendix).

(6). This viewpoint seems to suggest that, in analogy with Yang–Mills (or electromagnetic) field, we should regard the $\Gamma^\beta_{\lambda\mu}$'s instead of the metric, as potentials of the gravitational field and this lends some support to the suggestion of Yang and Killmister[5] that the source-free field equations of gravitation should be of the form $R_{\mu\alpha;\beta}=R_{\mu\beta;\alpha}$.

APPENDIX: THE REISSNER–NORDSTROM SOLUTION

In the case of combined electromagnetic and gravitational field, a connection on a U(1) bundle over M determines a connection on the principal frame bundle $L(M)$ according to the Einstein–Maxwell field equations.

The simplest example is the Reissner–Nordström solution,[6] where the metric is

$$ds^2 = -e^{2l(r)}dr^2 - r^2(d\theta + \sin^2\phi\, d\phi^2) + e^{2n(r)}dt^2,$$

with

$$e^{2l(r)} = \left(1 - \frac{2m}{r} + \frac{\chi q^2}{8\pi r^2}\right)^{-1}, \quad e^{2n(r)} = e^{-2l(r)},$$

where m,q represent mass and charge, respectively, of a static point charged particle generating a spherically symmetric electric potential given by $\phi_1 = \phi_2 = \phi_3 = 0$, $\phi_4 = q/r$, or $\phi_\alpha = \delta_{\alpha 4} q/r$. The connection components are

$$\Gamma^1_{11} = l'(r), \quad \Gamma^1_{22} = -re^{-2l(r)}, \quad \Gamma^1_{33} = \Gamma^1_{22}\cos^2\theta,$$

$$\Gamma^2_{33} = -\sin\theta\cos\theta, \quad \Gamma^2_{12} = \Gamma^3_{13} = 1/r, \quad \Gamma^3_{23} = 1/\tan\theta,$$

$$\Gamma^4_{14} = n'(r), \quad \Gamma^1_{44} = n'(r)e^{2[n(r)-l(r)]}.$$

If this solution is to serve as an example of our mapping theorem we must have $w^i_\alpha \equiv \phi_\alpha$, $G = \{e^{iu}\}$, and $G' = \mathrm{GL}(4)$. Consider as an example the following homomorphism of G into G':

$$f_G: e^{iu} \mapsto \begin{pmatrix} \cos u & -\sin u & 0 & 0 \\ \sin u & \cos u & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

so that

$$C^{\beta}_{i\mu} \equiv C^{\beta}_{\mu} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Since we are dealing with a Levi-Civita connection we have $\Gamma^\beta_{\nu\mu} - \Gamma^\beta_{\mu\nu} = 0$. Rewriting (6) as

$$\Gamma^\beta_{\nu\mu}(y) = C^{\beta}_{i\mu} w^i_\alpha(x) \frac{\partial x_\alpha}{\partial y_\nu}, \quad x_\alpha = x_\alpha(y),$$

we must then have

$$w^i_\alpha(x)\left(C^{\beta}_{i\mu}\frac{\partial x_\alpha}{\partial y_\nu} - C^{\beta}_{i\nu}\frac{\partial x_\alpha}{\partial y_\mu}\right) = 0,$$

which presents no problem. However, since C^β_μ is *antisymmetric* in β and μ for the above homomorphism f_G, $\Gamma^\beta_{\nu\mu}$ must also be *antisymmetric* in β and μ, which they are definitely not in the above case.

Thus the Reissner–Nordström solution cannot serve as an example of this simple mapping theorem for the above homomorphism.

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A local limit theorem for strongly dependent random variables and its application to a chaotic configuration of atoms

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We investigate one-dimensional chaotic configurations of atoms, which are generated by the Baker transformation or, equivalently, by the Bernoulli shift. The problem of calculating the distribution of the jth nearest-neighbor distances of these configurations is shown to be equivalent to the task of finding the limit distribution of the sum of the strongly dependent random variables $X_l:([0,1),\mu_L)\to[0,1)$, $x\to(2^l x)\bmod 1$ ($l\in\mathbb{N}_0$, μ_L is the Lebesgue measure). We prove the validity of a local limit theorem for this sequence of random variables and conclude, therefore, that the distribution density G_j of the jth nearest-neighbor distances is asymptotically (as $j\to\infty$) a Gaussian distribution, the width of which grows as $\sqrt{j}$. With the aid of this result, we prove that the pair distribution function G of our configurations, which is the sum of the G_j's, tends to unity in the limit of large distances.

I. INTRODUCTION

Central-limit and local-limit theorems for sums of independent random variables are well known in probability theory.[1,2] There has also been success in proving central limit theorems for sums of weakly dependent random variables, e.g., see Refs. 3 and 4. In this paper we are interested in the sum of the strongly dependent random variables

$$X_l:([0,1),\mu_L)\to[0,1),\qquad x\to(2^l x)\bmod 1 \tag{1.1}$$

($l\in\mathbb{N}_0$, μ_L is the Lebesgue measure). For sums of functions of these variables of the form

$$\sum_{l=0}^{j} f((2^l x)\bmod 1)=\sum_{l=0}^{j} f(X_l(x)), \tag{1.2}$$

Ibragimov[5] proved a central-limit theorem (convergence of the distribution function, not the density). For the special case of f as a characteristic function of an interval, Moskvin and Postnikov[6] showed the validity of a local-limit theorem. This result was generalized to a larger class of functions f by Rousseau-Egerle,[7] but our case, $f=$ identity, is excluded. We prove here this case in an elementary way in the sense that it does not presume knowledge of probability theory.

This local-limit theorem allows us to determine the asymptotic behavior of atomic pair-distribution functions of one-dimensional chaotic configurations of atoms, which are constructed by fixing the distances between neighboring atoms with the aid of the Baker transformation or the Bernoulli shift. The investigation of such configurations is motivated by the question of whether it is possible to interpret amorphous structures as a spatial analog to chaotic time evolution in dynamical systems. This question and a discussion of the physical significance of our results are published elsewhere[8]; here we give a mathematical formulation of the connection between the pair-distribution functions of these configurations and the random variables X_l defined in (1.1), and the proofs.

The paper is organized as follows: In Sec. II we first give the definitions of our chaotic configurations. Then we define the random variables D_j, which are essentially sums of the random variables X_l, and their distribution densities $A^{-1}G_j$. The crucial part of this section, the connection between the pair-distribution functions of our configurations and the densities of the random variables D_j, i.e., the identification of the distribution density ("function") of jth nearest-neighbor distances with G_j is given in Theorem 0b. Section III contains the following results: The above-mentioned identification allows us to apply the local-limit theorem (Theorem 1a) to our configurations (Theorem 1b). With this result it is possible to prove the convergence of the pair-distribution function G to a constant (which, in our units, is equal to unity) in the limit of large distances (Theorem 2). Section IV contains the proof of the local-limit theorem, and Sec. V applies it to demonstrate Theorem 2. Finally, in Sec. VI we give a short discussion of the results.

II. DEFINITIONS

By a configuration we mean the set of the positions of the atoms in a one-dimensional chain. We first specify the special configurations we want to look at (f^n denotes $f\circ f\circ\ldots\circ f$, n times).

Definition 1a: Baker configuration: Let $(\alpha,\beta)\in[0,1)^2$; $(A,B)\in\mathbb{R}^{+2}$, such that $B<2A$. Then we define

$$C_{\alpha,\beta}(A,B)=\{u_n\in\mathbb{R}\,|\,n\in\mathbb{Z},u_0=0,\ u_{n+1}-u_n=A+B\{(T^n(\alpha,\beta))_1-\tfrac{1}{2}\}\}, \tag{2.1}$$

where $T:[0,1)^2\to[0,1)^2$ is the Baker transformation

$$(T(x,y))_1=\begin{cases}2x, & \text{for } x\in[0,\frac{1}{2}),\\ 2x-1, & \text{for } x\in[\frac{1}{2},1);\end{cases} \tag{2.2}$$

$$(T(x,y))_2=\begin{cases}\frac{1}{2}y, & \text{for } x\in[0,\frac{1}{2}),\\ \frac{1}{2}(y+1), & \text{for } x\in[\frac{1}{2},1).\end{cases}$$

Definition 1b: Bernoulli configuration: Let $\gamma=\{\gamma_l\}_{l\in\mathbb{Z}}\in\{0,1\}^{\mathbb{Z}}$; $(A,B)\in\mathbb{R}^{+2}$, such that $B<2A$. Then we define

$$C_\gamma(A,B)=\{u_n\in\mathbb{R}\,|\,n\in\mathbb{Z},u_0=0,\ u_{n+1}-u_n=A+B\{\varphi(S^n(\gamma))-\tfrac{1}{2}\}\}, \tag{2.3}$$

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wnere

$$\varphi:\ \{0,1\}^{\mathbb{Z}}\to[0,1),$$
$$\gamma=\{\gamma_l\}_{l\in\mathbb{Z}}\mapsto\sum_{l=}^{\infty}\frac{\gamma_l}{2^l} \tag{2.4}$$

and

$$S:\ \{0,1\}^{\mathbb{Z}}\to\{0,1\}^{\mathbb{Z}},$$
$$\{\gamma_l\}_{l\in\mathbb{Z}}\mapsto\{\gamma_{l+1}\}_{l\in\mathbb{Z}} \tag{2.5}$$

is the Bernoulli shift.

Because of the well-known equivalence between Bernoulli shift S and Baker transformation T (see Refs. 9 and 10), we obtain, with

$$\alpha(\gamma)=\sum_{l=1}^{\infty}\frac{\gamma_l}{2^l},\quad \beta(\gamma)=\sum_{l=0}^{\infty}\frac{\gamma_{-l}}{2^{l+1}}, \tag{2.6}$$

the following identity between the Definitions 1a and 1b:

$$C_{\alpha(\gamma),\beta(\gamma)}(A,B)=C_{\gamma}(A,B)\,. \tag{2.7}$$

In the following, therefore, we limit our considerations to the more intuitive Definition 1a.

The construction of our configuration can be described as follows: The distances $v_n=u_{n+1}-u_n$ between neighboring atoms are in the interval $[A-B/2,\ A+B/2)$ of length B around the point A. For vanishing B, A is the lattice constant of the corresponding crystalline configuration; B limits the variation of the atomic distances around this value. It is clear, that the ratio B/A, the relative variation, is the important parameter of our model. The arbitrary fixation of $u_0=0$ has no influence to the results. The other parameter of the configurations is the initial point of iteration $(\alpha,\beta)\in[0,1)^2$. The first component of the nth point of iteration ($n\in\mathbb{Z}$) of the Baker transformation $T^n(\alpha,\beta)$ determines, according to (2.1), the distance

$$v_n=u_{n+1}-u_n=A+B\,((T^n(\alpha,\beta))_1-\tfrac{1}{2}). \tag{2.1'}$$

We now make the following assumptions.

Assumptions:

$\alpha\in[0,1)$, $\beta\in[0,1)$ normal numbers (see Niven[11]);

$$A\in\mathbb{R}^+,\ B\in\mathbb{R}^+,\quad B<2A; \tag{2.8}$$

$C_{\alpha,\beta}(A,B)=\{u_n\}_{n\in\mathbb{Z}}$, u_n as defined in (2.1).

The normality of α and β implies, according to its definition,[11] that the first components of the sequence of iteration points $(T^n(\alpha,\beta))_1$ are uniformly distributed in the unit interval:

$$\lim_{N\to\infty}(1/2N)\#\{l\in\mathbb{Z}\mid -N\leqslant l<N \text{ and}(T^{n+l}(\alpha,\beta))_1\in[x_L,x_R)\}=x_R-x_L\,, \tag{2.9}$$

for all $n\in\mathbb{Z}$ and all intervals $[x_L,x_R)\subset[0,1)$. (# means the cardinality of the set.) From (2.9) we conclude the following.

Theorem 0a: Mean atomic distance: Under the assumptions (2.8) we have

$$\lim_{N\to\infty}\frac{1}{2N}\sum_{l=-N}^{N-1}v_{n+l}=\lim_{N\to\infty}\frac{1}{2N}(u_{n+N}-u_{n-N})=A. \tag{2.10}$$

This theorem states that A is the mean atomic distance of our configuration if (2.8) is satisfied; it expresses the ergodicity of the Baker transformation T.

Proof: Let $\epsilon\in\mathbb{R}^+$, $n\in\mathbb{Z}$. Choose $m\in\mathbb{N}$, $N_0\in\mathbb{N}$ such that $B/2^{m+1}<\epsilon$,

$$\left|\frac{1}{2N}\#\left\{-N\leqslant l<N \text{ and } (T^{n+l}(\alpha,\beta))_1\in\left[\frac{k}{2^m},\frac{k+1}{2^m}\right)\right\}-\frac{1}{2^m}\right|<\frac{\epsilon}{B\cdot 2^m},\quad \text{for all } k\in\{0,1\ldots,2^m-1\},$$
$$\text{for all } N>N_0.$$

Then we obtain

$$\left|\frac{1}{2N}\sum_{l=-N}^{N-1}v_{n+l}-A\right|<B\frac{1}{2^{m+2}}+2^m\frac{\epsilon}{B\cdot 2^m}\frac{B}{2}<\epsilon.$$

Here, the first term bounds the effect of incomplete compensation of points within the intervals of length 2^{-m}, and the second term is the contribution of those points which are not in the "right" interval.

To characterize our configurations, we introduce the following functions.

Definition 2: Distribution functions (densities): Let $j\in\mathbb{N}$. Then we define

$$G_j:\mathbb{R}\to\mathbb{R}_0^+$$

by

$A^{-1}G_j$ is the probability density of the random variable D_j on the probability space $([0,1),\mu_L)$, (2.11)

$$D_j:[0,1)\to\mathbb{R}^+,$$
$$x\mapsto jA+B\sum_{l=0}^{j-1}\{(2^l x)\bmod 1-\tfrac{1}{2}\}, \tag{2.12}$$

here μ_L denotes the Lebesgue measure on the interval $[0,1)$ (we have introduced the factor A^{-1} in order to make G_j dimensionless).

Finally, we introduce

$$G=\sum_{j=1}^{\infty}G_j. \tag{2.13}$$

[As we will see later, for each R only a finite number of terms contribute to $G(R)$.]

By definition we then have

$$A^{-1}\int_{R_1}^{R_2}G_j(R)\,dR=\mu_L(D_j^{-1}([R_1,R_2))),\quad \forall[R_1,R_2)\subset\mathbb{R}. \tag{2.14}$$

Note that these functions D_j are essentially sums of the random variables X_l defined in (1.1),

$$D_j=j\left(A-\frac{B}{2}\right)+B\sum_{l=0}^{j-1}X_l, \tag{2.15}$$

and $A^{-1}G_j$ is therefore the probability density of such a sum. On the other hand, the functions D_j are related to the distances of jth nearest neighbors of our configurations $C_{\alpha,\beta}(A,B)$ in the following way [see (2.1) and (2.12)]:

$$D_j((T^n(\alpha,\beta))_1)=u_{n+j}-u_n,\quad \forall j\in\mathbb{N},\quad n\in\mathbb{Z}. \tag{2.16}$$

This connection allows us to give the following physical interpretation of the functions G_j and G.

Theorem 0b: Physical interpretation of G_j and G: Under the assumption (2.8) we have

$$A^{-1}\int_{R_1}^{R_2} G_j(R)\,dR$$

$$= \lim_{N\to\infty} (1/2N)\#\{l\in\mathbb{Z} \mid -N\leqslant l<N \text{ and } R_1\leqslant u_{n+l+j}-u_{n+l}<R_2\},$$

for all $j\in\mathbb{N}$, $n\in\mathbb{Z}$ and all $R_1\in\mathbb{R}$, $R_2\in\mathbb{R}$ with $R_1<R_2$; (2.17)

and

$$A^{-1}\int_{R_1}^{R_2} G(R)\,dR$$

$$= \lim_{N\to\infty} (1/2N)\#\{(l,m)\in\mathbb{Z}\times\mathbb{N} \mid -N\leqslant l<N \text{ and } R_1\leqslant u_{n+l+m}-u_{n+l}<R_2\},$$

for all $n\in\mathbb{Z}$ and all $R_1\in\mathbb{R}$, $R_2\in\mathbb{R}$ with $R_1<R_2$. (2.18)

The right-hand sides of these two equations are the relative frequencies of finding two jth nearest neighbors, or any two atoms, at a distance within the interval $[R_1, R_2)$ respectively. Therefore, we have the following physical interpretation of the functions G_j and G:

$A^{-1}G_j(R)$ is the distribution density of finding the jth nearest neighbor of an atom at distance R, (2.19)

$A^{-1}G(R)$ is the distribution of finding any two atoms at distance R. (2.20)

Or, in other words,

G is the pair-distribution function of our configuration. (2.21)

Proof: $D_j^{-1}([R_1,R_2))$ can be written as a union of a finite number of disjoint intervals $[x_L^i, x_R^i)$, because D_j is piecewise continuous:

$$D_j^{-1}([R_1,R_2)) = \bigcup_i [x_L^i, x_R^i).$$

By the aid of (2.14) we then find

$$A^{-1}\int_{R_1}^{R_2} G_j(R)\,dR = \mu_L\Big(\bigcup_i [x_L^i, x_R^i)\Big) = \sum_i (x_R^i - x_L^i). \tag{2.22}$$

On the other hand [from (2.16) and (2.9)],

$$\begin{aligned}
&(1/2N)\#\{l\in\mathbb{Z} \mid -N\leqslant l<N \text{ and } R_1\leqslant u_{n+l+j}-u_{n+l}<R_2\}\\
&= (1/2N)\#\{l\in\mathbb{Z} \mid -N\leqslant l<N \text{ and } D_j((T^{n+l}(\alpha,\beta))_1)\in[R_1,R_2)\}\\
&= (1/2N)\#\{l\in\mathbb{Z} \mid -N\leqslant l<N \text{ and } (T^{n+l}(\alpha,\beta))_1\in D_j^{-1}([R_1,R_2))\} \qquad (2.23)\\
&= \sum_i \frac{1}{2N}\#\{l\in\mathbb{Z} \mid -N\leqslant l<N \text{ and } (T^{n+l}(\alpha,\beta))_1\in[x_L^i, x_R^i)\}\\
&\to \sum_i (x_R^i - x_L^i), \quad \text{as } N\to\infty.
\end{aligned}$$

Then (2.17) follows immediately from (2.22) and (2.23), and (2.18) is now obvious.

The identification of the probability density $A^{-1}G_j$ of a sum of the random variables X_l defined by (1.1) and (2.15) with the distribution density of the jth nearest-neighbor distances of our configurations, which is given formally in (2.17) and intuitively in (2.19), allows us in the following section to apply the local-limit theorem (Theorem 1a) to our chaotic configurations.

III. RESULTS

In this section we state the local limit theorem (3.1), we give an obvious conclusion about the jth nearest-neighbor distances distributions (3.2), and, finally, we present a more indirect consequence about the pair-distribution function G (3.3). The proofs are given in Secs. IV and V.

A. Local limit theorem

We first give the formulation of the local limit theorem. The proof can be found in Sec. IV.

Theorem 1a: Local limit theorem: Let X_j, $j\in\mathbb{N}$ be the random variables on the probability space $([0,1), \mu_L)$ defined by

$$X_j(x) = (2^j x) \bmod 1 \tag{3.1}$$

[notice that $X_j = f\circ f\circ\ldots\circ f$ (j times), with $f(x) = (2x) \bmod 1$]. We define further

$$Y_j(x) = \sum_{l=0}^{j-1} (X_l(x) - \tfrac{1}{2}) = \sum_{l=0}^{j-1} (2^l x) \bmod 1 - \frac{j}{2}, \tag{3.2}$$

$$Z_j(x) = \frac{2}{\sqrt{j}}\, Y_j(x) = \frac{2}{\sqrt{j}} \sum_{l=0}^{j-1} (X_l(x) - \tfrac{1}{2}), \tag{3.3}$$

and let p_j be the probability density of Z_j. Then

$$\lim_{j\to\infty} p_j(z) = (1/\sqrt{2\pi}\,\exp(-z^2/2), \tag{3.4}$$

for all $z\in\mathbb{R}$, uniformly in every bounded z interval.

This theorem states, as do the limit theorems for independent and weakly dependent random variables mentioned in the Introduction, that the limit distribution of a sum of random variables $X_l - \frac{1}{2}$, with mean value zero and scaled by $j^{-1/2}$, is a Gaussian distribution.

B. jth nearest-neighbor distribution function G_j

From the connection

$$Z_j = (2/(B\sqrt{j}))(D_j - jA) \tag{3.5}$$

between the random variables Z_j (3.3) and D_j (2.12) we conclude the following relation between their probability densities p_j and $A^{-1}G_j$:

$$p_j(z) = (B\sqrt{j}/2A)\,G_j(jA + (B\sqrt{j}/2)z). \tag{3.6}$$

Therefore Theorem 1a is equivalent to the following theorem.

Theorem 1b: Asymptotic form of G_j:

$$\lim_{j\to\infty} \frac{B\sqrt{j}}{2A}\, G_j\Big(jA + \frac{B\sqrt{j}}{2}z\Big) = \frac{1}{\sqrt{2\pi}}\exp\Big(-\frac{z^2}{2}\Big), \tag{3.7}$$

for all $z\in\mathbb{R}$, uniformly in every bounded z interval.

Because of the physical interpretation of G_j of Theorem 0b [(2.17) and (2.19)], this is an interesting result concerning our chaotic configurations. It states, that the distribution function (density) of jth nearest-neighbor distances behaves asymptotically as a Gaussian distribution, centered at jA with a width which grows as $\sqrt{j}$.

Furthermore, from the proof in Sec. IV we get the following explicit formula for G_j:

$$G_j(R) = AN_j(R)/B(2^j - 1), \tag{3.8}$$

with

$$N_j(R) = \#\{x\in[0,1) | D_j(x) = R\}, \tag{3.9}$$

and with D_j according to (2.12).

Hence, G_j is a piecewise constant function, which is zero outside the interval $[j(A - B/2), j(A + B/2)]$. For small j, G_j can easily be calculated according to the above formula, but for large values of j this calculation becomes troublesome, because the number of steps of G_j grows exponentially with j. It is therefore useful that we can give the asymptotic form in (3.7).

C. Pair distribution function G

Because $G_j(R)$ is zero for R outside the interval $[j(A - B/2), j(A + B/2)]$, for each R only a finite number of terms (which depends on R) contribute to the sum (2.13), and therefore (3.8) allows us to calculate G. Nevertheless, it is very useful to have an analytic expression for its asymptotic behavior.

Theorem 2: Asymptotic behavior of G:

$$\lim_{R\to\infty} G(R) = 1. \tag{3.10}$$

Theorem 2 states that the oscillations of G go to zero, if R goes to infinity. This behavior is true for all allowed values of A and B ($B < 2A$), which influence only the speed of convergence, and it agrees very well with that expected for amorphous solids, as is discussed in Ref. 8. The proof of Theorem 2 is given in Sec. V.

IV. PROOF OF THEOREM 1

We establish here first the validity of formula (3.8) and then we prove the local-limit theorem (Theorem 1a).

Because the slope of Y_j (3.2) is constant

$$Y_j' = 2^j - 1 \quad \text{a.e.}, \tag{4.1}$$

and the probability density of the identity is $p = 1$, we get for the probability density q_j of Y_j

$$q_j(y) = M_j(y)/(2^j - 1), \tag{4.2}$$

where

$$M_j(y) = \#\{x\in[0,1) | Y_j(x) = y\}. \tag{4.3}$$

To get the corresponding expression for G_j we denote the probability densities of

identity, Y_j, Z_j, and D_j by

$$p, \quad q_j, \quad p_j, \quad \text{and} \quad A^{-1}G_j, \tag{4.4}$$

respectively [in accordance with the definitions of p_j (Theorem 1a) and G_j (2.11)]. From (3.3), (3.2), and (2.12) we obtain then

$$G_j(R) = \frac{A}{B} q_j\left(\frac{R - jA}{B}\right) = \frac{2A}{B\sqrt{j}} p_j\left(\frac{2(R - jA)}{B\sqrt{j}}\right). \tag{4.5}$$

Together with (4.2) and (4.3) this now leads to the formulas (3.8) and (3.9).

The proof of Theorem 1a is now given in three parts: First, we show that the probability density q_j (4.2) can be represented in a natural way by a binomial distribution plus a rest term [formula (4.2) together with Lemma 1], then we give an estimate of this rest term (Lemma 5), and finally, we use the local-limit theorem of de Moivre–Laplace (local-limit theorem for binomial distributions) to get a Gaussian distribution.

A. Part 1: Representation of M_j

To formulate the first statement, we need the following functions: For $j\in\mathbb{N}, m\in\{0,1,...j\}, x\in\mathbb{R}$ we define

$$n_m^j(x) = \#\left\{k\in\{0,1,...,2^j - 1\} \Big| \sum_{\nu=0}^{j-1} \sigma_\nu(k) = m \text{ and } \frac{k}{2^j} > x\right\}, \tag{4.6}$$

where $\sigma_\nu(k)\in\{0,1\}$ are the coefficients of the binary expansion of k:

$$k = \sum_{\nu=0}^{\infty} \sigma_\nu(k) 2^\nu. \tag{4.7}$$

Furthermore, we need for $j\in\mathbb{Z}$, $y\in\mathbb{R}$,

$$m(j,y) = [y + j/2] \tag{4.8}$$

where $[z]$ denotes the integer part of z. $\binom{j}{m}$ is the binomial coefficient, which we define to be zero for $m\in\mathbb{Z}\setminus\{0,1,...j\}$. We can give now the first step of the proof.

Lemma 1:

$$M_j(y) = \begin{cases} \binom{j}{m(j,y)} + R(j,y), & \text{for } y\in\left[-\frac{j}{2},\frac{j}{2}\right], \\ 0, & \text{for } y\notin\left[-\frac{j}{2},\frac{j}{2}\right], \end{cases} \tag{4.9}$$

with

$$R(j,y) = n_{m(j,y)+1}^{j-1}(x_0(y)) - n_{m(j,y)-1}^{j-1}(x_0(y)) + Q(j,y), \tag{4.10}$$

$$x_0(y) = \tfrac{1}{2} - y + [y + \tfrac{1}{2}], \quad |Q(j,y)| \leqslant 2.$$

Proof: We obtain this result in writing Y_j ($j > 1$) in the following form. For

$$x\in[k/2^{j-1}, (k+1)/2^{j-1}] \tag{4.11}$$

($j\in\mathbb{N}\setminus\{1\}$, $k\in\{0,1,...,2^{j-1} - 1\}$) and with

$$\Delta x = 2^{j-1}x - k = 2^{j-1}x - [2^{j-1}x]\in[0,1), \tag{4.12}$$

we can write

$$\begin{aligned} Y_j(x) &= Y_j^1(x) + Y_j^2(x), \\ Y_j^1(x) &= -k/2^{j-1} - \tfrac{1}{2} + (2 - 1/2^{j-1})\Delta x, \\ Y_j^2(x) &= \sum_{\nu=0}^{j-2} \sigma_\nu(k) - \frac{j-1}{2}. \end{aligned} \tag{4.13}$$

This decomposition allows an examination of the structure of the function Y_j: The graph of Y_j^1 consists of a set of parallel lines of slope $2^j - 1$, which are arranged in a strip of slope

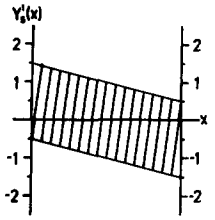

FIG. 1. First part of the decomposition of Y_5.

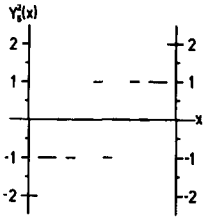

FIG. 2. Second part of the decomposition of Y_5.

-1 from $[-\frac{1}{2},\frac{3}{2}]$ at $x=0$ to $[-\frac{3}{2},\frac{1}{2}]$ at $x=1$ (compare Fig. 1). In Fig. 2 Y_j^2 spreads these lines out to j strips B^j_m, $m=0,1,\ldots,j-1$ parallel to the original one, B^j_m from $[-j/2+m,\ -j/2+m+2]$ at $x=0$ to $[-j/2+m-1,\ -j/2+m+1]$ at $x=1$ (see Fig. 3). Each strip B^j_m contains still $\binom{j}{m}^{-1}$ of the original lines, because this number is determined by the condition

$$\sum_{\nu=0}^{j-2}\sigma_\nu(k)=m,\quad k=[2^{j-1}x], \tag{4.14}$$

i.e., by the number of 1's in the binary decomposition of k.

The calculation of $M_j(y)$ (4.3) consists in counting the crossing points of the graph of Y_j with that of the constant function y. We first remark that only the three strips $B^j_{m(j,y)-1}$, $B^j_{m(j,y)}$, and $B^j_{m(j,y)+1}$ contribute [consider (4.12)].

Considering the segments of the graph of y that lie in these three different strips, we get Lemma 1.

Futhermore, we obtain from this proof the following rough estimate of G_j, which we will need in the next section to prove Theorem 2.

Lemma 2:

$$G_j(R)\begin{cases} <\dfrac{A}{B(2^j-1)}\left\{\binom{j-1}{m(j,R)-1}\right. \\ \quad\left.+\binom{j-1}{m(j,R)}+\binom{j-1}{m(j,R)+1}\right\}, \\ \quad \text{for } R\in[j(A-B/2),j(A+B/2)], \\ =0,\quad \text{for } R\notin[j(A-B/2),j(A+B/2)], \end{cases} \tag{4.15}$$

with

$$m(j,R)=[R/B-((2A-B)/2B)j]. \tag{4.16}$$

B. Part 2: Estimation of $R(j,y)$

According to (3.11) we are interested in an estimation of $R(j,y)$ for $y=(\sqrt{j}/2)z$ with fixed z and for large values of j. We get this estimate in three steps. First, we show in Lemma 3 that the lines within the strips $B^j_{m(j,y)}$ of Y_j (see the proof of Lemma 1) are asymptotically equidistributed in $[0,1)$ for large j and $y=(\sqrt{j}/2)z$. This result allows easily to conclude in Lemma 4 that $n^j_{m(j,(\sqrt{j}/2)z)}(x)$ is proportional to $(1-x)$ (for $j\to\infty$). From this we get the final upper bound of $R(j,(\sqrt{j}/2)z)$ in Lemma 5.

To formulate Lemma 3 we need the following notation: For $j\in\mathbb{N}$, $m\in\mathbb{N}_0$, $l\in\mathbb{N}_0$, $l\leqslant m\leqslant j$, $k\in\{0,1,\ldots,2^l-1\}$, we define

$$P^l_k(j,m)=\binom{j}{m}^{-1}\#\left\{n\in\{0,1,\ldots,2^j-1\}\,\middle|\, \sum_{\nu=0}^{j-1}\sigma_\nu(n)=m \text{ and } \frac{n}{2^j}\in\left[\frac{k}{2^l},\frac{k+1}{2^l}\right)\right\}. \tag{4.17}$$

Here, $P^l_k(j,m)$ gives the relative frequency of the numbers $n/2^j$, $n\in\{0,1,\ldots,2^j-1\}$, n with m 1's in its binary decomposition, to be in the interval $[k/2^l,(k+1)/2^l)$. This is equal to the relative frequency of the lines within the strip B^{j+1}_m to be in this interval, as is seen from the proof of Lemma 1. We define further

$$m(j,n_1,n_2,z)=[(j+n_1)/2+z\sqrt{j+n_1}/2]+n_2. \tag{4.18}$$

Now we can state equidistribution.

Lemma 3: Let $l\in\mathbb{N}_0$, $z_0\in\mathbb{R}^+$, $\epsilon_1\in\mathbb{R}^+$. Then there exists $j_1\in\mathbb{N}$ such that

$$\left|P^l_k(j,m(j,n_1,n_2,z))-1/2^l\right|<\epsilon_1, \tag{4.19}$$

for all $(j,k,n_1,n_2,z)\in\{(j,k,n_1,n_2,z)\in\mathbb{N}\times\{0,1,\ldots,2^{l-1}\}\times\{-1,0,1\}^2\times\mathbb{R}\,|\,j>j_1,|z|<z_0\}$.

Proof: If

$$m\geqslant l,\quad j-m\geqslant l, \tag{4.20}$$

i.e., if the integers n we count in (4.17) have at least l zeros and l 1's in their binary decomposition, we can give an explicit formula for P^l_k:

$$P^l_k(j,m)=\prod_{\mu=0}^{l-1}\left(\frac{\sigma_{l-1-\mu}(k)\{m+1-\Sigma_{\nu=0}^{\mu}\sigma_{l-1-\nu}(k)\}+(1-\sigma_{l-1-\mu}(k))\{j-m+1-\Sigma_{\nu=0}^{\mu}(1-\sigma_{l-1-\nu}(k))\}}{j-\mu}\right). \tag{4.21}$$

This formula is obtained in the following way: For $n/2^l$ to be in the interval $[k/2^l,(k+1)/2^l)$, l binary digits of n have to be equal to those of k. The factor with index μ of (4.21) gives the relative frequency of the binary digit $(\mu+1)$ of n to be equal to that of k if already μ digits are equal. The first term in each factor gives this quantity if the considered digit of k is 1, the second if it is zero. If we choose m according to (4.18), condition (4.20) is satisfied for sufficiently large j, and in inserting m into (4.21) we see that each factor converges to $\frac{1}{2}$ for $j\to\infty$ and Lemma 3 is proved.

As mentioned before, Lemma 3 can be used to draw conclusions concerning n^j_m.

Lemma 4: Let $z_0\in\mathbb{R}^+$, $\epsilon_2\in\mathbb{R}^+$. Then there exists $j_2\in\mathbb{N}$ such that

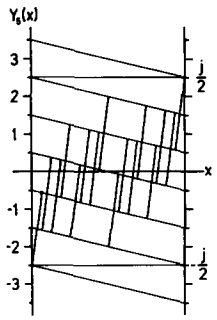

FIG. 3. Combinations of both parts Y_5^1 and Y_5^2 to Y_5.

$$\left| n^j_{m(j,n_1,n_2,z)}(x)\binom{j}{m(j,n_1,n_2,z)}^{-1} - (1-x)\right| < \epsilon_2, \tag{4.22}$$

for all $(j,n_1,n_2,z,x)\in\{(j,n_1,n_2,z,x)\in\mathbb{N}\times\{-1,0,1\}^2\times\mathbb{R}\times[0,1) \mid j>j_2, |z|<z_0\}$.

Proof: From the definitions (4.6) and (4.17), we conclude

$$\left| n^j_m(x)\binom{j}{m}^{-1} - \sum_{k=[2^l x]}^{2^l-1} P^l_k(j,m)\right| \leqslant P^l_{[2^l x]}(j,m). \tag{4.23}$$

By the aid of Lemma 3 we obtain

$$\left| n^j_{m(j,n_1,n_2,z)}(x)\binom{j}{m(j,n_1,n_2,z)}^{-1} - (1-x)\right| < \frac{2}{2^l} + (2^l+1)\epsilon_1, \tag{4.24}$$

for sufficiently large j. If we now choose l as big as $2/2^l < \epsilon_2/2$ and then ϵ_1 as small as $(2^l+1)\epsilon_1 < \epsilon_2/2$, Lemma 4 is proved with j_2 equal to the value of j_1 in Lemma 3 for this choice of ϵ_1.

Finally, we get the estimate of $R(j,(\sqrt{j}/2)z)$.

Lemma 5: Let $z_0\in\mathbb{R}^+$, $\epsilon_3\in\mathbb{R}^+$. Then there exists $j_3\in\mathbb{N}$ such that

$$\left| R\left(j,\frac{\sqrt{j}}{2}z\right)\right| < \binom{j}{[j/2+(\sqrt{j}/2)z]}\epsilon_3, \tag{4.25}$$

for all $(j,z)\in\{(j,z)\in\mathbb{N}\times\mathbb{R} \mid j>j_3, |z|<z_0\}$.

Proof: If we apply the preceding Lemma to $j-1$, $n_1=1$ and $n_2=\pm 1$ with

$$m(j,z) = [j/2+(\sqrt{j}/2)z], \tag{4.26}$$

we get

$$\begin{aligned} &|n^{j-1}_{m(j,z)+1}(x) - n^{j-1}_{m(j,z)-1}(x)| \\ &< \left|\binom{j-1}{m(j,z)+1} - \binom{j-1}{m(j,z)-1}\right| \\ &\quad + \epsilon_2\left\{\binom{j-1}{m(j,z)+1} + \binom{j-1}{m(j,z)-1}\right\} \end{aligned} \tag{4.27}$$

or (for sufficiently large j, $|z|<z_0$)

$$|n^{j-1}_{m(j,z)+1}(x) - n^{j-1}_{m(j,z)-1}(x)| < \binom{j}{m(j,z)}\epsilon_2(3+2\epsilon_2). \tag{4.28}$$

With this estimate and the definition (4.10) of $R(j,y)$, Lemma 5 follows.

C. Part 3: End of the proof

From (4.5), (4.2), Lemma 1, and Lemma 5 we conclude the following.

Lemma 6: Let $z_0\in\mathbb{R}^+$, $\epsilon_4\in\mathbb{R}^+$. Then there exists $j_4\in\mathbb{N}$ such that

$$\begin{aligned} &\left|p_j(z) - \frac{\sqrt{j}}{2}\binom{j}{[j/2+(\sqrt{j}/2)z]}2^{-j}\right| \\ &< \frac{\sqrt{j}}{2}\binom{j}{[j/2+(\sqrt{j}/2)z]}2^{-j}\epsilon_4, \end{aligned} \tag{4.29}$$

for all $(j,z)\in\{(j,z)\in\mathbb{N}\times\mathbb{R} \mid j>j_4, |z|<z_0\}$.

The approximation of the Gaussian distribution by the binomial distribution is described by the local-limit theorem of de Moivre–Laplace, which can be found in standard books on probability theory (e.g., Fisz,[2] p. 252).

Theorem (de Moivre–Laplace):

$$\lim_{j\to\infty}\left|\frac{\sqrt{j}}{2}\frac{1}{2^j}\binom{j}{k} - \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{z_{jk}^2}{2}\right)\right| = 0 \tag{4.30}$$

uniformly for all $k\in\mathbb{Z}$ where

$$z_{jk} = (2k-j)/\sqrt{j}. \tag{4.31}$$

We can reformulate this theorem in the following way.

Corollary: Let $\epsilon_5\in\mathbb{R}^+$. Then there exists $j_5\in\mathbb{N}$ such that

$$\left|\frac{\sqrt{j}}{2}\frac{1}{2^j}\binom{j}{[j/2+(\sqrt{j}/2)z]} - \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{z^2}{2}\right)\right| < \epsilon_5, \tag{4.32}$$

for all $(j,z)\in\{(j,z)\in\mathbb{N}\times\mathbb{R} \mid j>j_5\}$.

Lemma 6 and this corollary prove immediately Theorem 1b and therefore Theorem 1a.

V. PROOF OF THEOREM 2

Because G_j is zero outside $[j(A-B/2), j(A+B/2)]$, for each R, the sum (2.13) has only a finite number of terms, and we can write

$$G(R) = \sum_{j=[2R/(2A+B)]}^{[2R/(2A-B)]} G_j(R). \tag{5.1}$$

We now want to use the asymptotic form of G_j according to Theorem 1b to obtain the behavior of G for large values of R. To clarify the range of validity of the asymptotic approximation, we first write Theorem 1b in another form.

Theorem 1c: Let $z_0\in\mathbb{R}^+$, $\epsilon\in\mathbb{R}^+$. Then there exists $R_0\in\mathbb{R}^+$ such that

$$\left|G_j(R) - \frac{1}{\sqrt{2\pi}}\frac{2A}{B\sqrt{j}}\exp\left(-\frac{2(R-jA)^2}{B^2 j}\right)\right| < \frac{2A}{B\sqrt{j}}\epsilon, \tag{5.2}$$

for all $(j,R)\in\{(j,R)\in\mathbb{N}\times\mathbb{R}^+ \mid R>R_0$ and $R/A - (Bz_0/A)\sqrt{(R/A)} < j < R/A + (Bz_0/A)\sqrt{(R/A)}\}$.

Theorem 1c is easily deduced from Theorem 1b (3.7).

We see from Theorem 1c that an estimate of the sum (5.1) by the Gaussian approximations of G_j is only possible in a range of j values, which differ by not more than an amount or the order of $\sqrt{R/A}$ from the central value $j=[R/A]$. Therefore, it is natural to split the sum (5.1) into three parts in the following way:

$$S_1(R,z_0)=\sum_{j=[2R/(2A+B)]}^{[R/A]-[(Bz_0/2A)\sqrt{R/A}]-1} G_j(R),$$
$$S_2(R,z_0)=\sum_{j=[R/A]-[(Bz_0/2A)\sqrt{R/A}]}^{[R/A]+[(Bz_0/2A)\sqrt{R/A}]} G_j(R), \tag{5.3}$$
$$S_3(R,z_0)=\sum_{j=[R/A]+[(Bz_0/2A)\sqrt{R/A}]+1}^{[2R/(2A+B)]} G_j(R),$$
$$G(R)=S_1(R,z_0)+S_2(R,z_0)+S_3(R,z_0). \tag{5.4}$$

In Lemma 7, we determine the limit of the central part S_2 in the way described above. The other two parts are estimated in Lemma 8 by the aid of Lemma 2.

Lemma 7: Let $\epsilon\in\mathbb{R}^+$, $z_0\in\mathbb{R}^+$. Then there exists $R_1\in\mathbb{R}^+$ such that

$$\left|S_2(R,z_0)-\frac{1}{\sqrt{2\pi}}\int_{-z_0}^{z_0}\exp\left(-\frac{z^2}{2}\right)dz\right|<\frac{\epsilon}{6}, \tag{5.5}$$

for all $R>R_1$.

Proof: We denote the sum S_2 (5.3) with the asymptotic form (5.2) instead of G_j by $\hat{S}_2$. With

$$x=R/A,\quad l=j-[x], \tag{5.6}$$

we then obtain

$$\hat{S}_2(Ax,z_0)=\frac{1}{\sqrt{2\pi}}\sum_{l=-[(Bz_0/2A)\sqrt{x}]}^{[(Bz_0/2A)\sqrt{x}]}\left\{\frac{2A}{B\sqrt{x}}\times\exp\left(-\frac{((2A/B\sqrt{x})l)^2}{2}\right)h(x,l)\right\} \tag{5.7}$$

with

$$h(x,l)=\frac{\sqrt{x}}{\sqrt{[x]+l}}\exp\left(-\frac{2A^2}{B^2}\,\frac{x(x-[x])^2-2xl(x-[x])+l^2(x-[x])-l^3}{x([x]+l)}\right). \tag{5.8}$$

It is clear that $h(x,l)\to 1$ for $x\to\infty$ uniformly for l in the allowed range:

$$L(x)=\{l\in\mathbb{Z}|-[(Bz_0/2A)\sqrt{x}]\leqslant l\leqslant[(Bz_0/2A)\sqrt{x}]\}, \tag{5.9}$$

$$|h(x,l)-1|<\epsilon/25, \tag{5.10}$$

for sufficiently large x and $l\in L(x)$. Therefore, with

$$\tilde{S}_2(Ax,z_0)=\frac{1}{\sqrt{2\pi}}\sum_{l=-[(Bz_0/2A)\sqrt{x}]}^{[(Bz_0/2A)\sqrt{x}]}\frac{2A}{B\sqrt{x}}\times\exp\left(-\frac{((2A/B\sqrt{x})l)^2}{2}\right), \tag{5.11}$$

we have

$$|\hat{S}_2(Ax,z_0)-\tilde{S}_2(Ax,z_0)|<\tilde{S}_2(Ax,z_0)(\epsilon/25), \tag{5.12}$$

for sufficiently large x. But $\tilde{S}_2(Ax,z_0)$ is the Riemannian sum of $(1/\sqrt{2\pi})\exp(-z^2/2)$ $[\Delta z=2A/B\sqrt{x},\ z_l=(2A/B\sqrt{x})l]$ and converges to the integral of this function:

$$\left|\tilde{S}_2(Ax,z_0)-\frac{1}{\sqrt{2\pi}}\int_{-z_0}^{z_0}\exp\left(-\frac{z^2}{2}\right)dz\right|<\frac{\epsilon}{25}, \tag{5.13}$$

for sufficiently large x. From (5.12) and (5.13), we conclude

$$\left|\hat{S}_2(Ax,z_0)-\frac{1}{\sqrt{2\pi}}\int_{-z_0}^{z_0}\exp\left(-\frac{z^2}{2}\right)dz\right|<\left(1+\frac{\epsilon}{25}\right)\frac{\epsilon}{25}+\frac{\epsilon}{25}<\frac{\epsilon}{12}. \tag{5.14}$$

We have yet to estimate $|S_2-\hat{S}_2|$ with the aid of Theorem 1c (5.2). If we apply this theorem with $\epsilon/30z_0$ instead of ϵ, we get

$$|S_2(Ax,z_0)-\hat{S}_2(Ax,z_0)|<\frac{2A}{B}\,\frac{2[(Bz_0/2A)\sqrt{x}]+1}{\sqrt{[x]-[(Bz_0/2A)\sqrt{x}]}}\,\frac{\epsilon}{30z_0}<\frac{\epsilon}{12}, \tag{5.15}$$

for sufficiently large x. Lemma 7 is now a consequence of (5.14) and (5.15).

Finally, we estimate S_1 and S_3.

Lemma 8: Let $z_0\in\mathbb{R}^+$. Then there exists $R_2\in\mathbb{R}^+$ such that

$$S_1(R,z_0)<(c/z_0)\exp(-z_0^2/2),$$
$$S_3(R,z_0)<(c/z_0)\exp(-z_0^2/2), \tag{5.16}$$

for all $R>R_2$ with $c=\exp(A/B+6)$.

The proof of this lemma makes use only of Lemma 2 (4.19) and of Stirling's formula to estimate the binomial coefficients. It is troublesome but not interesting, and it is therefore omitted here. Theorem 2 now follows from Lemmas 7 and 8: To each $\epsilon>0$ we can choose z_0 such that

$$\left|\frac{1}{\sqrt{2\pi}}\int_{-z_0}^{z_0}\exp\left(-\frac{z^2}{2}\right)dz-1\right|<\frac{\epsilon}{6} \tag{5.17}$$

and

$$\frac{1}{z_0}\exp\left(\frac{A}{B}+6-\frac{z_0^2}{2}\right)<\frac{\epsilon}{3}. \tag{5.18}$$

We then conclude from (5.5) and (5.16)

$$|S_1(R,z_0)|<\epsilon/3,$$
$$|S_2(R,z_0)-1|<\epsilon/3, \tag{5.19}$$
$$|S_3(R,z_0)|<\epsilon/3,$$

for sufficiently large R, and Theorem 2 follows from (5.4).

VI. CONCLUSIONS

We have proved a local-limit theorem for the sum of the strongly dependent random variables

$$X_l:([0,1),\mu_L)\to[0,1)$$
$$x\mapsto(2^l x)\bmod 1, \tag{6.1}$$

(Theorem 1a).

With the aid of this theorem, we have demonstrated two important properties of the chaotic configurations according to Definition 1: First, the distribution function G_j of the jth nearest-neighbor distances becomes asymptotically a Gaussian distribution, centered at jA (A is the mean atomic distance) and with standard deviation

$$\sigma_j=(B/2)\sqrt{j}, \tag{6.2}$$

which grows as $\sqrt{j}$ (Theorem 1b). This statement reflects the absence of long-range order of our configurations, which is also confirmed by the second property, the convergence of

the pair-distribution function G to unity in the limit of large distances (Theorem 2).

Therefore, our configurations exhibit qualitatively the most characteristic feature of the structure of amorphous solids and our results fortify further efforts in the investigation of less simplified but more realistic chaotic configurations, which are stationary solutions of interaction potentials between the atoms and which have been the motivation to study the simplified configurations according to Definition 1 (see Ref. 8). The results concerning these configurations will be published later.

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Generalization of the diffusion equation by using the maximum entropy principle

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By using the so-called maximum entropy principle in information theory, one derives a generalization of the Fokker–Planck–Kolmogorov equation which applies when the n first transition moments of the process are proportional to Δt, while the other ones can be neglected.

I. INTRODUCTION

Consider a scalar valued Markovian stochastic process $x(t) \in R$, $t \in (t_0, +\infty)$ whose state probability density function $p(x,t)$ is given by the well-known so-called Fokker–Planck–Kolmogorov partial differential equation (FPK equation)

$$\dot{p}(x,t) = -(\alpha p)_x + \tfrac{1}{2}(\beta p)_{xx}, \quad \beta \geqslant 0 \tag{1}$$

where α and β denote two functions $\alpha(x,t)$ and $\beta(x,t)$ which are differentiable enough in order that Eq. (1) makes sense. The most standard ways to derive the FPK equation are the following.

(i) First, one may consider the Markovian process as being represented by the Ito stochastic differential equation

$$\dot{x}(t) = \alpha(x,t) + \sqrt{\beta(x,t)}\, w(t),$$

where $w(t)$ is a white noise with zero mean and unit variance, and then one determines $p(x,t)$ on using the Chapman–Kolmogorov equation.

(ii) Second, one may also assume that the Markovian process is defined by its conditional transition moments

$$E\{\Delta x/x,t\} = \alpha(x,t)\Delta t, \tag{2}$$

$$E\{(\Delta x - \overline{\Delta x})^2/x,t\} = \beta(x,t)\Delta t, \tag{3}$$

$$E\{(\Delta x - \overline{\Delta x})^n/x,t\} = o(\Delta t^2), \quad n \geqslant 3, \tag{4}$$

and then, by once more using the Chapman–Kolmogorov equation, one can get Eq. (1).

Another viewpoint, the information theoretic one, is as follows.[1]

Proposition 1: Assume that all the information we have at hand about the Markovian process is summarized in the knowledge of its transition moments (2) and (3); then, in the information theoretic framework, according to the maximum entropy principle,[2,3] all we can assume is that the probability density $p(x,t)$ is given by the FPK equation (1). □

Our main purpose, in the following, is to show that, by only using this maximum entropy principle, it is possible to derive a generalization of the FPK equation which applies when all the transition moments are proportional to Δt; a case which occurs, for instance, with some fluctuating density fields.

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II. A GENERALIZED DIFFUSION EQUATION

We state the following result.

Proposition 2: Consider a one-dimensional stochastic process $x(t)$ with the unknown probability density $p(x,t)$ and the transition probability density

$$p(x',t+\tau/x,t) =: q(z,\tau/x,t), \quad z := x' - x. \tag{5}$$

Assumption A1: Assume that for small τ, the value of the state x at $t+\tau$, say $x(t+\tau)$, depends upon $x(t)$ only.

Assumption A2: Assume that all the information we have at hand about this process is summarized in the knowledge of its first n transition moments

$$E\{z^j,\tau/x,t\} = \alpha_j(x,t)\tau, \quad j = 1,2,\ldots,n \tag{6}$$

where $\alpha_j(x,t)$ is continuous in t and differentiable w.r.t. x up to the jth order for every $x \in \mathbb{R}$.

Then, in the framework of the maximum entropy principle, $p(x,t)$ is given by the equation

$$\dot{p}(x,t) = \sum_{j=1}^{n} \frac{(-1)^j}{j!} \frac{\partial^j}{\partial x^j} [\alpha_j(x,t)p(x,t)]. \tag{7}$$

□

Proof: We decompose the proof in the following steps.

Step 1: The probability density $q(z,\tau/x,t)$ is unknown; and according to the maximum entropy principle, we shall define q as being that density which maximizes the conditional entropy

$$H(Z/x,t) = -\int_{-\infty}^{+\infty} q(z,\tau/x,t) \ln q(z,\tau/x,t)\, dz, \tag{8}$$

given the constraints (7) on the moments. A standard calculation yields

$$q(z,\tau/x,t) = \exp\left(\sum_{j=0}^{n} a_j(\tau) z^j\right). \tag{9}$$

The $a_j(\tau)$ functions should be determined by means of the conditions (6); but this is unnecessary since we need only their limiting values $\lim a_j(\tau)$, $\tau \to 0$. So we shall restrict ourselves to the calculation of the approximation

$$q(z,\tau) \cong q(z,0) + \tau \left(\frac{\partial q}{\partial z}\right)_{\tau=0}. \tag{10}$$

Step 2: First of all, one has necessarily

$$q(z,0) = \delta(z), \tag{11}$$

where $\delta(z)$ denotes the Dirac distribution.

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Step 3: This being so, Eq. (9) yields

$$\frac{\partial}{\partial\tau}q(z,\tau/x,t)=\left[-\sum_0^n a_j'(\tau)z^j\right]q(z,\tau/x,t), \tag{12}$$

where the prime denotes the derivative w.r.t. τ; and on integrating w.r.t. z, we obtain

$$\int_{-\infty}^{+\infty}\frac{\partial q}{\partial\tau}dz=-a_0'(\tau)-\tau\sum_1^n a_j'(\tau)\alpha_j(x,t). \tag{13}$$

As a result, there exist functions or generalized functions (in which case the derivatives are considered in the sense of distributions) $b_0(z,\tau)$, $b_j(z,\tau)$, $1\leqslant j\leqslant n$, such that

$$\frac{\partial}{\partial\tau}q(z,\tau/x,t)=b_0(z,\tau)+\sum_1^n\alpha_j(x,t)b_j(z,\tau). \tag{14}$$

Now, on substituting (11) and (14) into (10) we get

$$q(z,\tau)\cong\delta(z)+\tau c_0(z)+\tau\sum_1^n\alpha_j(x,t)c_j(z); \tag{15}$$

and the task is then to determine $C_0(z)$ and $c_j(z)$.

Step 4: We remark that, according to Eq. (11), the range of variation of z is small for small h, so that $c_j(z)$ is necessarily a distribution concentrated in 0, namely, according to Eq. (15), we should have

$$c_j(z)=k_j\delta^{(m_j)}(z),$$

where the constant k_j and the derivative order m_j is to be determined.

Step 5: Next, we use the moment conditions (6), $j=1,2,\ldots,n$ to finally obtain

$$q(z,\tau/x,t)\cong\delta(z)+\sum_{j=1}^n\frac{(-1)^j}{j!}\alpha(x,t)\delta^{(j)}(z). \tag{16}$$

Step 6: Assumption A1 provides the Chapman–Kolmogorov equation

$$p(x',t+\tau)=\int_{-\infty}^{+\infty}q(x'-x,t+\tau/x,t)p(x,t)dx, \tag{17}$$

and substituting (16) into (17) directly yields

$$p(x',t+\tau)=p(x',t)=\tau\sum_1^n\frac{(-1)^j}{j!}\frac{\partial}{\partial x'}[\alpha(x',t)p(x',t)] \tag{18}$$

as a direct consequence of the relation

$$\int_{-\infty}^{+\infty}f(x)\delta^{(j)}(y-x)dx=\left[\frac{d^jf}{dx^j}\right]_{x=y}.$$

By letting τ tend to zero in Eq. (18), we get Eq. (7). □

III. A FEW COMMENTS

(i) A generalization of the FPK equation has been proposed by Srinivasan and Vadusedan[4] in the form

$$\dot{p}=\sum_{j=1}^{\infty}\frac{1}{j!}\frac{\partial^j}{\partial x^j}(\alpha_j p)$$

to deal with the case where all the transition moments are proportional to Δt. This result certainly involves a mistake, because if we put $\alpha_1\neq 0$, $\alpha_2\neq 0$ and $\alpha_j=0, j\geqslant 3$, we do not obtain the usual FPK equation.

(ii) The milestone of our result is Assumption A1 which allows us to use the Chapman–Kolmogorov equation. This could be, of course, questionable; but our claim is that, for infinitely small τ, $x(t+\tau)$ should depend upon $x(t)$ only, which is physically very realistic. This assumption may be thought of as related to the characterization of the physical system itself, or merely as defining the framework in which we want to derive a modeling for the system. Equation (7) can be considered at least as a Markovian representation of the system under consideration.

(iii) In addition, we think that this result may add to the genuine meaning of the maximum informational entropy in physics.

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The Gibbs phenomenon in generalized Padé approximation

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The Gibbs phenomenon in generalized Padé approximation is discussed, and with the aid of some rational approximants the Gibbs constants are determined. In addition, the steepest of the rational approximants is calculated.

I. INTRODUCTION

If one approximates a discontinuous function by polynomials (or by Fourier series) it leads to an unusual property—the Gibbs phenomenon. The polynomials do not converge to the function near the discontinuity. The maximal value of the error is called the Gibbs constant. For example, it is well known that when we approximate the function sgn (x) in $(-1, +1)$ by Fourier series the Gibbs constant is

$$G=\frac{2}{\pi}\int_0^{\pi}\frac{\sin t}{t}\,dt-1=0.178\,979\,7\ldots.$$

Another important property of the approximation is the steepness. We call the value of the derivative of the approximant at the discontinuity the steepness. For the function sgn (x) the steepness is $(4/\pi)(n+1)$, for an n-term Fourier approximation. It is noted that both properties in a multidimensional generalization can appear in more difficult analytical features (rapid behavior of the trajectory in nonlinear system, strange attractors, etc.). It is desirable to obtain an approximation for which the Gibbs constant is as small as possible and the steepness is as high as possible.

Zygmund[1] proved that one can decrease the Gibbs constant by Cesaro's method of summing series, but as experimentally shown by Arfken[2] this method halves the steepness.

In this paper we consider some rational functions and we show that in our case the generalized Padé approximants have Gibbs constants smaller than G and their steepness is higher than Cn.

The paper is arranged as follows. In Sec. II we consider the generalized Padé approximation in the sense of Cheney[3]; in Sec. III we treat the same problem using the method of Clenshaw and Lord.[4] We provide proofs of the results of the previous sections in Sec. IV, and in Sec. V we present some calculations of the steepness following Cesaro's method of summing series.

II. APPROXIMANTS FOR sgn (x) BY CHENEY'S METHOD

Here and further we apply to a series representation for the function sgn (x) in the form

$$\operatorname{sgn}(x)=\begin{Bmatrix}-1, & -1\le x<0\\ +1, & 0<x\le 1\end{Bmatrix}=\sum_{n=0}^{\infty}C_n T_{2n+1}(x), \tag{1}$$

where $T_{2n+1}(x)$ is the Chebyshev polynomial and $C_n=(4/\pi)(-1)^n/(2n+1)$. The rationals

$$R_{n,m}(x)=\frac{\Sigma_{i=0}^{m}p_i T_{2i+1}(x)}{\Sigma_{i=0}^{n}q_i T_{2i}(x)},\quad n,m=0,1,2,\ldots, \tag{2}$$

which satisfy the relation

$$\left\{\sum_{i=0}^{n}q_i T_{2i}(x)\right\}\operatorname{sgn}(x)-\sum_{i=0}^{m}p_i T_{2i+1}(x)=O\left(T_{2n+2m+3}(x)\right), \tag{3}$$

are called the generalized Padé approximants.[3] The O term in (3) means a function for which the series in $T_i(x)$ begins with the term $T_{2n+2m+3}(x)$.

Next we shall list our main results. The solution of problem (3) in explicit form is

$$R_{n,m}(x)=A_{n,m}x\,\frac{{}_3F_2(-m,-n+\frac{1}{2},n+m+2;\frac{3}{2},\frac{3}{2};x^2)}{{}_3F_2(-n,-m-\frac{1}{2},n+m+\frac{3}{2};\frac{1}{2},1;x^2)}, \tag{4}$$

where the steepness A is

$$A_{n,m}=\frac{4}{\sqrt{\pi}}\cdot\frac{n!}{m!}\cdot\frac{\Gamma(m+\frac{3}{2})}{\Gamma(n+\frac{1}{2})}\,\frac{\Gamma(n+m+2)}{\Gamma(n+m+\frac{3}{2})}. \tag{5}$$

For $n=0$ we can get the classic result. In this case the approximating polynomial is

$$R_{0,m}(x)=A_{0,m}x\,{}_3F_2(-m,m+2,\tfrac{1}{2};\tfrac{3}{2},\tfrac{3}{2};x^2). \tag{6}$$

Its error function takes the highest maximum at the point $x=\alpha/m$, $m\to\infty$. This value is the Gibbs constant

$$G=(4/\pi)\alpha\,{}_1F_2(\tfrac{1}{2};\tfrac{3}{2},\tfrac{3}{2};-\alpha^2)-1.$$

Differentiating by α we get an equation for α:

$${}_0F_1(;\tfrac{3}{2};-\alpha^2)=\sin 2\alpha/2\alpha=0.$$

Its first zero is $\alpha=\pi/2$. The previous series considered in integral form gives the classical result

$$G=\frac{4}{\pi}\int_0^1\frac{\sin 2\alpha u}{2u}\,du-1=\frac{2}{\pi}\int_0^{\pi}\frac{\sin t}{t}\,dt-1.$$

The steepness is

$$A_{0,m}=(4/\pi)(m+1). \tag{7}$$

Second, we consider the case $m=0$, the reciprocal polynomial case. In this case the approximants are

$$R_{n,0}(x)=A_{n,0}x/{}_3F_2(-n,n+\tfrac{3}{2},-\tfrac{1}{2};\tfrac{1}{2},1;x^2). \tag{8}$$

Its error function takes its maximum at the point $x=\beta/n$ $n\to\infty$. By elementary calculations one can prove that β is the root of the equation

$$J_0(2\beta)=0,$$

where $J_0(x)$ is the Bessel function. From its first root we get

$$\beta=1.202\,412\,778\,8\ldots,$$

therefore the Gibbs constant is

$$G_{0,1}=\left(\int_0^{2\beta}\frac{J_1(u)}{u}\,du\right)^{-1}-1=0.051\,356\,067\ldots. \tag{9}$$

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That is, in this case the Gibbs constant is approximately 5%. The steepness is

$$A_{n,0} = 2n!(n+1)!/\Gamma(n+\tfrac{1}{2})\Gamma(n+\tfrac{3}{2}) = 2(n+1)a_n,$$

where $a_n \approx 1$ for moderate and large values of n. The most interesting case is $n = m$. The approximants are

$$R_{n,n}(x) = A_{n,n}x\,\frac{{}_3F_2(-n,-n+\tfrac{1}{2},2n+2;\tfrac{3}{2},\tfrac{3}{2};x^2)}{{}_3F_2(-n,-n-\tfrac{1}{2},2n+\tfrac{3}{2};\tfrac{1}{2},1;x^2)}, \quad (10)$$

where

$$A_{n,n} = \frac{2(2n+1)}{\sqrt{\pi}}\,\frac{\Gamma(2n+2)}{\Gamma(2n+\tfrac{3}{2})}.$$

The error function takes its maximal value at the point $x = \gamma/n^{3/2}$, $n\to\infty$. The constant γ is the root of the equation

$$\sum_{k=0}^{\infty}\frac{(-2\gamma^2)^k}{k!^2(\tfrac{3}{2})_k} = 0,$$

and its value $\gamma = 0.951\,020\,874\ldots$. The Gibbs constant is given by the formula

$$G_{1,1} = \frac{8\gamma}{\sqrt{2\pi}}\,\frac{{}_0F_2(;\tfrac{3}{2},\tfrac{3}{2};2\gamma^2)}{{}_0F_2(;\tfrac{1}{2},1;2\gamma^2)} - 1 = 0.008\,148\,902\ldots. \quad (11)$$

Semerdjiev and Nedelchev[5] performed a numerical experiment for determining $G_{1,1}$ enabling them to state that $G_{1,1}$ does not exceed 2%.

The steepest is

$$A_{n,n} = (4\sqrt{2}/\sqrt{\pi})\,n^{3/2}b_n,$$

where $b_n \approx 1$ for moderate ($n > 10$) and large values of n.

III. APPROXIMATIONS FOR sgn(x) BY THE CLENSHAW–LORD METHOD

Again, from series representation (1) we determine the rationals $S_{n,m}(x)$ by the method of Clenshaw and Lord[4]:

$$S_{n,m}(x) = \frac{\sum_{i=0}^{m} r_i T_{2i+1}(x)}{\sum_{i=0}^{n} s_i T_{2i}(x)}. \quad (12)$$

The coefficients r_i and s_i can be determined from the equality

$$\operatorname{sgn}(x) - S_{n,m}(x) = O(T_{2n+2m+3}(x)). \quad (13)$$

Our result is

$$S_{n,m}(x) = \frac{4}{\pi}(m+1)(2n+1)x \times \frac{{}_4F_3(-m,m+2,-n+\tfrac{1}{2},n+\tfrac{3}{2};\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2};x^2)}{{}_4F_3(-n,n+1,-m-\tfrac{1}{2},m+\tfrac{3}{2};\tfrac{1}{2},1,1;x^2)}. \quad (14)$$

First we consider the reciprocal polynomial approximants ($m = 0$)

$$S_{n,0}(x) = \frac{(4/\pi)(2n+1)x}{{}_4F_3(-n,n+1,-\tfrac{1}{2},\tfrac{3}{2};\tfrac{1}{2},1,1;x^2)}. \quad (15)$$

Its error function takes the maximal value at the point $x = \delta/n$, $n\to\infty$, where δ is the root of the equation,

$$J_0(\delta) = 2\delta J_1(\delta),$$

and $\delta = 0.940\,770\,564\ldots$. Its Gibbs constant is

$$G_{1,0} = 0.082\,417\,272\ldots. \quad (16)$$

The steepness is $4/\pi(2n+1)$.

The case $n = m$ presents powerful approximants. Here

$$S_{n,n}(x) = \frac{4}{\pi}(n+1)(2n+1)x \times \frac{{}_4F_3(-n,-n+\tfrac{1}{2},n+\tfrac{3}{2},n+2;\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2};x^2)}{{}_4F_3(-n,-n-\tfrac{1}{2},n+1,n+\tfrac{3}{2};\tfrac{1}{2},1,1;x^2)}. \quad (17)$$

The error function takes its maximal value at the point $x = \eta/n^2$, $n\to\infty$. The value of η is the root of the equation

$$\operatorname{ber}(2\sqrt{2\eta}) = 0,$$

its first root is $\eta = 1.014\,541\,594\ldots$. The Gibbs constant is

$$G_{1,1} = \frac{8\eta}{\pi}\,\frac{{}_0F_3(;\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2};\eta^2)}{{}_0F_3(;\tfrac{1}{2},1,1;\eta^2)} - 1 = 0.049\,325\,286\ldots. \quad (18)$$

The steepness is $(4/\pi)(n+1)(2n+1)$. This is the highest value in all cases.

IV. PROOFS

First we will prove formula (4). Let us consider a more generalized series expansion for sgn (x) like (1):

$$x^{2k}\operatorname{sgn}(x) = 2k!(\tfrac{1}{2})_k \sum_{j=0}^{\infty}\frac{T_{2j+1}(x)}{\Gamma(k+j+\tfrac{3}{2})\Gamma(k-j+\tfrac{1}{2})},$$

$$k = 0,1,2,\ldots.$$

Next, multiplying it by numbers q_k $(k = 0,1,\ldots,n)$, then summing these equations, we get

$$\left(\sum_{k=0}^{n} q_k x^{2k}\right)\operatorname{sgn}(x) = \frac{4}{\pi}\sum_{j=0}^{\infty}\frac{(-1)^j}{2j+1}T_{2j+1}(x)\sum_{k=0}^{n} q_k\,\frac{k!(\tfrac{1}{2})_k}{(\tfrac{3}{2}+j)_k(\tfrac{1}{2}-j)_k}.$$

We want to determine the coefficients in such a manner that the following equations are satisfied:

$$\sum_{k=0}^{n} q_k\,\frac{k!(\tfrac{1}{2})_k}{(\tfrac{3}{2}+j)_k(\tfrac{1}{2}-j)_k} = 0,$$

$$j = m+1, m+2,\ldots,m+n.$$

In this case the numerator polynomial will be

$$\frac{4}{\pi}\sum_{j=0}^{m}\frac{(-1)^j}{2j+1}T_{2j+1}(x)\sum_{k=0}^{n} q_k\,\frac{k!(\tfrac{1}{2})_k}{(\tfrac{3}{2}+j)_k(\tfrac{1}{2}-j)_k}.$$

To solve the previous equations let us suppose for a moment that

$$q_k = (-n)_k(-m-\tfrac{1}{2})_k(n+m+\tfrac{3}{2})_k/k!^2(\tfrac{1}{2})_k.$$

Consider now the sum

$$S = \sum_{k=0}^{n}\frac{(-n)_k(-m-\tfrac{1}{2})_k(n+m+\tfrac{3}{2})_k}{k!(\tfrac{3}{2}+j)_k(\tfrac{1}{2}-j)_k} = {}_3F_2(-n,-m-\tfrac{1}{2},n+m+\tfrac{3}{2};\tfrac{3}{2}+j,\tfrac{1}{2}-j;1).$$

S is a Saalschütz-type hypergeometric sum and therefore it is summable by factorial functions. Really,[6]

$$S = (1+m-j)_n(-1-m-n-j)_n \times [(\tfrac{1}{2}-j)_n(-\tfrac{1}{2}-j-n)_n]^{-1}.$$

It is not difficult to see that all products differ from zero except the first one. Further, when j runs from $m+1$ to $m+n$ then $1+m-j$ runs from 0 to $-n+1$ by -1. Therefore, $S=0$ for all j ($j=m+1,\ldots,m+n$). We have thus proved the form of the denominator polynomial. To get the explicit form of the numerator polynomial we apply the value of S for $j=0,1,\ldots,m$:

$$Z=\frac{4}{\pi}\sum_{j=0}^{m}\frac{(-1)^j}{2j+1}T_{2j+1}(x)\times\frac{(1+m-j)_n(-1-m-n-j)_n}{(\frac{1}{2}-j)_n(-\frac{1}{2}-n-j)_n}.$$

Taking the power form of the Chebyshev polynomial

$$(1/x)T_{2j+1}(x)=(2j+1)(-1)^j\,{}_2F_1(-j,j+1;\tfrac{3}{2};x^2),$$

we get

$$Z=\frac{(n+m)!\Gamma(n+m+2)}{(\frac{1}{2})_n(\frac{3}{2})_n m!\Gamma(m+2)}\frac{4}{\pi}x\times\sum_{j=0}^{m}(2j+1)\,{}_2F_1(-j,j+1;\tfrac{3}{2};x^2)\times\frac{(-m)_j(n+m+2)_j(\frac{1}{2}-n)_j}{(-n-m)_j(m+2)_j(\frac{3}{2}+n)_j}.$$

Let us transform Z to the power form in x^2:

$$Z=\frac{4}{\pi}x\frac{(n+m)!(n+m+1)!}{(\frac{1}{2})_n(\frac{3}{2})_n m!(m+1)!}\times\sum_{i=0}^{m}(-4x^2)^i\frac{(-m)_i(n+m+2)_i(\frac{1}{2}-n)_i}{(-n-m)_i(m+2)_i(\frac{3}{2}+n)_i}W,$$

where

$$W=\sum_{j=0}^{m-i}\frac{(2i+1)_j}{j!}\times\frac{(-m+i)_j(n+m+i+2)_j(\frac{1}{2}-n+i)_j(\frac{3}{2}+i)_j}{(-n-m+i)_j(m+2+i)_j(\frac{3}{2}+n+i)_j(\frac{1}{2}+i)_j}.$$

The sum W is an ${}_5F_4$ hypergeometric function which one can sum by theorem of Dougall[7]:

$$W=(-1)^m\times\frac{\Gamma(i+m+2)\Gamma(-\frac{1}{2}-i)\Gamma(\frac{3}{2}+n+i)n!(-n-m)_i}{\Gamma(2i+2)\Gamma(-\frac{1}{2}-m)\Gamma(\frac{3}{2}+n+m)(n+m)!}.$$

By elementary calculations we get the required result:

$$Z=\frac{4}{\sqrt{\pi}}\frac{n!}{m!}\frac{\Gamma(m+\frac{3}{2})}{\Gamma(n+\frac{1}{2})}\frac{\Gamma(n+m+2)}{\Gamma(n+m+\frac{3}{2})}x\times\sum_{i=0}^{m}\frac{(-m)_i(-n+\frac{1}{2})_i(n+m+2)_i}{i!(\frac{3}{2})_i(\frac{3}{2})_i}x^{2i}.$$

Proof of the form of Gibbs constants for the cases $m=0$ and $m=n$ can be obtained by elementary analysis. Here we omit the details. The proof of the results of Sec. III is analogous with the previous one.

V. CESARO'S METHOD OF SUMMING SERIES FOR sgn (x) AND THE STEEPNESS

It is well known that if we have a series

$$\sum_{\nu=0}^{\infty}a_\nu,$$

its Cesaro's sum is defined by the formula

$$C_n^\alpha=\sum_{\nu=0}^{n}a_\nu\frac{(-n)_\nu}{(-n-\alpha)_\nu}.$$

Here α is a positive parameter. It is well known that if $\alpha=1$, C_n^α is Fejér's arithmetic mean and in this case the Gibbs phenomenon does not occur. (The case $\alpha=0$ gives the original series.)

Next we will prove that if $\alpha>\alpha_0=0.439\,551\,2893\ldots$, then, again, the Gibbs phenomenon does not occur.

Consider again the series (1), thus

$$a_\nu=(4/\pi)[(-1)^\nu/(2\nu+1)]T_{2\nu+1}(x).$$

By short, elementary calculation we get

$$C_n^\alpha(x)=\frac{4}{\pi}\frac{n+1+\alpha}{1+\alpha}x\sum_{j=0}^{n}\frac{(-n)_j(n+\alpha+2)_j(\frac{1}{2})_j}{(\frac{3}{2})_j(1+\alpha/2)_j(\frac{3}{2}+\alpha/2)_j}x^{2j}.$$

Its error function has the maximum at the point $x=s/n$, $n\to\infty$. The maximum is

$$G_\alpha(s)=\frac{4}{\pi}\frac{s}{1+\alpha}\sum_{k=0}^{\infty}\frac{1}{2k+1}\frac{(-s^2)^k}{(1+\alpha/2)_k(\frac{3}{2}+\alpha/2)_k}-1=\frac{2}{\pi}\int_0^1(1-t)^\alpha\frac{\sin 2st}{t}\,dt-1.$$

By determining the value s we get the equation

$$\sum_{k=0}^{\infty}\frac{(-s^2)^k}{(1+\alpha/2)_k(\frac{3}{2}+\alpha/2)_k}=0,$$

or in integral form

$$\int_0^1(1-t)^\alpha\cos 2st\,dt=0,$$

The solutions α and s of the equation $G_\alpha(s)$ and of the previous equation are

$$\alpha=0.439\,551\,2893\ldots,$$

$$s=2.025\,782\,092\ldots.$$

Note: Gronwall[8] also determined the values α and s, but the stated precision of his results is incorrect. The steepness in Cesaro's method is $(4/\pi)(n+1+\alpha)/(1+\alpha)$. For $\alpha=1$, the steepness is $(4/\pi)(n+2)/2$. It is halved corresponding to

TABLE I. Gibbs constant and the steepness.

	Cheney's method		Method of Clenshaw and Lord		
Fourier series	Reciprocal polynomial	Rational	Reciprocal polynomial	Rational	Cesaro's sum
18%	5.1%	0.8%	8.2%	4.9%	$18\% \le G \le 0\%$
$(4/\pi)\,n$	$2n$	$(4\sqrt{2}/\sqrt{\pi})\,n^{3/2}$	$(8/\pi)\,n$	$(8/\pi)\,n^2$	$(4/\pi)n/(1+\alpha)$

$\alpha = 0$. Thus, we have proved that Cesaro's method of summing series decreases the Gibbs constant, but it also decreases the steepness.

VI. CONCLUSIONS

As a means of summarizing our results, we have listed in Table I the Gibbs constants and their steepness corresponding to the methods used.

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Energy levels of a two-dimensional anharmonic oscillator: Characteristic function approach

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The eigenlevels of a two-dimensional quartic anharmonic oscillator are identified as the zeros of a "characteristic function" derived from the resolvent. Numerical values are obtained by means of Padé approximants.

I. INTRODUCTION

In this work we report on an approximation algorithm for obtaining the eigenvalues of Schrödinger operators. The eigenvalues of the system $H\psi = E\psi$ are approximated by the zeros of Padé approximants of a "characteristic function"

$$\lambda(E) = (\phi,\phi)/(\phi,(H-E)^{-1}\phi), \tag{1.1}$$

where ϕ is a suitable trial function in L^2. The approach has its roots in the resolvent operator techniques of Weinstein,[1] Löwdin,[2] and Masson,[3] and $\lambda(E)$ is closely related to the well-known Weinstein function.

As an illustration of the method we will investigate the energy levels of a two-dimensional anharmonic oscillator with a positive quartic anharmonicity. It is characterized by the Hamiltonian

$$\begin{aligned} H &= H_0 + kV_A \\ &= \frac{1}{2}\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \omega_1^2 x^2 + \omega_2^2 y^2\right) \\ &\quad + k(a_{11}x^4 + 2a_{12}x^2y^2 + a_{22}y^4) \end{aligned} \tag{1.2}$$

where ω_i^2, a_{ij} $(i,j = 1,2)$, and k describe the interaction potential and are given as system parameters ($k > 0$, $a_{11}a_{22} - a_{12}^2 > 0$).

The anharmonic eigenvalue problem provides a convenient testing ground for the present approach. It is a prominent example of a class of singular perturbation problems. The energy levels of H in (1.2) are not analytic in the coupling parameter k. The Rayleigh–Schrödinger (RS) perturbation series in k, near the known energy levels of H_0, have a zero radius of convergence and the regular perturbation approach becomes inadequate. Interest in the physics of anharmonic oscillators *per se* and studies of the analytic properties of the divergent perturbative series and of their resummation techniques helped to create an extensive literature on anharmonic eigenvalues. Thus a wide spectrum of approximate methods and data exist for comparison purposes.

We have already obtained encouraging results for the one-dimensional problem.[4] The characteristic function method yielded a higher number of accurate digits for eigenvalues than the resummation techniques directly applied to RS series. It did compete well also with other nonperturbative approximation schemes, in particular for low to moderate quantum numbers.

The abundance of the studies of one-dimensional anharmonic eigenvalue problems does not carry over to multidimensional problems and there are few reported results. On the other hand, an important asset of the characteristic function approach is that it generalizes to multidimensional problems in a straightforward manner due to the scalar form of (1.1). Thus we choose the two-dimensional anharmonic oscillator as a critical test problem.

In Sec. II we briefly describe the characteristic function method. On the example of the anharmonic oscillator, we discuss its relation to other approximation methods and consequently the motivation for it. In Sec. III we construct a characteristic function for the anharmonic oscillator. The values for the energy levels are given in Sec. IV. In that section we also discuss how to obtain approximation error bounds directly from the information on the zeros and poles of the relevant Padé approximants. We close the section with a numerical example. Section V concludes the paper with a discussion of the results. There we compare our results with those of Hioe *et al.*[5] We observe that the characteristic function approach offers a robust and efficient approximation scheme for low to moderate eigenlevels of complicated potentials.

II. ANHARMONIC OSCILLATOR

A review of anharmonic oscillator problems is outside the scope of this work. However we may outline the main approaches in three groups: perturbative methods which emphasize the resummation of the divergent RS series; nonperturbative methods which try to obtain "best" approximate wave functions by variational, recursive, or iterative techniques; and asymptotic WKB methods.

In order to apply the summability methods one has to determine the analytic behavior of the perturbation series. This might prove to be difficult for multidimensional and complicated potentials. Nevertheless, Padé and Borel summation methods have been used effectively to extract eigenvalue information from these divergent series.[6,7] These methods have been very useful in illuminating the analytic properties of the RS series. However their convergence rate is relatively slow. Due to the asymptotic character of these series, summability methods are confined to the small values of the perturbation parameter [e.g., k small in (1.2)] and to the lowest quantum numbers.

For high quantum numbers WKB methods yield in one dimension rather good numerical results. Their extension to multidimensional problems is, however, quite laborious. It is

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also known that the WKB methods yield low accuracy at small quantum numbers.[8,9]

In the one-dimensional problem, Hill determinant methods have been effective for the full range of quantum numbers and coupling constants k (see Ref. 10). First one represents the eigenfunctions by

$$\psi = e^{-\gamma x^2} \sum c_N x^N . \tag{2.1}$$

Then by substituting (2.1) into the original equation one obtains infinite Hill determinants for the determination of the c_N's. In the one-dimensional case, by exploiting special recursive relations among the c_N's various determinant truncation schemes have been devised. Looking for the zeros of increasingly larger determinants, one obtains better estimates on the eigenvalues in an iterative way. The extension of these special techniques to multidimensional problems, however, requires the handling of very large determinants.

The work of Hioe *et al.*[5,9] on anharmonic oscillators is most extensive. They have been able to combine various methods suited for different regimes of the coupling parameter k and quantum numbers. Thus they obtain approximate analytical expressions for various eigenvalue regimes. They extended their approach also to a pair of anharmonic oscillators which are essentially equivalent to a two-dimensional anharmonic oscillator. Their analysis of energy-level crossing and their extensive numerical tables provide useful comparison data. To obtain high accuracy by this method, however, still involves dealing with large determinants or high-order WKB expansions.

The characteristic function method is a hybrid algorithm. It utilizes resummation techniques (Padé), not, however, on eigenvalue perturbation series but on a properly chosen convergent series derived from the resolvent operator. The eigenvalue problem of a linear operator H,

$$H\psi = E\psi , \tag{2.2}$$

is transformed by operator projection techniques into finding the zeros of

$$\Delta(E) = (\phi,\phi)/(\phi,(H-E)^{-1}\phi) , \tag{2.3}$$

where ϕ is one of the normalized basis functions which span the Hilbert space under consideration. [A more detailed account of (2.3) is given in Ref. 11.]

For the present problem, noting that H is positive definite, we modify (2.2) and (2.3) and identify the eigenvalues of H as the poles of the following reciprocal characteristic function:

$$f(E) = (\phi,(I-EH^{-1})^{-1}\phi)/(\phi,\phi) = \sum \Delta_N E^N , \tag{2.4}$$

where

$$\Delta_N = (\phi,H^{-N}\phi)/(\phi,\phi) . \tag{2.5}$$

The positive anharmonic oscillator has a purely discrete spectrum. Thus an equivalent representation of (2.4) is

$$f(E) = \sum \frac{d_i^2}{1-E/E_i} , \quad \sum d_i^2 = 1 , \tag{2.6}$$

where the E_i denote the eigenvalues and the d_i are defined by the projection relation

$$\phi = \sum d_i \psi_i . \tag{2.7}$$

Utilizing the representation in (2.7) and (2.5) we deduce

$$\Delta_N = E_1^{-N} \sum d_i^2 \left(\frac{E_i}{E_1}\right)^{-N} \tag{2.8}$$

and consequently we observe that

$$\Delta_{N+1}/\Delta_N < 1/E_1 . \tag{2.9}$$

The algorithm consists now of approximating (2.4) by Padé approximants using only a finite number of the "spectral coefficients," Δ_N's. In some cases it might be difficult to work with H^{-N} in the evaluation of Δ_N's in (2.5). To avoid this difficulty we introduce the transformation

$$\phi = H^{2M}\varphi , \tag{2.10}$$

where φ is a closed family of functions under H. Now (2.5) becomes

$$\Delta_N = (\varphi,H^{2M-N}\varphi)/(\varphi,H^{2M}\varphi) . \tag{2.11}$$

Thus for sufficiently high M in the computation of the Δ_N's, we will have to deal only with positive powers of H.

With the general outline of the method in perspective, now we can discuss the motivation for and the relative advantages of the present approach. In the first place, we are approximating a function with a known analytic structure. The mereomorphic character of $f(E)$ in (2.4) is particularly suited for rational Padé approximants. By (2.4) and (2.9) we also observe that $f(E)$ is a convergent Stieltjes series. Padé approximation theory for such a series is well developed and there exist strong theorems on their convergence properties (see Ref. 12, Chap. 17). The Padé summability of $f(E)$ is guaranteed. Second, the poles of $f(E)$ are relatively insensitive to the details of trial functions as long as they are closed under H and the trial functions are included in symmetry subspaces of the relevant eigenfunctions. Thus be focusing on the eigenvalues, the characteristic function approach offers larger flexibility in the choice of trial functions. Of course the more information one includes on the asymptotics of eigenfunctions in the formation of φ, the better the convergence rate one obtains. Finally we note that the scalar form of $f(E)$ lends itself to an easy generalization to multidimensional problems.

The relative insensitivity of the characteristic function approach to the choice of the trial function provides ground for a robust approximation scheme. Further it is a controlled approximation method, one can extract information about error bounds directly from the Padé table utilizing the properties of Stieltjes series. A restriction of the method is, however, that it is confined to moderately low quantum numbers. This is due to the fact that $f(E)$ is a series expansion around the origin.

For interacting many-body systems it is the lower energy levels that are of the most interest. For such states and for complicated potentials the simple form of the resolvent operator presents the characteristic function approach as an efficient eigenvalue approximation scheme where the implementation of other methods may prove to be quite laborious. In the following section we construct the function $f(E)$ for the anharmonic oscillator.

III. CHARACTERISTIC FUNCTION

In order to build $f(E)$ for the anharmonic oscillator first we have to choose a suitable trial function and then evaluate the spectral coefficients as defined by (2.11). To this end we utilize the normalized wave functions of one-dimensional harmonic oscillators

$$\phi_n = \pi^{-1/4} 2^{-n/2} (n!)^{-1/2} H_n(x) e^{-x^2/2}, \tag{3.1}$$

whose pairwise products

$$u_{m,n}(x,y) = \phi_m(x)\phi_n(y) \tag{3.2}$$

span the relevant Hilbert space. Within this basis set, $H^M u_{m,n}$ $(M = 0,1,...)$ has a particularly simple representation. For the H given by (1.2), by repeated use of standard recurrence relations among the Hermite polynomials, one can show that it is given by (we assume henceforth the summation convention on repeated indices)

$$H^M u_{m,n} = C^{(M)}_{j,k} u_{m+2j,n+2k}, \quad |j|,|k| < 2M. \tag{3.3}$$

Further by noting that $H^{M+1} u_{m,n} = H(H^M u_{m,n})$ and that the $u_{m,n}$'s in (3.2) are closed under H we obtain a convenient recursive relation for the determination of the $C_{j,k}$'s in the form

$$C^{(M+1)}_{j,k} = g_{r,s} C^{(M)}_{j+2r,k+2s}, \quad |r|,|s| < 2, \tag{3.4}$$

with

$$C^{(0)}_{0,0} = 1$$
$$C^{(M)}_{j,k} = 0, \quad |j| + |k| > 2M + 1. \tag{3.5}$$

By this choice of trial functions the evaluation of the spectral coefficients becomes an algebraic routine. The inner products in (2.11) are easily calculated by (3.3) and by the orthonormality of ϕ_n's, e.g.,

$$(u_{m,n}, H^M u_{m,n}) = C^{(M)}_{0,0}. \tag{3.6}$$

In the present problem before we embark on the calculation of the spectral coefficients we introduce the transformation $(x,y,\psi) \to (\alpha X, \beta Y, \bar{\psi})$, to incorporate some asymptotic scaling for large values of the coupling parameter k and (1.2) becomes

$$\begin{aligned}\bar{H}\bar{\psi} = \Big\{\Big[2\Big(&-\alpha^{-2}\frac{\partial^2}{\partial X^2} - \beta^{-2}\frac{\partial^2}{\partial Y^2} \\ &+ \omega_1^2 \alpha^{-4}\beta^{-2} X^2 + \omega_2^2 \alpha^{-2}\beta^{-4} Y^2\Big)\Big]^{-1} \\ &+ k(a_{11}\alpha^{-6}\beta^{-2} X^4 + 2a_{12}\alpha^{-4}\beta^{-4} X^2 Y^2 \\ &+ a_{22}\alpha^{-2}\beta^{-6} Y^4)\Big\}\bar{\psi} \\ = (E/\alpha^2\beta^2)\bar{\psi} = \bar{E}\bar{\psi}.\end{aligned} \tag{3.7}$$

The next step is to establish the recursive relation among the $C^{(M)}_{j,k}$'s. Here we introduce the scaling

$$B^{(M)}_{j,k} = C^{(M)}_{j,k} / [(m+2j)!(n+2k)!]^{1/2} \tag{3.8}$$

to avoid very large numbers in (3.4). For the particular Hamiltonian $\bar{H}$ we then obtain a recursive relation among the $B^{(M)}_{j,k}$'s:

$$B^{(M+1)}_{j,k} = G_{r,s} B^{(M)}_{j+2r,k+2s}, \quad |r|,|s| < 2, \tag{3.9}$$

where

$$\begin{aligned}
&G_{-2,0} = A_{11}, \quad G_{2,0} = MJ(4)A_{11}, \\
&G_{-1,-1} = A_{12}, \quad G_{1,1} = MJ(2)NK(2)A_{12}, \\
&G_{0,-2} = A_{22}, \quad G_{0,2} = NK(4)A_{22}, \\
&G_{1,-1} = MJ(2)A_{12}, \quad G_{-1,1} = NK(2)A_{12}, \\
&G_{-1,0} = W_1 + 4A_{11}(m - \tfrac{1}{2}) + 2A_{12}(n + \tfrac{1}{2}), \\
&G_{0,-1} = W_2 + 4A_{22}(n - \tfrac{1}{2}) + 2A_{12}(m + \tfrac{1}{2}), \\
&G_{1,0} = (W_1 + 4A_{11}(m + \tfrac{3}{2}) + 2A_{12}(n + \tfrac{1}{2}))MJ(2), \\
&G_{0,1} = (W_2 + 4A_{22}(n + \tfrac{3}{2}) + 2A_{12}(m + \tfrac{1}{2}))NK(2), \\
&G_{0,0} = (m + \tfrac{1}{2})W_3 + (n + \tfrac{1}{2})W_4 + 4[\tfrac{3}{2}A_{11}(\tfrac{1}{2} + mj + mj^2) \\
&\qquad + (m + \tfrac{1}{2})(n + \tfrac{1}{2})A_{12} + \tfrac{3}{2}A_{22}(\tfrac{1}{2} + nk + nk^2)],
\end{aligned} \tag{3.10}$$

with

$$\begin{aligned}
&A_{11} = ka_{11}/4\alpha^6\beta^2, \quad mj = m + 2j, \\
&A_{12} = ka_{12}/4\alpha^4\beta^4, \quad nk = n + 2k, \\
&A_{22} = ka_{22}/4\alpha^2\beta^6, \quad MJ(r) = (mj + r)!/mj!, \\
&\qquad\qquad NK(r) = (nk + r)!/nk!, \\
&W_1 = (1 - \alpha^4)/4\alpha^4\beta^2, \quad W_3 = (1 - \alpha^4)/4\alpha^2\beta^4, \\
&W_2 = (1 + \alpha^4)/2\alpha^4\beta^2, \quad W_4 = (1 + \alpha^4)/2\alpha^2\beta^4.
\end{aligned}$$

For the trial function now we set

$$\psi^{\pm} = 1/2(u_{m,n}(x,y) \pm u_{n,m}(x,y)), \tag{3.11}$$

whose form yields different symmetry subspaces depending on whether m and n have the same or different parity. Consideration of these subgroups provides valuable insight into energy level crossings and degeneracies.

By (2.11) and (3.11) the relevant spectral coefficients are given as

$$\Delta^{\pm}_N = \delta^{\pm}_{2M-N}/\delta^{\pm}_{2M}, \tag{3.12}$$

where

$$\begin{aligned}\delta^{\pm}_N = 1/4[&C^{(M)}_{0,0}(m,n) + C^{(M)}_{0,0}(n,m) \\ &\pm (C_{-q,q}(m,n) + C_{q,-q}(n,m))],\end{aligned} \tag{3.13}$$

with $q = (m-n)/2$ and $C_{q,-q} = 0$ if q is not an integer.

The next step after obtaining the spectral coefficients is the formation of Padé approximants to $f(\bar{E})$. The Padé approximant $[L/M]_g$ to the formal power series $g = \Sigma a_n x^n$ is defined as the ratio of two polynomials $P_L(x)$ and $Q_M(x)$ of orders L and M,

$$[L/M]_g = P_L(x)/Q_M(x), \tag{3.14}$$

which satisfy the condition

$$\left| \frac{P_L(x)}{Q_M(x)} - \sum^{L+M} a_N x^N \right| = O(x^{L+M+1}), \tag{3.15}$$

with

$$Q_M(0) = 1.$$

In the present problem $f(\bar{E})$ is a convergent Stieltjes series. The poles of Padé approximants will converge uniquely to its poles, hence to the eigenvalues of $\bar{H}$ (see Ref. 3). With increasing M the poles of $[M/M]$ will provide tighter upper bounds for the energy levels. There are no explicit error bounds on the location of the poles. However one can derive *a posteriori* bound estimates as will be shown in the next

section. There we also tabulate the energy levels for some critical parameter values and compare our results with those of Hioe *et al.*

IV. NUMERICAL RESULTS AND ERROR BOUNDS

In the numerical implementation of the steps as summarized in Sec. III, the scaling parameters α and β could be utilized as optimization parameters. However, since we were not interested in fine tuning the trial function we took $\alpha=\beta$ for simplicity and initially we set $\alpha^2\sim 4k^{1/3}$. We altered α when necessary so as only to avoid any over- or underflows in the spectral coefficients of (2.11). In forming the Padé approximants we used the NAG (Mark 9) double precision routine, E02RAF.

In extracting information from the Padé table one has to be cautious about the accumulated round-off errors and the "defects"—the unstable pole-zero pairs of the approximants (see Ref. 13, p. 58). Here too, the structure of the Stieltjes series provides convenient checkpoints, i.e., we have that (i) the poles of the $[M+J/M]$, $J\geqslant -1$ Padé approximants are on the negative real axis; (ii) the poles of successive approximants interlace; (iii) the roots of the numerator also interlace those of the denominator; etc. (see Ref. 12, Chap. 16). Hence, if the general positioning of the zeros and poles of the approximants are not compatible with the Stieltjes character of the series we can easily discard information from these Padé sequences.

With respect to the "defects" we have to be more careful. Since we were not aiming at the close approximation of the eigenfunctions by the trial functions the residues of the poles of $f(\bar{E})$ [i.e., d_i^2 in (2.6)] were in general very small. This particular structure of the $f(\bar{E})$ will yield then the close pole-zero pairs. These are, however, genuine singularities, they are stable and thus easily distinguished from the unstable "defects."

In order to obtain the eigenvalues we utilized either 33 or 43 spectral coefficients. We could form Padé approximants up to the order [16/16] or [21/21]. To monitor the convergence rates we also obtained lower-order Padé approximants.

We looked for the poles of the $[l,m]$ and $[l,m]^*$ approximants ($l+m+1=p<2M+1$) which are formed by utilizing either the first p or the latter p spectral coefficients of $f(\bar{E})$ (i.e., $\Delta_{2M+1-p},\ldots,\Delta_{2M+1}$). We observed that the sequence $[M-n/M-n]^*$, $n=M,\ M-1,\ldots$ provided a smoother converging sequence in comparison with the $[M-n/M-n]$ $n=M,M-1,\ldots$ sequence (compare $B_{M,1}$ and $B^*_{M,1}$ in Table IV later). Hence after the initial screening of the Padé table against numerical pitfalls, we recorded the conforming digits of two consecutive diagonal approximants (i.e., $[M/M]^*$, $[M-1,M-1]^*$) as significant digits for the energy levels. They are given in Tables I–III along with the results of Hioe, *et al.*[5]

Additional checks on the reliability are provided by the stability of the results with respect to the small variations of α at a given order of $[M/M]$ Padé approximants. It is however also possible to derive error bounds by utilizing the two-sided Padé inequalities for Stieltjes series. Below we give a numerical example on how to obtain error bounds for the ground level. The example lends credence to our rule of thumb of picking the conforming digits of consecutive diagonal approximants as significant digits.

The Stieltjes inequalities given in Ref. 12, p. 243, when adopted to our notation, yield

TABLE I. Energy eigenstates for $\omega_1=\omega_2=1$, $a_{11}=a_{22}=1$.

	a_{12} \ k	1	5	50	500	5000
$E_{0,0}$:		1.724 184 069 2603	2.674 676 409 703	5.511 798 964 39	11.756 694 59	25.274 022 474 05
	1	1.724 2	2.674 7	5.511 8	11.757	25.274
		1.607 541 310	2.449 174 1	4.999 417 6	10.639 789	22.861 609
	0	1.690 75	2.449 2	4.999 5	10.640	22.862
		1.443 775	2.105 880	4.184 19	8.843 39	18.972 5
	−1	1.443 8	2.105 9	4.184 3	8.843 7	18.973
$E_{0,1}$:		3.830 323 856 2968	6.069 112 369 4	12.639 925 716 7	27.027 427 8	58.133 690 484 1
	1	3.830 4	6.069 2	12.640	27.028	58.134
		3.541 66	5.524 09	11.414 81	24.363 3	52.382 5
	0	3.541 7	5.524 2	11.414 81	24.364	52.383
		3.066 591	4.513 5	8.983	18.933 94	40.72
	−1	3.066 6	4.513 6	8.983 0	18.984	40.724
$E_{1,1}$:		6.213 815 078 277	9.968 450 186 999	20.884 372 171 99	44.716 717 018	96.210 280 600 9
	1	6.214 0	9.968 7	20.885	44.718	96.213
		5.475 784 5	8.599 003	17.830 192	38.086 83	81.903 317
	0	5.475 9	8.599 1	17.830	38.087	81.904
		4.210 52	5.984 7	11.632	24.441 4	52.344
	−1	4.210 6	5.984 8	11.637	24.438	52.350

TABLE II. Ground levels for $\omega_1 = \omega_2 = 1$, $a_{22} = 1$.

		k				
a_{11}	a_{12}	1	5	50	500	5000
0.8	2	1.691 301 58 1.691 3	2.611 6768 2.611 7	5.369 253 5.369 3	11.446 272 11.446	23.733 76 24.604
	0	1.568 914 1.568 9	2.373 376 2.373 4	4.825 98 4.826 0	10.261 15 10.261	22.043 4 22.044
0.4	2	1.612 296 5 1.612 3	2.455 659 2.445 7	5.011 169 5.011 1	10.663 7 10.664	22.912 54 22.913
	0	1.472 543 1.472 5	2.176 15 2.176 2	4.365 40 4.365 4	9.250 91 9.250 9	19.888 30 19.859

$$[M/M] < f(E) < [M/M] \times \frac{1-(E/R)P_M^{-1}(E)Q_M^0(E)/Q_M^{-1}(M)P_M^0(R)}{1-(E/R)Q_M^{-1}(E)Q_M^0(R)/Q_M^{-1}(R)Q_M^0(E)} = S_M(E), \quad 0<E<R, \tag{4.1}$$

where

$$[L/M] = [M+J/M] = \frac{P_L^{(J)}}{Q_M^{(J)}} = \frac{\Sigma_{n=0}^{L} P_{L,n}^{(J)} E^n}{\Sigma_{n=0}^{M} Q_{M,n}^{(J)} E^n} = \frac{\Pi_{n=1}^{L}(1-E/A_{L,n}^{(J)})}{\Pi_{n=1}^{M}(1-E/B_{M,n}^{(J)})}, \tag{4.2}$$

where $A_{L,n}$ and $B_{M,n}$ correspond to the zeros and poles of the

TABLE III. Energy eigenstates for $k = 1$, $\omega_1 = \omega_2 = 0$, $a_{12} = 0$, $a_{11} = a_{12} = 1$.

l $2n+l+1$	0 $E_{0,2}^{+}$	1 $E_{0,1}^{+}$	2 $E_{0,2}^{-}, E_{1,3}^{+}$	3 $E_{1,2}^{+}$	4 $E_{1,3}^{-}$
1	1,447 149 753 78 1.477				
2		3.398 150 176 027 3.398			
3	6.003 386 085 78 6.007		5.624 339 349 5.625		
4		8.704 538 139 8.70		8.696 861 8.11	
5	11.802 433 630 1 12.5		11.534 749 11.5		10.758 265 165 10.8
6		14.977 808 37 14.9		14.626 328 14.5	
7	18.458 819 47 19.2		18.245 419 18.2		17.616 153 17.6
8		21.999 601 21.9		21.774 8 21.6	
9	25.791 808 03 26.5		25.611 50 25.5		25.076 18 25.0
10		29.634 8 29.4		29.446 6317 29.2	
11	33.694 556 34.4		33.536 33.4		33.066 9 33.0
12		37.798 37.5		37.666 37.3	
13	42.097 48 42.7		41.95 41.6		41.532 41.3

function $f(E)$ and $P_{L,n}$ and $q_{M,n}$ are various coefficients in the polynomials which form the Padé approximants. In (4.1) and (4.2), R is the radius of convergence for the series which is equal to the ground level E_1. Since both $f(E)$ and $S_M(E)$ do have poles at R the inequality does not provide tight bounds near R. With increasing M, however, S_M and $[M/M]$ define consecutive inclusion regions which become smaller (see Ref. 12, Chap. 17), hence we note that

$$S_{M+1}(E) < S_M(E), \quad 0 < E < R. \tag{4.3}$$

Now if we define

$$Z_M(R) = \lim_{E \to R} (R - E) S_M(E) \tag{4.4}$$

from (4.3) we derive

$$Z_{M+1}(R) < Z_M(R), \tag{4.5}$$

where

$$Z_M(R) = ([M/M](R) - [M-1/M](R))/(1 + W_{1,M}(R)), \tag{4.6}$$

with

$$W_{K,M}(R) = R \sum_{n=K}^{M} \frac{b_{M,n} - B_{M,n}}{(b_{M,n} - R)(B_{M,n} - R)} \tag{4.7}$$

and

$$\frac{(b_M - B_M)R}{(b_M - R)(B_M - R)} < \frac{(b_{M+1} - B_{M+1})R}{(b_{M+1} - R)(B_{M+1} - R) D_{M+1}(R)} + Y_M(R), \tag{4.8}$$

where

$$Y_M(R) = [1 + W_{2,M+1}(R) - D_M(R) \times (1 + W_{2,M}(R))]/D_M(R), \tag{4.9}$$

with

$$D_M(E) = ([M+1/M+1](E) - [M/M](E))/([M/M](E) - [M-1/M](E)) \tag{4.10}$$

$$= \frac{\rho_M E^2 \prod_{n=1}^{M} (1 - E b_{M,n})(1 - E/B_{M,n})}{\prod_{n=1}^{M+1} (1 - E/b_{M+1,n})(1 - E/B_{M+1,n})} \tag{4.11}$$

and

$$\rho_M = q^{(-1)}_{M+1,M+1} p^{(0)}_{M+1,M+1} / q^{(-1)}_{M,M} p_{M,M}.$$

$D_M(E)$ is a positive, monotone increasing function of (E) $(b_{M,n} > b_{M+1,n}$, $B_{M,n} > B_{M+1,n}$, $\rho_M > 0)$. In the interval $0 < E < B_{M+1,1}$ it increases from zero to infinity. On the other hand as $M \to \infty$, $B_{M,1} \to R$, hence for some critical $M = M_c$ we will have

$$D_{M_c}(R) > 1 \quad \text{and} \quad Y_{M_c}(R) < 0. \tag{4.12}$$

In the sequel we will conjecture that such a critical order of approximation is reached when a sufficient uniformity in the upper bounds for the eigenlevels is reached. Rigorous checks of (4.12) can be accomplished by substituting moderately tight lower bound estimates in (4.11).

When (4.12) holds, (4.8) can be simplified into a contracting sequence of error bounds, i.e.,

$$(b_{M+1,1} - R)(B_{M+1,1} - R) < \epsilon_M (b_{M,1} - R)(B_{M,1} - R), \tag{4.13}$$

with

$$\epsilon_M = (b_{M,1} - B_{M,1})/(b_{M+1,1} - B_{M+1,1}) < 1. \tag{4.14}$$

In the following we present a numerical example for the parameter values of $a_{11} = 1$, $a_{12} = 0$, $a_{22} = 0$, $k = 5$ in (1.2), a case for which we can compare our error estimates with actual errors (we utilize the 16-digit results given in Ref. 10). In Table IV we list some information relevant to the evaluation of (4.8) and (4.14), i.e., $b_{M,1}$, $B_{M,1}$, $B^*_{M,1}$, $N_{2,M}$, ρ_M, ϵ_M, D_M, where $B^*_{M,1}$ are the upper bounds obtained from $[M/M]^*$ approximants. Utilizing the conjecture (4.12) and Table IV we first obtain a rough estimate (i.e., assuming $D_M = 1$, $Y_M < 0$, $R > 1$)

$$(B_{16,1} - R)^2 < \epsilon_{14}\epsilon_{15}(b_{14,1} - 1)^2 \sim 14 \times 10^{-12}. \tag{4.15}$$

Now we can assert that at least five digits of $B_{16,1}$ are correct. We can revise our estimates on $(b_{15,1} - R)$ and $(b_{14,1} - R)$ and obtain

$$(B_{16,1} - R)^2 < 6 \times 10^{-14}. \tag{4.16}$$

By (4.16) we get a new round of estimates for D_{14}, D_{15}, and $(B_{16,1} - R)$. Finally, we obtain, by repeated use of (4.8),

$$(B_{16,1} - R) < 10^{-13}. \tag{4.17}$$

In the present example $R = 1.224\,558\,703\,665\,9195$ and hence

$$(B_{16,1} - R) \sim 0.55 \times 10^{-13}. \tag{4.18}$$

From Table IV we read

$$B_{15,1} - B_{16,1} = 0.16 \times 10^{-13} \tag{4.19}$$

and observe that (4.17) and (4.18) are consistent and they are also in tune with our rule of thumb of taking the conforming digits of consecutive upper bounds as significant digits. Further we note that the true values of $D_{14}(R)$ and $D_{15}(R)$ (Table IV) are rather large, conforming in this case with our conjecture of (4.12).

V. CONCLUSIONS

In Tables I and II we observe that the characteristic function method yields a high number of accurate digits for

TABLE IV. Auxiliary quantities for determining the error bounds from (4.8)–(4.14).

M	$b_{M,1}$	$B_{M,1}$	$B^*_{M,1}$	$W_{2,M}$	ρ_M	ϵ_M	D_M
14	1.31	1.225 2	1.224 587 036 060 0	2.5×10^{-3}	1.2×10^{-5}	1.5×10^{-5}	1.2×10^{3}
15	1.224 588 5	1.224 587 044	1.224 587 036 059 4	4.5×10^{-3}	6×10^{-6}	10^{-6}	1.8×10^{6}
16	1.224 587 036 073	1.224 587 036 059 25	1.224 587 036 059 25	5.9×10^{-3}			

the eigenvalues. Moreover these results have been obtained by means of very simple trial functions. The results are particularly good for $a_{12}=1$ and they become less precise as $a_{12}\to -1$. That is related to the fact that our circularly symmetric trial functions fail to reflect the symmetries of the anharmonic interaction potential as $a_{12}\to -1$. In our example we have $V_A \sim k(x^2-y^2)^2$ for $a_{12}=-1$ and $V_A \sim k(x^2+y^2)^2$ for $a_{12}=1$. As we mentioned earlier the results are not sensitive to the details of the trial functions, however the choice of proper symmetry subgroups is crucial for good convergence rates in operator projection techniques.

In Table III for the circularly symmetric case we tabulate our results in a form compatible with the notation of Hioe *et al.*[5] We do not duplicate here their excellent analysis of energy level crossings. However by selecting different m, n, and signs in (3.11) we could order our eigenvalues according to the quantum numbers. For example, the higher-order poles, i.e., the excited states of $E^{+}_{0,2}$, correspond to $l=0$ and $2n+1$ quantum numbers. Here we observe that the characteristic function provides good estimates for quite a number of excited states. In addition we note that the form of the spectral coefficients in (3.13) guides us in interpreting the energy degeneracies, e.g., we can tell directly that $E^{-}_{0,2}$ and $E^{+}_{1,3}$ energy levels will be identical (Table III).

Finally in Sec. III we gave an example of how to obtain error bounds. The information is directly acquired from the already calculated Padé approximants.

In the present work we wanted to present the characteristic function method as a simple, self-contained eigenvalue approximation scheme. We expect it to be useful in obtaining the low quantum number excited states of complicated potentials. The results on the two-dimensional anharmonic oscillator encourage us in applying the algorithm to more complex systems.

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Ion-acoustic dispersion relation with direct fractional approximation for $Z'(s)$

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A direct fractional approximation for the derivative Z' of the plasma dispersion function $Z(s)$ has been obtained by using the modified asymptotic Padé method. The dispersion relation for the ion-acoustic wave and for the ion-beam instability has been solved by the use of that fractional approximation yielding satisfactory results. A comparison is given between the dispersion relations calculated with (a) our approximation, (b) other approximations to Z', and (c) the exact function.

I. INTRODUCTION

Lately, new methods[1-3] to find fractional approximations have been published which lead to accurate approximations for the plasma dispersion function $Z(s)$ defined as a Hilbert transform of the Gaussian[4,5]

$$Z(s)=\sqrt{\pi}\int_{-\infty}^{\infty} dt\, e^{-t^2}(t-s)^{-1},$$

for $\operatorname{Im} s>0$ and analytic continuation of this for $\operatorname{Im} s<0$.

This function is commonly found in dispersion equations of plasma waves.[4,6,7] Thus, it seems advantageous to analyze the goodness of any approximation within the dispersion equation rather than in the plasma dispersion function $Z(s)$. However, the dispersion relation is originally written as a function of $Z'(s)$; $Z'(s)$ can be obtained in a simple way by means of the differential equation or alternatively by deriving the function $Z(s)$. The latter is a cumbersome method if a fractional approximation is used to obtain $Z(s)$. On the other hand, the former method yields undesirably large errors for $Z'(s)$.

These considerations led us to seek direct approximations to $Z'(s)$ and to analyze the accuracy of these approximations in the dispersion relation. Direct approximation for $Z'(s)$ denotes here that the parameters of the fractional approximations are determined by the expansions for $Z'(s)$ instead of those for $Z(s)$. Using in both cases the same number of terms of the expansions, the accuracy for $Z'(s)$ is much better with the direct approximation method. Furthermore, the solution of the ion-acoustic dispersion relation with our approximation is simple and sufficiently accurate for most of the experimental and theoretical needs. When the approximation $\hat{Z}'(s)$ found here is used, the dispersion equation reduces to a simple equation instead of the integrotranscendental equation which is usually obtained when the exact $Z'(s)$ is used. If the previous approximations are used the corresponding dispersion equation is more cumbersome and the result would be of much lower accuracy.

The analysis has also been extended to the dispersion equation for the ion-beam instability, with satisfactory results.

The material is arranged in the following way. The direct approximation to $Z'(s)$ is obtained in the next section and compared with the previous ones. In Sec. III the ion-acoustic dispersion relation is solved using the exact and approximated functions and the results are compared. The analysis of the ion beam–plasma system is also included. The last section is devoted to the conclusions.

II. DIRECT FRACTIONAL APPROXIMATION FOR $Z'(s)$

Let us consider fractional approximations to $Z'(s)$ of the type

$$\hat{Z}'(s)=P_n(s)/Q_{n+2}(s)=\tilde{P}_n(1/s)/s^2\tilde{Q}_{n+2}(1/s), \tag{1}$$

where $P_n(s)$, $\tilde{P}_n(1/s)$, $Q_{n+2}(s)$, $\tilde{Q}_{n+2}(1/s)$ are polynomials of the nth and $(n+2)$th degree, respectively. In order to ensure the right asymptotic behavior the degree of the denominator must exceed the numerator's degree in two units.

For $n=4$ the explicit expressions for $P_n(s)$, $\tilde{P}_n(1/s)$, $Q_{n+2}s)$, and $\tilde{Q}_{n+2}(1/s)$ are

$$P_4(s)=p_0+p_1s+p_2s^2+p_3s^3, \tag{2}$$

$$\tilde{P}_4(1/s)=p_3+p_2(1/s)+p_1(1/s^2)+p_0(1/s^3), \tag{3}$$

$$Q_6(s)=1+q_1s+q_2s^2+q_3s^3+q_4s^4+q_5s^5, \tag{4}$$

$$\tilde{Q}_6\left(\frac{1}{s}\right)=q_5+q_4\frac{1}{s}+q_3\frac{1}{s^2}+q_2\frac{1}{s^3}+q_1\frac{1}{s^4}+\frac{1}{s^5}. \tag{5}$$

Here the p's and q's are parameters to be determined.

The data we require to perform our calculations is contained in the following potential and asymptotic expansions:

$$Z'(s)=-2i\sqrt{\pi}se^{-s^2}-2+4s^2-\tfrac{8}{3}s^4\pm\cdots, \tag{6}$$

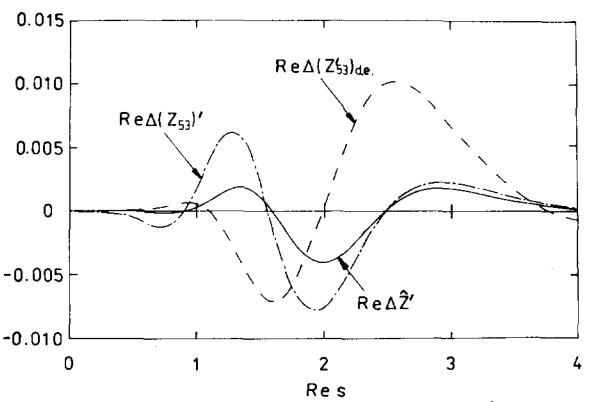

FIG. 1. Real parts of $\Delta Z'(s)\equiv Z'_{\text{approx}}-Z'$ for real s. $\Delta\hat{Z}'$ (direct approximation), $\Delta(Z_{53})'$ (derivative of Z_{53}), and $\Delta(Z'_{53})_{\text{de}}$ [calculated by using the differential equation $Z'_{53}=-2(1+sZ_{53})$]. Z_{53} and Z'_{53} are taken from Ref. 1. Z' is the exact function.

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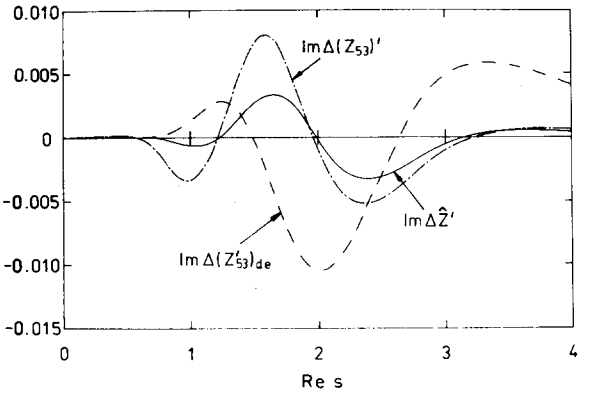

FIG. 2. Imaginary parts of $\Delta Z'(s)$ for $\Delta\hat{Z}'$, $\Delta(Z_{53})'$, and $\Delta(Z'_{53})_{de}$.

$$\tilde{Z}'(s) = \frac{1}{s^2} + \frac{3}{2}\frac{1}{s^4} + \cdots, \tag{7}$$

where we have taken the same number of terms in the power series and asymptotic expansions as that used in the calculation of $Z_{53}(s)$ (Ref. 1).

The coefficients p_i and q_i are calculated by equating the coefficients of the rationalized expansions

$$Z'(s)Q_{n+2}(s) = P_n(s), \tag{8}$$

$$s^2\tilde{Z}'(1/s)\tilde{Q}_{n+2}(1/s) = \tilde{P}_n(1/s). \tag{9}$$

From (8) six linear equations are obtained, which together with the three equations from (9) form a system of nine linear equations in nine unknowns which leads to the following approximation:

$$\hat{Z}'(s) = (-2 + 1.5869is + 0.5957s^2 - 0.0978is^3) \times (1 - 2.5659is - 2.8458s^2 + 1.7336is^3 + 0.5957s^4 - 0.0978is^5)^{-1}. \tag{10}$$

The difference between this approximation and the exact function is shown in Figs. 1 and 2 (real and imaginary part, respectively). The approximation $(Z_{53})'$ and $(Z'_{53})_{de}$ calculated from derivation of $Z_{53}(s)$ and from the differential equation, respectively, are included. The first method of calculation of Z' is cumbersome for it involves the derivative of a polynomial fraction, but it is more accurate than using the differential equation. In any case, the method presented here of direct approximation to $Z'(s)$ yields an error 2.5 times less than the previous one; in addition, calculation is easier.

III. THE ION-ACOUSTIC DISPERSION RELATION

The normalized dispersion relation for the ion-acoustic wave is

$$Z'(s) - 2(1/\Theta + k^2) = 0, \tag{11}$$

where $s \equiv v_\phi/a_i = w/(k\sqrt{2})$ is the phase velocity normalized to the thermal speed of the ions a_i, w is measured in units of w_{pi} (ion plasma frequency), and k is measured in units of k_{Di} (ion Debye length). Here we have normalized as in Ref. 4. Here, Θ is the electron-to-ion temperature in the plasma.

By using the fractional approximation (1) the integro-transcendental equation (11) for the damping wave reduces to

$$[P(s^*)]^* - [4i\sqrt{\pi}se^{-s^2} + 2/\Theta + 2k^2][Q(s^*)]^* = 0, \tag{12}$$

where we have used the extension of the approximation from the upper to the lower complex half-plane (see Ref. 1, p. 281, second column, second paragraph).

This equation in w has been solved by means of the approximation (10) for a plasma having $\Theta = 20$. The results (thin solid line) are shown in Fig. 3(a) together with the values of w obtained by the exact function (thick solid line) for comparison. In ordinary size plots both curves differ very slightly. From the experimental point of view the accuracy seems to be sufficient.

In this figure we also include the solution of the dispersion relation, which is obtained by using $(Z_{53})'$—as a derivative of Z_{53}—and by using $(Z'_{53})_{de}$—from the differential equation using Z_{53} of Ref. 1 (dot-segmented and segmented lines, respectively). With these approximations the results are not as satisfactory as in the case in which $\hat{Z}'$ is used. Discrepancies happen to be noticeable in certain regions. The approximations to $Z'(s)$ obtained from the differential equation $(Z'_{53})_{de} \equiv -2(1 + sZ_{53})$ show a large discrepancy for small values of k $(0 < k \lesssim 0.4)$ resulting in a Landau damping much larger than the true one (the normalized damping is $\gamma/w_{pi} \equiv \sqrt{2}k$ Im s). This is due mainly to the fact that the function $(Z'_{53})_{de}$ does not correctly approximate the imaginary part of Z' for real $s \gtrsim 2.7$. In Fig. 2 it can be seen that $\mathrm{Im}(Z'_{53})_{de}$ is positive and the relative error is large [Im Z' for the exact Z' is negative and very small so that $(\Delta Z'_{53})_{de} \cong (Z'_{53})_{de}$]. For this reason Im s has to take larger negative values to reduce to zero Im Z' in Eq. (11).

We have also calculated with the three approximations to Z' [viz., $\hat{Z}'$, $(Z_{53})'$, and $(Z'_{53})_{de}$] the dispersion relation for the beam–plasma instability for a beam with the following

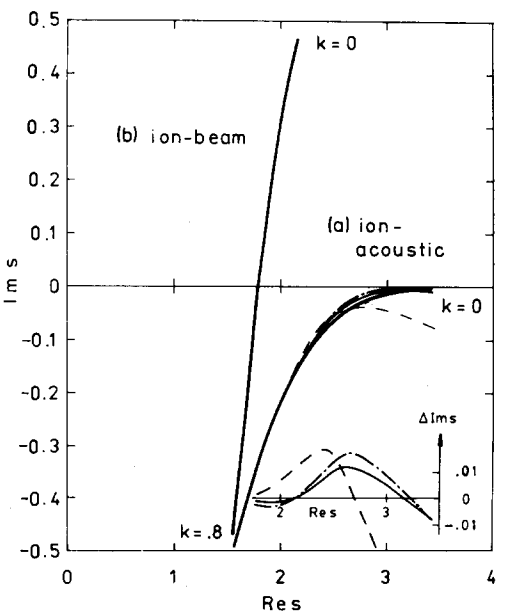

FIG. 3. (a) Dispersion relation for the ion-acoustic wave calculated by using the exact Z' function (———), the approximation $\hat{Z}'$ (———), the derivative $(Z_{53})'$ of Z_{53} (- · -), and $(Z'_{53})_{de}$ (– –). Temperature ratio $T_e/T_i = 20$. Inset: Differences Δ Im s between the approximated and the exact damping rate. (b) Dispersion relation for the ion-beam instability. [Beam parameters: $T_b/T_i = 1$, $n_b/n_0 = 0.20$, $v_b/a_i = 2.0$. a_i is the ion thermal velocity $(2T_i/M)^{1/2}$.] Here the curves are indistinguishable from the exact dispersion relation.

parameters: ion density ratio $n_b/n_0 = 0.2$, normalized drift velocity = 2.0, and ion temperature ratio $T_b/T_i = 1.0$. The approximating curves cannot be distinguished from the exact curve (thick solid line) in Fig. 3(b) since in this case $1.5 < \mathrm{Re}\, s < 2.5$, so that Im Z' is much larger than the difference between the approximations and the exact function.

IV. CONCLUSIONS

We have demonstrated that in order to obtain an acceptable solution of the ion-acoustic wave dispersion equation it is more advantageous using direct approximations to the function $Z'(s)$ instead of approximating $Z(s)$ and then calculating $Z'(s)$. In addition we have presented an approximation to $Z'(s)$ which allows the resolution of the dispersion equation in a way which is both simple and sufficiently accurate for most of the experimental and theoretical needs. The dispersion equation for the ion-acoustic wave becomes in this case a simple equation which can be easily solved even with a desk calculator. The maximum error for the real part of the phase velocity is $\Delta\, \mathrm{Re}\, s = 0.02$ (for $k = 0$, which means $\mathrm{Re}\, s = 3.42$). The maximum error in the imaginary part is $\Delta\, \mathrm{Im}\, s = 0.012$ (for $k = 0.23$, which means $\mathrm{Im}\, s = -0.035$). In the resolution of the dispersion equation for a beam–plasma system the accuracy obtained is better.

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Lie–Bäcklund symmetries of certain nonlinear evolution equations under perturbation around their solutions

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A generalization of the Lie–Bäcklund (LB) theory for coupled evolution equations is discussed. As a consequence, the direct connection between the LB symmetries and constants of motion of these systems is also established. Furthermore, as an application of this theory we investigate the existence of infinitely many commuting LB symmetries of certain nonlinear evolution equations under perturbation around their solutions. Then the corresponding constants of motion are derived, which are in agreement with the known results.

I. INTRODUCTION

It is well known that the geometrical interpretation and invariance under various groups of transformations of many completely integrable Hamiltonian systems have received much attention in recent years.[1–10] Such exactly solvable systems possess various properties in common such as Bäcklund transformations, infinitely many conservation laws, N-soliton solutions, etc.[1–4] It has become possible in the past few years to establish that the above properties are basically due to the existence of the so-called generalized Lie–Bäcklund (LB) symmetries possessing certain bi-Hamiltonian structures.[9,11–18] In particular, there exists a one-to-one correspondence between the LB symmetries and local constants of motion for the Hamiltonian systems.

Apart from the study of single-component evolution equations, there has also been a growing interest in understanding the symmetries of coupled nonlinear evolution equations.[19] However, the recent studies on the LB symmetries of such coupled systems are rather *ad hoc* in nature and no systematic LB symmetry approach seems to have been developed to handle these systems conveniently. In the present paper we develop the theory of LB symmetries for coupled nonlinear evolution equations in a natural way.

It is well known[20] that nonlinear evolution equations under perturbation around their solution give rise to a set of coupled nonlinear evolution equations. As an application of our theory we consider this perturbed class of nonlinear evolution equations as a specific example. Case and Roos[20] proved that when a completely integrable Hamiltonian system is perturbed about a particular solution the resulting equations to all orders of perturbation are completely integrable Hamiltonian systems. It is generally believed that the existence of infinitely many constants of motion which are in involution is the primary evidence for the complete integrability of the system and that there exist certain deep connections between the existence of infinitely many constants of motion and LB symmetries.[21–23] This prompts one to search for the existence of infinitely many LB symmetries for the Hamiltonian equations under perturbation around their solution as well, the analysis of which we carry out in this paper.

The organization of the paper is as follows. Section II of the present paper begins with a brief account of the basic concepts and facts about the theory of LB invariance and Hamiltonian formalism for coupled nonlinear evolution equations generalized in a natural way in the following four stages: (a) We state necessary and sufficient conditions for the existence of a LB symmetry for coupled equations; (b) the definitions of a conserved covariant, strong symmetry, and hereditary symmetry appropriate for coupled systems are given; (c) a direct connection between the conserved covariants and LB symmetries through the Hamiltonian formalism is shown; and (d) as a consequence of the above facts, we give the derivation of a relation connecting the strong symmetry and its adjoint.

The method which we present in Sec. II for obtaining the LB symmetries is applied in Sec. III for Hamiltonian systems under perturbation around their solutions. The most general form of the ith perturbed Hamiltonian is given. We present further the general structure of the strong symmetry and the symplectic operator for arbitrary order of the perturbed evolution equations. Finally, in Sec. IV we illustrate our theory with the help of a class of well-known soliton equations involving Korteweg–de Vries (KdV), modified Korteweg–de Vries (mKdV), sine–Gordon (sG), nonlinear Schrödinger (NLS), and derivative nonlinear Schrödinger (DNLS) equations. Furthermore, we show that one can derive infinitely many vector-valued LB symmetries for the above soliton equations under the perturbation around their solutions and that infinitely many vector-valued local constants of motion for these systems can be derived in agreement with the results of Case and Roos.[20] It may be mentioned that a similar connection also exists for nonlocal constants of motion, which we have planned to discuss elsewhere.

II. LIE–BÄCKLUND INVARIANCE AND HAMILTONIAN FORMALISM FOR COUPLED SYSTEMS

In this section, we tersely discuss some basic definitions and notations of LB theory and develop the consequences for coupled evolution equations. We consider a C^∞ manifold M with local coordinates (x,t) and its tangent space S and cotangent space S^*, in which all the C^∞ functions defined vanish at $x = \pm\infty$. In a simple geometrical sense the theory of LB symmetries mainly deals with the local study of the differentiable manifold of solutions of the evolution equations and

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the fact that every typical fiber of the tangent bundle in S defines the boundaries of the symmetry mapping in S. Similar study in the cotangent space S^* explains the conservation laws.[9] It is assumed throughout this paper that the various functions defined are C^∞. We will assume the above facts throughout the paper without explicitly stating them further.

We consider now the following vector-valued functions:

$$(u) = (u^{(0)},u^{(1)},...,u^{(n)}) \in S, \tag{2.1a}$$

$$(u_k) = (u_k^{(0)},u_k^{(1)},...,u_k^{(n)}) \in S, \quad k = 0,1,2,...,\infty, \tag{2.1b}$$

where the partial derivatives are denoted by

$$u_0^{(i)} = u^{(i)}, \quad u_k^{(i)} = \frac{\partial^k u^{(i)}}{\partial x^k}, \tag{2.1c}$$

$$u_{kt}^{(i)} = \frac{\partial u_k^{(i)}}{\partial t} \in S, \quad i = 0,1,2,...,n; \quad k = 1,2,...,\infty.$$

We define the ring of functions $G^{(i)}(u)$ and a corresponding vector-valued function $G(u)$ in S, in such a way that

$$G(u) = (G^{(0)}(u),G^{(1)}(u),...,G^{(n)}(u)), \tag{2.1d}$$

where

$$\{G^{(i)}(u) | G^{(i)}(u) = G^{(i)}(u,u_1,u_2,...) \in S\}. \tag{2.1e}$$

At this stage we consider the vector-valued evolution equation

$$\Omega = u_t + K(u) = 0, \tag{2.2a}$$

where

$$\Omega = (\Omega^{(0)},\Omega^{(1)},...,\Omega^{(n)}), \tag{2.2b}$$

$$K(u) = (K^{(0)}(u),K^{(1)}(u),...,K^{(n)}(u)). \tag{2.2c}$$

We note that the component form of Eq. (2.2a) reads as

$$\Omega^{(i)} \equiv u_t^{(i)} + K^{(i)}(u) = 0, \quad i = 0,1,2,...,n, \tag{2.2d}$$

in S. For our further discussions of the LB symmetries, we need the following definitions. We define the total derivative operators

$$D \equiv \begin{cases} D_x = \sum_{i=0}^{n} \sum_{k=0}^{\infty} u_{k+1}^{(i)} \dfrac{\partial}{\partial u_k^{(i)}}, & (2.3a) \\ D_t = \sum_{i=0}^{n} \sum_{k=0}^{\infty} u_{kt}^{(i)} \dfrac{\partial}{\partial u_k^{(i)}}, & (2.3b) \end{cases}$$

and the Lie–Bäcklund (LB) operator

$$X(\eta) = \sum_{i=0}^{n} (D_t \eta^{(i)}) \frac{\partial}{\partial u_t^{(i)}} + \sum_{i=0}^{n} \sum_{k=0}^{\infty} (D^k \eta^{(i)}) \frac{\partial}{\partial u_k^{(i)}}, \tag{2.4a}$$

where the vector-valued generalized LB symmetries are

$$\eta(u) = (\eta^{(0)}(u),\eta^{(1)}(u),...,\eta^{(n)}(u)) \in S. \tag{2.4b}$$

We note that with each of the component equations (2.2d), $u_t^{(i)} + K^{(i)}(u) = 0$, a $\eta^{(i)}$ is associated. We further assume that η does not depend on x and t explicitly for the systems under study. The LB operator $X(\eta)$ in (2.4a) leaves Eq. (2.2a) invariant[23] iff

$$X(\eta)\Omega|_{\Omega=0} \doteq 0, \tag{2.5}$$

where $\doteq$ stands for the restriction to solutions of Eq. (2.2a). Equation (2.5) provides an algorithm for finding η as the solution of a system of linear overdetermined equations.

Now the Fréchet derivative of the vector-valued function $K(u)$ at $u \in S$ in the direction of $(v) = (v^{(0)},v^{(1)},...,v^{(n)})$ is defined by

$$K'(u)[v] = \frac{\partial K}{\partial \epsilon}(u + \epsilon v)|_{\epsilon=0}, \quad u,v \in S. \tag{2.6}$$

It is clear that the operator $K'(u)$ is an $(n+1)\times(n+1)$ matrix given by

$$K'(u) = (K_j^{(i)'}), \quad i,j = 0,1,2,...,n, \tag{2.7}$$

where

$$K_j^{(i)'} = \sum_{k=0}^{\infty} \frac{\partial K^{(i)}}{\partial u_k^{(j)}} D^k, \quad i,j = 0,1,2,...,n. \tag{2.8}$$

We further define the Fréchet derivative of an $(n+1)\times(n+1)$ matrix operator-valued function $\Phi(u)$ by

$$\Phi'(u)[v]w = \frac{\partial \Phi}{\partial \epsilon}(u + \epsilon v)w|_{\epsilon=0}, \tag{2.9}$$

where the operator

$$\Phi'(u) = (\Phi_j^i(u)), \quad i,j = 0,1,2,...,n \tag{2.10}$$

is also an $(n+1)\times(n+1)$ matrix. In the above definitions v and w are arbitrary functions of (u), (u_1), (u_2),... .

In what follows we define the necessary and sufficient condition for the existence of the LB symmetry for Eq. (2.2), wherein we have generalized the definitions of the $n = 1$ case.[13,14] By assumption (2.2) is analytic in the space S and let $u(t)$ be the solution of (2.2a). Then for every initial time t_0 and for every initial condition $\eta(t_0) = \eta_0$, $\eta_0 \in S$, $\eta(t)$ is unique[13] for the invariant equation (2.5).

Definition 1: A vector-valued function $\eta: S \to S$ is called a LB symmetry of (2.2a) iff it satisfies

$$X(\eta)K = X(K)\eta. \tag{2.11}$$

This is a necessary and sufficient condition for the existence of LB symmetry for the initial value problem (2.2a). In the component form, for (2.2d), the condition (2.11) reads as

$$X(\eta)K^{(i)} = X(K)\eta^{(i)}, \quad i = 0,1,2,...,n. \tag{2.12}$$

Definition 2: The vector-valued map $\{\gamma: S \to S^* | \gamma(u) = (\gamma^{(0)}(u),\gamma^{(1)}(u),...,\gamma^{(n)}(u)) \in S^*\}$ is a conserved covariant of (2.2a) iff the following condition holds:

$$\gamma'[K] + (K')^+[\gamma] = 0, \tag{2.13a}$$

where $(K')^+$ denotes the adjoint of K' with respect to the inner product $\langle\ ,\ \rangle$ as defined below. For the given vector-valued conserved covariants f and vector-valued symmetries of g we define

$$\langle f,g \rangle = \int_{-\infty}^{\infty} fg^T dx = \int_{-\infty}^{\infty} \left(\sum_{r=0}^{n} f^{(r)} g^{(r)} \right) dx. \tag{2.13b}$$

Furthermore, the Fréchet derivative of γ,

$$\gamma' = (\gamma_j^{(i)'}), \tag{2.13c}$$

where

$$\gamma_j^{(i)'} = \sum_{k\geq 0} \frac{\partial \gamma^{(i)}}{\partial u_k^{(j)}} D^k, \quad i,j = 0,1,2,...,n, \tag{2.13d}$$

is an $(n+1)\times(n+1)$ matrix-valued operator. In deriving (2.13a) we have used the fact that $\gamma' = \gamma'^+$ (since γ is the conserved covariant).

Definition 3: Let the $(n+1)\times(n+1)$ matrix operator-valued function Φ be a map of the vector-valued symmetries $\eta_l(u) = (\eta_l^{(0)}(u),\eta_l^{(1)}(u),...,\eta_l^{(n)}(u))^T$ in such a way[11] that

$$\{\Phi: S \to S \,|\, \eta_{l+1} = \Phi\eta_l, \eta_l \in S\}, \quad l = 1,2,...,\infty. \tag{2.14}$$

Then the operator Φ is a strong symmetry iff it satisfies the condition

$$\Phi'[K]v - [K',\Phi]v = 0, \tag{2.15}$$

where v is an arbitrary vector function of $(u),(u_1),(u_2),...$. It is worth noting that the operator Φ plays a fundamental role as it generates an infinite number of new vector-valued LB symmetries η_{l+1} from the known ones η_l, $l = 1,2,3,...,\infty$.

Definition 4: The map $\Phi: S \to S$ is called a hereditary operator iff Φ satisfies[11,13]

$$\Phi'[\Phi w]v - \Phi'[\Phi v]w - \Phi\Phi'[w]v + \Phi\Phi'[v]w = 0, \tag{2.16}$$

where v and w are functions of $(u),(u_1),...$.

Furthermore, the hereditary property (2.16) of Φ allows us to associate with (2.2) a hierarchy of matrix-valued evolution equations[11]

$$u_t + \Phi^m u_1 = 0, \quad m = 0,1,2,...,\infty. \tag{2.17}$$

Since the x-translation symmetry (see Sec. IV below) is the first of the matrix-valued LB symmetry (η_1) then using (2.14),(2.17) can also be written as

$$u_t + \eta_{m+1} = 0, \quad m = 0,1,2,...,\infty. \tag{2.18}$$

After establishing the existence of infinitely many commuting LB symmetries of (2.2), it is of immediate importance to investigate the associated conserved quantities. Let the constants of motion for the system of equations (2.2) be defined by the functional

$$I_l = \int_{-\infty}^{\infty} \rho_l(x,(u),(u_1),...)dx, \quad l = 1,2,...,\infty. \tag{2.19}$$

Then the corresponding vector-valued conserved covariants

$$\gamma_l(u) = (\gamma_l^{(0)}(u),\gamma_l^{(1)}(u),...,\gamma_l^{(n)}(u))^T \tag{2.20}$$

can be written as

$$\gamma_l = \operatorname{grad} I_l \Leftrightarrow (\gamma_l^{(i)}) = \left(\frac{\delta I_l}{\delta u^{(i)}}\right), \tag{2.21}$$

$$i = 0,1,2,...,n, \quad l = 1,2,3,...,\infty.$$

More explicitly (2.21) can be written as

$$(\gamma_l^{(0)}(u),\gamma_l^{(1)}(u),\gamma_l^{(2)}(u),...,\gamma_l^{(n)}(u)) = \left(\frac{\delta I_l}{\delta u^{(0)}}, \frac{\delta I_l}{\delta u^{(1)}}, ..., \frac{\delta I_l}{\delta u^{(n)}}\right). \tag{2.22}$$

Now the equations of motion (2.2) can always be written in the Hamiltonian form[8,24]

$$u_t + J\frac{\delta \mathcal{H}}{\delta u} = 0 \Leftrightarrow (u_t^{(i)}) = -J\frac{\delta \mathcal{H}}{\delta u^{(i)}} = -K^{(i)}, \quad i = 0,1,2,...,n, \tag{2.23}$$

where J is an $(n+1)\times(n+1)$ skew-symmetric matrix operator.

Furthermore, it follows from the fact that Eqs. (2.2) admit strong and hereditary symmetry and so we have the infinite hierarchy of evolution Eqs. (2.17), which gives us that any of the constants of motion of (2.2) can be used as a Hamiltonian. Then, by writing the hierarchy (2.17) in the Hamiltonian form,

$$u_t + J\frac{\delta I_{m+1}}{\delta u} = u_t + J\gamma_{m+1} = 0, \quad m = 0,1,2,...,\infty. \tag{2.24}$$

Comparing (2.18) and (2.24) we obtain the matrix relation

$$J\gamma_{m+1} = \eta_{m+1}, \quad m = 0,1,2,...,\infty, \tag{2.25a}$$

connecting the vector-valued conserved covariants and the vector-valued LB symmetries. We infer from (2.25a) that the operator J maps conserved covariants into symmetries. Using (2.14), Eq. (2.25a) may be rewritten as

$$J\gamma_{m+1} = \eta_{m+1} = \Phi\eta_m = \Phi J\gamma_m, \tag{2.25b}$$

and hence

$$J\gamma_{m+1} = L\gamma_m, \tag{2.25c}$$

where $L = \Phi J$ is a symplectic operator.

In the light of the results obtained above, we derive a recursive relation for the conserved covariants through the adjoint of the strong symmetry. By definition, the matrix-valued adjoint operator Φ^+ satisfies the condition

$$\langle f,\Phi g\rangle = \langle \Phi^+ f,g\rangle. \tag{2.26}$$

As we mentioned earlier, I_l is a constant of motion of (2.2), so that it implies that this is true for the whole hierarchy (2.17). From this fact we have $dI_l/dt = I_l'(u_t) = 0 \Leftrightarrow \langle\gamma_l,K\rangle = 0$, as well as $\langle\gamma_l,\Phi^m K\rangle = 0$, $m = 0,1,2,...$. From (2.26) we also have the relation $\langle\gamma_l,\Phi^m K\rangle = \langle(\Phi^+)^m\gamma_l,K\rangle$, and therefore

$$\gamma_{l+m} = (\Phi^+)^m\gamma_l, \quad m = 0,1,2,...,\infty, \quad l = 1,2,3,...,\infty, \tag{2.27}$$

are also the conserved covariants of (2.2). Finally, from (2.25) and (2.27) we readily establish that

$$\Phi\eta_l = \Phi J\gamma_l = \eta_{l+1} = J\gamma_{l+1} = J\Phi^+\gamma_l, \tag{2.28}$$

so that

$$J\Phi^+ = \Phi J, \tag{2.29}$$

which connects the strong symmetry and its adjoint through the symplectic operator J.

III. LB SYMMETRIES OF THE HAMILTONIAN SYSTEMS UNDER PERTURBATION AROUND THEIR SOLUTIONS

Now we consider the evolution equations resulting from the completely integrable Hamiltonian systems under perturbation around their solutions as a set of specific examples of the previous section and discuss the existence of LB symmetries and consequences. For this purpose we concentrate on a one-component, completely integrable nonlinear evolution equation of the Hamiltonian type in the form

$$w_t = \overline{K}(w), \tag{3.1}$$

where $\overline{K}(\cdot)$ is a nonlinear operator and w is a one-component (real or complex) function. For convenience we consider in this section only a real w. It is straightforward to extend these ideas for complex cases (see Sec. IV below).

If $\mathcal{H}(w)$ is the appropriate Hamiltonian for (3.1), then the corresponding equation of motion is

$$w_t = [w,\mathscr{H}] = \overline{K}(w), \tag{3.2}$$

with the Lie bracket defined by

$$[F_i,F_j] = \int_{-\infty}^{\infty} dy \frac{\delta F_i}{\delta w} J_1 \frac{\delta F_j}{\delta w}, \tag{3.3}$$

where J_1 is a symplectic operator, which is linear and antisymmetric. Then, given a solution $w^{(0)}$ of Eq. (3.2) (for example, the soliton solution), we look for a solution close to it in the form

$$W = w^{(0)} + \Delta w, \tag{3.4}$$

where

$$\Delta w = \sum_{r=1}^{n} \epsilon^r w^{(r)} \in S, \tag{3.5}$$

where $\epsilon \in R$ is a small parameter and r denotes the order of the perturbation. Then by using (3.4) in (3.1) we can write the evolution equations to each order in ϵ as[20]

$$w_t^{(i)} = [w^{(i)},\mathscr{H}_i]_i, \quad i = 0,1,2,...,n, \tag{3.6}$$

where

$$\mathscr{H}_i = \mathscr{H}_i((w_0),(w_1),...), \tag{3.7}$$

$$w_k = \frac{\partial^k w}{\partial x^k} = (w_k^{(0)},w_k^{(1)},...,w_k^{(n)}),$$

$$w = w_0, \quad k = 0,1,2,...,\infty, \tag{3.8}$$

and the ith Poisson bracket on the right-hand side of (3.6) is defined by

$$[F_l,F_{l'}]_i = \int_{-\infty}^{\infty} dy \frac{\delta F_l}{\delta w^{(i)}} J_1 \frac{\delta F_{l'}}{\delta w^{(i)}},$$

$$i = 0,1,2,...,n. \tag{3.9}$$

We note further that the explicit analysis of (3.6) is facilitated by assigning a weight n to $w^{(n)}$ and its derivatives and requiring that each term in the equation derived from it must have equal weight.

The Hamiltonian functional $\mathscr{H}_i$ in (3.6) may be obtained by Taylor-expanding the Hamiltonian functional $\mathscr{H}(W)$,

$$\mathscr{H}[w^{(0)} + \Delta w] = \sum_{N=0}^{\infty} I^N \left(\frac{[\Delta w]^N}{N!} \frac{\delta^N \mathscr{H}[w^{(0)}]}{\delta w^N} \right), \tag{3.10}$$

where

$$I^1\left(\Delta w \frac{\delta \mathscr{H}}{\delta w}\right) = \int_{-\infty}^{\infty} dx_1 \, \Delta w(x_1) \frac{\delta \mathscr{H}}{\delta w(x_1)},$$

$$I^2\left([\Delta w]^2 \frac{\delta^2 \mathscr{H}}{\delta w^2}\right)$$

$$= \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \, \Delta w(x_1) \Delta w(x_2) \times \frac{\delta^2 \mathscr{H}}{\delta w(x_1) \delta w(x_2)}, \tag{3.11}$$

etc. On substituting (3.5) into (3.10) and equating the ϵ^{2i} coefficient in the expansion of the functional $\mathscr{H}(W)$ we obtain[20]

$$\mathscr{H}_i = \sum_{n_j}^{2i} \sum_{n=1}^{2i} \frac{I^N([w^{(1)}]^{n_1}[w^{(2)}]^{n_2}...[w^{(N)}]^{n_N}(\delta^N \mathscr{H}/\delta w^N))}{n_1! n_2! ... n_N!}, \tag{3.12}$$

where the first summation over n_j denotes the summation over all possible combinations of $n_1,n_2,...,n_n$ with $\Sigma_{j=1}^{2i} n_j = N$, n_j and N are integers, and $2i = n_1 + 2(n_2) + 3(n_3) + \cdots + N(n_N)$.

In order to associate the evolution equations (3.6) with the system of coupled evolution equations (2.2), we identify

$$w^{(i)} \leftrightarrow u^{(i)}, \tag{3.13a}$$

$$[w^{(i)},\mathscr{H}_i]_i \leftrightarrow -K^{(i)}. \tag{3.13b}$$

It is then possible to use the results of Sec. II straightaway with appropriate modifications.

We further note that the coupling of the field variables in the case of perturbed evolution equations (3.6) is such that the equation for $w^{(i)}$ contains all the perturbed variables $(w^{(0)},w^{(1)},...,w^{(i-1)},w^{(i)})$ but not the later ones, $(w^{(i+1)},...,w^{(n)})$. As a consequence, the ith component $\eta^{(i)}$ of the vector-valued LB symmetry η_l will not involve functions $w^{(i+j)}$, $j \geq 1$. Then it is possible to determine the LB symmetries of the ith perturbed equations in conjunction with all the previously known LB symmetries. Correspondingly, for perturbed evolution equations any conserved functional assumes the vector-valued form $I_l = (I_l^{(0)},...,I_l^{(n)})$, $l = 1,2,...,\infty$. Then the associated conserved covariants corresponding to I_l can be written as

$$\gamma_l \equiv (\gamma_l^{(0)},\gamma_l^{(1)},...,\gamma_l^{(n)}) = \left(\frac{\delta I_l^{(n)}}{\delta w^{(n)}}, \frac{\delta I_l^{(n)}}{\delta w^{(n-1)}}, ..., \frac{\delta I_l^{(n)}}{\delta w^{(0)}} \right), \tag{3.14}$$

so that the corresponding terms on either side of Eq. (3.14) have equal weights. Stated simply (3.14) implies that for the nth perturbed equation, the component form of the conserved covariant γ_l corresponding to $w^{(i)}$ is given by $\gamma_l^{(n-j)} = \delta I_l^{(n)}/\delta w^{(j)}$. We can easily check that this vector-valued conserved covariant γ_l satisfies condition (2.13a) with the definition of the inner product taking the form

$$\langle f,g \rangle = \int_{-\infty}^{\infty} fg^T dx = \int_{-\infty}^{\infty} \sum_{r=0}^{n} f^{(r)} g^{(n-r)} dx, \tag{3.15}$$

where f,g are vector-valued conserved covariants and symmetries, respectively, of the perturbed evolution equation (3.6). The symplectic operator J in (2.29) is also a matrix-valued operator with the diagonal elements equal to the symplectic operator of the unperturbed system and zero elsewhere. It may be noted that in the above, the order of the matrix-valued operator is equal to the order of the perturbation. With the above identifications all the further discussion given in Sec. II follows here also. Thus we can discuss the LB symmetries for the evolution equation resulting from the coefficients of nth order of the perturbation ϵ^n straightaway from the LB theory of (2.2) discussed earlier in Sec. II.

From these LB symmetries it is often possible to construct the strong symmetry for the perturbed evolution equations of any order such that the strong symmetry takes the form of an $(n+1)\times(n+1)$ matrix operator-valued function $\Phi^{(n)}$. When this operator operates on the vector-valued LB symmetry $\eta_l = (\eta_l^{(0)}(w),\eta_l^{(1)}(w),...,\eta_l^{(n)}(w))$, it generates further symmetries from the known ones satisfying the relation

$$\eta_{l+1} = \Phi^{(n)} \eta_l, \quad l = 1,2,...,\infty, \tag{3.16}$$

where now

$$\eta_l(w) = (\eta_l^{(0)}(w), \eta_l^{(1)}(w), \ldots, \eta_l^{(n)}(w)), \tag{3.17}$$

$$\Phi^{(n)} = \begin{bmatrix} a_{11} & 0 & 0 & \cdots & 0 \\ a_{21} & a_{22} & 0 & \cdots & 0 \\ a_{31} & a_{32} & a_{33} & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ a_{n+11} & a_{n+12} & a_{n+13} & \cdots & a_{n+1\,n+1} \end{bmatrix},$$

$$a_{ii} = \Phi^{(0)}(w^{(0)}), \quad i = 1,2,\ldots,n,$$
$$a_{ij} = a_{i+1,j+1}, \quad i,j = 1,2,\ldots,n, \tag{3.18a}$$

and

$$a_{n+1,1} = \left(\frac{1}{m_1!m_2!\cdots m_N!}\Phi^{(0)^{m_1+\cdots+m_r\ \text{times}}}(w^{(0)}) \times [(w^{(1)})^{m_1}(w^{(2)})^{m_2}\cdots(w^{(N)})^{m_N}]\right),$$
$$r = 1,2,\ldots,N, \quad N = m_1 + m_2 + \cdots + m_N,$$
$$n = m_1 + 2(m_2) + \cdots + N(m_N). \tag{3.18b}$$

From the results of Sec. II, Eq. (2.27), the conserved covariants for the perturbed evolution equations can be directly obtained from the relation

$$\gamma_{l+1} = \Phi^{(n)^+}\gamma_l, \quad l = 1,2,3,\ldots,\infty, \tag{3.19}$$
$$\gamma_l(w) = (\gamma_l^{(0)}(w), \gamma_l^{(1)}(w), \ldots, \gamma_l^{(n)}(w)),$$

and $\Phi^{(n)^+}$ can be obtained from the relation

$$J\Phi^{(n)^+} = \Phi^{(n)}J, \tag{3.20}$$

where the $(n+1)\times(n+1)$ matrix operator

$$J = \operatorname{diag}[J_1, J_1, \ldots, J_1], \tag{3.21}$$

and J_1 is the symplectic operator of the unperturbed case. The corresponding constants of motion can be derived from the relation $\operatorname{grad} I_l = \gamma_l$ [see Sec. II, Eqs. (2.21) and (2.22)].

IV. EXAMPLES: SOLITON EQUATIONS

In this section, we wish to apply our theory developed in Secs. II and III to some of the completely integrable Hamiltonian systems under perturbation around their solution explicitly. We show that these systems admit LB symmetries at every order of perturation by solving the appropriate LB invariant equations so that we can construct a strong and hereditary symmetry operator which satisfies conditions (2.15) and (2.16). It is also pointed out how the conserved covariants and constants of motion, which are in involution with respect to the appropriate Poisson brackets and symplectic operators, can be derived. These results are in full agreement with Ref. 20.

A. The Korteweg–de Vries (KdV) equations

We consider the KdV equation in the form

$$U_t = -\partial_x\{U^2 + 2U_2\}. \tag{4.1}$$

It can be written in the Hamiltonian form (3.2) with

$$\mathcal{H} = \int_{-\infty}^{\infty}(U^3/3 - U_1^2)dx \tag{4.2}$$

and the symplectic operator J_1 [in (3.3)] defined by

$$J_1 = -\partial_x = -D. \tag{4.3}$$

We now consider the perturbation of (4.1),

$$U \equiv u^{(0)} + \Delta u = u^{(0)} + \sum_{k=1}^{n}\epsilon^k u^{(k)} \in S, \tag{4.4}$$

where $\epsilon \in R$ is a small real parameter and the given solution $u^{(0)}$ in (4.4) is, for example, the soliton solution of (4.1) or equivalently of (3.6). Then the perturbed evolution equations to order ϵ^i become

$$u_t^{(i)} + 2u_3^{(i)} + 2\sum_{0<j<i} u^{(j)}u_1^{(i-j)} = 0, \quad i = 0,1,2,\ldots,n. \tag{4.5}$$

Here the unperturbed solution $u^{(0)}$ obeys the KdV equation

$$u_t^{(0)} = -\partial_x\{u^{(0)^2} + 2u_2^{(0)}\}. \tag{4.6}$$

It is then clear that the LB operator $X(\eta)$ in (2.4a) leaves the system (4.5) invariant iff

$$D_t\eta^{(i)} + 2D^3\eta^{(i)} + 2\sum_{0<j<i}(u_1^{(i-j)}\eta^{(j)} + u^{(j)}D\eta^{(i-j)}) = 0, \quad i = 0,1,2,\ldots,n, \tag{4.7}$$

hold.

In order to find the LB symmetries associated with the ith perturbed equations (4.5), we have to consider this in conjunction with the LB symmetries associated with the evolution equations of preceding orders of perturbation. To prove the existence of an infinite number of commuting vector-valued symmetries η_l, $l = 1,2,\ldots,\infty$, as in the case of the evolution equation with a single variable, it is generally enough to find one vector-valued LB symmetry apart from the already known space and time translation LB symmetries, provided we can construct the strong and hereditary operator.[11,13]

1. The first-order perturbation

a. LB symmetries. Considering now the first-order case in (4.5),

$$u_t^{(1)} + 2u_3^{(1)} + 2u^{(0)}u_1^{(1)} + 2u^{(1)}u_1^{(1)} = 0, \tag{4.8}$$

we now find its infinitely many commuting LB symmetries and obtain the corresponding constants of motion which are in involution and then show the possible generalization of these results to any order of perturbation.

In order to find the LB symmetries of (4.8) we have to consider this in conjunction with the LB symmetries of (4.6). By solving the LB invariant equation [$i = 0$ in (4.7)]

$$D_t\eta^{(0)} + 2D^3\eta^{(0)} + 2u^{(0)}D\eta^{(0)} + 2u_1^{(0)}\eta^{(0)} = 0, \tag{4.9}$$

where

$$\eta^0 = \eta^0(u^{(0)}, u_1^{(0)}, u_2^{(0)}, \ldots), \tag{4.10}$$

recursively we can obtain the LB symmetries of the unperturbed equation (4.6). For example, we have the following first three LB symmetries of (4.6)[11]:

$$\eta_1^{(0)} = u_1^{(0)}, \tag{4.11}$$
$$\eta_2^{(0)} = 2u_3^{(0)} + 2u^{(0)}u_1^{(0)}, \tag{4.12}$$
$$\eta_3^{(0)} = 4u_5^{(0)} + \tfrac{40}{3}u_1^{(0)}u_2^{(0)} + \tfrac{20}{3}u^{(0)}u_3^{(0)} + \tfrac{10}{3}(u^{(0)})^2u_1^{(0)}. \tag{4.13}$$

Using the above three LB symmetries it is possible to construct the strong and hereditary symmetry $\Phi^{(0)}$ of (4.6) which satisfies conditions (2.15) and (2.16). This operator $\Phi^{(0)}$ is known[11] to be given by

$$\Phi \equiv \Phi^{(0)} = 2D^2 + \tfrac{4}{3}u^{(0)} + \tfrac{2}{3}u_1^{(0)}D^{-1}, \tag{4.14}$$

where

$$D^{-1}w(x) = \int_{-\infty}^{x} w(y)dy, \tag{4.15}$$

and it generates an infinite number of commuting LB symmetries $\{\eta_l^{(0)}\}$, $l = 1,2,...,\infty$ for (4.6).

The action of the LB operator (2.4a) on the first-order perturbation equation (4.8) gives the corresponding LB invariant equation [$i = 1$ in (4.7)],

$$D_t\eta^{(1)} + 2D^3\eta^{(1)} + 2u^{(0)}D\eta^{(1)} + 2u^{(1)}D\eta^{(0)} + 2u_1^{(1)}\eta^{(0)} + 2u_1^{(0)}\eta^{(1)} = 0. \tag{4.16}$$

Obviously the first two LB symmetries corresponding to space and time translation invariance are

$$\eta_1^{(1)} = u_1^{(1)}, \tag{4.17}$$

$$\eta_2^{(1)} = 2u_3^{(1)} + 2u^{(0)}u_1^{(1)} + 2u_1^{(0)}u^{(1)}. \tag{4.18}$$

To find a generalized LB symmetry we follow the procedure as given below.[11,18] Let us denote $\eta_3^{(1)} = \xi$. We search for a

$$\xi = \xi(u^{(0)},u_1^{(0)},u_2^{(0)},u_3^{(0)}u_4^{(0)},u_5^{(0)},u^{(1)},u_1^{(1)},u_2^{(1)},u_3^{(1)},u_4^{(1)},u_5^{(1)}) \tag{4.19}$$

with unit weight. Substituting (4.19) in (4.16) and eliminating $u_{it}^{(0)}$ and $u_{it}^{(1)}$, $i = 0,1,2,3,4,5$ by using (4.6) and (4.8), we collect the coefficients of $u_7^{(1)},u_7^{(0)},u_6^{(1)},u_6^{(0)}$ (noting that the coefficients of $u_8^{(1)}$ and $u_8^{(0)}$ are canceled away). Then equating each of these coefficients to zero, we obtain $D\xi_{u_5^{(1)}} = 0$, $D\xi_{u_4^{(1)}} = 0$. Solving these equations we have

$$\xi = a_1u_5^{(1)} + a_2u_4^{(1)} + A(u^{(0)},u_1^{(0)},u_2^{(0)},u_3^{(0)},u^{(1)},u_1^{(1)},u_2^{(1)},u_3^{(1)}), \tag{4.20}$$

where a_1 and a_2 are integration constants. Using (4.20) again in (4.16), we obtain

$$DA_{u_3^{(0)}} = 2a_1u_1^{(1)} - \tfrac{4}{3}u_1^{(1)} + \tfrac{1}{3}a_2u^{(1)}, \quad DA_{u_3^{(1)}} = \tfrac{5}{3}a_1u_1^{(0)}. \tag{4.21}$$

Solving (4.21), we get $a_2 = 0$ and

$$A = 2a_1u^{(1)}u_3^{(0)} - \tfrac{4}{3}u^{(1)}u_3^{(0)} + \tfrac{5}{3}a_1u_1^{(0)}u_3^{(1)} + a_3u_3^{(1)} + B(u^{(0)},u_1^{(0)},u_2^{(0)},u^{(1)},u_1^{(1)},u_2^{(1)}),$$
$$a_3 = \text{const.} \tag{4.22}$$

Again substituting (4.22) in (4.16), we obtain

$$DB_{u_2^{(0)}} = 3a_1u_2^{(1)} + \tfrac{4}{3}u_2^{(1)}, DB_{u_2^{(1)}} = \tfrac{10}{3}a_1u_2^{(0)}, \tag{4.23}$$

and so $a_1 = 4$, $a_3 = 0$, and

$$B = \tfrac{40}{3}u_1^{(1)}u_2^{(0)} + \tfrac{40}{3}u_1^{(0)}u_2^{(1)} + a_4u_2^{(1)} + C(u^{(0)},u_1^{(0)},u^{(1)},u_1^{(1)}), \tag{4.24}$$

where a_4 is again an integration constant.

Repeating the same procedure further, we obtain

$$DC_{u_1^{(0)}} = \tfrac{20}{3}u^{(0)}u_1^{(1)} + \tfrac{20}{3}u_1^{(0)}u^{(1)}, DC_{u_1^{(1)}} = \tfrac{20}{3}u^{(0)}u_1^{(0)}. \tag{4.25}$$

Solving (4.25), we find $a_4 = 0$ and

$$C = \tfrac{20}{3}u^{(0)}u_1^{(0)}u^{(1)} + \tfrac{10}{3}u^{(0)2}u_1^{(1)} + a_5u_1^{(1)} + D(u^{(0)},u^{(1)}), \tag{4.26}$$

where a_5 is an integration constant. By similar arguments we can show tht $a_4 = a_5 = 0$ and hence the final form of the generalized LB symmetry is

$$\eta_3^{(1)} = \xi = 4u_5^{(1)} + \tfrac{20}{3}u_3^{(0)}u^{(1)} + \tfrac{20}{3}u^{(0)}u_3^{(1)} + \tfrac{40}{3}u_2^{(0)}u_1^{(1)} + \tfrac{40}{3}u_1^{(0)}u_2^{(1)} + \tfrac{20}{3}u^{(0)}u_1^{(0)}u^{(1)} + \tfrac{10}{3}(u^{(0)})^2u_1^{(1)}. \tag{4.27}$$

This symmetry is a solution of (4.16) in conjunction with (4.13).

Now from the above first three LB symmetries of zeroth- and first-order equations, namely $(\eta_1^{(0)},\eta_2^{(0)},\eta_3^{(0)})$ and $(\eta_1^{(1)},\eta_2^{(1)},\eta_3^{(1)})$ we can construct an operator

$$\Phi^{(1)} = \begin{bmatrix} \Phi^{(0)}(u^{(0)}) & 0 \\ \Phi^{(0)\prime}(u^{(1)}) & \Phi^{(0)}(u^{(0)}) \end{bmatrix} = \begin{bmatrix} 2D^2 + \frac{4}{3}u^{(0)} + \frac{2}{3}u_1^{(0)}D^{-1} & 0 \\ \frac{4}{3}u^{(1)} + \frac{2}{3}u_1^{(1)}D^{-1} & 2D^2 + \frac{4}{3}u^{(0)} + \frac{2}{3}u_1^{(0)}D^{-1} \end{bmatrix}, \tag{4.28}$$

which satisfies the strong symmetry condition (2.15)

$$\Phi^{(1)\prime}[K]\Psi - [K',\Phi^{(1)}]\Psi = 0,$$
$$K = (K^{(0)},K^{(1)})^T, \quad \Psi = (\Psi_1,\Psi_2)^T, \tag{4.29a}$$

where

$$K^{(0)} = -2u_3^{(0)} - 2u^{(0)}u_1^{(0)},$$
$$K^{(1)} = -2u_3^{(1)} - 2u^{(0)}u_1^{(1)} - 2u^{(1)}u_1^{(0)}. \tag{4.29b}$$

This operator $\Phi^{(1)}$ generates an infinite number of LB symmetries of both Eqs. (4.6) and (4.8) in such a way that

$$\begin{pmatrix} \eta_{l+1}^{(0)} \\ \eta_{l+1}^{(1)} \end{pmatrix} = \Phi^{(1)} \begin{pmatrix} \eta_l^{(0)} \\ \eta_l^{(1)} \end{pmatrix}, \quad l = 1,2,...,\infty, \tag{4.30}$$

where $\Phi^{(1)}$ is given by (4.28) and $\eta_l^{(0)}$ and $\eta_l^{(1)}$ are LB symmetries of (4.6) and (4.8), respectively. Similarly, we can find the values of each term in (2.16) by taking the Fréchet derivatives of $\Phi^{(1)}$ along the direction of v, w, $\Phi^{(1)}v$, and $\Phi^{(1)}w$ and prove that (2.16) is satisfied and hence $\Phi^{(1)}$ is a hereditary symmetry as well.

b. Constants of motion. It is known that for Hamiltonian systems, the LB symmetries and constants of motion are interrelated.[21,22] In Sec. IVA1a we found that infinitely many commuting LB symmetries exist, and from these symmetries we can easily deduce the corresponding constants of motion.

We note from (2.29) that the strong symmetry $\Phi^{(1)}$ and its adjoint satisfy the relation

$$J\Phi^{(1)+} = \Phi^{(1)}J = L, \tag{4.31}$$

where

$$J = \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix} \tag{4.32}$$

is symplectic and D is the total derivative operator. Since the operator J is also invertible, we can immediately write down the adjoint of $\Phi^{(1)}$ from (4.31) as

$$\Phi^{(1)+} = \begin{bmatrix} 2D^2 + \frac{4}{3}D^{-1}u^{(0)}D + \frac{2}{3}D^{-1}u_1^{(0)} & 0 \\ \frac{4}{3}D^{-1}u^{(1)}D + \frac{2}{3}D^{-1}u_1^{(1)} & 2D^2 + \frac{4}{3}D^{-1}u^{(0)}D + \frac{2}{3}D^{-1}u_1^{(0)} \end{bmatrix}. \tag{4.34}$$

Then from the relation (2.27) we can find the infinitely many conserved covariants in such a way that

$$\begin{pmatrix} \gamma_{l+1}^{(0)} \\ \gamma_{l+1}^{(1)} \end{pmatrix} = \Phi^{(1)+} \begin{pmatrix} \gamma_l^{(0)} \\ \gamma_l^{(1)} \end{pmatrix}, \quad l = 1,2,\ldots,\infty. \tag{4.35}$$

The first few conserved covariants of Eqs. (4.6) and (4.8), respectively, may be written as follows:

$$\gamma_1^{(0)} = u^{(0)}, \tag{4.36}$$

$$\gamma_2^{(0)} = 2u_2^{(0)} + (u^{(0)})^2, \tag{4.37}$$

$$\gamma_3^{(0)} = 4u_4^{(0)} + \tfrac{20}{3}u^{(0)}u_2^{(0)} + \tfrac{10}{3}(u_1^{(0)})^2 + \tfrac{10}{9}(u^{(0)})^3, \tag{4.38}$$

etc., and

$$\gamma_1^{(1)} = u^{(1)}, \tag{4.39}$$

$$\gamma_2^{(1)} = 2u_2^{(1)} + 2u^{(0)}u^{(1)}, \tag{4.40}$$

$$\gamma_3^{(1)} = 4u_4^{(1)} + \tfrac{20}{3}u^{(1)}u_2^{(0)} + \tfrac{20}{3}u^{(0)}u_2^{(1)} + \tfrac{20}{3}u_1^{(0)}u_1^{(1)} + \tfrac{10}{3}(u^{(0)})^2u^{(1)}, \tag{4.41}$$

etc. It can also be verified that the $\gamma_l = (\gamma_l^{(0)},\gamma_l^{(1)})^T$, $l = 1,2,\ldots,\infty$ in (4.36)–(4.41) satisfy relation (2.13a) with K defined as in (4.29b). The associated constants of motion can then be written straightforwardly[18] using the one-to-one correspondence between the conserved covariants and constants of motion given in (2.22), which are exactly the same as in Ref. 20.

Finally, these constants of motion are also seen to be in involution with respect to the Poisson bracket

$$[F,G] = \int_{-\infty}^{\infty} \left(\frac{\delta F}{\delta u^{(1)}}, \frac{\delta F}{\delta u^{(0)}}\right) J \begin{pmatrix} \delta G/\delta u^{(1)} \\ \delta G/\delta u^{(0)} \end{pmatrix}, \tag{4.42}$$

where J is as given in (4.32). In fact, using the skew symmetry of J, L, and Eqs. (2.25a), (4.31), and the inner-product definition (3.15) we get

$$\Phi^{(1)+} = J^{-1}\Phi^{(1)}J. \tag{4.33}$$

From (4.28) and (4.32) we find that

$$\begin{aligned} [I_l^{(1)},I_{l'}^{(1)}] &= \langle \gamma_l^{(1)}, J\gamma_{l'}^{(1)} \rangle = -\langle J\gamma_l^{(1)}, \gamma_{l'}^{(1)} \rangle \\ &= -\langle L\gamma_{l-1}^{(1)}, \gamma_{l'}^{(1)} \rangle = \langle \gamma_{l-1}^{(1)}, L\gamma_{l'}^{(1)} \rangle \\ &= \langle \gamma_{l-1}^{(1)}, J\gamma_{l'+1}^{(1)} \rangle = \cdots \\ &= \langle \gamma_{(l'-l)/2}^{(1)}, J\gamma_{(l'-l)/2}^{(1)} \rangle, \qquad \text{(4.43a)} \\ &\quad \text{if } l'-l \text{ is even} \\ &= \langle \gamma_{(l'+l-1)/2}^{(1)}, L\gamma_{(l'+l-1)/2}^{(1)} \rangle, \qquad \text{(4.43b)} \\ &\quad \text{if } l'-l \text{ is odd.} \end{aligned}$$

Since both L and J are skew symmetric we conclude that $[I_l^{(1)},I_{l'}^{(1)}] = 0$. Similarly, we can easily prove that $[I_l^{(0)},I_{l'}^{(0)}] = 0$. Thus we have an infinite number of LB symmetries and constants of motion which are in involution for the first-order perturbed evolution equation as well, and therefore it is completely integrable in this sense.

2. Arbitrary order of perturbation

As a generalization of the above results to all orders of perturbation, Eq. (4.5), it is possible to extend the results and to find an infinite number of LB symmetries and constants of motion straightaway using the various definitions (2.3)–(2.29) we have discussed in Sec. II.

Considering the arbitrary nth perturbed evolution equation, we note that as a generalization of the strong symmetry $\Phi^{(1)}$ in (4.28) we have an $(n+1)\times(n+1)$ matrix operator-valued function $\Phi^{(n)}$ such that it generates new symmetries from the known ones satisfying the relation

$$\eta_{l+1} = \Phi^{(n)}\eta_l, \quad l = 1,2,\ldots,\infty, \tag{4.44}$$

where now

$$\eta_l(u) = (\eta_l^{(0)}(u),\eta_l^{(1)}(u),\ldots,\eta_l^{(n)}(u)),$$

and

$$\Phi^{(n)} = \begin{bmatrix} \Phi^{(0)}(u^{(0)}) & 0 & 0 & \cdots & 0 \\ \Phi^{(0)\prime}(u^{(1)}) & \Phi^{(0)}(u^{(0)}) & 0 & \cdots & 0 \\ \Phi^{(0)\prime}(u^{(2)}) & \Phi^{(0)\prime}(u^{(1)}) & \Phi^{(0)}(u^{(0)}) & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \Phi^{(0)\prime}(u^{(n)}) & \cdot & \cdot & \cdots & \Phi^{(0)}(u^{(0)}) \end{bmatrix}. \tag{4.45}$$

We can easily see that Eq. (4.45) is a particular case of Eq. (3.18). Now, using relation (2.27) we can find the conserved covariants in such a way

$$\gamma_{l+1} = \Phi^{(n)+}\gamma_l, \quad l = 1,2,3,\ldots,\infty, \tag{4.46}$$

$$\gamma_l(u) = (\gamma_l^{(0)}(u),\gamma_l^{(1)}(u),\ldots,\gamma_l^{(n)}(u)), \tag{4.47}$$

and $\Phi^{(n)+}$ can be obtained from the relation

$$J\Phi^{(n)+} = \Phi^{(n)}J, \tag{4.48}$$

where the $(n+1)\times(n+1)$ matrix is

$$J = \begin{bmatrix} D & 0 & 0 & \cdots & 0 \\ 0 & D & 0 & \cdots & 0 \\ 0 & 0 & D & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ 0 & 0 & 0 & \cdots & D \end{bmatrix}. \tag{4.49}$$

From these conserved covariants we can find the corre-

sponding constants of motion by using the relation grad $I_l = \gamma_l$ [see Eq. (2.21)]. Thus we can establish that an infinite number of vector-valued LB symmetries exist and that the corresponding constants of motion are in involution for any order of perturbation as well; thereby establishing the complete integrability.

B. Potential modified KdV equation (PmKdV)

We consider the potential modified KdV equation in the form

$$U_t = -U_3 - U_1^3/2. \tag{4.50}$$

The Hamiltonian for this equation is

$$\mathscr{H} = \int_{-\infty}^{\infty} \left\{ -\frac{U_2^2}{2} + \frac{U_1^4}{8} \right\} dx, \tag{4.51}$$

and the corresponding symplectic operator J_1 [in Eq. (3.3)] is given as $J_1 = \partial_x^{-1} = D^{-1}$. Substituting the perturbation expansion (4.4) in (4.50) and collecting the coefficients of ϵ^i, getting each of them individually equal to zero, the resulting ith-order perturbed PmKdV (perturbation around the solution of the PmKdV) equation is of the form

$$u_t^{(i)} + u_3^{(i)} + \frac{1}{2} \sum_{\substack{0<j,k<i,\\ i>(j+k)}} u_1^{(k)} u_1^{(j)} u_1^{(i-j-k)} = 0,$$
$$i = 0,1,2,\ldots,n. \tag{4.52}$$

Equation (4.52) may also be obtained by using Eqs. (3.6), (3.12), and (4.51). The unperturbed (soliton) solution $u^{(0)}$ satisfies the PmKdV equation

$$u_t^{(0)} = -u_3^{(0)} - u_1^{(0)^3}/2. \tag{4.53}$$

The action of the LB operator (2.4a) on (4.52) gives rise to the following LB invariant equation:

$$D_t \eta^{(i)} + D^3 \eta^{(i)} + \frac{1}{2} \left[\sum_{\substack{0<j,k<i\\ i>(j+k)}} (u_1^{(k)} u_1^{(j)} D\eta^{(i-j-k)} + 2u_1^{(k)} u_1^{(i-j-k)} D\eta^{(j)}) \right] = 0,$$
$$i = 0,1,2,\ldots,n. \tag{4.54}$$

The LB invariant equation for (4.53) can be written in the form [$i = 0$ in (4.54)]

$$D_t \eta^{(0)} + D^3 \eta^{(0)} + \tfrac{3}{2} u_1^{(0)^2} D\eta^{(0)} = 0. \tag{4.55}$$

We can solve this invariant equation as outlined in the previous example. We have the following first three LB symmetries[11]:

$$\eta_1^{(0)} = u_1^{(0)}, \tag{4.56a}$$
$$\eta_2^{(0)} = u_3^{(0)} + u_1^{(0)^3}/2, \tag{4.56b}$$
$$\eta_3^{(0)} = u_5^{(0)} + \tfrac{5}{2} u_1^{(0)^2} u_3^{(0)} + \tfrac{5}{2} u_1^{(0)} u_2^{(0)^2} + \tfrac{3}{8} u_1^{(0)^5}. \tag{4.56c}$$

From this sequence of LB symmetries we can generate infinitely many further symmetries by the strong symmetry[11]

$$\Phi \equiv \Phi^{(0)} = D^2 + u_1^{(0)^2} - u_1^{(0)} D^{-1}(u_2^{(0)}), \tag{4.57}$$

which satisfies condition (2.15) and (4.44) [with $n = 0$ in (4.44)]. In addition, the operator $\Phi^{(0)}$ is hereditary by condition (2.16).

The first-order perturbation PmKdV takes the form

$$u_t^{(1)} = \{ -u_3^{(1)} - \tfrac{3}{2} u_1^{(0)^2} u_1^{(1)} \}. \tag{4.58}$$

Then the corresponding LB invariant equation is in the form [$i = 1$ in Eq. (4.54)]

$$D_t \eta^{(1)} + D^3 \eta^{(1)} + 3u_1^{(0)} u_1^{(1)} D\eta^{(0)} + \tfrac{3}{2} u_1^{(0)^2} D\eta^{(1)} = 0. \tag{4.59}$$

To find the generalized symmetry $\eta^{(1)}$ of (4.59) we have followed the same procedure as in the case of solving the invariant equation (4.13). We have obtained the following first three LB symmetries of (4.58):

$$\eta_1^{(1)} = u_1^{(1)}, \tag{4.60a}$$
$$\eta_2^{(1)} = u_3^{(1)} + \tfrac{3}{2} (u_1^{(0)})^2 u_1^{(1)}, \tag{4.60b}$$
$$\eta_3^{(1)} = u_5^{(1)} + 5u_1^{(0)} u_3^{(0)} u_1^{(1)} + \tfrac{5}{2} u_1^{(0)2} u_3^{(1)} + \tfrac{5}{2} u_2^{(0)^2} u_1^{(1)} + 5u_1^{(0)} u_2^{(0)} u_2^{(1)} + \tfrac{15}{8} u_1^{(0)^4} u_1^{(1)}. \tag{4.60c}$$

From the sets of LB symmetries in (4.56) and (4.60) we can easily construct the operator

$$\Phi^{(1)} = \begin{bmatrix} \Phi^{(0)}(u^{(0)}) & 0 \\ \Phi^{(0)\prime}(u^{(1)}) & \Phi^{(0)}(u^{(0)}) \end{bmatrix} = \begin{bmatrix} D^2 + u_1^{(0)^2} - u_1^{(0)} D^{-1}(u_2^{(0)}) & 0 \\ 2u_1^{(0)} u_1^{(1)} - u_1^{(1)} D^{-1}(u_2^{(0)}) - u_1^{(0)} D^{-1}(u_2^{(1)}) & D^2 + u_1^{(0)^2} - u_1^{(0)} D^{-1}(u_2^{(0)}) \end{bmatrix}, \tag{4.61}$$

satisfying conditions (2.15) and (2.16) [for $n = 1$ in Eq. (3.16)]. Hence $\Phi^{(1)}$ is strong as well as a hereditary symmetry operator. Thus we conclude that infinitely many commuting LB symmetries exist for the first-order perturbed PmKdV equation (4.58) [in conjunction with Eq. (4.53)].

As before, from the infinitely many commuting LB symmetries we can generate the corresponding constants of motion. For this purpose we use the relation

$$J\Phi^{(1)+} = \Phi^{(1)} J = L, \tag{4.62}$$

where now

$$J = \begin{pmatrix} D^{-1} & 0 \\ 0 & D^{-1} \end{pmatrix}, \tag{4.63}$$

and $\Phi^{(1)}$ is as given in (4.61). By using the relations (4.35), (4.62), and (4.63), we can derive the first few conserved covariants as

$$\gamma_1^{(0)} = -u_2^{(0)}, \quad \gamma_2^{(0)} = -u_4^{(0)} - \tfrac{3}{2} u_1^{(0)^2} u_2^{(0)}, \tag{4.64}$$
$$\gamma_3^{(0)} = -u_6^{(0)} - 10u_1^{(0)} u_2^{(0)} u_3^{(0)} - \tfrac{5}{2} u_1^{(0)^2} u_4^{(0)} - \tfrac{5}{2} u_2^{(0)^3} - \tfrac{15}{8} u_1^{(0)^4} u_2^{(0)}, \tag{4.65}$$

and

$$\gamma_1^{(1)} = -u_2^{(1)},$$

$$\gamma_2^{(1)} = -u_4^{(1)} - 3u_1^{(0)}u_2^{(0)}u_1^{(1)} - \tfrac{3}{2}u_1^{(0)^2}u_2^{(1)}, \tag{4.66}$$

$$\begin{aligned}\gamma_3^{(1)} = &-u_6^{(1)} - \tfrac{15}{2}u_1^{(0)^3}u_2^{(0)}u_1^{(1)} - 10u_3^{(1)}u_1^{(0)}u_2^{(0)} \\ &- \tfrac{15}{8}u_1^{(0)^4}u_2^{(1)} - \tfrac{5}{2}u_4^{(1)}u_1^{(0)^2} - \tfrac{15}{2}u_2^{(1)}u_2^{(0)^2} \\ &- 10u_2^{(1)}u_1^{(0)}u_3^{(0)} - 10u_1^{(1)}u_2^{(0)}u_3^{(0)} \\ &- 5u_1^{(1)}u_4^{(0)}u_1^{(0)}.\end{aligned} \tag{4.67}$$

Now, again using the conserved covariants in the sets (4.64)–(4.67) and by Eq. (2.21) we can derive the associated involutive constants of motion explicitly as in Ref. 20. Finally, the generalization of this theory to any order of perturbed evolution equation is analogous to the previous example and so we do not present the details here.

C. Sine–Gordon equation (sG)

We consider the sG equation in the form

$$U_t = D^{-1}\sin U. \tag{4.68}$$

The associated Hamiltonian is

$$\mathscr{H} = \int_{-\infty}^{\infty}(1-\cos U)dx, \tag{4.69}$$

and the symplectic operator J_1 in (3.3) is given by $J_1 = D^{-1}$. The zeroth- and first-order perturbed sG equations are

$$u_t^{(0)} = D^{-1}\sin u^{(0)}, \tag{4.70}$$

$$u_t^{(1)} = D^{-1}[u^{(1)}\cos u^{(0)}], \tag{4.71}$$

respectively. Recently Kaliappan and Lakshmanan[25] have pointed out that the PmKdV and sG equations possess the same set of infinitely many local LB symmetries. The LB invariant equation for (4.70) is

$$D_tD_x\eta^{(0)} - \eta^{(0)}\cos u^{(0)} = 0. \tag{4.72}$$

Solving this recursively as outlined before we have the following first three LB symmetries[10]:

$$\eta_1^{(0)} = u_1^{(0)}, \tag{4.73a}$$

$$\eta_2^{(0)} = u_3^{(0)} + \tfrac{1}{2}u_1^{(0)^3}, \tag{4.73b}$$

$$\eta_3^{(0)} = u_5^{(0)} + \tfrac{5}{2}u_1^{(0)^2}u_3^{(0)} + \tfrac{5}{2}u_1^{(0)}u_2^{(0)^2} + \tfrac{3}{8}u_1^{(0)^5}, \tag{4.73c}$$

etc. And the strong and hereditary symmetry for (4.70) is given by[10]

$$\Phi \equiv \Phi^{(0)} = D + u_1^{(0)^2} - u_1^{(0)}D^{-1}(u_2^{(0)}). \tag{4.74}$$

We can see that Eqs. (4.73) and (4.74) are identical with Eqs. (4.56) and (4.57). From this fact it is clear that for any order of perturbation, the corresponding LB symmetries of PmKdV and sG are equal.

Furthermore, we can derive the constants of motion for the sG equation using the constants of motion of PmKdV (4.66) itself. This can be done explicitly in the following way.[20] The sine–Gordon equation is symmetric in the variables x and t. This property leads to the conclusion that for each sine–Gordon conservation law

$$\partial_t T + \partial_x X = 0,$$

there is a corresponding conservation law

$$\partial_t T' + \partial_x X' = 0,$$

where the prime denotes interchanging the x and t derivatives and then elimination of the t derivatives using the equation of motion (4.68). For example,

$$\partial_t(u_1^2/2) = u_1u_{1t} = u_1\sin u = \partial_x(1-\cos u), \quad U = u,$$

$$\partial_t(1-\cos u) = \sin u u_t = u_{xt}u_t = \partial_x(u_t^2/2).$$

Thus from the latter equation we arrive at the constant $I_{\mathrm{sG}} = \int_{-\infty}^{\infty}(1-\cos u)dx$ of the sG equation from the constant $I_{\mathrm{PmKdV}} = \int_{-\infty}^{\infty}(u_1^2/2)dx$. Similarly we can calculate other constants from the constants of PmKdV. Since this is also true for the perturbed sine–Gordon equation, we do not proceed with our analysis further for this case.

D. Nonlinear Schrödinger equation (NLS)

We consider the NLS equation in the form

$$U_t - i\{U_2 + 2U^2\bar{U}\} = 0, \tag{4.75}$$

where the bar denotes the complex conjugate, as well as the complex conjugate form of (4.75). Equation (4.75) can be written in the Hamiltonian form (3.2) as

$$\mathscr{H} = \int_{-\infty}^{\infty}\{\bar{U}_1U_1 - (U\bar{U})^2\}dx, \tag{4.76}$$

and the Poisson bracket is defined as

$$[F_i,F_j] = i\int_{-\infty}^{\infty}\left\{\frac{\delta F_i}{\delta\bar{U}}\frac{\delta F_j}{\delta U} - \frac{\delta F_i}{\delta U}\frac{\delta F_j}{\delta\bar{U}}\right\}dx. \tag{4.77}$$

If we substitute the perturbation (4.4) into (4.75) and collect the coefficients of ϵ^j, putting each of them individually equal to zero, then the perturbed equations are of the form

$$u_t^{(j)} - i\left\{u_2^{(j)} + 2\sum_{0<k,l<j}u^{(k)}\bar{u}^{(l)}u^{(j-k-l)}\right\} = 0,$$
$$j = 0,1,2,\ldots,n, \tag{4.78}$$

and the associated complex conjugate form. Hereafter we will omit the latter from further consideration for simplicity, as its treatment will be analogous to that of (4.78). The unperturbed (soliton) solution $u^{(0)}$ satisfies the equation

$$u_t^{(0)} - i\{u_2^{(0)} + 2(u^{(0)})^2\bar{u}^{(0)}\} = 0. \tag{4.79}$$

Before obtaining the LB invariant equations corresponding to the evolution equations (4.78), we generalize the definitions of total differentials and LB operators given in Eqs. (2.3) and (2.4) for complex valued functions:

$$\hat{D} \equiv \hat{D}_x = \sum_{j=0}^{n}\sum_{m=0}^{\infty}\left(u_{m+1}^{(j)}\frac{\partial}{\partial u_m^{(j)}} + \bar{u}_{m+1}^{(j)}\frac{\partial}{\partial\bar{u}_m^{(j)}}\right), \tag{4.80a}$$

$$\hat{D}_t = \sum_{j=0}^{n}\sum_{m=0}^{\infty}\left(u_{mt}^{(j)}\frac{\partial}{\partial u_m^{(j)}} + \bar{u}_{mt}^{(j)}\frac{\partial}{\partial\bar{u}_m^{(j)}}\right), \tag{4.80b}$$

and

$$\begin{aligned}X(\eta) = &\sum_{j=0}^{n}(\hat{D}_t\eta^{(j)})\frac{\partial}{\partial u_t^{(j)}} + \sum_{j=0}^{n}\sum_{m=0}^{\infty}(\hat{D}^m\eta^{(j)})\frac{\partial}{\partial u_m^{(j)}} \\ &+ \sum_{j=0}^{n}(\hat{D}_t\bar{\eta}^{(j)})\frac{\partial}{\partial\bar{u}_t^{(j)}} + \sum_{j=0}^{n}\sum_{m=0}^{\infty}(\hat{D}^m\bar{\eta}^{(j)})\frac{\partial}{\partial\bar{u}_m^{(j)}}.\end{aligned} \tag{4.81}$$

With these as our new definitions we can obtain the explicit

form of the invariant equations of (4.78) by using Eqs. (4.80), (4.81), and (2.5) as

$$\hat{D}_t\eta^{(j)} - i\left\{\hat{D}^2\eta^{(j)} + 2\sum_{\substack{0<k,l<j \\ k+l<j}}(u^{(k)}\bar{u}^{(l)}\eta^{(j-k-l)} + u^{(k)}u^{(j-k-l)}\bar{\eta}^{(l)} + \bar{u}^{(l)}u^{(j-k-l)}\eta^{(k)})\right\} = 0, \quad j = 0,1,2,\ldots,n. \tag{4.82}$$

Then the LB invariant equation for the unperturbed case ($j = 0$) is

$$\hat{D}_t\eta^{(0)} - i\{\hat{D}^2\eta^{(0)} + 4\bar{u}^{(0)}u^{(0)}\eta^{(0)} + 2u^{(0)2}\bar{\eta}^{(0)}\} = 0. \tag{4.83}$$

It is known[9] that Eq. (4.83) has infinitely many solutions, which in turn are the LB symmetries of (4.79). The first three of them are

$$\eta_1^{(0)} = u_1^{(0)}, \tag{4.84a}$$

$$\eta_2^{(0)} = +i(u_2^{(0)} + 2u^{(0)2}\bar{u}^{(0)}), \tag{4.84b}$$

$$\eta_3^{(0)} = -(u_3^{(0)} + 6u^{(0)}u_1^{(0)}\bar{u}^{(0)}). \tag{4.84c}$$

The strong and hereditary symmetry of (4.79) is[9] given by

$$\Phi \equiv \Phi^{(0)} = \hat{D} + 2u^{(0)}\hat{D}^{-1}\{\bar{u}^{(0)}(\cdot) - u^{(0)}(\bar{\cdot})\}. \tag{4.85}$$

Then $\Phi^{(0)}$ generates the sequence in (4.84) into infinitely many sequences in such a way that $\Phi^{(0)}$ satisfies the relation

$$\eta_{l+1}^{(0)} = \Phi^{(0)}(i\eta_l^{(0)}), \quad l = 1,2,\ldots,\infty. \tag{4.86}$$

By the hereditary property of the strong symmetry these symmetries are mutually commuting.

Next, we consider the first-order perturbation equation of (4.75) ($j = 1$) in Eq. (4.78). This reads

$$u_t^{(1)} - i\{u_2^{(1)} + 4u^{(1)}\bar{u}^{(0)}u^{(0)} + 2u^{(0)2}\bar{u}^{(1)}\} = 0. \tag{4.87}$$

The associated LB invariant equation for (4.87) can be obtained from (4.82) (for $j = 1$) as

$$\hat{D}_t\eta^{(1)} - i\{\hat{D}^2\eta^{(1)} + 4\bar{u}^{(0)}u^{(0)}\eta^{(1)} + 4\bar{u}^{(0)}u^{(1)}\eta^{(0)} + 4\bar{u}^{(1)}u^{(0)}\eta^{(0)} + 2u^{(0)^2}\bar{\eta}^{(1)} + 4u^{(0)}u^{(1)}\bar{\eta}^{(0)}\} = 0. \tag{4.88}$$

By solving this equation and its complex conjugate as outlined for (4.8) we have the first three LB symmetries

$$\eta_1^{(1)} = u_1^{(1)}, \tag{4.89a}$$

$$\eta_2^{(1)} = +i\{u_2^{(1)} + 4u^{(0)}\bar{u}^{(0)}u^{(1)} + 2u^{(0)^2}\bar{u}^{(1)}\}, \tag{4.89b}$$

$$\eta_3^{(1)} = -\{u_3^{(1)} + 6\bar{u}^{(0)}u_1^{(0)}u^{(1)} + 6u^{(0)}u_1^{(0)}\bar{u}^{(1)} + 6u^{(0)}\bar{u}^{(0)}u_1^{(1)}\}, \tag{4.89c}$$

and the complex conjugates. Using the LB symmetries in Eqs. (4.84) and (4.89) we are able to find the strong and hereditary symmetry operator

$$\Phi^{(1)} = \begin{bmatrix} \hat{D} + 2u^{(0)}\hat{D}^{-1}\{\bar{u}^{(0)}(\cdot) - u^{(0)}(\bar{\cdot})\} & 0 \\ 2u^{(1)}\hat{D}^{-1}\{\bar{u}^{(0)}(\cdot) - u^{(0)}(\bar{\cdot})\} + 2u^{(0)}\hat{D}^{-1}\{\bar{u}^{(1)}(\cdot) - u^{(1)}(\bar{\cdot})\} & \hat{D} + 2u^{(0)}\hat{D}^{-1} \times \{\bar{u}^{(0)}(\cdot) - u^{(0)}(\bar{\cdot})\} \end{bmatrix}, \tag{4.90}$$

satisfying Eqs. (2.15) and (2.16). Thus we have shown that infinitely many commuting LB symmetries exist for the first-order perturbed NLS equation (4.87) also (in conjunction) with (4.79). From the definitions (2.19)–(2.21) we define the constants of motion and conserved covariant of the first-order perturbed NLS as follows:

$$I_l^{(1)} = \int_{-\infty}^{\infty} \rho_l(x,u^{(0)},\bar{u}^{(0)},u^{(1)},\bar{u}^{(1)}, u_1^{(0)},\bar{u}_1^{(0)},u_1^{(1)},\bar{u}_1^{(1)},\ldots)dx, \tag{4.91}$$

and

$$(\gamma_l^{(1)},\bar{\gamma}_l^{(1)},\gamma_l^{(0)},\bar{\gamma}_l^{(0)}) = \left(\frac{\delta I_l^{(1)}}{\delta\bar{u}^{(0)}}, \frac{\delta I_l^{(1)}}{\delta u^{(0)}}, \frac{\delta I_l^{(1)}}{\delta\bar{u}^{(1)}}, \frac{\delta I_l^{(1)}}{\delta u^{(1)}}\right). \tag{4.92}$$

Using these relations in (2.25) and (2.27) along with the LB symmetries (4.84) and (4.89) we can find the corresponding conserved covariants with (2×2) diagonal matrix J having diagonal elements i. We list below the first few of them:

$$\gamma_1^{(0)} = -iu_1^{(0)}, \quad \gamma_2^{(0)} = (u_2^{(0)} + 2u^{(0)^2}\bar{u}^{(0)}), \tag{4.93}$$

$$\gamma_3^{(0)} = i(u_3^{(0)} + 6\bar{u}^{(0)}u^{(0)}u_1^{(0)}), \tag{4.94}$$

etc., and

$$\gamma_1^{(1)} = -iu_1^{(1)}, \tag{4.95}$$

$$\gamma_2^{(1)} = (u_2^{(1)} + 4u^{(0)}\bar{u}^{(0)}u^{(1)} + 2u^{(0)^2}\bar{u}^{(1)}),$$

$$\gamma_3^{(1)} = i(u_3^{(1)} + 6u_1^{(0)}\bar{u}^{(0)}u^{(1)} + 6u^{(0)}u_1^{(0)}\bar{u}^{(1)} + 6u^{(0)}\bar{u}^{(0)}u_1^{(1)}), \tag{4.96}$$

etc., and their complex conjugates. Furthermore, conserved covariants can be generated by using (2.27), (2.29), and(4.90). The associated infinitely many commuting constants of motion can then be obtained from (4.91)–(4.96) and thereby the complete integrability of the system can be proved.

Generalizing the above results straightforwardly it is possible to find the infinitely many LB symmetries and constants of motion for all orders of the perturbed NLS equation (4.82) also. Now the strong symmetry operator, as before, is an $(n+1)\times(n+1)$ matrix operator defined by (3.16) with $\Phi^{(0)}$ as given in (4.85). The recursive relations for LB symmetries and the conserved covariants are as in (3.14) and (3.17). But the conserved covariants γ_l now read as

$$\text{grad } I_l = \gamma_l = (\gamma_l^{(0)},\gamma_l^{(1)},\ldots,\gamma_l^{(n)}), \tag{4.97}$$

or

$$\text{grad } I_l = \left(\frac{\delta I_l^{(n)}}{\delta\bar{u}^{(n)}}, \frac{\delta I_l^{(n)}}{\delta\bar{u}^{(n-1)}}, \ldots, \frac{\delta I_l^{(n)}}{\delta\bar{u}^{(0)}}\right) \tag{4.98}$$

and its complex conjugate. In addition, we note that the operator J in (2.29) now takes the form

$$J = \text{diag}[i,i,\ldots,i]. \tag{4.99}$$

E. Derivative NLS equation (Kaup and Newell)[26]

We take the DNLS equation in the form

$$iU_t + U_2 + i(\bar{U}_1U^2) + 2i\bar{U}UU_1 = 0 \tag{4.100}$$

and its complex conjugate. This equation can be written in the Hamiltonian form (3.2), by choosing

$$\mathscr{H} = -i\int_{-\infty}^{\infty}\left(U\bar{U}_1 + \frac{i}{2}U^2\bar{U}^2\right)dx \tag{4.101}$$

and the symplectic operator J_1 as

$$J_1 = \partial_x = \hat{D}. \tag{4.102}$$

As in the previous examples, substituting the perturbation form (4.4) into the DNLS equation (4.100) and equating each coefficient of ϵ^j equal to zero, we have

$$iu_t^{(j)} + u_2^{(j)} + i\sum_{\substack{0<k,l<j\\ k+l>j}}(u^{(k)}u^{(l)}\bar{u}_1^{(j-k-l)} + 2iu^{(k)}u_1^{(l)}\bar{u}^{(j-k-l)}) = 0, \quad j = 0,1,2,\ldots,n. \tag{4.103}$$

In the above, $u^{(0)}$ then satisfies the DNLS equation

$$iu_t^{(0)} + u_2^{(0)} + i(\bar{u}_1^{(0)}u^{(0)^2}) + 2i\bar{u}^{(0)}u^{(0)}u_1^{(0)} = 0. \tag{4.104}$$

From the invariant condition (2.5) and using the definitions (4.80) and(4.81), we get the LB invariant equation corresponding to Eqs. (4.103) in the form

$$i\hat{D}_t\eta^{(j)} + \hat{D}^2\eta^{(j)} + i\sum_{0<k,l<j}(u^{(k)}u^{(l)}\hat{D}\bar{\eta}^{(j-k-l)} + 2u^{(k)}\bar{u}_1^{(j-k-l)}\eta^{(l)} + 2u_1^{(l)}\bar{u}^{(j-k-l)}\eta^{(k)} + 2u^{(k)}\bar{u}^{(j-k-l)}\hat{D}\eta^{(l)} + 2u^{(k)}u_1^{(l)}\bar{\eta}^{(j-k-l)}) = 0, \quad j = 0,1,2,\ldots,n. \tag{4.105}$$

For $j = 0$ in (4.105) we obtain the LB invariant equation for the unperturbed case, Eq. (4.104),

$$i\hat{D}_t\eta^{(0)} + \hat{D}^2\eta^{(0)} + 2iu^{(0)}\bar{u}^{(0)}\hat{D}\eta^{(0)} + 2i\eta^{(0)}\times(u_1^{(0)}\bar{u}^{(0)} + u^{(0)}\bar{u}_1^{(0)}) + iu^{(0)^2}\hat{D}\bar{\eta}^{(0)} + 2iu^{(0)}u_1^{(0)}\bar{\eta}^{(0)} = 0. \tag{4.106}$$

The first few LB symmetries[9] are

$$\eta_1^{(0)} = u_1^{(0)}, \tag{4.107a}$$

$$\eta_2^{(0)} = i(u_2^{(0)} + i\bar{u}_1^{(0)}u^{(0)^2} + 2iu^{(0)}\bar{u}^{(0)}u_1^{(0)}), \tag{4.107b}$$

$$\eta_3^{(0)} = -u_3^{(0)} - 3iu^{(0)}\bar{u}^{(0)}u_2^{(0)} - 3iu^{(0)}u_1^{(0)}\bar{u}_1^{(0)} + 3u^{(0)^3}\bar{u}^{(0)}\bar{u}_1^{(0)} - 3iu_1^{(0)^2}\bar{u}^{(0)} + \tfrac{9}{2}u^{(0)^2}\bar{u}^{(0)^2}u_1^{(0)}. \tag{4.107c}$$

The associated strong symmetry[9] satisfying (2.15), which generates the above sequence (4.107) into infinitely many sequences is given by

$$\Phi^{(0)} \equiv \hat{D}\,[i - u^{(0)}\hat{D}^{-1}\{\bar{u}^{(0)}(\cdot) + u^{(0)}(\bar{\cdot})\}], \tag{4.108}$$

which also satisfies the hereditary condition (2.16). Thus Eq. (4.104) has infinitely many commuting LB symmetries.

Next, we consider the first-order perturbed DNLS equation from (4.103) [for the value $j = 1$ in (4.103)]

$$iu_t^{(1)} + u_2^{(1)} + 2iu^{(0)}\bar{u}_1^{(0)}u^{(1)} + iu^{(0)^2}\bar{u}_1^{(1)} + 2iu^{(0)}\bar{u}^{(0)}u_1^{(1)} + 2iu^{(0)}u_1^{(0)}\bar{u}^{(1)} + 2iu_1^{(0)}\bar{u}^{(0)}u^{(1)} = 0. \tag{4.109}$$

The corresponding LB invariant equation can be obtained from (4.105) (for $j = 1$) as

$$i\hat{D}_t\eta^{(1)} + \hat{D}^2\eta^{(1)} + 2i(u^{(0)}u^{(1)}\hat{D}\bar{\eta}^{(0)} + u^{(0)}\bar{u}^{(1)}\hat{D}\eta^{(0)} + \bar{u}^{(0)}u^{(1)}\hat{D}\eta^{(0)} + \tfrac{1}{2}u^{(0)^2}\hat{D}\bar{\eta}^{(1)} + u^{(0)}\bar{u}^{(0)}\hat{D}\eta^{(1)} + \bar{u}^{(0)}u_1^{(1)}\eta^{(0)} + u^{(0)}\bar{u}_1^{(1)}\eta^{(0)} + u^{(0)}u_1^{(1)}\bar{\eta}^{(0)} + \bar{u}_1^{(0)}u^{(1)}\eta^{(0)} + u_1^{(0)}\bar{u}^{(1)}\eta^{(0)} + u_1^{(0)}u^{(1)}\bar{\eta}^{(0)} + \bar{u}^{(0)}u_1^{(0)}\eta^{(1)} + u^{(0)}\bar{u}_1^{(0)}\eta^{(1)} + u^{(0)}u_1^{(0)}\bar{\eta}^{(1)}) = 0. \tag{4.110}$$

Proceeding as in the previous cases, we get the first three LB symmetries as

$$\eta_1^{(1)} = u_1^{(1)}, \tag{4.111a}$$

$$\eta_2^{(1)} = iu_2^{(1)} - 2\bar{u}_1^{(0)}u^{(0)}u^{(1)} - u^{(0)^2}\bar{u}_1^{(1)} - 2\bar{u}^{(0)}u^{(0)}u_1^{(1)} - 2u_1^{(0)}u^{(0)}\bar{u}^{(1)} - 2\bar{u}^{(0)}u_1^{(0)}u^{(1)}, \tag{4.111b}$$

$$\eta_3^{(1)} = -u_3^{(1)} - 3i[u_1^{(0)^2}\bar{u}^{(1)} + 2\bar{u}^{(0)}u_1^{(0)}u_1^{(1)} + u^{(0)}u_2^{(0)}\bar{u}^{(1)} + u^{(0)}\bar{u}^{(0)}u_2^{(1)} + \bar{u}^{(0)}u_2^{(0)}u^{(1)} + u^{(0)}u_1^{(0)}\bar{u}_1^{(1)} + u_1^{(0)}\bar{u}_1^{(0)}u^{(1)} + u^{(0)}u_1^{(1)}\bar{u}_1^{(0)}] + \tfrac{9}{2}[u^{(0)^2}\bar{u}^{(0)^2}u_1^{(1)} + 2u^{(0)}\bar{u}^{(0)^2}u_1^{(0)}u^{(1)} + 2u^{(0)^2}\bar{u}^{(0)}u_1^{(0)}\bar{u}^{(1)}] + 3[u^{(0)^3}\bar{u}^{(0)}\bar{u}_1^{(1)} + u^{(0)^3}\bar{u}_1^{(0)}\bar{u}^{(1)} + 3u^{(0)^2}u_1^{(0)}\bar{u}^{(0)}\bar{u}^{(1)}]. \tag{4.111c}$$

Using the LB symmetries in (4.107) and (4.111) we can construct the operator $\Phi^{(1)}$ satisfying the relation (2.14)

$$\Phi^{(1)} = \begin{bmatrix} \hat{D}\,[i - u^{(0)}\hat{D}^{-1}\{\bar{u}^{(0)}(\cdot) + u^{(0)}(\bar{\cdot})\}] & 0 \\ -\hat{D}\,[u^{(1)}\hat{D}^{-1}\{\bar{u}^{(0)}(\cdot) + u^{(0)}(\cdot)\} + u^{(0)}\hat{D}^{-1}\{\bar{u}^{(1)}(\cdot) + u^{(1)}(\bar{\cdot})\}] & \hat{D}\,[i - u^{(0)}\hat{D}^{-1}\times\{\bar{u}^{(0)}(\cdot) + u^{(0)}(\cdot)\}] \end{bmatrix}. \tag{4.112}$$

It might be noted that the operator $\Phi^{(1)}$ satisfies [in conjunction with (4.104)] the appropriate conditions (2.15) and (2.16) and therefore it is the strong and hereditary symmetry of (4.109). Thus we have infinitely many commuting LB symmetries for the first-order perturbed DNLS equation (4.109).

The conserved covariants corresponding to the LB symmetries in (4.107) and (4.111) follow straightforwardly from the relation (2.25) with $J = \mathrm{diag}\,(\hat{D},\hat{D})$

$$\gamma_1^{(0)} = u^{(0)}, \tag{4.113a}$$

$$\gamma_2^{(0)} = i(u_1^{(0)} + (i/2)\bar{u}^{(0)}u^{(0)^2}), \tag{4.113b}$$

$$\gamma_3^{(0)} = -u_2^{(0)} - 3iu^{(0)}u_1^{(0)}\bar{u}^{(0)} + \tfrac{3}{2}u^{(0)^3}\bar{u}^{(0)^2}, \tag{4.113c}$$

etc., and

$$\gamma_1^{(1)} = u^{(1)}, \tag{4.114a}$$

$$\gamma_2^{(1)} = i(u_1^{(1)} + i\bar{u}^{(0)}u^{(0)}u^{(1)} + iu^{(0)^2}\bar{u}^{(1)}), \tag{4.114b}$$

$$\gamma_3^{(1)} = -u_2^{(1)} - 3i[\bar{u}^{(0)}u_1^{(0)}u^{(1)} + u^{(0)}u_1^{(0)}\bar{u}^{(1)} + u_1^{(1)}\bar{u}^{(0)}u^{(0)}] + \tfrac{9}{2}u^{(0)^2}\bar{u}^{(0)^2}u^{(1)} + 3u^{(0)^3}\bar{u}^{(0)}\bar{u}^{(1)}, \tag{4.114c}$$

etc., and their complex conjugates. As before, using Eqs. (4.42) and (4.43) with $J = \mathrm{diag}(\hat{D},\hat{D})$, we can obtain the constants of motion which are in involution. Thus infinitely many constants of motion and LB symmetries exist for the first-order perturbed DNLS equation (4.109) [in conjunction with (4.104)].

For any order of the perturbed DNLS equation (4.103), as before, we can find the strong symmetry operator, which is an $(n+1)\times(n+1)$ matrix operator-valued function which generates further new symmetries, and its adjoint which generates further new conserved covariants with the $(n+1)\times(n+1)$ skew-symmetric matrix operator $J = \mathrm{diag}[\hat{D},\hat{D},\ldots,\hat{D}]$. Finally, the corresponding commuting constants of motion can be obtained by using the relation (4.97). Hence we conclude that it is possible to find infinitely many LB symmetries and constants of motion for any order of perturbation of the DNLS equation.

V. CONCLUSIONS

In this paper we have developed an applicable technique for establishing the existence of infinitely many LB symmetries and constants of motion for coupled evolution equations. We have pointed out that there exists a one-to-one correspondence between LB symmetries and conserved covariants, where the symplectic operator J plays an important role. We have also shown that the conserved covariants can be obtained by considering the adjoint of the strong symmetry operator. We have presented important relations between the strong symmetry and its adjoint [see Eq. (2.29)] and further consequences have been discussed.

As examples, we considered the completely integrable systems under perturbation around their solutions. The Hamiltonian structure of these perturbed systems has been presented explicitly. Then we have shown the possible form of the strong and hereditary symmetry operator for any order of perturbation.

Finally, we have applied our technique to the specific examples of equations like the KdV, PmKdV, sG, NLS, and DNLS equations. We showed explicitly that infinitely many commuting LB symmetries and constants of motion exist for these completely integrable Hamiltonian systems under perturbation around their solution. Thus we conclude from the theory of LB symmetries that if the original system is a completely integrable Hamiltonian system, then the perturbed systems are also completely integrable.

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Theorem on linearized Hamiltonian systems

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Many nonlinear field equations can be written in Hamiltonian form. Thus the equation $\partial_t u = K(u)$ can be written $\partial_t u = [u, H]$, where H is an appropriate functional and $[\ ,\ ]$ is a Poisson bracket. Frequently one is interested in the solution of the equation linearized about a given solution, i.e., the equation $\partial_t \tau = K'(\tau)$, where $K'(\tau) = (d/d\epsilon) K(u + \epsilon\tau)|_{\epsilon=0}$. It is known that if a functional I is a constant of motion then $\tau = [u, I]$ is a solution. Recently, more general solutions of this form have been found. To prove these results, it is very useful to have the answer to the following question: If I_i, I_j are two functionals, and $K_i = [u, I_i]$, what is $K_i'(K_j)$? The answer is $K_i'(K_j) = [[u, I_i], I_j]$. Previously, this was proved assuming that canonical coordinates can be introduced. Here a proof is given without any such assumption.

I. INTRODUCTION

There is considerable current interest in Hamiltonian formulations of nonlinear evolution equations.[1] By this we mean systems of the form

$$\partial_t u = K(u) = [u, H]. \tag{1}$$

Here $u(x) \equiv (u_1(x), u_2(x), \ldots, u_n(x))$, $x \equiv (x_1, \ldots, x_m)$, H is a suitable functional, and $[\ ,\ ]$ is a Poisson bracket satisfying the antisymmetry and Jacobi conditions.

Frequently one is interested in the solution of Eq. (1) linearized around a particular solution,

$$\partial_t \tau = K'\tau, \tag{2}$$

where $K'\tau$ is the Gateaux derivative

$$K'\tau = \frac{d}{d\epsilon} K(u + \epsilon\tau)|_{\epsilon=0}. \tag{3}$$

It is known[2] that if $[H, I] = 0$, then $\tau = [u, I]$ is a solution of Eq. (2). More general solutions of the linearized equation have been found which are of this form but for which I is not a constant of motion. This leads us to the following question: Consider two functionals I_1, I_2 with "symmetries"[3,4] $K_i = [u, I_i]$, what is $K_1' K_2$? The answer is given by the following.

Theorem:

$$K_1' K_2 = [[u, I_1], I_2]. \tag{4}$$

Recently,[5] we have proved this assuming that canonical coordinates can be introduced. This certainly suffices for most (if not all) of the known completely integrable Hamiltonian systems. (Examples are the KdV equation, the sine–Gordon equation, and the nonlinear Schrödinger equation.)

Here we want to give two new proofs which do not invoke canonical coordinates. There are two reasons.

(a) It seems inelegant to invoke canonical coordinates.

(b) There are some Hamiltonian systems[1] for which it is not known if global canonical coordinates can be constructed.

The first new proof involves a particular assumption which may or may not be equivalent to the canonical coordinate assumption. The proof is, however, very perspicuous and particularly short.

The second new proof does not make any extra assumptions. It does require more technical details.

After giving the proofs some simple applications of the theorem are indicated.

II. SOME DEFINITIONS

All known Hamiltonian systems appear to be specializations of the following general form: We introduce a bilinear form $\langle v, w\rangle = \int (v, w) dx$. The Poisson bracket of two functionals $F_i[u]$, $F_j[u]$ is taken to be

$$[F_i, F_j] = \int \left(\frac{\delta F_i}{\delta u}, L_u \frac{\delta F_j}{\delta u}\right) dx. \tag{5}$$

Here L_u is to be antisymmetric so that

$$[F_i, F_j] = -[F_j, F_i] \tag{6}$$

and L_u is to be such that the Jacobi condition

$$[[F_i, F_j], F_k] + [[F_j, F_k], F_i] + [[F_k, F_i], F_j] = 0 \tag{7}$$

is satisfied.

(Note: If L is independent of u this is automatically fulfilled in virtue of the antisymmetry. The general condition on L_u is given in Ref. 3.) The functional derivatives are defined by

$$\frac{d}{d\epsilon} F[u + \epsilon\delta u]|_{\epsilon=0} = \int \left(\frac{\delta F}{\delta u(x)}, \delta u(x)\right) dx. \tag{8}$$

III. A SIMPLE PROOF

Assume L independent of u. (It seems likely that in this case we can always introduce canonical coordinates—by introducing the Fourier transform of u. However, we will make no use of this here.)

We have $K_1(u) = [u, I_1(u)]$. Since L is independent of u we have $K_1(u + \epsilon\tau) = [u + \epsilon\tau, I_1(u + \epsilon\tau)]$ and then

$$K_1'\tau = \frac{d}{d\epsilon} K_1(u + \epsilon\tau)|_{\tau=0}$$

$$= [\tau, I_1(u)] + \left[u, \int \left(\frac{\delta I_1}{\delta u}, \tau\right) dx'\right]. \tag{9}$$

If we choose $\tau = [u, I_2]$, then $\tau = L_u(\delta I_2/\delta u)$, and

$$K_1'[u, I_2] \equiv K_1' K_2 = [[u, I_2], I_1] + \left[u, \int \left(\frac{\delta I_1}{\delta u}, L_u \frac{\delta I_2}{\delta u}\right) dx\right].$$

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But from the definition of Eq. (5),

$$\int\left(\frac{\delta I_1}{\delta u}, L_u\frac{\delta I_2}{\delta u}\right)dx = [I_1, I_2],$$

$$\therefore K_1' K_2 = [[u, I_2], I_1] + [u, [I_1, I_2]]. \tag{10}$$

The Jacobi identity [Eq. (7)] then yields the theorem

$$K_1' K_2 = [[u, I_1], I_2]. \tag{4}$$

IV. THE GENERAL PROOF

Let L_u be arbitrary (except, of course, that antisymmetry and Jacobi be satisfied).

We directly compute the right-hand side of Eq. (4). To do this, we need $(\delta/\delta u(x'))[u(x), I_1]$. First $[u(x), I_1]$ is expressed as a functional by

$$[u(x), I_1] \equiv K_1(u(x)) = \int \delta(x - x') K_1(u(x'))dx'. \tag{11}$$

Then

$$\frac{d}{d\epsilon}K_1(u(x) + \epsilon\delta u(x)) = \int \delta(x - x') K_1' \delta u(x')dx' \tag{12}$$

$$= \int (\tilde{K}_1' \delta(x - x'), \delta u(x'))dx' \tag{13}$$

(where $\tilde{}$ denotes adjoint).

From the definition of Eq. (8) it is then seen that

$$(\delta/\delta u(x'))[u(x), I_1] = \tilde{K}_1' \delta(x - x') \tag{14}$$

$$\therefore [[u, I_1], I_2] = \int\left(\tilde{K}_1' \delta(x - x'), L_u\frac{\delta I_2}{\delta u'}\right)dx'$$

$$= \int\left((\delta(x - x')), K_1' L_u\frac{\delta I_2}{\delta u}\right)dx'$$

$$= K_1' L_u(\delta I_2/\delta u) \equiv K_1' K_2. \tag{15}$$

V. SIMPLE APPLICATIONS

(1) Suppose $I_1 = H$, and $[H, I_2] = 0$. From Eq. (10) we read

$$K_1' [u, I_2] = [[u, I_2], H], \tag{16}$$

but $[[u, I_2], H] \equiv \partial_t [u, I_2]$. We conclude that $\tau = [u, I_2]$ satisfies Eq. (2) (the known result).

(2) What is the relation between $K_1' [u, I_2]$ and $K_2' [u, I_1]$? We have

$$K_1' [u, I_2] = [[u, I_1], I_2], \tag{17}$$

and similarly

$$K_2' [u, I_1] = [[u, I_2], I_1]. \tag{18}$$

Substracting and using the Jacobi identity yields

$$K_1' [u, I_2] - K_2' [u, I_1] = [u, [I_1, I_2]]. \tag{19}$$

(a) If $[I_1, I_2] = 0$ we see

$$K_1' [u, I_2] = K_2' [u, I_1]. \tag{20}$$

(b) In Refs. 3 and 4, Lie algebras of symmetries are introduced using as Lie product

$$\{K_i K_j\} = K_i' K_j - K_j' K_i. \tag{21}$$

From Eq. (19) it is seen that

$$\{K_i K_j\} = [u, [I_i, I_j]]. \tag{22}$$

Thus this Lie algebra is isomorphic to the algebra of the associated functionals with the Poisson bracket as the Lie product.

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Exact solution for the spatially inhomogeneous nonlinear Kac model of the Boltzmann equation

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We study the spatially inhomogeneous Kac model of the nonlinear Boltzmann equation in $1+1+1$ dimensions (velocity v, time t, position x). We obtain an exact solution which is the product of a Maxwellian with a time-dependent width by a second-order polynomial in the velocity variable. The solution satisfies a specular reflection condition at the boundary $x = x_0$. The position $x_0 - x$ appears linearly and only in the odd part of the velocity distribution, the range of $x_0 - x$ being arbitrarily large but finite in order to maintain the positivity of the distribution. The local density is spatially homogeneous. Further, a particular linear relation between the moments of the cross section must be satisfied. The most general Maxwellian width has two relaxation times and their ratio is a function of the moments of the cross sections. Depending on whether this ratio is larger than or smaller than 1 we find contraction or expansion. The solution relaxes towards a Maxwellian equilibrium solution. Studying the Tjon overpopulation effect of high velocity particles, we find that it depends weakly on the initial condition, and strongly on both the microscopic model of cross section and on the ratio of the two relaxation times. We give a simple criterion (linked to the distinction between contraction and expansion) for the existence of the effect. Theoretically and numerically we test its validity and its failure.

I. INTRODUCTION

It is a common belief that the discovery of exact solutions can help towards a better understanding of the Boltzmann equation.

For the homogeneous distributions, with Maxwell interaction, first Bobylev,[1] then Krook and Wu[2] have found an exact solution (hereafter called the BKW even velocity mode) relaxing towards a Maxwellian equilibrium solution. Previously Nikol'skii[3] had defined a transformation generating exact inhomogeneous solutions from homogeneous ones. Applying this method to the BKW even mode, first Bobylev[1] and then Tenti and Hui[4] have discussed the associate inhomogeneous solution. Unfortunately this solution is going to zero when the time increases up to infinity. In fact, in the homogeneous case with Maxwell interaction, there exists an infinite number of closed solutions[3–5] (only the BKW even mode satisfies the physical requirements of homogeneous distributions), for which one can apply the Nikol'skii transform. Unfortunately, for Maxwell interactions, the inhomogeneous solutions constructed with the Nikol'skii method cannot relax towards a Maxwellian equilibrium state.[3,4] A first question arises: *Is there any exact inhomogeneous solution relaxing towards a Maxwellian?*

Another useful property of these exact solutions is that one can easily study the Tjon[6] overpopulation effect of high velocity particles. In the homogeneous Maxwell interaction case, with even velocity distribution alone, Hauge and Praestgaard[7] have defined a criterion explaining that the existence of the effect depends uniquely on the initial distributions. *For more general distributions* (inhomogeneous and including odd velocity parts) *is it always true that the effect depends only on the initial distributions?*

In order to answer partially these questions we investigate the simplest model: the Kac[8] model which, due to its simplicity, must be considered more as a mathematical frame than a physical one.

The Kac model in $1+1+1$ dimensions depends on the three variables v,t,x (velocity v, time t, position x), and the distribution function, when no external force is present, satisfies the equation

$$(\partial_t + v\,\partial_x) f(v) = \nu \int_{-\pi}^{+\pi} \sigma(\theta) \int_{-\infty}^{+\infty} (f(v')f(w') - f(v)(w))\,dw\,d\theta, \tag{1.1}$$

$$v' = v\cos\theta - w\sin\theta, \quad w' = v\sin\theta + w\cos\theta,$$

$$\sigma(\theta) = \sigma(-\theta),$$

where $f(v)$ means $f(v,t,x)$, $\sigma(\theta)$ is the scattering cross section, and ν is a constant. When the gradient term $v\,\partial_x$ is absent, $f = f(v,t)$ is the spatially homogeneous solution. Ernst[9] recognizes that the even velocity part f^+ of $f = f^+ + f^-$ ($f^\pm$ even and odd in v) has a BKW even mode solution, but he associates trivial odd parts f^- to form complete closed solutions. In fact there exists[10] a nontrivial odd $f^-(v,t)$ closed solution, partner to the BKW even mode, and also a whole class of nontrivial and nonexplicit $f^-(v,t)$ associated odd solutions.

On the other hand, while the BKW even mode alone forbids the existence of the Tjon effect, the addition of nontrivial odd parts $f^-(v,t)$ gives the possibility to recover the effect (with or without a force term present[10]). We find out that the effect depends on both the microscopic $\sigma(\theta)$ model and the initial condition $f(v,0)$.

The aim of this paper is to try to obtain, in the inhomogeneous case, an explicit solution $f(v,x,t)$ and to study the possible associated Tjon effect. We require that f relaxes towards the Maxwellian distribution $\exp(-v^2/2)$ when $t \to \infty$ and define a reduced distribution function

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$F(v,t,x) = f(v,t,x)/f(v,\infty,x)$. Our main result is that there exists such a solution:

$$F = e^{-(v^2/2)(\Delta^{-1}-1)}\Delta^{-3/2}\left[\left(\frac{1-y}{1+y}\right)\Delta + \frac{y}{2\lambda}\partial_y\Delta + v2C_2\frac{(x_0-x)\,y}{(1+y)^2} - \frac{v^2}{2}y\,\partial_y \log\Delta\right], \tag{1.2a}$$

$$y = C_1 e^{-C_2 t}, \quad \Delta = \Delta(y),$$

with C_1, C_2 arbitrary constants, $C_2 > 0$, the moments $\tau_m = \int_{-\pi}^{+\pi}\sigma(\theta)(\cos\theta)^m\,d\sigma$, $\sigma_{2n} = \int_{-\pi}^{\pi}\sigma(\theta)(\cos\theta\sin\theta)^{2n} \times d\theta > 0$ of $\sigma(\theta)$ being such that they satisfy the relations

$$\sigma_2 - \tau_1 + \tau_3 = 0, \quad \lambda(\tau_0 - \tau_1) = \sigma_2, \quad \lambda \in]0,2[,$$
$$C_2 = \nu(\tau_0 - \tau_1), \tag{1.2b}$$

and the time-dependent Maxwellian width $\Delta^{-1}(y)$ satisfies a second-order linear differential equation

$$(4\lambda + (1+y)(\lambda - 1 - y(\lambda+1))\partial_y - y(1+y)^2\partial_{y^2}^2)\Delta(y) = 0. \tag{1.2c}$$

We require $\Delta(y) \underset{y\to 0}{\longrightarrow} 1$ in order that $F \underset{t\to\infty}{\longrightarrow} 1$ (or f relaxes towards a Maxwellian). In the one spatial dimensional Kac model we have the energy conservation $v^2 + w^2 = v'^2 + w'^2$ but not the momentum conservation $v + w \neq v' + w'$. It is interesting for the solution (1.2) to discuss the hydrodynamical equations $(\partial N_i/\partial t) + \operatorname{div} J_i = 0$, $N_i = \int f v^i\,dv$, $J_i = \int f v^{i+1}\,dv$, $n = 0$ and 2. The local density $N_0 = (1-y)/(1+y) = N_0(t)$ being independent of x, is uniform in the space while the current J_0 is linear in x. For the solution (1.2) we find $\partial_t N_0 = y(2C_2)/(1+y)^2$ having the same sign as y or C_1, and we have contraction or dilatation depending on whether y is positive or negative. Similar properties hold both for $N_2(t)$ such that $\partial_t N_2 = 3\Delta\,\partial_t N_0$ and for J_2.

In Sec. II, from (1.1) we deduce the exact solution (1.2). Let us put $d = (x_0 - x)c_2$ fixed, the solution can be written $F(v,t,x) = F^+(v,t) + dF^-(v,t)$ with $F^+(F^-)$ even (odd) velocity functions. From transformations of both the relative position $x_0 - x$ and time t variables, we obtain invariance properties for the solutions F.

Let us define x_0', x', $c_2' > 0, t'$, keep C_1 (in y) and d fixed, then with an obvious notation for F we find

$$d = c_2(x_0 - x) = c_2'(x_0' - x'),$$
$$c_2 t = c_2' t', \quad (x_0 - x)(x_0' - x') > 0, \tag{1.3a}$$
$$F(v,t,x;x_0 - x, c_2; c_1, d) = F(v,t,x;x_0' - x', c_2'; c_1, d);$$
$$d = c_2(x_0 - x) = -c_2'(x_0' - x'),$$
$$c_2 t = c_2' t', \quad (x_0 - x)(x_0' - x') < 0, \tag{1.3b}$$
$$F(v,t,x;x_0 - x, c_2; c_1, d) = F(-v,t,x;x_0' - x', c_2'; c_1, d).$$

This means that it is sufficient to study F for a chosen finite interval $x_0 - x$ and, using the scaling properties (1.3a) and (1.3b), obtain results for arbitrarily large but finite other intervals $x_0' - x'$. Of course, due to the positivity constraint $F > 0$, these intervals cannot go up to $\pm\infty$. We remark that the specular reflection condition $F^-(v,t,x_0) = 0$ is satisfied at the boundary $x = x_0$ and $F(v,t,x_0) = F(-v,t,x_0)$. We notice also that the F solutions for $(x_0 - x, v)$ and $(x - x_0, -v)$ are the same. Using all these invariances we can study the solutions for $x \gtrless x_0$ and deduce the corresponding ones for $x \lesseqgtr x_0$.

In Sec. II we also check that (1.2) is a solution of the Laguerre moments system associated with (1.1). At the end we construct $\sigma(\theta)$ models which satisfy the linear moment relations (1.2b).

In Sec. III we determine the time-dependent Maxwellian width $\Delta(y)$, solutions of (1.2c), and study the positivity property of F. Here, $\sigma(\theta) > 0$ requires $\lambda \in]0,2[$ and first we study $\lambda \neq 1$, where the general solution has no $\log y$ term. If we adopt the language of potential theory, the most general solution is $\Delta = \Delta_s + C_3\Delta_R$, where $\Delta_s = 1 + \Sigma a_n y^n$ and $\Delta_R = |y|^{-1}(1 + \Sigma d_n y^n)$, $|y| < 1$ are the two independent "singular" and "regular" solutions of (1.2c) when $y \to 0$. For $C_3 = 0$, we find that the positivity of F at $t = 0$ requires $\lambda < 1$ in the expansion case ($y < 0$ or $C_1 < 0$) and $\lambda > 1$ in the contraction case ($y > 0$ or $C_1 > 0$). If we add a Δ_R component, then C_3 is restricted by the condition $F > 0$ at $t = 0$. For the positivity of F at $t \neq 0$, we show in the contraction case ($y > 0$), that it is sufficient to have $F > 0$ at $t = 0$, whereas in the expansion case ($y < 0$) the positivity is violated if $C_3 > 0$. For $\lambda = 1$, where a $\log y$ term is present, a similar study can be done.

In Sec. IV, for all these different Maxwellian widths Δ, in order to study the Tjon effect, we seek the asymptotic behaviors when $t \to \infty$ (or $y \to 0$) of the reduced distribution $F(v,t,x)$ and investigate both the sign and the size of $F - 1$. If the $F - 1 > 0$ values are appreciable then we conclude that the Tjon effect exists.

First, we study the simplest case $\Delta \equiv \Delta_s$ having *only one relaxation time* $c_2^{-1} = T_s$ and establish a criterion

$$\text{crit.} = \tau_0 - \tau_1 - \sigma_2 \tag{1.4}$$

saying that $F - 1 > 0$ if crit. > 0 (or $\lambda < 1$) and $F - 1 < 0$ if crit. < 0 (or $\lambda > 1$). On the other hand, for $\lambda < 1$, the $F - 1 > 0$ values decrease when λ increases. Combining these two results, we find appreciable Tjon effect in the contraction case for $\lambda < \frac{3}{4}$.

Second, we introduce Δ_R, and for the general $\Delta = \Delta_s + C_3\Delta_R$, $\Delta - 1$ has two different relaxation times: $T_s = c_2$ coming from $\Delta_s - 1$ and $T_R = (\lambda c_2)^{-1}$ coming from Δ_R. In the expansion case $\lambda > 1$ we still have no effect while in the contraction $\lambda < 1$, the effect disappears for important $C_3 < 0$ contributions. The effect depends weakly on the initial distributions but strongly on $\sigma(\theta)$ and on the existence of two relaxation times.

Third, we compare the exact solution with the one obtained from the linearized formalism.

II. DETERMINATION OF AN EXACT INHOMOGENEOUS SOLUTION

Different methods can be used for the search of closed solutions. We can either try the direct substitution of an appropriate ansatz into (1.1) or investigate the differential system for the Laguerre moments of $f(v,t,x)$. Writing f as a sum of even and odd velocity parts $f = f^+(v,t,x) + f^-(v,t,x)$, Eq. (1.1) becomes

$$\partial_t f^+ + v\,\partial_x f^- = \int_{-\pi}^{+\pi} d\theta\,\sigma(\theta)\int_{-\infty}^{+\infty} dw(f^+(w')f^+(v') - f^+(v)f^+(w)), \tag{2.1a}$$

$$\partial_t f^- + v\,\partial_x f^+ = \int_{-\pi}^{+\pi} d\theta\,\sigma(\theta)\int_{-\infty}^{+\infty} dw(f^+(w')f^-(v') - f^+(w)f^-(v)). \tag{2.1b}$$

We start with an ansatz solution product of a Maxwellian, with $b(x,t)$ width, by an arbitrary polynomial

$$\sqrt{2\pi}f^+ = e^{-b(t,x)v^2/2}\sum_0^{n_+}\alpha_{2n}(t,x)\left(\frac{v}{\sqrt{2}}\right)^{2n},$$
$$\sqrt{2\pi}f^- = e^{-bv^2/2}\sum_0^{n_-}\alpha_{2n+1}(t,x)\left(\frac{v}{\sqrt{2}}\right)^{2n+1}. \tag{2.2}$$

A. Restrictions on both the polynomials and the width of Eq. (2.2)

We substitute (2.2) into (2.1a) and (2.1b) and integrate over w,θ. Then (2.1a) and (2.1b) become, respectively, an even and odd v polynomial. The coefficients of the polynomials depend on both $b,\alpha_{2n},\alpha_{2n+1}$, and their derivatives, and on the moments

$$\tau_m = \int_{-\pi}^{+\pi}\sigma(\theta)\cos\theta^m\,d\theta,$$
$$\sigma_{2n} = \int_{-\pi}^{+\pi}\sigma(\theta)(\cos\theta\sin\theta)^{2n}\,d\theta > 0$$

of the cross section $\sigma(\theta)$. The coefficient of the highest v power v^{2n_+} is proportional to $\alpha_{2n}^2\sigma_{2n} > 0$ on the rhs of (2.1a) and the corresponding one of $v^{2n_+ + 2n_- + 1}$ in (2.1b) is $\alpha_{2n_+}\alpha_{2n_-+1}\int_{-\pi}^{+\pi}\sigma(\theta)(\sin\theta)^{2n_+}(\cos\theta)^{2n_-+1}$, which can vanish.

Comparing the highest degrees of both polynomials on the lhs and the rhs, we find the constraints

$$\sup(n_+ + 1, n_- + 2) = 2n_+, \tag{2.3a}$$
$$\sup(2n_- + 3, 2n_+ + 3) \leqslant 2n_+ + 2n_- + 1. \tag{2.3b}$$

First, $f > 0$ for $|v|$ large requires $n_- < n_+$. Second, if the sup is $n_+ + 1$ in (2.3a) then $n_+ = 1$, $n_- = 0$, if it is $n_- + 2$ then $2 - n_+ = n_+ - n_- > 0$, still $n_+ = 1$, $n_- = 0$. Third, these values lead to an impossibility: $\sup(3,5) \leqslant 3$ into (2.3b) unless $\partial b/\partial x \equiv 0$, or $b \equiv b(t)$ with $\sup(3,3) \leqslant 3$. The only possible ansatz (2.2) is

$$\sqrt{2\pi}f^+ = e^{-b(t)v^2/2}(\alpha_0(t,x) + \alpha_2(t,x)(v^2/2)),$$
$$\sqrt{2\pi}f^- = e^{-b(t)v^2/2}(v/\sqrt{2})\alpha_1(x,t). \tag{2.2'}$$

Let us notice that if we have allowed $n_- \geqslant n_+$ (or f violating positivity when $v \to \pm\infty$) then the discussion would be different (see, for instance, a similar discussion for the stationary case[11]).

B. The system of nonlinear partial differential equations

We have five unknown functions $b,\alpha_0,\alpha_2,\alpha_1,\sigma$ and five relations (three coming from the vanishing of the coefficients of $[v^2/2]^2$, $[v^2/2]$, $[v^0]$ in (2.1a) and two from $[v/\sqrt{2}]$, $[v/\sqrt{2}]^3$ in (2.1b)).

The first relation coming from $[v]^4$ is

$$\alpha_2 = -(b^{1/2}/v\sigma_2)b_t \to \alpha_2 \equiv \alpha_2(t), \quad \alpha_{2x} = 0. \tag{2.4a}$$

If, for a t value $b_t > 0$, then $\alpha_2 < 0$, $f^+ < 0$ for large v, (2.2') violates positivity. The second, deduced from $[v]^0$, is $\alpha_{0t} = \frac{3}{4}\nu\sigma_2\alpha_2^2 b^{-5/2}$, leading to $\alpha_0(t,x) = \overline{\alpha}_0(t) + \overline{\alpha}_0(x)$. We see that α_0 is a sum of two terms depending either on x or t. Instead of writing separately the coefficients of $[v^0]$ and $[v^2]$ we choose the sums of $(b/2)[v^2/2] + b^2[v^0]$ and $\frac{3}{2}b[v^2/2] + b^2[v^0]$, because, as we shall see, they have a physical interpretation:

$$\partial_t N_0 + \partial_x J_0 = 0, \quad N_0 = \int f\,dv, \quad J_0 = \int fv\,dv,$$
$$N_0 = (\overline{\alpha}_0(t) + \overline{\alpha}_0(x))b^{-1/2} + (\alpha_2(t)/2)b^{-3/2}, \tag{2.4b}$$
$$J_0 = \alpha_1 b^{-3/2}/\sqrt{2};$$
$$\partial_t N_2 + \partial_x J_2 = 0, \quad N_2 = \int fv^2\,dv, \quad J_2 = \int fv^3\,dv,$$
$$N_2 = (\overline{\alpha}_0(t) + \overline{\alpha}_0(x))b^{-3/2} + \tfrac{3}{2}\alpha_2(t)b^{-5/2}, \tag{2.4c}$$
$$J_2 = \alpha_1 3b^{-5/2}\sqrt{2} = (3/b)J_0.$$

N_0,N_2 are, respectively, the local density and energy while J_0,J_2 are the corresponding components of the current. These relations represent conservation laws. If in (2.1a) we multiply by the invariants $1, v^2$ and integrate over v, then as is well known, the collision term contributions vanish. We find $\partial_t\int f^+\,dv + \partial_x\int vf^- = 0$, $\partial_t\int f^+v^2\,dv + \partial_x\int v^3f^- = 0$, which are, respectively, (2.4a) and (2.4b).

It remains to study the odd v polynomial obtained after substitution of (2.2') into (2.1b) and integration. Taking into account (2.4a) and the relations between $\alpha_0,\alpha_1,\alpha_2$ and N_0,J_0, the coefficients of $[v/\sqrt{2}]$, $[v/\sqrt{2}]^3$ give the two last equations

$$\partial_t J_0 + b^{-1}\partial_x N_0 + \nu(\tau_0 - \tau_1)J_0N_0 = 0, \tag{2.4d}$$
$$\sigma_2 - \tau_1 + \tau_3 = 0. \tag{2.4e}$$

Relation (2.4e) for the moments of $\sigma(\theta)$ is the same relation as in the homogeneous case.[10] Similarly in (2.4d), if $\alpha_{0x} = 0$, $N_0 = 1$, we find again the homogeneous relation. Here [see the conservation law (2.4b)], $N_0(x,t)$ is not a constant. We have four relations (2.4a)–(2.4d) for the determination of four quantities $b(t)$, $\alpha_2(t)$, $\overline{\alpha}_0(t) + \overline{\alpha}_0(x)$ or $N_0(x,t)$, and $\alpha_1(x,t)$ or $J_0(x,t)$. We want to simplify the formalism and try to reduce the number of independent relations which apply to independent quantities. From (2.4b) and (2.4c) we find $3b^{-1} \times \partial_t N_0 = \partial_t N_2$, $N_2 = N_0 b^{-1} + \alpha_2 b^{-5/2}$, eliminate α_2 with (2.4a), and obtain a first equation [equivalent to (2.4c)] in which only N_0 and b are present:

$$2b^{-1}\partial_t N_0 - N_0\,\partial_t b^{-1} - (1/\sigma_2\nu)\partial_t^2 b^{-1} = 0. \tag{2.4c'}$$

Noticing from (2.4b) that N_0 can be written $N_0(x,t) = \overline{N}_0(t) + \overline{\alpha}_0(x)b^{-1/2}$ and substituting into (2.4c'), we find that the two terms proportional to $\overline{\alpha}_0(x)$ cancel each other and consequently (2.4c') is an x-independent equation. For the determination of the possible x dependences of J_0 and N_0 we look at the two equations (2.4b) and (2.4d) and eliminate J_0. A compatibility condition $(\partial_{xt}^2 - \partial_{tx}^2)J_0(x,t) \equiv 0$ can be deduced from the two equations (see Appendix A). Taking advantage of the decomposition $N_0 = \overline{N}_0 + \overline{\alpha}_0(x)b^{-1/2}$, we can write a sum of terms which are functionals of $\overline{\alpha}_0(x)$ only with time-dependent coefficients. We find that the only possibility is $\overline{\alpha}_0 \equiv 0$ and $N_0 \equiv N_0(t)$ must satisfy a differential equation

$$\partial_t \log \partial_t N_0(t) = (\tau_1 - \tau_0)\nu N_0(t), \quad \partial_x \alpha_0 \equiv \partial_x N_0 \equiv 0. \tag{2.4d'}$$

In conclusion, we first obtain $N_0(t)$ in (2.4d') and second, substituting into (2.4c'), we determine the class of $b(t)$ solutions. The two remaining equations (2.4a) and (2.4b) give both $\alpha_2, \alpha_0 = b^{1/2}[N_0 + b_t(2\sigma_2 \nu b)^{-1}]$ and $J_0(x,t) = (x_0 - x)\partial_t N_0 + J_0(x_0,t)$, $\alpha_1 = \sqrt{2} J_0 b^{3/2}$. We choose $J_0(x_0,t) \equiv 0$ in order that f satisfies a specular reflection boundary condition at an arbitrary x_0 value. The solution f can be written

$$f\sqrt{2\pi} = b^{3/2} e^{-bv^2/2}\left[b^{-1}\left(N_0 + \frac{b_t}{2\nu\sigma_2 b}\right) + v(x_0 - x)N_{0t} - \frac{v^2}{2}\frac{b_t}{\nu\sigma_2 b}\right]. \tag{2.5}$$

In this way, Eqs. (2.4c'), (2.4d'), and (2.5) give the only exact solution of Kac's model corresponding to the general ansatz family written down in (2.2a). Let us emphasize the very important fact that the solution (2.5) cannot represent an extension of the complete BKW homogeneous solution. Although in (2.4c') if $N_0 \equiv \text{const} = 1$, we find the same Maxwellian width $b(t) = (1 - c_1 e^{-\nu c_2 t})^{-1}$ as in the KWB solution; $N_0 = \text{const}$ is not a solution of (2.4d'). Here (2.4d') represents the compatibility condition between (2.4b) and (2.4d) when we eliminate J_0 (or α_1). In the homogeneous case, due to the mass conservation law, $\partial_x J_0 = 0$ and J_0 (or α_1) does not appear in (2.4b). In that case (2.4b) and (2.4d) represent two decoupled equations which determine separately N_0 and J_0 (or α_1).

C. Some general considerations for the possible $N_0(t)b^{-1}(t)$

The general solution of (2.4c') depends on two arbitrary constants c_1, c_2 and can be written

$$N_0(t) = \frac{c_2}{\nu(\tau_0 - \tau_1)}\left(\frac{1-y}{1+y}\right),$$
$$y = c_1 e^{-c_2 t}, \quad c_2 > 0, \quad y \underset{t\to\infty}{\to} 0. \tag{2.6}$$

A solution corresponds to a fixed sign (y): $y \gtrless 0$ if $c_1 \gtrless 0$. Let us define $\Delta(y) = b^{-1}$, substitute (2.6) into (2.4c') and obtain, in the y variable, a second-order differential equation depending on a parameter λ linked to the moments of $\sigma(\theta)$,

$$\left(\frac{4\lambda}{y(1+y)^2} + \left(\frac{\lambda(1-y)}{y(1+y)} - \frac{1}{y}\right)\partial_y - \partial_{y^2}^2\right)\Delta(y) = 0, \tag{2.4c''}$$
$$\lambda(\tau_0 - \tau_1) - \sigma_2 = 0.$$

The definition of $\lambda\left[\int_{-\pi}^{+\pi}\sigma(\theta)(1-z)(z^2(1+z) - \lambda)d\theta = 0\right]$, $z = \cos\theta$, and the positivity of $\sigma(\theta)$ lead to the restriction $0 < \lambda < 2$. The solution f written down in (2.5) can be expressed in terms of $\Delta(y), y$ alone. Requiring at equilibrium a Maxwellian behavior $f\sqrt{2\pi} \underset{t\to\infty}{\simeq} e^{-v^2/2}$, we obtain a relation between the relaxation time c_2^{-1}, the constant ν of the collision term, and the moment $\tau_0 - \tau_1$ of $\sigma(\theta)$:

$$f(v,t,x) = \frac{e^{-v^2/2\Delta^{-1}}}{\sqrt{2\pi}}\Delta^{-3/2}\left[\left(\frac{1-y}{1+y}\right)\Delta + \frac{y}{2\lambda}\partial_y\Delta + v\frac{2c_2\,dy}{(1+y)^2} - \frac{v^2}{2}\frac{y}{\lambda}\frac{\partial_y\Delta}{\Delta}\right] \underset{t\to\infty}{\to} \frac{e^{-v^2/2}}{\sqrt{2\pi}},$$
$$\Delta(y) \underset{y\to 0}{\to} 1, \quad y\,\partial_y\Delta \underset{y\to 0}{\to} 0, \quad 1 = \nu(\tau_0 - \tau_1)c_2^{-1},$$
$$d = c_2(x_0 - x), \quad \lambda = \sigma_2/(\tau_0 - \tau_1). \tag{2.5'}$$

The reduced distribution function $F = f/f(t\to\infty)$ is just the solution (1.2a) and (1.2b) written down in the Introduction. In Sec. III we study both the solutions $\Delta(y)$ of (2.4c") and the corresponding properties of $f(v,t,x)$ given by (2.5'). As explained in the Introduction, for a given solution with c and d fixed, f in (2.5') leads to a family of solutions with $c_2, x_0 - x, t$ varying in such a way that $c_2(x - x_0) = c_2'(x' - x_0')$, $c_2 t = c_2' t'$.

Can we only have solutions with time dependence provided by the variable $y = c_1 e^{-c_2 t}$? There exist also solutions with another time dependence, but they do not lead to Maxwellian asymptotic distributions. From the general solution (2.6), putting $c_1 = -e^{-c_2 t_0}$ and taking the limit $c_2 \to 0$, we find a power-type solution $N_0(t) = [2/\nu(\tau_0 - \tau_1)][1/(t + t_0)]$ of (2.4d'). Substituting it into (2.4c'), $\Delta = b^{-1}$ is the solution of the equation $(4\lambda + 2\lambda(t + t_0)\partial_t + (t + t_0)^2\partial_{t^2}^2)\Delta = 0$ and $\Delta \not\to 1$. We find $\Delta = c^+(t_0 + t)^{\rho^+} + c^-(t_0 + t)^{\rho^-}$, $\rho^{\pm} = \frac{1}{2} - \lambda \pm \frac{1}{2}\sqrt{1 + 4\lambda^2 - 20\lambda}$ and substituting into (2.5) we have not found solutions which do not violate either $f > 0$ or $\sigma(\theta) > 0$.

D. Laguerre moments

In order to check the validity of the formalism leading to (2.5'), (2.4c"), we can determine the Laguerre moments of F and verify that they are also solutions of the differential system satisfied by the Laguerre moments. Let us define for the reduced distribution $F(v,t,x)$ of (2.5') the moments $D_n^{\pm}$

$$F(v,t,x) = \sum_n\left[(-1)^n D_n^+(t) L_n^{(-1/2)}\left(\frac{v^2}{2}\right) + \frac{v}{\sqrt{2}}(-1)^n D_n^-(x,t) L_n^{1/2}\left(\frac{v^2}{2}\right)\right]. \tag{2.7}$$

With the help of the generating functionals of the $L_n^{\pm 1/2}$ we can (see Appendix B) find the Laguerre moments of the solution (2.5'):

$$D_n^+ = \left(\frac{1-y}{1+y}\right)(\Delta - 1)^n - \frac{y}{\lambda}n(\Delta - 1)^{n-1}\partial_y\Delta,$$
$$D_n^- = \sqrt{2}(x_0 - x)[2c_2 y(\Delta - 1)^n/(1+y)^2]. \tag{2.8}$$

In the spatially homogeneous case, Kac[8] and Ernst[9] (using the Fourier transform) have given the equations for the Hermite moments. In the inhomogeneous case, when the gradient term $v\,\partial_x$ is present, one can directly obtain[10] the equations for the Laguerre moments. Let us assume

$$f^+\sqrt{2\pi}e^{v^2/2} = \sum L_n^{-1/2}\left(\frac{v^2}{2}\right)(-1)^n D_n^+,$$
$$f^-\sqrt{2\pi}e^{v^2/2} = \frac{v}{\sqrt{2}}\sum L_n^{1/2}\left(\frac{v^2}{2}\right)(-1)^n D_n^-, \tag{2.9}$$

substitute into (1.1), and find for the $D_n^{\pm}$,

$$\partial_t D_n^+ \sqrt{2}\,\partial_x((n+\tfrac{1}{2})D_n^- + D_{n-1}^-) = \sum_0^n D_q^+ D_{n-q}^+ C_n^q B_{qn},$$

$$B_{on} = \tau_{2n} - \tau_0, \quad B_{qn} = \sum_0^q (-1)^m C_q^m \tau_{2(n+m-q)}, \tag{2.10}$$

$$\partial_t D_n^- + \sqrt{2}\,\partial_x(D_n^+ + D_{n+1}^+) = \sum_0^n D_q^+ D_{n-q}^- C_n^q E_{qn},$$

$$E_{on} = \tau_{2n+1} - \tau_0, \tag{2.11}$$

$$E_{qn} = \sum_0^q (-1)^m C_q^m \tau_{2(n-m+q)+1}.$$

By direct substitution of the $D_n^{\pm}$ written down in (2.8), if Δ satisfies (2.4c″) and if the relations $c_2 = \nu(\tau_0 - \tau_1)$, $\sigma_2 = \tau_1 - \tau_3 = \lambda(\tau_0 - \tau_1)$ hold, then the reader can verify that the $D_n^{\pm}$ are solutions of the system (2.10) and (2.11).

E. $\sigma(\theta)$ models

We want to construct explicit cross sections $\sigma(\theta)$ such that both the moment relations

$$\sigma_2 - \tau_1 + \tau_3 = 0, \quad \sigma_2 - \lambda(\tau_0 - \tau_1) = 0, \quad \lambda \in]0,2[\tag{2.12}$$

are satisfied. We remark that the first relation in (2.12) cannot hold if the $\sigma(\theta)$ satisfy the special symmetry $\sigma(\theta) = \sigma(\pi - \theta)$. We choose a very simple family where σ is a sum of δ distribution functions,

$$\sigma(\theta) = \frac{1}{2}\sum_{i=1}^{2} \mu_i(\delta(\theta - \theta_i) + \delta(\theta + \theta_i)),$$
$$\tau_0 = \mu_1 + \mu_2, \quad \mu_i > 0. \tag{2.13a}$$

The θ_i are arbitrary and lead to the following system:

$$\sum_1^1 \mu_i A_i = 0, \quad A_i = (1 - z_i^2)(z_i - z_i^2), \quad \cos\theta_i = z_i,$$
$$\sum_1^2 \mu_i C_i = 0, \quad C_i = (1 - z_i)(z_i(1 + z_i) - \lambda). \tag{2.13b}$$

We fix $\mu_1 > 0$ and z_1, $0 < |z_1| < 1$. The compatibility condition $A_1C_2 - A_2C_1 = 0$ determines z_2 with constraint $0 < |z_2| < 1$ and we find $\mu_2 = \mu_1 A_1/A_2$. A simpler case can be obtained for $0 < \lambda < 1$ because we can choose $z_1 = \sqrt{\lambda}$ and $z_2 = -z_1$ leading to the model

$$\sigma(\theta) = (\mu_1/2)[\delta(\theta - \theta_1) + \delta(\theta + \theta_1) + [(1 - \sqrt{\lambda})/(1 + \sqrt{\lambda})](\delta(\theta - \pi + \theta_1) + \delta(\theta + \pi - \theta_1))]. \tag{2.13c}$$

One can also consider smooth $\sigma(\theta)$ models $\sigma = \cos(\theta/2)\Sigma_1^{\mu}\mu_i(\cos\theta)^{m-1}$, $\mu \geqslant 3$.

In Sec. IV we illustrate the properties of the reduced distribution F with many examples. When $0 < \lambda < 1$, we always choose the $\sigma(\theta)$ model (2.13a) and (2.13c) with $\mu_1 = 1$, $\mu_2 = (1 - \sqrt{\lambda})(1 + \sqrt{\lambda})^{-1}$, $z_1 = \sqrt{\lambda}$, $z_2 = -z_1$ such that the knowledge of λ determines entirely $\sigma(\theta)$. When $\lambda \in [1,2[$, we choose $\sigma(\theta)$ given by (2.13b), $\mu_1 = 1$, and must determine numerically the couple (z_1,z_2) satisfying $A_1C_2 - A_2C_1 = 0$ and then deduce μ_2.

F. Equations when a force term $\Lambda(t,x)\partial_v f$ is present

Let us add $\Lambda(x,t)\partial_v f^{\pm}$, respectively, to the lhs of (2.1a) and (2.1b), assume an ansatz of the (2.2) type, verify that (2.2′) with $b = b(t)$ is still the only possible one, and, substituting (2.2′) into (2.1a) and (2.1b) find the five independent relations (2.14a)–(2.14e) which generalize (2.4a)–(2.4e). The first one (2.14a) is identical with (2.4a) leading to $\alpha_2 = \alpha_2(t)$. The second, $\partial_t N_0 + \partial_x J_0 = 0$, assuming that N_0 and J_0 are partial derivatives of the same $U(t,x)$ function, becomes

$$N_0 = U_x, \quad J_0 = -U_t. \tag{2.14b}$$

The three others are different than the (2.4) ones,

$$2b^{-1}U_{xt} - U_x\,\partial_t b^{-1} - (\sigma_2\nu)^{-1}\partial_{t^2}^2 b^{-1} = 2\nu J_0^2(\tau_1 - \tau_3 - \sigma_2), \tag{2.14c}$$

$$b^{-1}U_{xx} - U_{tt} + \nu(\tau_1 - \tau_0)U_x U_T = \nu(\tau_1 - \tau_3 - \sigma_2)U_x U_T, \tag{2.14d}$$

$$(\sigma_2 - \tau_1 + \tau_3)\nu J_0 = \Lambda, \tag{2.14e}$$

but reduce to them if $\sigma_2 - \tau_1 + \tau_3 = 0$.

Here we only want to verify that the exact inhomogeneous solution for $\Lambda \equiv 0$ presented before and the exact homogeneous one with $\Lambda(t) \neq 0$ obtained recently[10] are easily deduced from the system (2.14c)–(2.14e).

(i) First, we assume $\Lambda \equiv 0$, $U = x\bar{N}_0(t) + M_0(t)$ ($\bar{N}_0$, M_0 unknown functions) and substitute into the system (2.14). It is trivial to verify that (2.4c′), (2.4d), and (2.4e) are satisfied with $N_0 = \bar{N}_0(t)$ and $M_0(t) = \text{const}$, $N_0(t)$, which means $U = (x_0 - x)\bar{N}_0(t)$ or the solution Eq. (2.5) for $f(v,t,x)$.

(ii) Second, we assume $\Lambda \equiv \Lambda(t) \neq 0$, $U = x - V(t)$ and substitute into (2.14). We find $N_0 = 1$, $J_0 = V_t = \text{const}\, e^{-\nu\tau_F}$, $\tau_F = \tau_0 - \sigma_2 - \tau_3$, $b^{-1} = 1 + \text{const}_1 \times e^{-\nu\sigma_2 t} + \text{const}_2\, e^{-2\nu\tau_F t}$, which, for $\nu = 1$, is the solution given in Ref. 10.

III. SOLUTIONS FOR THE MAXWELLIAN WIDTH $\Delta^{-1}(t) = b(t)$ AND POSITIVITY PROPERTIES OF $F(v,t,x)$

We rewrite (2.4c″) as

$$\left[\frac{4\lambda}{y(1+y)^2} + \left(\frac{\lambda(1-y) - (1+y)}{y(1+y)}\right)\partial_y - \partial_{y^2}^2\right]\Delta(y) = 0,$$
$$0 < \lambda < 2, \quad y = C_1 e^{-C_2 y}, \tag{3.1}$$

and study both the different classes of Δ, when the λ parameter is varying between 0 and 2, and the positivity properties of F.

A. Solutions of the Maxwellian width Δ^{-1}

This second-order differential equation has a singularity of the Fuchsian type at $y = 0$. The two roots of the indicial equation are 0 and λ and, if $\lambda \neq 1$, we do not need a log y term in the solution.

1. $\lambda \neq 1$

Let us define, as in the framework of potential theory, the fundamental "singular" solution Δ_s and "regular" solution Δ_R at $y = 0$, where the coefficients satisfy a three-term recurrence relation

$$\Delta_s = \sum_0^\infty a_n y^n, \quad a_0 = 1, \quad a_1 = \frac{4\lambda}{1-\lambda},$$

$$a_{n+2} = \frac{a_n n(\lambda+n) + a_{n+1}(2(n+1)^2 - 4\lambda)}{(n+2)(\lambda-n-2)}, \quad n \geqslant 0,$$

$$\Delta_R = y^\lambda \sum_0^\infty d_n y^n, \quad d_0 = 1, \quad d_1 = \frac{2\lambda(2-\lambda)}{\lambda+1}, \tag{3.2}$$

$$d_{n+2} = \frac{dn(2\lambda^2 + 3\lambda n + n^2) + 2d_{n+1}((\lambda+n)^2 + 2n + 1)}{-(n+2)(\lambda+n+2)}. \tag{3.2'}$$

From the general theory of differential equations, we know that these expansions are valid for $|y| < 1$, up to the nearest singularity $y = -1$ of the coefficients of Eq. (3.1). If y has the sign of C_1, and if $C_1 < 0$, we replace y^λ by $(-y)^\lambda$ in the definition of Δ_R. The general "singular" solution $\underset{y\to 0}{\Delta \to 1}$ is

$$\Delta_G = \Delta_s + C_3 \Delta_R, \tag{3.3}$$

with C_3 an arbitrary constant.

2. $\lambda = 1$

In this case Δ_s and Δ_G contain a logarithmic term

$$\Delta_s = \sum_0^\infty e_n y^n + 4(\log y)\Delta_R, \quad e_0 = 1, \quad e_1 = 0,$$

$$e_{n+2} = -\frac{1}{(n+1)(n+2)}\{2e_{n+1}(n^2+2n-1) + n(n+1)e_n + 4(2n+1)(d_{n-1} + 2d_n) + 4(2n+3)d_{n+1} + 8d_n\}, \tag{3.4a}$$

where Δ_R is the solution equation (3.2') for $\lambda = 1$, $\log y$ being replaced by $\log(-y)$ if $y < 0$. The general "singular" solution $\to 1$ when $y \to 0$ is

$$\Delta_G = \Delta_s + C_3 \Delta_R. \tag{3.4b}$$

B. Positivity property

1. $t = 0$

We rewrite (1.2a) and study the positivity of the quadratic v polynomial which appears at the right:

$$F\Delta^{3/2} = e^{-(v^2/2)(\Delta^{-1}-1)}[\bar{\alpha}_0 + v\bar{\alpha}_1 + (v^2/2)\bar{\alpha}_2],$$
$$y = C_1 e^{-C_2 t}, \quad \Delta > 0,$$
$$\bar{\alpha}_0 = \frac{1-y}{1+y}\Delta + \frac{y}{2\lambda}\partial_y \Delta, \quad \alpha_2 = -\frac{y}{\lambda}\partial_y \log \Delta, \tag{3.5}$$
$$\bar{\alpha}_1 = 2(x_0 - x)C_2 y/(1+y)^2.$$

The positivity of the even velocity part of F requires $\bar{\alpha}_0 > 0$ and $\bar{\alpha}_2 > 0$. We note that at $t = 0$, C_2 and $(x - x_0)$ enter only as a product $d = (x_0 - x)C_2$ into the odd part. It follows that if we choose both C_1 and λ such that $\bar{\alpha}_0 > 0$, $\bar{\alpha}_2 > 0$, and d is sufficiently small then the rhs of (3.5) remains positive for $v \in [-\infty, +\infty]$. Let us first consider the fundamental singular solution $\Delta_s = 1 + \Sigma a_n y^n$ with $\lambda \neq 1$. A necessary condition for $\bar{\alpha}_2 > 0$ is $-y\Delta_y = -C_1 a_1[1 + \Sigma_2^\infty n(a_n/a_1)C_1^{n-1}] > 0$ or $C_1 a_1 < 0$ if 1 is the dominant term in the bracket. On the other hand, when $y \to 0$ or $t \to \infty$ $\bar{\alpha}_2 \simeq -(a_1 C_1/\lambda)e^{-C_2 t}$ and still we have that $-a_1 C_1 = 4\lambda C_1/(\lambda - 1)$ must be positive. Consequently we must have $C_1 < 0$ ($C_1 > 0$) for $\lambda < 1$ ($\lambda > 1$) or $\lambda < 1$ ($\lambda > 1$) corresponds to an expansion (contraction).

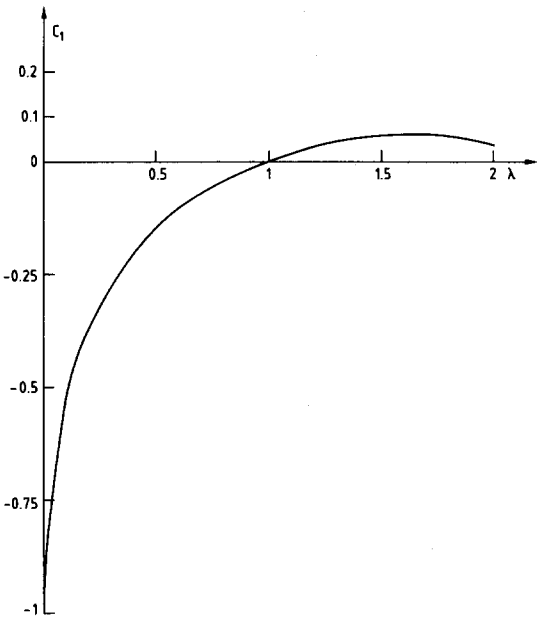


FIG. 1. C_1, λ domain when $F^+ > 0$ at $t = 0$. For other figures, plot of $F(v,t,x)$ vs v.

In Fig. 1, we plot the curve $C_1(\lambda)$ vs λ, limiting the positivity domain of the even velocity part of F at $t = 0$. Adding the odd part and a new parameter $d = C_2(x_0 - x)$ then there exists in the three-dimensional space (λ, C_1, d) a domain where $F > 0$ at $t = 0$.

Second, for the complete singular solution $\Delta_s + C_3\Delta_R$, it is clear that we can choose $|C_3|$ sufficiently small such that F is positive at $t = 0$ in a domain of the four-dimensional space (λ, C_1, d, C_3).

For $\lambda = 1$, the positivity condition at $t = 0$ can be satisfied if we choose sufficient small C_1 positive or negative values.

2. $t \neq 0$

We recall that in order to maintain the positivity for F at $t = 0$, $d = C_2(x_0 - x)$ must remain finite. Consequently when $|x| \to \infty$ the positivity is violated. We cannot simply apply the usual argument[12] assuring the positivity at $t \neq 0$. We assume x fixed, $F > 0$ at $t = 0$ and study $t \neq 0$.

(i) However, modifying slightly this argument, one can still prove the positivity in the contraction case ($y > 0$ or $C_1 > 0$ or $\lambda > 1$). When only f^- contains x, f_x^- is independent of x, one can rewrite (1.1) with $-vf_x^-(v) = v^2 e^{-bv^2/2} b^{3/2} N_{0,t} \geqslant 0$ if $y \geqslant 0$:

$$f_t(v) = -vf_x^-(v) + \nu \int\int \sigma(\theta)(f(v')f(w') - f(v)f(w))dw\, d\theta, \tag{3.6}$$

where x is a fixed parameter. We prove *ab absurdo* that $f > 0$ at $t \neq 0$ if both $f > 0$ at $t = 0$ and $-vf_x^- > 0$ for $v \in [-\infty, +\infty]$, $t > 0$. Let (v_0, t_0) be the values where $f > 0$ is violated for the first time. By continuity we have at a slightly earlier time $t_0 - a$; $f(v_0, t_0 - a) = 0$, $f(v, t_0 - a) > 0$, for $v \neq v_0$.

Then in (3.6), the rhs is positive at $(v,t)=(v_0,t_0-a)$ and the lhs being $\partial_t(f(v_0,t))_{t=t_0-a}>0$ contradicts the assumption $f(v_0,t_0)<0$. Of course if $-vf_x^-<0$, the solution can still remain positive because the above condition is not a necessary condition.

(ii) In the expansion case ($y<0, C_1<0, \lambda<1$) we still have positivity at $t\neq 0$ if Δ is reduced to Δ_s. The dominant term in the bracket of (3.5) is $\bar{\alpha}_2 v^2$. For t large, with $\bar{\alpha}_2$ having the positive sign of $C_1/(\lambda-1)$, we can always manage the odd part such that the bracket remains positive for $t=0$.

(iii) Always in the expansion case ($C_1<0, \lambda<1$), we consider now the general $\Delta=\Delta_s+C_3\Delta_R$. We look at $b=\Delta^{-1}$ and its derivative $b_t \simeq C_2C_3\lambda(-y)^\lambda$ when t is large.

For t very large, the Maxwellian width $b\simeq 1-C_3(-y)^\lambda<1$ (or >1) if $C_3>0$ (or $C_3<0$), $b\underset{t\to\infty}{\longrightarrow}1^-$ if $C_3>0$ (or 1^+ if $C_3<0$). This means that for t sufficiently large the distribution function will decrease less (or more) than the Maxwellian if $C_3>0$ (or $C_3<0$). Consequently in (2.5) the derivative $b_t>0$ and $\alpha_2<0$ if $C_3>0$ (or $b_t<0$, $\alpha_2>0$ if $C_3<0$) and t large. It follows that depending on whether $C_3>0$ or <0, for t and $|v|$ sufficiently large we must find a violation (or not) of the positivity property of f or F.

So with these C_3 positive parameter values we can construct examples of distributions which are positive at $t=0$, tend to the Maxwellian for $t\to\infty$, but nevertheless will violate positivity above some t critical value. The theoretical discussion occurs with the time dependence of the Maxwellian width $b(t)$ which decreases down to a $b_{\min}<1$ for $t=t_1$ and increases afterwards up to $b\to 1^-$. At this minimum $b_t=0$ for $t=t_1$, $\alpha_2(t_1)$ vanishes and changes sign afterwards leading to a violation of positivity. At this t_1 value, f^+ is a pure Gaussian or a Maxwellian $\exp-(v^2/2)b_{\min}$ and f a Gaussian multiplied by a first-order v polynomial. Consequently in Eq. (2.1a) the collision term for the even part vanishes [or the rhs of (2.1a)] but not the odd one [rhs of (2.1b)]. The positivity violation occurs for t values a little bit less than t_1 (depending on the x_0-x_1 values). All the above discussion was mainly with the even part f^+, when we include f^- there exists a small shift of the violation.

For the numerical study we choose $\lambda=\frac{1}{2}$, $C_1=-0.1$ (or $y<0$), $x_0-x=1$, and for C_3 positive varying values. For $C_3>1.7$, the positivity is violated at $t=0$ but if we choose a smaller x_0-x value, the positivity would be violated for larger C_3 value.

For $C_3=0.5$, we plot the relaxation curves in Fig. 2. There exist different successive regimes: for $0\leqslant t\leqslant 0.5$, the positivity $F>0$ is satisfied and $F\to 0$ for large $|v|$; for $0.51\leqslant t\leqslant 0.86$, F is still positive but $F\to\infty$; and for $0.86<t<\infty$, F violates positivity and $|F|\to\infty$ when $|v|\to\infty$. At the critical value $t\#0.8520$ a double zero appears for $v\#68$. Let us consider the curve $b(t)$. At $t=0$, $b(0)=1.35$, then $b(t)$ decreases, crosses $b=1$ at $t=0.5$, still decreases to a minimum $b_{\min}=0.98$, $\alpha_2=b_t=0$ at $t=0.86$ and increases towards 1 for higher t values.

We have verified the persistence of the phenomenon described here for other $\lambda<1$ and $C_3>0$ values.

(iv) $\lambda=1$. Being as t is large we have $\Delta_s\simeq 1+4y\log|y|$, $\bar{\alpha}_2\simeq -4y(1+\log|y|)$, and the Gaussian term in (3.5) is $\exp((v^2/2)4y\log|y|)$.

If $y>0$ (or $C_1>0$) the Gaussian term and F tend to zero when $|v|\to\infty$, t being large but fixed, $\bar{\alpha}_2v^2>0$ and the solution remains positive for large t, $|v|$.

On the contrary if $y<0$ (or $C_1<0$), the Gaussian and F tend to infinity, $\bar{\alpha}_2v^2$ becomes negative and F violates positivity. We find the same phenomenon as in the previous $\lambda<1$, $C_3>0$ case.

In conclusion, in order to construct distributions not violating positivity, we can choose in the contraction case ($\lambda\geqslant 1, C_1\geqslant 0$), either $C_3>0$ or $C_3<0$, and in the expansion or dilatation case ($\lambda<1, C_1<0$) we must restrict to $C_3<0$.

IV. RELAXATION TOWARDS EQUILIBRIUM AND TJON EFFECT

By construction, the reduced distribution function $F\to 1$ when $t\to\infty$ or $y\to 0$, $|v|$ being fixed [equivalently $f\to$Maxwellian $e^{-v^2/2}(2\pi)^{-1/2}$]. We study the asymptotic behavior $y\to 0$ (or $t\to\infty$) of F corresponding to the different classes of Δ solutions: namely $\lambda\neq 1$ and $\lambda=1$, $\Delta=\Delta_s$ and

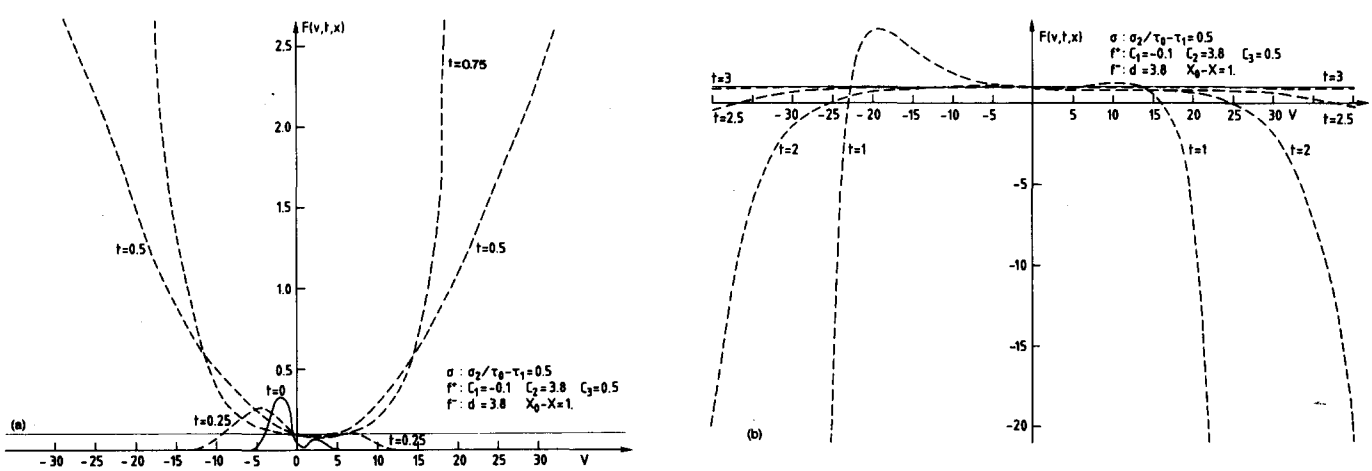


FIG. 2. (a) $\lambda=0.5$, $C_1=-0.1$, $C_2=3.8$, $C_3=0.5$, $x_0-x=1$ and $t\leqslant 0.75$; (b) like (a) but $t\geqslant 1$.

Δ_G, and establish the connections with the existence or non-existence of the Tjon effect.

A. Tjon overpopulation effect

When we look at the relaxation towards equilibrium, either $F \to 1$ in a monotonic way from below (no effect) or there exist high velocity particles for which, at intermediate times, F is substantially larger than 1. Equivalently, when the effect exists, it may produce, at intermediate times, a population of high velocity particles, larger than the one present at initial time or at equilibrium. A necessary (but not sufficient) condition for the existence of the effect is the displacement of the last positive $v_+(t)$ or negative $v_-(t)$ zero of $F(v,x,t) - 1$ when t increases.

B. $\lambda = \sigma_2(\tau_0 - \tau_1)^{-1} \neq 1$ and $\Delta = \Delta_s = 1 + \Sigma a_n y^n$ having one relaxation time

This is the most simple case because F is analytic in y at $y = 0$ and we only have to consider the first-order correction in y (for $|v|$ large but fixed). We find $\Delta_s \simeq 1 + a_1 y$, $F - 1 \simeq y(\partial F/\partial y)(y = 0) \simeq y[(v^2/2)a_1(1 + 1/\lambda) + 2C_2 v(x - x_0)]$, $a_1 = 4\lambda/(1 - \lambda)$ or

$$(F - 1)(e^{C_2 t}/2) \simeq C_1[-v^2 + C_2 v(x_0 - x)]. \tag{4.1}$$

On the one hand, recalling that $C_1 \gtrless 0$ if $\lambda \gtrless 1$, it follows that $F - 1 < 0$ if $\lambda > 1$ and $F - 1 > 0$ if $\lambda < 1$. Consequently, we define a criterion which corresponds to microscopic conditions on $\sigma(\theta)$

$$\text{crit.} = \tau_0 - \tau_1 - \sigma_2, \tag{4.2}$$

and we conclude that if crit. > 0 (or $\lambda < 1$) the relaxation for F towards 1 is from above, $F > 1$, whereas if crit. < 0 (or $\lambda > 1$) it is from below, $F < 1$. On the other hand the rhs of (4.1) is proportional to $|C_1|$ which means that the importance of the effect will depend on how large are the C_1 parameters. If although positive, the rhs of Eq. (41.) is too small, then there is no effect. Due to the positivity constraint at $t = 0$ (Fig. 1), we see that when $\lambda < 1$, the maximum $-C_1$ parameter value decreases when λ increases. In conclusion we expect to find the Tjon effect for $\lambda < 1$ but decreasing when λ increases and it must have disappeared when $\lambda \to 1$. With this result in mind let us discuss numerical examples obtained with the simple $\sigma(\theta)$ given by (2.13a) and (2.13b) if $\lambda > 1$ and (2.13a) and (2.13c) if $\lambda < 1$. Numerically we observe that the effect disappears for $\lambda > 0.75$. In Fig. 3(a) we present the relaxation curves for $\lambda = 0.1$ where the effect is present and in Fig. 4 those for $\lambda = 1.5$ where it is absent. Modifying the initial conditions does not change the results concerning the existence of the effect [see Fig. 3(b) with $\lambda = 0.5$].

C. $\lambda \neq 1$ and $\Delta = \Delta_s + C_3\Delta_R$ having two relaxation times

Here the analysis becomes more complex because $\Delta \simeq 1 + a_1 y + C_3|y|^\lambda$ with two independent decreasing terms when $t \to \infty$. Equivalently we have two relaxation times $T_s \simeq C_2^{-1}$ for the y term and $T_R = (\lambda C_2)^{-1}$ for $|y|^\lambda$. If $\lambda > 1$, then $T_R < T_s$ and $\Delta \simeq 1 + a_1 y$, we expect that $C_3\Delta_R$ is a small perturbation which does not modify very much the above analysis with $\Delta_R \equiv 0$. If $\lambda < 1$, then $T_s < T_R$, the important contribution can come from Δ_R, $\Delta_s - 1$ being now the perturbation, Δ_R becoming more and more important when λ decreases. In both cases, F is no longer analytic at $y = 0$.

1. $\lambda > 1$

$$\Delta \underset{y \to 0}{\simeq} 1 + a_1 y, \quad b \simeq 1 + \frac{4\lambda}{\lambda - 1} y \geqslant 1 \text{ for } y > 0,$$

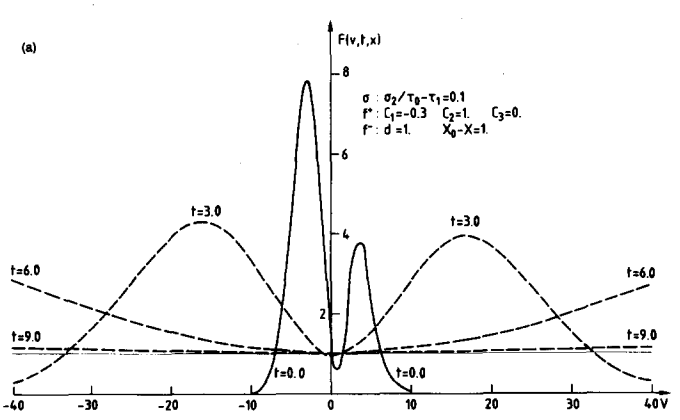
we still obtain the approximation (4.1) predicting no effect and we have numerically checked this result.

2. $\lambda < 1$

We consider sufficiently small $C_3 < 0$ values such that $F(v,t,x) > 0$ for all t; in view of a possible Tjon effect, we study the behavior of F for $(-y)$ small. In Δ we do not retain only the $(-y)^\lambda$ term. We have $\Delta = 1 + a_1 y + C_3(-y)^\lambda$, $y\Delta y/\lambda \simeq a_1 y/\lambda + C_3(-y)^\lambda$, substitute into (3.5), and obtain for the dominant contributions the terms present in (4.1) with a supplementary term proportional to $(C_3)^2$:

$$F - 1 \simeq -\tfrac{1}{2}(v^2/2)^2(C_3)^2(-y)^{2\lambda} + 2y[-v^2 + vC_2(x_0 - x)],$$
$$-y = -C_1 e^{-C_2 t} > 0. \tag{4.3}$$

In (4.3) we have neglected the term proportional to $v^3|y|^{1+\lambda}$ both for simplicity in the discussion and the fact that $|y|^{1+\lambda} \ll |y|^{2\lambda}$ for $\lambda < 1$ and $|y|$ small. On the one hand, for



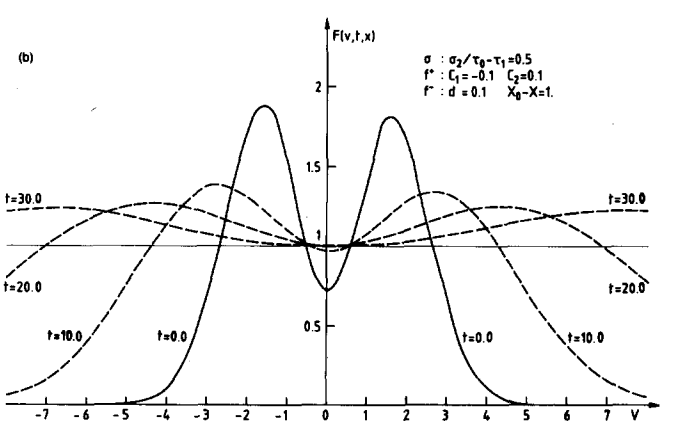


FIG. 3. (a) $\lambda = 0.1$, $C_1 = -0.3$, $C_2 = 1.0$, $C_3 = 0$, $x_0 - x = 1$; (b) $\lambda = 0.5$, $C_1 = -0.1$, $C_2 = 0.1$, $C_3 = 0$, $x_0 - x = 1$.

$(-y)$ close to zero we have two competitive terms (or two relaxation times T_s, $T_R/2$) and the dominant one is coming either from $(-y)^{2\lambda}$ if $\lambda < \frac{1}{2}$ or y if $\lambda > \frac{1}{2}$. For $\lambda < \frac{1}{2}$ we find $F-1 \simeq -\frac{1}{2}(v^2/2)^2 C_3^2 (-y)^{2\lambda} < 0$ without Tjon effect. For $\lambda > \frac{1}{2}$, $F-1 \simeq 2y[-v^2 + vC_2(x_0 - x)] > 0$, as in the above $C_3 = 0$ case. So the Tjon effect must decrease when λ decreases.

On the other hand, the rhs of (4.3) has in factor the sup of $|y|$, $|y|^{2\lambda}$ or $|C_1|$, $|C_1|^{2\lambda}$ and we recall that as in the $C_3 = 0$ case the $|C_1|$ available values decrease when λ increases. So, in an opposite way to the previous argument, the Tjon effect must decrease when λ increases.

Further, the magnitude of C_3 is another important parameter. If $|C_3|$ is very small, for t not too large we can expect to find results similar to the $C_3 = 0$ case, whereas for important C_3 values the two corresponding relaxation pictures can be very different.

In conclusion, except for $|C_3|$ small and for intermediate t values, we do not expect to find the Tjon effect when $C_3 \Delta_R$ is present in Δ. As an illustration we consider a case $\lambda = \frac{1}{4}$ where the effect exists for $C_3 = 0$ and take increasing $-C_3$ values. For $C_3 = -0.1$ and $0 \leqslant t \leqslant 3$ we still have substantial $F > 1$ values for not too large $|v|$ intervals, but for higher times where the term proportional to $(-y)^{2\lambda}$ dominates, the last $v_{\pm}(t)$ zero of $F-1$ does not move, we do not observe the effect, and the relaxation is from below. For the largest $-C_3 = 0.45$ value the Tjon effect disappears (Fig. 5).

In conclusion, although the criterion (4.2) fails when an important $C_3 \Delta_R$ term is present, the numerical examples agree very well with the theoretical analysis of this subsection.

D. $\lambda = 1$ or $\tau_0 - \tau_1 - \sigma_2 = 0$ and $\Delta = \Delta_s$ given in (3.4a) with one relaxation time

(i) First this is the λ value for which the criterion (4.2) gives nothing. If $C_1 \gtrless 0$ (or $y \gtrless 0$), we choose $\log(y)$ and $\log(-y)$; in other words $\Delta_s = 1 + \Sigma e_n y^n + 4y(\log|y|)\Sigma d_n y^n$, $y = C_1 e^{-C_2 t}$. However, we recall that the positivity at $t \neq 0$ is always satisfied if $F > 0$ at $t = 0$ and if $y > 0$ (contraction).

(ii) Second we restrict to C_1 and y positive values. From (3.5) we find for the dominant terms, when $t \to \infty$ or $y \simeq 0^+$ and $|v|$ large

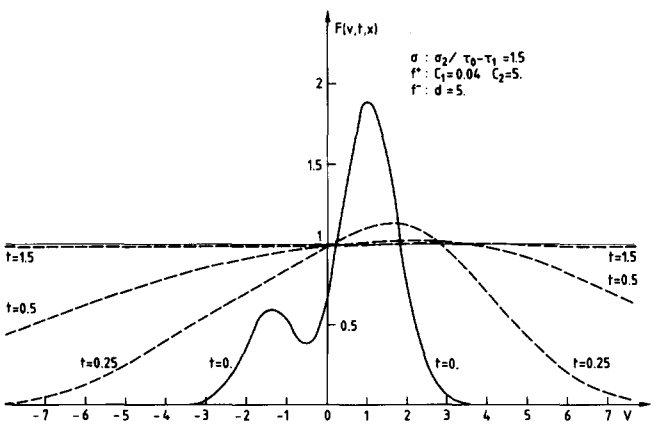


FIG. 4. $\lambda = 1.5$, $C_1 = 0.04$, $C_2 = 5.0$, $C_3 = 0$, $x_0 - x = 1$.

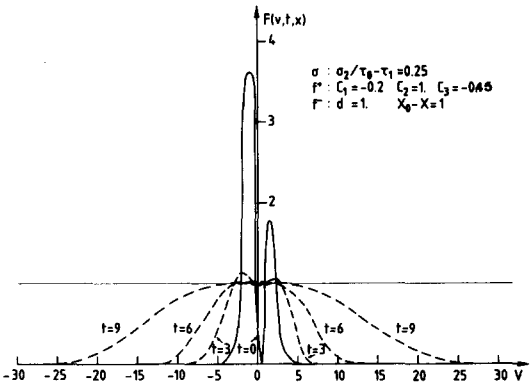


FIG. 5. $\lambda = 0.25$, $C_1 = -0.2$, $C_2 = 1.0$, $C_3 = -0.45$, $x_0 - x = 1$.

$$F-1 \simeq -2y[v^2 - 2C_2(x_0 - x)v + v^4 y(\log y)^2], \quad y > 0, \tag{4.4}$$

and predict that in general $F-1 < 0$ or the Tjon effect is nonexistent. Of course, if the odd part is sufficiently important, a moving zero can appear in the bracket, but since the $F-1$ values are small there is no effect.

(iii) Finally we consider the (3.4b) general solution $\Delta_G = \Delta + C_3 \Delta_R$ and $y > 0$. In this case $\Delta \simeq 1 + 4y \log y + C_3 y$ and $C_3 y$ is a perturbation which must not affect the asymptotic behavior found in (ii) very much. Analyzing the asymptotic $F-1$ behavior we still find the same dominant terms as in (4.4), while those proportional to C_3 are weaker.

E. Linearized versus nonlinear formalisms

Comparing in both homogeneous and inhomogeneous solutions the nonlinear with the linearized ones we have found different properties.

In the Boltzmann homogeneous case, for Maxwell interaction and even velocity distributions, due to the conservation laws of mass and energy, the Laguerre moments $D_0^+ = 1$, $D_1^+ = 0$ lead to linear equations for D_2^+, D_3^+. Consequently all these four moments are identical with their linearized ones. Further, for higher D_n^+ moments [taking into account the positivity of the moments of $\sigma(\theta)$], their linearized part gives the dominant contribution when $t \to \infty$. Seeking, for v^2 and t varying, significant nonlinear contributions, we recall that they were found only for small t and v^2 large (see the review papers[7-9]). In the homogeneous Kac model, the same situation occurs for f^+. Add now $f^-(v,t)$, still due to $D_0^+ = 1$, $D_1^+ = 0$, the moments D_0^-, D_1^- satisfy linear equations and are identical with their linearized partners. [For higher D_n^-, $n \geqslant 2$, a rigorous discussion is more delicate because new odd moments τ_m of $\sigma(\theta)$, not necessarily positive, are introduced which do not allow, without precising $\sigma(\theta)$, an easy estimation of the D_n^- decrease when t increases. For simplicity, in general in the following we neglect this problem.] In conclusion, the first moments $D_0^{\pm}, D_1^{\pm}, D_2^+, D_3^+$ which give the dominant contributions are identical in both nonlinear and linearized formalisms. Further, in both cases we can always construct solutions with the same initial conditions (i.c.).

In the inhomogeneous nonlinear and linearized formalisms, the main differences are that these first Laguerre moments are different, we cannot, in general, define solutions with the same i.c. and the linearized solutions have always two relaxation times.

Let us define $F = 1 + g$, $g = g^+ + g^-$, eliminate from the collision term the product of the two $g^\pm$'s, expand in a Laguerre series $L_n^{\mp(1/2)}(v^2/2)$ with moments $(-1)^n d_n^\pm$, assume $\partial_x g^+ = 0$, and find for the $d_n^\pm$ the solutions written down in Table I. Further we assume that the spatial dependence is linear: $d_n^-(x,0) = (x_0 - x) d_n^-(0)$. Although for d_n^- and d_n^+ $n \geqslant 2$, arbitrary constants are available, this is not true for d_0^+, d_1^+. Consequently the nonlinear and linearized solutions cannot coincide at $t = 0$ (in the homogeneous case $d_0^+ = d_1^+ = 0$ and this problem does not occur). Now we compare our exact solution with its linearized version, beginning with the two ratios d_0^+/d_0^- and $(D_0^+ - 1)/D_0^-$ that we multiply by $\sqrt{2}\, c_2(x - x_0)$. The first is a constant equal to 1 and the second a function $1 + y$ different for any t values except $t = \infty$. Exactly the same difficulty occurs for the relative estimate of $d_1^\pm/D_1^\pm$.

In Table I we estimate the dominant contributions of both $D_n^\pm, d_n^\pm$ for the first Laguerre moments (they are identical in the homogeneous case) and seek whether they can coincide when $t \to \infty$. For $n = 0, \pm$ and $n = 1, +$ we find a condition on $d_0^-(0)$ and a good agreement. For other moments while the exact moments have either pure c_2^{-1} relaxation time ($c_3 = 0$) or a mixing of c_2^{-1} and $(\lambda c_2)^{-1}$ relaxation times ($c_3 \neq 0$), on the contrary the linearized ones never have pure C_2^{-1}. Consequently, for the exact solution with $C_3 = 0$, there does not exist any connection between the two formalisms, the ratios of the two corresponding moments going either to zero or infinity (for $\lambda = 1$, the situation is the same because $\log y$ factors are present only in the exact solution). A similar situation arises for $C_3 \neq 0$, $\lambda > 1$. On the contrary for $C_3 = 0$, $\lambda < 1$, these ratios tend to 1 if we fix the arbitrary constants $d_1^-(0)$ or $d_2^+(0)$ or $d_3^+(0)$. Trying to understand these different features between the two formalisms we remark that the $D_n^\pm$ satisfy *coupled* first-order equations leading for $D_n^+, n \geqslant 1$, to second-order linear differential equations of the Fuchs type (always with two independent fundamental solutions). On the contrary, the linearization procedure decouples the equations, leads to first-order equations for $d_n^\pm$, and makes it difficult to reproduce one class of solutions (in the homogeneous case both $D_n^\pm$ and $d_n^\pm$ satisfy first-order linear equations). In Table I, for d_2^+, d_3^+ we have neglected the contributions coming from d_2^-, d_3^- which introduce the moments τ_5 and τ_7 not present in the exact solu-

TABLE I. Laguerre moments for the linearized solutions, comparison between nonlinear ($D_n^\pm$) and linearized ($d_n^\pm$) moments, and an asymptotic estimate of the linearized solution.

$$d_n^-(x,t) = d_n^-(x,0) e^{\nu E_{0n} t}, \quad d_n^+(t) = -\sqrt{2}\left(\frac{n+\frac{1}{2}}{\nu E_{0n}} \partial_x d_n^-(x,t) + \frac{n}{\nu E_{0n-1}} \partial_x d_{n-1}^-(x,t)\right), \quad n = 0, 1$$

$$d_n^+(t) = e^{\lambda_n t}\left[d_n^+(0) - \sqrt{2}\int_0^t e^{-\lambda_n t'}\left(\left(n+\frac{1}{2}\right)\partial_x d_n^-(x,t') + n\,\partial_x d_{n-1}^-(x,t')\right) dt'\right], \quad n \geqslant 2, \quad \lambda_n = \nu(B_{0n} + B_{nn})$$

$$d_n^-(x,0) = (x_0 - x) d_n^-(0), \quad \sigma_2 - \tau_1 + \tau_3 = 0, \quad C_2 + \nu E_{00} = 0, \quad \lambda = \sigma_0/(\tau_0 - \tau_1), \quad y = C_1 e^{-c_2 t}$$

$$\frac{d_0^-}{x_0 - x} = d_0^-(0) e^{-C_2 t}, \quad d_0^+ = -\frac{d_0^-(0)}{\sqrt{2} C_2} e^{-c_2 t}, \quad d_1^+ = -\frac{\sqrt{2}}{C_2} d_0^-(0) e^{-C_2 t} + \text{const}\, e^{-C_2(1+\lambda)t}, \quad \frac{D_0^-}{x_0 - x} \underset{t \to \infty}{\simeq} 2\sqrt{2} C_2 y$$

$$D_0^+ - 1 \simeq -2y, \quad D_1^+ \simeq -4y; \quad \frac{d_0^+}{D_0^+ - 1} \to 1, \quad \frac{d_1^+}{D_1^+} \to 1, \frac{d_0^-}{D_0^-} \to 1, \quad \text{if } d_0^-(0) = 2\sqrt{2} C_2 C_1$$

$$\frac{d_1^-}{x_0 - x} = d_1^-(0) e^{-C_2(1+\lambda)t}$$

$$\frac{D_1^-}{x_0 - x} \simeq 2\sqrt{2} C_2 \sup(a_1 y^2, C_3 y^{1+\lambda}), \quad \text{if } \lambda = 1 \simeq 2\sqrt{2} C_2 y^2 \log y$$

$$\frac{d_1^-}{D_1^-} \to \begin{cases} 1, & \text{if } C_3 \neq 0, \quad \lambda < 1, \quad d_1^-(0) = 2\sqrt{2} C_2 C_3 |C_1|^{1+\lambda} \\ 0, & \text{if } C_3 = 0, \quad \lambda > 1 \quad \text{or} \quad C_3 \neq 0, \quad \lambda > 1 \\ \infty, & \text{if } C_3 = 0, \quad \lambda < 1 \\ 0, & \text{if } \lambda = 1 \end{cases}$$

$$d_2^+ \simeq \sup(\text{const}_1\, e^{-2C_2\lambda t}, \text{const}_2\, e^{-C_2(1+\lambda)t})$$

$$D_2^+ \simeq -\sup\left(a_1^2 y^2 \frac{(2-\lambda)}{\lambda}, C_3^2 y^{2\lambda}\right) \simeq -16 y^2 (\log y)^2, \quad \text{if } \lambda = 1$$

$$\frac{d_2^+}{D_2^+} \to \begin{cases} 1, & \text{if } C_3 \neq 0, \quad \lambda < 1, \\ & d_2^+(0) + 2\,\frac{1}{C_2(1-\lambda)} = -(C_3)^2 |C_1|^{2\lambda} \\ 0, & \text{if } C_3 = 0, \quad \lambda < 1 \quad \text{or } C_3 \neq 0, \quad \lambda > 1 \\ \infty, & \text{if } C_3 = 0, \quad \lambda > 1 \\ 0, & \text{if } \lambda = 1 \end{cases}$$

$$d_3^+ \simeq e^{-3\lambda C_2 t} d_3^+(0)$$

$$D_3^+ \simeq -\sup\left(a_1^3 y^3 \left(\frac{3-\lambda}{\lambda}\right), 2C_3^3 y^{3\lambda}\right) \simeq -128 y^3 (\log y)^3, \quad \text{if } \lambda = 1$$

$$\frac{d_+^3}{D_3^+} \to \begin{cases} 1, & \text{if } C_3 \neq 0, \quad \lambda < 1, \quad d_3^+(0) = 2C_3^3 |C_1|^{3\lambda} \\ 0, & \text{if } C = 0, \quad \lambda < 1 \quad \text{or } C_3 \neq 0, \quad \lambda > 1 \\ \infty, & \text{if } C_3 = 0, \quad \lambda > 1 \\ 0, & \text{if } \lambda = 1 \end{cases}$$

$$F - 1 \simeq e^{-C_2 t}\left[-\frac{d_0^-(0) v^2}{\sqrt{2} C_2} + \frac{v^4}{8}\left(d_2^+(0) + \frac{2\sqrt{2} d_1^-(0)}{C_2(1-\lambda)}\right) e^{-C_2(2\lambda - 1)t}\right] \begin{cases} > 0, & \text{if } \frac{1}{2} < \lambda < 1 \\ < 0, & \text{if } \lambda > 1 \\ < 0, & \text{if } \lambda < \frac{1}{2}, \quad C_3 \neq 0 \\ ?, & \text{if } \lambda < \frac{1}{2}, \quad C_3 = 0 \end{cases}$$

tion. If we choose for $\lambda < 1$ the (2.13c) $\sigma(\theta)$ models we have verified that the estimations given are correct for d_2^- and for d_3^- if further $\lambda < 0.3$. If $\lambda = 1$, $C_3 = 0$ or $\neq 0$, we find a discrepancy for d_1^-, d_2^+, d_3^+. In Table I we write down an asymptotic estimate of g taking v large but finite and $t \to \infty$ (we neglect d_n^- for $n > 2$). Only the contributions coming from d_1^+ and d_2^+ (if $\lambda < \frac{1}{2}$) remain. If $\lambda > \frac{1}{2}$, $F - 1$ has the sign of $-d_0^-(0)$ (or $-C_1$) and if $\lambda < \frac{1}{2}$ it has the sign of the constant of the v^4 term. If $C_3 \neq 0$ this constant is $-C_3^2 |C_1|^{2\lambda} < 0$, whereas if $C_3 = 0$ we have no information about it.

This analysis suggests that we remain careful when dealing with linearized formalisms and that we not forget that the time-independent constant $F - g = 1$ represents the conservation law of mass in the homogeneous case and only an asymptotic constraint in the inhomogeneous one. We could think to define new approximations of the nonlinear formalism: for instance, eliminate all products of two Laguerre moments except those containing D_0^+ or except those containing either D_0^+ or D_0^-.

V. CONCLUSION

In this paper we have determined an exact inhomogeneous solution of Kac's model relaxing towards a Maxwellian, and with the following properties.

(i) The time dependence is of the exponential type and defines a new variable $y = C_1 \exp -C_2 t$. The Maxwellian width is only time dependent and can have two relaxation times $T_s = C_2^{-1}$ and T_R.

(ii) The relative position $x_0 - x$ enters only in the odd velocity part of the distribution and linearly. When $x_0 - x$ is too large the distribution function violates positivity, and scaling variables corresponding to invariance property can be defined. The local density is uniform in the space or $N_0 \equiv N_0(t)$, the current is proportional to $(x_0 - x)$. The derivative $\partial_t N_0$ having the same sign as y (or C_1), we have either contraction $y > 0$ or dilatation $y < 0$. [We remark that the Nikol'skii solutions have also $N_0 = N_0(t)$.]

(iii) The moments of the cross section must satisfy a linear relation, the cross section must be asymmetric $[\sigma(\theta) \neq \sigma(\pi - \theta)]$, and it is useful to introduce a parameter $\lambda = \sigma_2(\tau_0 - \tau_1)^{-1}$, $T_R = (\lambda C_2)^{-1}$ and a criterion $\tau_0 - \tau_1 - \tau_2$. The positivity of the solution requires $C_1 < 0$, $\lambda < 1$ (expansion) or $C_1 > 0$, $\lambda \geqslant 1$ (contraction).

(iv) The asymptotic behavior of the reduced distribution F explains quite well the existence or nonexistence of the Tjon effect. In the more general case we have

$$F - 1 \simeq |y| [2 \operatorname{sgn}(\lambda - 1)(-v^2 + vC_2(x_0 - x)v) - \tfrac{1}{2}(v^2/2)^2 C_3^2 |y|^{2\lambda - 1}],$$

with two relaxation times T_s and $T_{R/2}$. If the Maxwellian width has only one relaxation time ($C_3 = 0$), we find $F - 1 > 0 (< 0)$ in the expansion case $y < 0$ or $\lambda < 1$ or crit. > 0 (in the contraction case $y > 0$ or $\lambda \geqslant 1$ or crit. $\leqslant 0$). Due to the positivity constraint $F > 0$, for $\lambda < 1$ we find that the maximum of these $F - 1 > 0$ values decreases when λ increases and practically we observe that the effect occurs only for $\lambda < 0.75$. If the Maxwellian width has two relaxation times T_s, $T_R/2$, for important T_R contributions we find in the whole $0 < \lambda < 2$ interval that the effect is not present.

Is it possible to improve the properties of the present one-dimensional spatial solution? Perhaps we can define other spatial boundaries at the x values where $F(v,x,t=0)$ begins to violate positivity and require supplementary boundary conditions.[13]

ACKNOWLEDGMENTS

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APPENDIX A: COMPATIBILITY $J_{0,xt} - J_{0,tx} = 0$

We write the equations for $J_{0,x}, J_{0,t}$

$$J_{0,t} = -b^{-1} N_{0x} + J_0 \nu(\tau_1 - \tau_0) N_0, \quad J_{0,x} = N_{0,t}. \tag{A1}$$

Define $\varphi = \nu(\tau_1 - \tau_0)$, $N_0(x,t) = \overline{N}_0(t) + \overline{\alpha}_0(x) b^{-1/2}$, write the compatibility $J_{0,xt} = J_{0,tx} = 0$ or

$$N_{0,tt} - b^{-1} N_{0,xx} - \varphi N_0 N_{0,t} + \varphi J_0 N_{0,x} = 0, \tag{A2}$$

and eliminate J_0 by integrating (A1):

$$J_0(x,t) = J_0(x_0,t) + (x_0 - x)\overline{N}_{0,t} - (b^{-1/2})_t \int_{x_0}^{x} \overline{\alpha}_0(x')dx'.$$

Finally the compatibility condition can be written as a sum of $\overline{\alpha}_0(x)$ functionals such that the coefficients depend only on $b(t), \overline{N}_0, J_0(x_0,t)$:

$$\begin{aligned} 0 = {} & A(t) - \overline{\alpha}_{0,xx} b^{-3/2} + \overline{\alpha}_0 \varphi (b^{-1/2})_{tt} (\overline{N}_0 b^{-1/2})_t \\ & + \left(\overline{\alpha}_0^2 - \overline{\alpha}_0 \int_{x_0}^{x} \overline{\alpha}_0(x')dx'\right)(\varphi b^{-1/2})(b^{-1/2})_t \\ & + \varphi \overline{\alpha}_{0,x} b^{-1/2} J_0(x_0,t) + \varphi \overline{\alpha}_{0,x}(x_0 - x) b^{-1/2} \overline{N}_0(t), \end{aligned} \tag{A3}$$

$$A(t) = \overline{N}_{0,tt} - \varphi \overline{N}_0 \overline{N}_{0,t}.$$

Let us exclude the trivial cases for $\overline{\alpha}_0$. If $\overline{\alpha}_0 = \text{const}$, then we redefine $\overline{N}_0$, if $\overline{\alpha}_0 = \text{constant } x$ then in (A3) on the rhs when $x \to \infty$ we have a term $x^2 b^{-1/2} \varphi \partial_t b^{-1/2}$ which cannot be canceled. Otherwise $\overline{\alpha}_{0xx} \not\equiv 0$ and all x functions in (A3) are nontrivial. First, we must have $A(t) \equiv 0$ and we substitute the general solution written down in Sec. II: $\overline{N}_0 = C_2 \varphi^{-1}(1 - y)/(1 + y)$, $\lim_{t \to \infty} \overline{N}_{0,t}$, $\overline{N}_{0tt}$ being zero. For Maxwellian behavior when $t \to \infty$ we must have $b \to 1$, $b_t \to 0$ and from (2.4c'), $b_{tt} \to 0$. In (A4) we take the limit $t \to \infty$ and find

$$0 \equiv -\overline{\alpha}_{0,xx} + \overline{\alpha}_{0,x} \varphi J_0(x_0, \infty). \tag{A4}$$

Still requiring asymptotic Maxwellian behavior for the distribution function, $J_0(x_0, \infty)$ cannot be infinite. If it is zero we are back with $\overline{\alpha}_0 = \text{const}_1 + x\ \text{const}_2$. Otherwise $\overline{\alpha}_0 = \text{const}_1 + e^{x\ \text{const}_2}$. Substituting into (A4) we have, when $x \to \infty$, a term $x\, e^{x\ \text{const}_2}$ which cannot be canceled. In conclusion the only possibility is $\overline{\alpha}_{0x} \equiv 0$.

APPENDIX B: LAGUERRE EXPANSION FOR THE SOLUTION (1.2a)

We recall

$$F=\Delta^{-3/2}\exp\left(-\frac{v^2}{2}(\Delta^{-1}-1)\right)\left[\Delta\left(\frac{1-y}{1+y}\right)+\frac{y}{\lambda}\left(\frac{1}{2}\partial_y\Delta-\frac{v^2}{2}\frac{\partial_y\Delta}{\Delta}\right)+v(x_0-x)\frac{2C_2y}{(1+y)^2}\right], \quad \text{(A5)}$$

$$\exp\left(-\frac{v^2}{2}(\Delta^{-1}-1)\right)=\Delta^{1\pm1/2}\sum(1-\Delta)^n L_n^{\pm1/2}\left(\frac{v^2}{2}\right), \quad |\Delta-1|<1, \quad \text{(A6)}$$

$$\exp\left(-\frac{v^2}{2}(\Delta^{-1}-1)\right)\left(\frac{1}{2}\partial_y\Delta-\frac{v^2}{2}\frac{\partial_y\Delta}{\Delta}\right)=\Delta^{3/2}\sum n(1-\Delta)^{n-1}\partial_y\Delta L_n^{(-1/2)}\left(\frac{v^2}{2}\right), \quad \text{(A7)}$$

and substituting into F we find the Laguerre expansion

$$F=\sum L_n^{(-1/2)}\left(\frac{v^2}{2}\right)\left[\left(\frac{1-y}{1+y}\right)(1-\Delta)^n+\frac{y}{\lambda}n(1-\Delta)^{n-1}\partial_y\Delta\right]+2C_2\frac{vy}{(1+y)^2}(x_0-x)\sum L_n^{1/2}\left(\frac{v^2}{n}\right)(1-\Delta)^n. \quad \text{(A8)}$$

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Infinitesimal transformations about soliton solutions of sine–Gordon and modified Korteweg–de Vries equations

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Infinitesimal transformations about n-soliton solutions of sine-Gordon and modified Korteweg–de Vries equations are obtained using respective Bäcklund transformations. We also obtain the eigenfunctions of corresponding generalized Zakharov–Shabat systems.

I. INTRODUCTION

Nonlinear evolution equations (NLEE) like the Korteweg–de Vries (KdV), modified Korteweg–de Vries (MKdV), sine–Gordon (SG), and cubic Schrödinger have been extensively studied for the past 15 years or so. Associated with these nonlinear equations are certain eigenvalue equations involving linear differential operators. Such a linear eigenvalue system is the Zakharov–Shabat[1] (ZS) two component equations and their generalizations given by Ablowitz *et al.* (AKNS).[2] These linear systems are of primary importance in the solution of the above nonlinear equations via the inverse scattering transform method wherein one constructs the soliton solutions of the NLEE starting with asymptotic forms of solutions of the linear system of equations.

We can ask the reverse question: Whether it is possible to obtain in a simple way solutions of the linear equations knowing the soliton solutions of the NLEE. The answer turns out to be yes.[3] One of the aims of the present paper is to obtain the solutions of SG and MKdV equations. The above search for solutions is intimately tied with the solution of the problem of obtaining the infinitesimal transformations (IT's) about n-soliton solutions of the SG and MKdV equations. These IT's are themselves closely linked with the conservation laws for the above NLEE systems.[4] The IT's are given in terms of squares of eigenfunctions of the generalized ZS systems.[5,6] Once the IT's are obtained, we can just read off the solutions of the generalized ZS systems.

The content of the present paper is as follows. In Sec. II we restrict ourselves to the SG equation. In Sec. II A, we set up a differential equation of the IT's using the Bäcklund transformation. In Sec. II B, this is solved explicitly to get an IT about a one-soliton solution. This IT is found to be in the form of a sum of squares of the eigenfunctions of the corresponding generalized ZS equations. Using this, one constructs an IT, y_n, about the n-soliton solution σ_n. In II C, we show that the IT's so obtained are eigenfunctions of the operators $T(\sigma)$ and that one can also generate an infinite number of IT's about a given soliton solution using these operators $T(\sigma)$.

In Sec. III, we obtain analogous results for the MKdV equation.

II. SINE–GORDON EQUATION

We begin by defining[3,4] an infinitesimal transformation (IT) about any solution $u(x,t)$ of the equation

$$u_t = K(u), \tag{2.1}$$

as a function $y(x,t)$ such that $u(x,t) + \epsilon y(x,t)$, $\epsilon \ll 1$ is also a solution of Eq. (2.1). Here K is, in general, a nonlinear operator.

A. Differential equation for IT

The SG equation, in light-cone coordinates, is

$$\sigma_{xt} = \sin\sigma, \tag{2.2}$$

where the subscripts denote partial differentiation. Using the definition of IT, we find that IT, $y(x,t)$, about $\sigma(x,t)$ satisfies the differential equation

$$y_{xt} = y\cos\sigma. \tag{2.3}$$

We now relate the IT's about two different solutions $\sigma(x,t)$ and $\sigma'(x,t)$ using the Bäcklund transformation (BT). The first half of the BT for the SG equation is[7]

$$\sigma'_x + \sigma_x = 2a\sin((\sigma' - \sigma)/2). \tag{2.4}$$

If $z(x,t)$ is an IT about $\sigma'(x,t)$ and $y(x,t)$ is an IT about $\sigma(x,t)$, then using Eq. (2.4) we find that $z(x,t)$ and $y(x,t)$ are related by the equation

$$z_x + y_x = a\cos((\sigma' - \sigma)/2)\cdot(z - y). \tag{2.5}$$

The second half of the BT does not yield any new information and consequently we do not consider it here.

Equation (2.5) is the basic equation from which the explicit form of the IT's is derived. To carry through this program we begin with the trivial solution $\sigma(x,t) = 0$ of Eq. (2.2). For this solution Eq. (2.3) reduces to

$$y_{xt} = y. \tag{2.6}$$

The plane wave solutions of Eq. (2.6) are

$$y^k = \exp[\pm 2i(kx - \omega t)], \tag{2.7}$$

with the dispersion relation $\omega k = \frac{1}{4}$. Denoting an IT about $\sigma(x,t) = 0$ by y_0^k, we have

$$y_0^k = \exp[\pm 2i(kx - \omega t)]. \tag{2.8}$$

We now use Eq. (2.5) repeatedly starting with $\sigma(x,t) = 0$ and $y_0^k(x,t)$ given by Eq. (2.8) to obtain an IT about $\sigma_n(x,t)$.

B. IT about an n-soliton solution

Equation (2.5) may be written for the soliton solutions as

$$y_{nx} + y_{(n-1)x} = a_n\cos((\sigma_n - \sigma_{n-1})/2)\cdot(y_n - y_{n-1}). \tag{2.9}$$

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Here $y_i(x,t)$ is an IT about an i-soliton solution, $\sigma_i(x,t)$. From Eq. (2.9) is follows that $y_1(x,t)$ satisfies the equation

$$y_{1x} + y_{0x} = a_1 \cos((\sigma_1 - \sigma_0)/2) \cdot (y_1 - y_0).$$

Hence,

$$y_{1x}^k + e^{\pm 2ikx} = a_1 \cos(\sigma_1/2)(y_1^k - e^{\pm 2ikx}). \tag{2.10}$$

Here and subsequently we drop the term $e^{\mp 2i\omega t}$ in t, since it is always present. The one-soliton solution of the SG equation is[8]

$$\sigma_1(x,t) = 4 \tan^{-1} e^{\mp 2\theta_1}, \quad \theta_1 = -\eta_1 x - t/4\eta_1 + \theta_{10}, \tag{2.11}$$

where η_1 and θ_{10} are constants, the upper (lower) sign in Eq. (2.11) and in subsequent equations refers to soliton (antisoliton) solutions. Using Eq. (2.11), we solve Eq. (2.10) to get

$$y_1^k = [1/(k^2 + \eta_1^2)]\,[(\psi_1'(1))^2 + (\psi_2'(1))^2], \tag{2.12a}$$

or

$$y_1^k = [1/(k^2 + \eta_1^2)]\,[(\phi_1'(1))^2 + (\phi_2'(1))^2], \tag{2.12b}$$

where

$$\psi_1'(1) = e^{ikx}(\mp \eta_1 \sin(\sigma_1/2)), \tag{2.13a}$$

$$\psi_2'(1) = e^{ikx}(ik \pm \eta_1 \cos(\sigma_1/2)), \tag{2.13b}$$

and

$$\phi_1'(1) = e^{-ikx}(ik \mp \eta_1 \cos(\sigma_1/2)), \tag{2.14a}$$

$$\phi_2'(1) = e^{-ikx}(\mp \eta_1 \sin(\sigma_1/2)), \tag{2.14b}$$

with a_1 set equal to $\pm 2\eta_1$. The sets $\{\psi_1'(1),\psi_2'(1)\}$ and $\{\phi_1'(1),\phi_2'(1)\}$ satisfy the generalized ZS equations or ZS/AKNS equations[2]

$$\begin{aligned} v_{1x} + i\zeta v_1 &= q v_2, \\ v_{2x} - i\zeta v_2 &= -q v_1, \end{aligned} \tag{2.15}$$

$$q = -\frac{1}{2}\frac{\partial \sigma}{\partial x} = \mp 2\eta_1 \sin\frac{\sigma_1}{2}, \quad \zeta = k. \tag{2.16}$$

The $\psi_i'(1)$'s and $\phi_i'(1)$'s are linearly independent solutions of the ZS/AKNS equations. The argument 1 indicates that these functions refer to one-soliton or one-antisoliton solutions.

The above IT about a one-soliton was obtained by actual integration. To obtain an IT about a two-soliton solution σ_2, using the above method, requires the explicit form for solution σ_2. The latter is quite complicated and consequently the integration becomes very involved. It is, however, possible to obtain an IT about a two-soliton solution without really knowing the explict form of σ_2. We just conjecture it and verify that our conjecture satisfies all the requisite properties.

We conjecture that an IT about a two-soliton solution $\sigma_2(x,t)$ is

$$y_2^k = \left[\prod_{i=1}^{2}(k^2 + \eta_i^2)\right]^{-1}[(\psi_1'(2))^2 + (\psi_2'(2))^2], \tag{2.17a}$$

or

$$y_2^k = \left[\prod_{i=1}^{2}(k^2 + \eta_i^2)\right]^{-1}[(\phi_1'(2))^2 + (\phi_2'(2))^2], \tag{2.17b}$$

where

$$\psi_1'(2) = [\psi_1'(1)(-ik \pm \eta_2 \cos[(\sigma_2 - \sigma_1)/2]) + \psi_2'(1)(\mp \eta_2 \sin[(\sigma_2 - \sigma_1)/2])], \tag{2.18a}$$

$$\psi_2'(2) = [\psi_1'(1)(\pm \eta_2 \sin[(\sigma_2 - \sigma_1)/2]) + \psi_2'(1)(ik \pm \eta_2 \cos[(\sigma_2 - \sigma_1)/2])], \tag{2.18b}$$

and

$$\phi_1'(2) = [\phi_1'(1)(ik \mp \eta_2 \cos[(\sigma_2 - \sigma_1)/2]) \pm \phi_2'(1)(\eta_2 \sin[(\sigma_2 - \sigma_1)/2])], \tag{2.19a}$$

$$\phi_2'(2) = [\phi_1'(1)(\mp \eta_2 \sin[(\sigma_2 - \sigma_1)/2]) - \phi_2'(1)(ik \pm \eta_2 \cos[(\sigma_2 - \sigma_1)/2])]. \tag{2.19b}$$

We now convince ourselves that Eq. (2.17) is indeed an IT about $\sigma_2(x,t)$. For this purpose we can explictly verify that $(\psi_1'(2),\psi_2'(2))$ and $(\phi_1'(2),\phi_2'(2))$ satisfy Eq. (2.15) with

$$q = -\frac{1}{2}\frac{\partial \sigma_2}{\partial x} = \left(\mp 2\eta_2 \sin\frac{\sigma_2 - \sigma_1}{2} \pm 2\eta_1 \sin\frac{\sigma_1}{2}\right), \tag{2.20}$$

which is the "field" appropriate for two solitons (upper sign) or two antisolitons (lower sign). Also Eqs. (2.17a) and (2.17b) satisfy Eq. (2.9) with $y_n = y_2$, IT about a two-soliton solution σ_2, and $y_{n-1} = y_1$, IT about a one-soliton solution σ_1. It is now straightforward to generalize and obtain an IT about an n-soliton solution σ_n. It is

$$y_n^k = \left[\prod_{i=1}^{n}(k^2 + \eta_i^2)\right]^{-1}[(\psi_1'(n))^2 + (\psi_2'(n))^2], \tag{2.21a}$$

or

$$y_n^k = \left[\prod_{i=1}^{n}(k^2 + \eta_i^2)\right]^{-1}[(\phi_1'(n))^2 + (\phi_2'(n))^2], \tag{2.21b}$$

where $\{\psi_1'(n),\psi_2'(n)\}$ and $\{\phi_1'(n),\phi_2'(n)\}$ satisfy the ZS/AKNS equations with

$$q = -\frac{1}{2}\frac{\partial \sigma_n}{\partial n} = \mp\left[2\eta_n \sin\frac{\sigma_n - \sigma_{n-1}}{2} - 2\eta_{n-1} \times \sin\frac{\sigma_{n-1} - \sigma_{n-2}}{2} + \cdots + (-)^{l-1} 2\eta_1 \sin\frac{\sigma_1}{2}\right], \tag{2.22}$$

where l stands for the l th term in the bracket and

$$\psi_1'(n) = \psi_1'(n-1)(-ik \pm \eta_n \cos[(\sigma_n - \sigma_{n-1})/2]) + \psi_2'(n-1)(\mp \eta_n \sin[(\sigma_n - \sigma_{n-1})/2]), \tag{2.23a}$$

$$\psi_2'(n) = \psi_1'(n-1)(\pm \eta_n \sin[(\sigma_n - \sigma_{n-1})/2]) + \psi_2'(n-1)(ik \pm \eta_n \cos[(\sigma_n - \sigma_{n-1})/2]), \tag{2.23b}$$

and

$$\phi_1'(n) = \phi_1'(n-1)(ik \mp \eta_n \cos[(\sigma_n - \sigma_{n-1})/2]) + \phi_2'(n-1)(\pm \eta_n \sin[(\sigma_n - \sigma_{n-1})/2]), \tag{2.24a}$$

$$\phi_2'(n) = \phi_1'(n-1)(\mp \eta_n \sin[(\sigma_n - \sigma_{n-1})/2]) + \phi_2'(n-1)(-ik \mp \eta_n \cos[(\sigma_n - \sigma_{n-1})/2]). \tag{2.24b}$$

Needless to say, one verifies that Eq. (2.21) satisfies Eq. (2.9) with the ψ's and ϕ's satisfying the ZS/AKNS equations with q given by Eq. (2.22). Once again, the upper (lower) sign in

the above equations (2.22)–(2.24) refer to an n-soliton (n-antisoliton) system.

We write

$$\psi'(j)=\begin{pmatrix}\psi_1'(j)\\ \psi_2'(j)\end{pmatrix} \quad \text{and} \quad \phi'(j)=\begin{pmatrix}\phi_1'(j)\\ \phi_2'(j)\end{pmatrix}.$$

Then the eigenfunctions

$$\psi(j)=\frac{\psi'(j)}{\Pi_{l=1}^{j}(ik-\eta_l)} \quad \text{and} \quad \phi(j)=\frac{\phi'(j)}{\Pi_{l=1}^{j}(ik-\eta_l)}$$

have the standard asymptotic behaviors

$$\psi(j)\to\begin{pmatrix}0\\ 1\end{pmatrix}e^{ikx}, \quad x\to+\infty; \quad \phi(j)\to\begin{pmatrix}1\\ 0\end{pmatrix}e^{-ikx}, \quad x\to-\infty.$$

The localized solutions of the ZS/AKNS equations are obtained for the values of k which correspond to the poles of transmission coefficients. For a SG equation these values of k either lie on the imaginary axis or are symmetrically placed about the imaginary axis. Since we are restricting ourselves here to purely soliton (or antisoliton) solutions the corresponding values of k lie on the imaginary axis only. For an n-soliton system there are precisely n such imaginary values. We take them to be

$$k=i\kappa_r, \quad r=1,2,\ldots,n.$$

Even in this case, Eq. (2.21) is an IT about an n-soliton $\sigma_n(x,t)$.

C. Generator of an infinite set of IT's about a given soliton solution

In the preceding subsection, starting with an IT about the zero-soliton solution, we have successively obtained IT's about the 1-,2-,..., n-soliton solutions in terms of the sum of squares of eigenfunctions of the corresponding ZS/AKNS equations. It is well known[4] that for a *given* $\sigma(x,t)$, Eq. (2.3) has an infinite number of solutions. We now obtain a recurrence formula[9] for an IT about a given soliton solution and thus obtain an infinite number of IT's about a specific soliton solution. In the process we also obtain an eigenoperator[10] for the IT's y_n^k.

For the above purpose we start with the eigenvalue equations[2]

$$L\begin{pmatrix}\psi_1^2\\ \psi_2^2\end{pmatrix}=\zeta\begin{pmatrix}\psi_1^2\\ \psi_2^2\end{pmatrix}, \tag{2.25a}$$

$$L^{A}\begin{pmatrix}\phi_2^2\\ -\phi_1^2\end{pmatrix}=\zeta\begin{pmatrix}\phi_2^2\\ -\phi_1^2\end{pmatrix}, \tag{2.25b}$$

where L and L^A are given in Ref. 2. Using Eqs. (2.25) and (2.15) we get

$$\begin{aligned}T_\psi(\sigma)(\psi_1^2+\psi_2^2)&\equiv\frac{1}{4}\left[-\frac{\partial^2}{\partial x^2}+\sigma_x\int_x^\infty dx_1\,\sigma_{x_1}\frac{\partial}{\partial x_1}\right](\psi_1^2+\psi_2^2)\\&=k^2(\psi_1^2+\psi_2^2),\end{aligned} \tag{2.26a}$$

$$\begin{aligned}T_\phi(\sigma)(\phi_1^2+\phi_2^2)&\equiv\frac{1}{4}\left[\frac{\partial^2}{\partial x^2}+\sigma_x\int_{-\infty}^x dx_1\,\sigma_{x_1}\frac{\partial}{\partial x_1}\right](\phi_1^2+\phi_2^2)\\&=-k^2(\phi_1^2+\phi_2^2).\end{aligned} \tag{2.26b}$$

It may be emphasized that the σ appearing in the above equations is the same σ for which $\{\psi_1,\psi_2\}$ and $\{\phi_1,\phi_2\}$ are solutions of the ZS/AKNS equations. Specifically,

$$T_\psi(\sigma_n)y_{n,\psi}^k=k^2y_{n,\psi}^k, \tag{2.27a}$$

$$T_\phi(\sigma_n)y_{n,\phi}^k=-k^2y_{n,\phi}^k, \tag{2.27b}$$

where $y_{n,\psi}^k$ and $y_{n,\phi}^k$ are IT's about an n-soliton solution expressed in terms of ψ's and ϕ's, respectively.

To obtain the recursion relation we first note that if Y is a solution of Eq. (2.3) with a given σ, then $T_\phi(\sigma)Y$ and $T_\psi(\sigma)Y$ are also solutions of Eq. (2.3) with the same σ.

The above result enables us to generate new IT's about a given $\sigma(x,t)$. To be specific, consider an n-soliton solution $\sigma_n(x,t)$. We already have two distinct IT's about the n-solition solution given by $y_{n,\psi}^k$ and $y_{n,\phi}^k$. From each of these we can generate an infinity of new IT's. For purposes of illustration consider $y_{n,\psi}^k$. We operate on this by $T_\phi(\sigma_n)$. The resulting function is then an IT about σ_n in view of the statement made in the preceding paragraph. Thus $Y_1=T_\phi(\sigma_n)y_{n,\psi}^k$ is an IT. We now operate on Y_1 with $T_\phi(\sigma_n)$, which would then give a new IT Y_2. In this way an infinite set of IT's can be generated.

III. MODIFIED KORTEWEG–DE VRIES EQUATION

As the method of obtaining IT's about an n-soliton solution in this case is exactly the same as for the SG equation, we limit ourselves by just quoting the main results. The MKdV equation is

$$q_t+6q^2q_x+q_{xxx}=0. \tag{3.1}$$

If $q=-W_x$ then

$$W_t+2W_x^3+W_{xxx}=0. \tag{3.2}$$

If $y(x,t)$ is an IT about a solution $W(x,t)$ of Eq. (3.2), then $y(x,t)$ satisfies the equation

$$y_t+6W_x^2y_x+y_{xxx}=0. \tag{3.3}$$

We use Eq. (3.3) to obtain an IT about the trivial solution $W(x,t)=0$.

The first half of the BT for Eq. (3.2) is[11]

$$W_x+W_x'=2\eta\sin(W-W'), \tag{3.4}$$

and gives the following equation connecting the two IT's $z(x,t)$ and $y(x,t)$ about the solutions $W'(x,t)$ and $W(x,t)$, respectively:

$$z_x+y_x=2\eta\cos(W-W')\cdot(y-z). \tag{3.5}$$

We find that the result for an IT about an n-soliton solution of a MKdV equation is

$$y_{n,\psi}^k=\left[\prod_{i=1}^{n}(k^2+\eta_i^2)\right]^{-1}[(\psi_1'(n))^2+(\psi_2'(n))^2], \tag{3.6a}$$

or

$$y_{n,\phi}^k=\left[\prod_{i=1}^{n}(k^2+\eta_i^2)\right]^{-1}[(\phi_1'(n))^2+(\phi_2'(n))^2], \tag{3.6b}$$

where

$$\begin{aligned}\psi_1'(n)=\{\psi_1'(n-1)[&-ik-\eta_n\cos(W_n-W_{n-1})]\\&+\psi_2'(n-1)[\eta_n\sin(W_n-W_{n-1})]\},\end{aligned} \tag{3.7a}$$

$$\psi_2'(n) = \{ -\psi_1'(n-1)[\eta_n \sin(W_n - W_{n-1})] + \psi_2'(n-1)[ik - \eta_n \cos(W_n - W_{n-1})]\}, \tag{3.7b}$$

and

$$\phi_1'(n) = \{\phi_1'(n-1)[ik + \eta_n \cos(W_n - W_{n-1})] - \phi_2'(n-1)[\eta_n \sin(W_n - W_{n-1})]\}, \tag{3.8a}$$

$$\phi_2'(n) = \{\phi_1'(n-1)[\eta_n \sin(W_n - W_{n-1})] - \phi_2'(n-1)[ik - \eta_n \cos(W_n - W_{n-1})]\}. \tag{3.8b}$$

Here $\{\psi_1'(n),\psi_2'(n)\}$ and $\{\phi_1'(n),\phi_2'(n)\}$ satisfy Eq. (2.15) with $\zeta = k$ and

$$q = [2\eta_n \sin(W_n - W_{n-1}) - 2\eta_{n-1} \sin(W_{n-1} - W_{n-2}) + \cdots + (-)^{l-1} 2\eta_1 \sin(W_1/2)],$$

where, as before in Eq. (2.22), l stands for the l th term in the bracket. The IT's $y^k_{n,\phi}$ and $y^k_{n,\psi}$ satisfy the following eigenvalue equations:

$$T_\psi(W) y^k_{n,\psi} = k^2 y^k_{n,\psi}, \tag{3.9a}$$

$$T_\phi(W) y^k_{n,\phi} = -k^2 y^k_{n,\phi}, \tag{3.9b}$$

where the operators are given by

$$T_\psi(W) = \left[-\frac{1}{4}\frac{\partial^2}{\partial x^2} + W_x \int_x^\infty dx_1 \, W_{x_1} \frac{\partial}{\partial x_1} \right], \tag{3.10a}$$

$$T_\phi(W) = \left[\frac{1}{4}\frac{\partial^2}{\partial x^2} + W_x \int_\infty^x dx_1 \, W_{x_1} \frac{\partial}{\partial x_1} \right]. \tag{3.10b}$$

These operators can be used to generate new IT's about a given solution in the same manner as described for the SG equation.

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Bifurcations in the slow-fluctuation technique

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In the slow-fluctuation method, the bifurcations between solutions of a conservative, autonomous, nonlinear oscillatory system can be found by an essentially algebraic, systematic study of constant-amplitude motions and root parities. This is shown for simple systems with sufficient detail to indicate the extensions needed in the treatment of more complex systems. An example from celestial mechanics is given.

I. INTRODUCTION

We have developed the main aspects of the slow-fluctuation method in two previous papers, hereafter referred to as SF[1] and STAB.[2] One of our more important results was that in conservative, autonomous, nonlinear oscillatory systems of several degrees of freedom (d.f.'s) there are generally no purely periodic motions; instead, a plethora of constant-amplitude (c-a) motions usually exists. These as well as all variable-amplitude motions can be calculated by means of a single polynomial, called $f(\bar{p}_1)$.

In a third paper, hereafter referred to as PAR,[3] we introduced the notion of the parity of the roots of f. Being a discrete attribute, it furnishes many technical advantages, much as if the tools of proof had been augmented by another conservation theorem. In PAR we showed specifically how root parity helped to develop a natural, mathematical classification of all solutions, and to explore the subtleties of phase behavior in the dynamical neighborhood of c-a solutions.

We now turn to solutions of variable amplitude. In practice, one should certainly like to know how to classify them, quickly and simply if possible, according to criteria which in a commonsense way emphasize outstanding and important features. Given the variety of possible systems, it is as well to glance at a few of them to see what notions of "importance" are feasible.

We have elsewhere published a study[4] of a system with two d.f.'s, coupling of $q_1^2 q_2^2$ type, and exact resonance $\omega_1 = \omega_2$. All its solutions were bounded, and the variable-amplitude ones fell into three neatly distinct classes, even–even, even–odd, and odd–odd (cf. PAR, Sec. IV B), separated by unstable c-a motions at certain critical parameter values. In conformity with current usage with regard to conspicuous, qualitative changes of behavior, we spoke of "bifurcation" values. There were two such bifurcations: one with respect to an integration constant (in fact, the c_1 type described in Fig. 1 below), the other with respect to a system parameter which allows either the even–even or the odd–odd class but not both. On the other hand, consider the elastic pendulum[5]: amidst the richness of its solutions, including the stable cup and cap c-a motions, all change is smooth and gradual except for the rather obvious bifurcation where the suspension motion becomes unstable and the class of "nontrivial $c_1 = 0$" motions appears suddenly. Yet, when in the elastic-pendulum Hamiltonian we make one mass negative, as we do below in Sec. V, we always find four sharply distinct classes of motions bordered by c-a motions and by exceptional low-amplitude motions in different ways. In either of these cases, somewhat similar to Ref. 4, there are system parameter bifurcations in the form of sign and parity changes.

It would be idle to conclude that "apparently anything can happen"; it rather seems certain that the c-a motions should be taken as the skeleton of classification. This is a truism in abstract phase space, but it was not obvious that in real situations, too, the types of actual motions which most readily meet the eye should be closely related to c-a motions in various ways.

In the present paper we follow this lead. The parameters determining the c-a motions are, of course, exactly the integration constants $\alpha_2,\ldots,\alpha_n, E$ which we have to employ anyway (see PAR); hence their bifurcation values must be sought. [Phase shifts and a shift in the zero of time cannot cause any qualitative differences between representative solutions and others (c.f. PAR, Sec. II), hence they can be entirely left out of the bifurcation context.] We find that when we look at the simplest cases they exhibit characteristics which deserve to be defined formally, and are susceptible to generalization. We also find that root parity is an indispensable tool, and that skew roots of the first order need to be carefully considered where they exist, as we did in many previous instances.

Thus we outline a corpus of general theorems, parity arguments, and procedural rules which are adequate to deal with the simpler systems, and point the way toward the treatment of more complex systems. In the interest of brevity, we have strictly confined ourselves to physical, oscillatory systems (as defined in PAR, Sec. III D). We have also left out momentum-dependent couplings because the definition of root parity in such systems seems to lead to complications. As for system parameter bifurcations, we have not touched them in any generality because we are doubtful that there are any simple, clear types of them beyond the transparent parity-switch and sign-change cases mentioned above. Lastly, we emphasize that we say nothing about *quantitative* aspects of classification such as amplitude modulation ranges; the calculation of the roots of f is an algebra-

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ic and/or numerical task rather different from the *qualitative* one that we pursued.

II. THE c_1 BIFURCATIONS

A. The parameter c_1

The polynomial $f(\bar{p}_1)$ has been defined in SF, Eq. (3.9). We rewrite it here with some adaptations introduced in PAR, Eqs. (3.1) and (3.2) as

$$f(\bar{p}_1) = \overline{F}(\bar{p}_1,\alpha)^2 - \overline{P}(\bar{p}_1,\alpha,E)^2,$$
$$\overline{P} = c_1 - (\epsilon + b_1)\bar{p}_1 - \cdots - b_m \bar{p}_1^m, \tag{2.1}$$
$$c_1 = E - \sum_2^n \omega_i \alpha_i - b_0,$$

where $\overline{F}$ is given explicitly in PAR, Eq. (3.5), and the b_i are polynomials in system parameters and the α's (see STAB, Sec. III A).

Any root of f satisfies

$$\overline{P} = +\overline{F} \quad \text{and/or} \quad \overline{P} = -\overline{F}. \tag{2.2}$$

Thus, at a fixed set of integration constants $\alpha_2,\ldots,\alpha_n$, E all roots of f can be obtained graphically from the intersections of curves representing the two sides of Eqs. (2.2); for formal examples, see PAR, Sec. III D, while an application to plasma physics can be found in Ref. 6. The constant E occurs in Eqs. (2.1) in only one place, in the constant term c_1 of polynomial $\overline{P}$; therefore a variation of E at constant α will only shift the $\overline{P}$ curve vertically while the $\pm\overline{F}$ curves remain fixed. The accompanying variation of the roots of f then becomes especially transparent. At constant α, it makes no difference whether we vary E or c_1, and because of some formal conveniences we choose the latter. Thus we begin with a discussion of the roots of f as c_1 is varied at constant α.

Following the detailed exposition in PAR, a root of f is called even or odd, respectively, if either the first or the second Eq. (2.2) is fulfilled. If both are fulfilled, the root is called skew; then (and only then) $\overline{F} = 0$ holds, and with it $\overline{P} = 0$.

Thus, a skew root $\overline{P} = \Gamma$ obeys the equation $\overline{F}(\Gamma,\alpha) = 0$, which does not contain E, or c_1. In physical systems $\bar{p}_1$ is real, and therefore we are primarily interested in real roots Γ. In an oscillatory system, Γ must also lie in a certain non-negative interval, the domain of $\bar{p}_1$; see PAR, Sec. III D for detail. A solution of $\overline{F}(\Gamma,\alpha) = 0$ can be a first-order skew root of f only in systems which permit exceptional low-amplitude conditions; it can be a second-order skew root of f at any given set of values $\alpha_2,\ldots\alpha_n$ provided c_1 is chosen right, although this value of c_1 does not necessarily correspond to a physically possible system energy; and it will in general not be a higher-order root of f unless the α's have certain particular values (and/or unless system parameters have special values, as in STAB, Fig. 5, where the triple skew root at the origin requires exact resonance $\epsilon = 0$).

Alternatively, consider a root which is not skew. It requires an intersection of $\overline{P}$ with $\pm\overline{F}$ at $\overline{F} \neq 0$; this may be a simple crossing of two curves, or it may be a contact of possibly high order and then the root is multiple. In the latter case, some special value of c_1 is required. If the domain of $\bar{p}_1$ is finite, all this is easy to see. Since $\overline{P}$ and $\overline{F}$ are continuous and smooth over the domain, and $\overline{F} = 0$ holds at both endpoints, we can always find a c_1 such that $\overline{P}$ intersects the $\pm\overline{F}$ curves, and another c_1 such that there is no intersection; hence there exists an intermediate value where the curves touch. This contact will normally be of the second order, but at particular values of the α's (and/or system parameters) which yield the right curve shapes it can be of higher order. With a half-infinite domain, particular values of the α's (and parameters) will generally be required even for second-order contact, in addition to the right c_1.

It emerges from this survey that at an *arbitrary* set of α values we may normally expect the physically relevant roots of f to be single and of definite parity. Keeping the α's fixed, we may often expect to find second-order roots by varying c_1, but higher-order roots generally require special values of the α's (and/or system parameters) in addition to special values of c_1. We arrange the following discussions accordingly, with the α's fixed in one instance and variable in the other, and omitting explicit mention of system parameters which are always assumed fixed.

B. Discontinuous change of amplitude modulation

Consider a set of fixed α values such that there can be more than two real, single roots of f in the domain of $\bar{p}_1$. Figure 1(a) sketches a typical case, with amplitude modulation between R_1 and R_2. Now vary c_1 through some interval. Since f depends on c_1 in a continuous way, only continuous deformations of the graph of f are possible. It can happen, amongst other things, that a third root R_3 approaches R_2 and at a certain value $c_1 = c_1^*$ coalesces with it, as in Fig. 1(b). Moreover, it can happen that under further change of c_1 the double root $R_2 = R_3$ becomes complex, and the graph of f lifts off the axis as in Fig. 1(c). The modulation range of $\bar{p}_1$ then increases abruptly to the next real root if there is one; or if there is none, monotonic growth $\bar{p}_1 \to \infty$ takes place ("explosive instability"). For examples, see Fig. 1 of Ref. 4, and also Ref. 6.

Owing to this discontinuous change of the modulation range, c_1^* constitutes a bifurcation value of c_1 where the system motion mutates from one type to another in phase space as well as in configuration space. In the literature,[8] such a critical value is often called a separatrix.

At the bifurcation, there is a double root $R_2 = R_3$ which cannot be skew. Indeed at any skew root $R = \Gamma$ we have

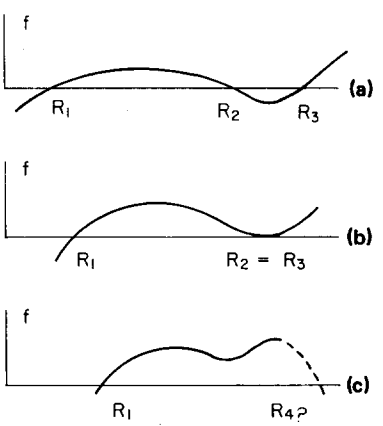

FIG. 1. Discontinuous change in the range of $\bar{p}_1(t)$ under monotonic change of c_1 at constant $\alpha_2,\ldots,\alpha_n$. (a) Modulation between R_1 and R_2; R_3 is near R_2 and has the same, definite parity. (b) Aperiodic modulation, or unstable Case (II) c-a motion, when $R_2 = R_3$ and $c_1 = c_1^*$. (c) Modulation between R_1 and some new turning point R_4, if any.

$\bar{F} = \bar{P} = 0$, and if we now vary c_1 at constant α, $\bar{F} = 0$ continues to hold at $\bar{p}_1 = \Gamma$ so that $f(\Gamma) < 0$ results according to Eq. (2.1); thus the minimum in the graph of f cannot lift off the axis as in Fig. 1(c) but must sink below it as in Fig. 1(a), and there is no abrupt change of the modulation range. Incidentally, a multiple root of definite parity, such as the $R_2 = R_3$ of Fig. 1, can never lie at an endpoint of the domain of $\bar{p}_1$; as discussed in PAR, Sec. III C, at an endpoint one or more (resonant) system amplitudes $\bar{p}_i$ must vanish, with them $\bar{F}$ vanishes, and hence any root at the endpoint is skew.

Clearly it is crucial that at the bifurcation the graph of f touches the $\bar{p}_1$ axis from above, or in equivalent terms, that the c-a motion at the multiple root be orbitally unstable. Conversely, whenever a multiple root of definite parity with an unstable c-a motion occurs in the domain of $\bar{p}_1$, it must lie in the interior of the domain as has just been remarked, and therefore it can separate adjacent modulation ranges. These two statements hold not only for the second-order root described by Fig. 1, but for roots of higher order as well. In any case, there will be contact between the $\bar{P}$ curve and the $\pm\bar{F}$ curves which graphically determine the roots. However, with a contact of higher order it is not generally possible to say how it must evolve under a vertical shift of the $\bar{P}$ curve, i.e., under a change of c_1; what kind of bifurcation results is, therefore, a matter for separate study in each such case. Still, for a second-order contact as in Fig. 1 a universal evolution does take place: if a change of c_1 first merges two simple intersections, then further change in the same direction will remove the contact altogether. We can therefore without restriction state the following theorem.

Theorem: Whenever in an oscillatory system orbitally unstable Case (II) c-a motion exists at a double root of $f(\bar{p}_1)$, the corresponding value $c_1 = c_1^*$ marks a bifurcation in the sense that under variation of c_1 at constant $\alpha_2,...\alpha_n$ a discontinuous change of amplitude modulation range occurs at $c_1 = c_1^*$.

C. Discontinuous change of phase function

It is possible for a root marking the end of a modulation range to change parity as c_1 is varied. According to PAR, Sec. III B, a change between even and odd involves an intermediary skew stage. This skew root could be of any order from the first up. We again leave cases of order three and higher for *ad hoc* investigation on account of their multifarious nature, and begin with the second order.

Figure 2(a) sketches a type case. Beyond the modulation range from R_1 to R_2, there is some other single root R_3, and between R_2 and R_3 there is a zero Γ of $\bar{F}$. It can happen that, as c_1 is varied, R_2 and R_3 approach each other, and at a value $c_1 = c_{1\Gamma}$ coalesce into a skew double root at Γ; see Fig. 2(b) and the Theorem of PAR, Sec. III D. Under further change of c_1 the graph of f cannot lift off the axis, as has been shown for any skew root in the previous section; the next stage is therefore as in Fig. 2(c).

The distinctive feature of the process is that the parities of R_2 and R_2' are necessarily opposite. For the proof, the unstable nature of the double root in Fig. 2(b) is again crucial. Suppose first that the zero of $\bar{F}$ at Γ is of the first order; then for instability the slope of $\bar{P}$ at Γ must be less than that of $\bar{F}$ in

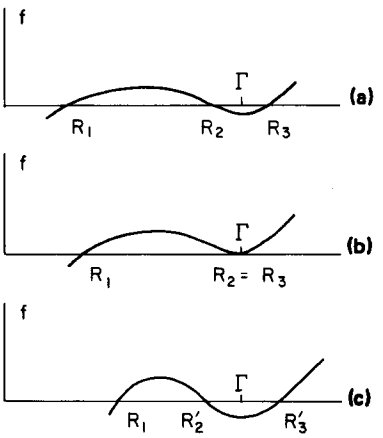

FIG. 2. The change in turning point near a second-order skew root Γ under monotonic change of c_1 at constant $\alpha_2,...,\alpha_n$. (a) Modulation between R_1 and R_2. (b) Aperiodic modulation, or unstable Case (I) c-a motion, when $R_2 = R_3$ and $c_1 = c_{1\Gamma}$. (c) Modulation between R_1 and R_2'; R_2 and R_2' have definite, opposite parities (proof by means of Fig. 3).

amount, according to STAB, Eq. (3.12). Graphically, the situation is as in Fig. 3, and it is seen at once that vertical shifts of the $\bar{P}$ curve through Γ produce roots R_2 and R_2' of opposite parities. Next suppose that Γ is a zero of $\bar{F}$ of order $\frac{3}{2}$ or higher. If $\bar{P}$ has a first-order zero at Γ when $c_1 = c_{1\Gamma}$, then the quoted criterion for instability cannot be met, but if $\bar{P}$ has a zero of second or higher order, then Γ is a root of $f = \bar{F}^2 - \bar{P}^2$ of order at least three, contrary to hypothesis. Hence the configuration of Fig. 3 is the only relevant one (except for mirror versions thereof). Incidentally, note that it makes no difference how the $\pm\bar{F}$ curves pass through Γ, as unbroken straight lines, or with kinks as for the "confluence of two exceptional low-amplitude conditions" of PAR, Fig. 5; in the latter case, interestingly enough, R_2 and R_3 are of the same parity (and so are R_2' and R_3').

The difference in parity implies that the combined phase function $\bar{q}_1(t)$ differs at R_2 and R_2' by an odd multiple of π. This discontinuity as c_1 passes through $c_{1\Gamma}$ is again properly a bifurcation, but it is conspicuous in phase space

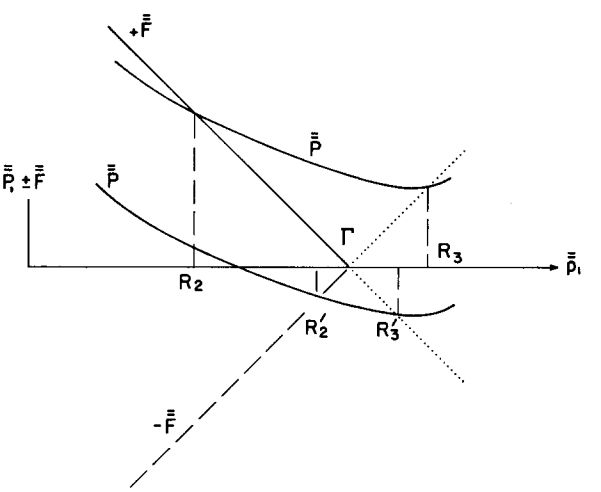

FIG. 3. The origin of the roots in Fig. 2. The $\pm\bar{F}$ curves have a first-order zero at Γ (which may lie at an endpoint of the domain of $\bar{p}_1$ or not). The $\bar{P}$ curve has a slope at Γ smaller in amount than that of $\bar{F}$, so that the c-a motion at the second-order skew root Γ is unstable. Under vertical shift through Γ, the $\bar{P}$ curves yield roots R_2 and R_2' of opposite parities.

rather than in configuration space. In particular, when one d.f. almost goes to rest, as in so many motions neighboring to an unstable Case (I), the variability of its phase is not reduced (cf. PAR, Sec. IV D, Theorem 5); thus, while nothing remains to be seen along the coordinate axis, the phase discontinuity at $c_{1\Gamma}$ stands out. How severe the discontinuity is in general can be appreciated from the fact that, as long as the parity of the lower modulation limit R_1 does not change at $c_{1\Gamma}$, too, the change in parity at the upper limit entails a change from a purely periodic phase function $\bar{q}_1(t)$ to one which steadily grows by π during any half-period of the modulation; cf. the Theorem in PAR, Sec. IV A.

In summary, we have Theorem 1.

Theorem 1: Whenever in an oscillatory system unstable Case (I) c-a motion exists at a double root of $f(\bar{p}_1)$, the corresponding value $c_1 = c_{1\Gamma}$ marks a phase space bifurcation in the sense that under variation of c_1 at constant $\alpha_2,...,\alpha_n$ a discontinuous change of the combined phase $\bar{q}_1(t)$ takes place at $c_1 = c_{1\Gamma}$; the change amounts to an odd multiple of π at the modulation turning point next to the skew root.

It remains to look briefly at a skew root Γ of the first order (which marks an "exceptional low-amplitude condition," and cannot lie in the interior of the domain; see SF and PAR). The origin of such a root is described in PAR, Fig. 1, where we read off at once that the sequence under variation of c_1 will be as in Fig. 4 (which has been drawn for Γ at a lower endpoint of the domain). Again there is a change of parity for the root which passes through the skew one, and a corresponding phase discontinuity at the critical $c_1 = c_{1\Gamma}$, just like the one discussed above. The phase behavior at the critical value, with the root configuration of Fig. 4(b), is not simple, cf. PAR, Sec. IV E, but this is not relevant to the occurrence of a bifurcation as c_1 passes through $c_{1\Gamma}$. In short, we have Theorem 2.

Theorem 2: Whenever in an oscillatory system a first-order skew root of $f(\bar{p}_1)$ lies at an endpoint of the domain of $\bar{p}_1$, the corresponding value $c_1 = c_{1\Gamma}$ marks a phase space bifurcation of the kind described in Theorem 1.

III. THE α BIFURCATIONS

The c_1 bifurcations at second-order roots are associated with instability because in the (phase space) neighborhood of an orbitally *stable* c-a motion there are by definition no discontinuities. The pertaining stability criteria STAB (3.12) and (3.14) do not contain E, and therefore do not depend on c_1. Thus, under a change of c_1 at constant α it cannot happen that a double root changes its stability character and thereby makes a c_1 bifurcation appear or disappear. It can happen under a change of $\alpha_2,...,\alpha_n$, though, and this is one example of an α bifurcation.

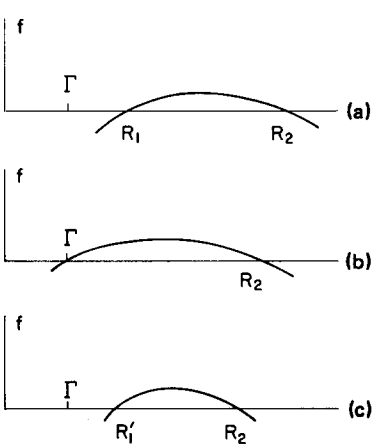

FIG. 4. The change in turning point near a first-order skew root Γ under monotonic change of c_1 at constant $\alpha_2,...,\alpha_n$. R_1 and R_1' have opposite parities (proof from PAR, Fig. 1).

A precisely analogous possibility exists at higher-order roots, but we shall again not treat these because of their variety.

The α's also determine the endpoints of the domain of $\bar{p}_1$; see PAR, Sec. III C. It can therefore happen that under a change of one or more α's there is an exchange of roles between the d.f.'s as to which of them will have its amplitude modulation reach right out to a domain endpoint. A typical case is the passing of an "exceptional low-amplitude condition" from one d.f. to another, with a confluence of two such conditions in between. The attendant phase space complexities are summarily described by Fig. 4 of PAR, and are exemplified by the much-discussed "case of the three interacting waves."[6] This, and analogous α bifurcations involving higher-order skew roots, whether intrinsically complicated or not, are very easy to spot in any given system. In the interest of brevity we abstain from further discussion of such fairly obvious cases.

At any rate, α bifurcations are associated with the appearance of orbital instabilities, just like c_1 bifurcations. For the summary description of the dynamical stability of an oscillatory system we introduced in STAB an n-dimensional space spanned by $\bar{p}_1,...,\bar{p}_n$. In this $\bar{p}$ space, any system motion is represented by a segment of some straight line having given slopes; for a c-a motion the segment contracts into a point. The points representing all c-a motions of a particular class form an object which we called the "existence surface" of the class; the existence surfaces for Cases (I) and (II) at second-order roots are reciprocal to each other in the sense that (essentially) one marks the stability boundaries on the other.

For the present purposes, we subject the $\bar{p}$ space to the linear transformation SF, Eqs. (3.3) and (3.4), to obtain a space spanned by $\bar{p}_1, \alpha_2,...,\alpha_n$. In this $\bar{p}_1, \alpha$ space any system motion is represented by a segment of some straight line parallel to the $\bar{p}_1$ axis. The transformation is affine and thus puts no strain on the imagination; all geometrical terms from STAB may be taken over verbatim.

Since we confine ourselves to α bifurcations associated with stability changes of second-order roots, we should find them in general at intersections of second-order existence surfaces for a Case (I) and a Case (II), where in general there will be found the c-a motions associated with (skew) roots of at least the third order. An exhaustive study of third-order roots looks uninviting, but somewhat contrary to expectations, general results of a helpful nature do exist. We present several of these in the following, both for practical application, and to show the way towards possible extensions.

A. Intersection of I- and II-existence surfaces

For a Case (I) c-a motion it is required that $\overline{P} = \overline{F} = 0$ and that $\overline{F}^2$ have a root of at least the seond order. For a Case

(II), at a root of definite parity, $\overline{\overline{P}} = \pm \overline{\overline{F}} \neq 0$ is required together with

$$\frac{\partial \overline{\overline{P}}}{\partial \bar{p}_1} = \pm \frac{\partial \overline{\overline{F}}}{\partial \bar{p}_1} \tag{3.1}$$

to guarantee that the root is multiple.

Where a I-existence surface intersects a II-existence surface, the condition $\overline{\overline{P}} = \overline{\overline{F}} = 0$ is augmented by Eq. (3.1), which must hold in the intersection by continuity of the first derivatives, given that $\overline{\overline{F}}^2$ has at least a double root there. It follows that $f = \overline{\overline{F}}^2 - \overline{\overline{P}}^2$ has in the intersection a root of order higher than two. It could be of order four or higher, of course, but in that case, in addition to (3.1),

$$\frac{\partial^2 \overline{\overline{P}}}{\partial \bar{p}_1^2} = \pm \frac{\partial^2 \overline{\overline{F}}}{\partial \bar{p}_1^2} \tag{3.2}$$

must hold to guarantee the high order.

If on the other hand Eq. (3.2) does not hold, the root of f in the intersection can only be of order three. Note also that Eq. (3.2) is identical with STAB, Eq. (3.19), which describes the "supplementary stability boundary" of the II-existence surface; if this equation is not fulfilled at the intersection in question, the possible complication of a supplementary boundary is absent. Thus, this case is intrinsically simple. We pick from it the simplest of its variants, and for the rest of this section make the following assumption.

Least-complexity assumption: A I- and a II-existence surface intersect in a set C such that (a) C represents triple roots only, (b) in some neighborhood of C both existence surfaces represent double roots only, and (c) no $\overline{\overline{F}} = 0$ sheets corresponding to *single* skew roots pass through the said neighborhood of C.

Here part (c) excludes not only the parity complications displayed in PAR, Figs. 1 and 4; it also excludes that $\overline{\overline{F}}$ is not differentiable at $\bar{p}_1 = \Gamma$. Hence the word "intersection" may be taken in the narrow sense that either existence surface passes through C continuously and with a smooth tangent. However, we do not require that any of the multiple roots correspond to physically possible motions; they may well lie outside the domain of $\bar{p}_1$.

We now prove several results which are best formulated in $\bar{p}_1$, α space. They hold for physical, oscillatory systems.

Lemma 1: Under least-complexity conditions, at points of C neither of the intersecting existence surfaces has a tangent parallel to the $\bar{p}_1$ axis.

Proof: (I) Consider the explicit expression for $\overline{\overline{F}}$ in PAR, Eq. (3.5): a I-existence surface $\overline{\overline{F}} = 0$ is seen always to consist of planes $\bar{p}_1 = 0$ and $\alpha_j = -g_j \bar{p}_1$, none of which contains a parallel to the $\bar{p}_1$ axis, together with plane and/or curved sheets arising from a polynomial $\overline{\overline{Q}}(\bar{p}_1, \alpha)$, if there is one; therefore, if $\partial \overline{\overline{F}} / \partial \bar{p}_1 = 0$ were possible in C, this could only happen because of $\partial \overline{\overline{Q}} / \partial \bar{p}_1 = 0$. In C, the surface $\overline{\overline{F}} = 0$ also fulfills Eq. (3.1). If $\partial \overline{\overline{F}} / \partial \bar{p}_1 = 0$ were possible there, $\partial \overline{\overline{P}} / \partial \bar{p}_1 = 0$ would follow; then both polynomials $\overline{\overline{Q}}$ and $\overline{\overline{P}}$ have in C zeros of at least the second order, and hence the root of f in C is of at least the fourth order, contrary to hypothesis. (II) The II-existence surface fulfills Eq. (3.1). Where it has a $\bar{p}_1$-parallel tangent, the $\bar{p}_1$-derivative equation (3.2) must hold, too, but in C this cannot be the case, by hypothesis. Q.E.D.

Theorem 1: Under least-complexity conditions, and in the said neighborhood of C, if D is a point of the intersecting existence surfaces but not in C, then there exists a point E on the other existence surface but not in C, having the same coordinates $\alpha_2, \ldots, \alpha_n$ and such that for the double roots at D and E the graph of $f(\bar{p}_1)$ has opposite curvature.

Corollary: If both D and E lie in the domain of $\bar{p}_1$, then the corresponding c-a motions have opposite orbital stability.

Proof: By Lemma 1, a straight line parallel to the $\bar{p}_1$ axis, not passing through C but coming sufficiently close to it, must intersect both existence surfaces at neighboring points, say D and E. The possible situations are depicted in Fig. 5. Corresponding to a point in C, the graph of $f(\bar{p}_1)$ has for a certain small range of $\bar{p}_1$ values the configuration of Fig. 6(a), by hypothesis. At D or E, with α values outside C, the configuration of f can only be as in Fig. 6(b) or 6(c), by the continuity of f under changes of the α's. One of the double roots at D and E is skew, the other has definite parity, by hypothesis. If we keep the α's constant and vary only c_1, the skew root can only split into two real, single roots by a Theorem in PAR, Sec. III D; the corresponding f has the configuration of Fig. 6(d). This holds whether we decrease or increase c_1 from its value $c_{1\Gamma}$ at the skew root. Let us vary c_1 in that sense which should eventually lead to the other double root, which is not skew. Figuratively speaking: we *can* pass from the skew end of the interval DE in Fig. 5 into its interior, where the corresponding values of c_1 yield three real, distinct roots of f as in Fig. 6(d), and by continuity of f under changes of c_1 we *can* continue to the other end of the interval, where there is another double root of f, but with definite parity. Since the skew root at the outset is not formed from a confluence of low-amplitude conditions, it follows from the theorem just quoted that it necessarily splits into an even and an odd single root (cf. also Fig. 3 above!). Furthermore, since no single skew root can occur in the vicinity, by assumption, all single roots must conserve their parities under change of c_1. If the double root at the other end were again formed by coalescence of the said two single roots, it would therefore be skew, contrary to hypothesis. Rather, it must be formed by coalescence with the third one of the three real roots; thus, in Fig. 6(d) it is the middle root which under monotonic change of c_1 moves from the configuration of Fig. 6(b) to that of 6(c),

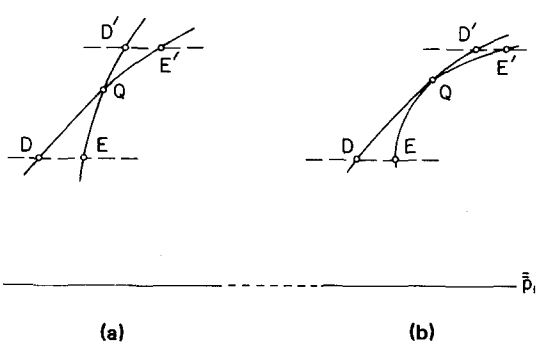

FIG. 5. The two existence surfaces meeting at a point $Q \in C$, (a) at an angle, and (b) with contact. The figure is a projection from n-dimensional space into some plane containing the $\bar{p}_1$ axis, and the resultant two-dimensional curves are schematic only.

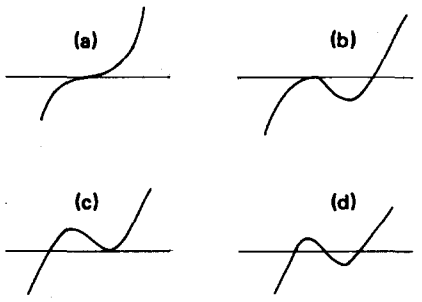

FIG. 6. The splitting of a third-order root of $f(\bar{p}_1)$ in the vicinity of C (schematic, with analogous mirror images). At any point in C, the graph of f has the form (a). If then a set of values $\alpha_2,\ldots,\alpha_n$ outside C is chosen and kept constant, under change of c_1 the graph takes the forms (b) for a value of c_1 on one existence surface, (c) for a value on the other existence surface, and (d) in the interval between. That the sequence is (b)–(d)–(c) (or reverse), without complex roots is proved in the text.

or the reverse. Q.E.D. The Corollary follows trivially from STAB, Sec. III C.

Incidentally, it follows that in Fig. 6(d) the outer roots necessarily have opposite parities. Another small detail becomes clear which has further uses: when the skew double root at Γ is split by a change of c_1, none of the three resultant real roots in Fig. 6(d) can under a further change c_1 move *across* the abscissa $\bar{p}_1 = \Gamma$. In fact, Γ can only be a *double* root of $f = \overline{F}^2 - \overline{P}^2$ because Γ remains a single root of $\overline{F}$ when c_1 is changed while the α's are kept constant. It follows that of the three separate roots in Fig. 6(d) at least two must lie on the same side of Γ as the *other* double root, for the latter needs to be formed by a coalescence of two such roots. This allows us to clarify an ambiguity remaining in Theorem 1 by the following.

Lemma 2: Under the conditions of Theorem 1, and assuming the configuration of Figs. 5 and 6, with D to the left of E on a parallel to the $\bar{p}_1$ axis, and with the cubic part of $f(\bar{p}_1)$ increasing towards the right, the graphs 6(b) and 6(c) are associated with D and E, respectively. This is analogous for mirror versions of the figures.

Proof: The proof is by contradiction. Interchange the graphs, assigning Fig. 6(c) to D and 6(b) to E, and then pass from D to E and back to D by changes of c_1. In such a complete cycle, each of the outer roots in the intermediate configuration 6(d) needs to move across one double root in order to make a coalescence of that outer root with the middle root possible at the *other* double root, as is required by the root parities. However, one of the double roots is skew and therefore cannot be crossed by a single root under a change of c_1 alone, as has been noted above; hence this assignment is impossible. This is analogous for the mirror versions.

Theorem 2: Under the conditions of Theorem 1, if the two existence surfaces meet in C with different or equal $\bar{p}_1$ derivatives, then C divides each surface into parts where $f(\bar{p}_1)$ at the double roots has opposite curvatures or the same curvature, respectively.

Proof: In Fig. 5 assume for the sake of argument that D and E are associated with Figs. 6(b) and 6(c), respectively. Figure 5(a) corresponds to the case of different $\bar{p}_1$ derivatives with the points D' and E on one surface, and D and E' on the other. Figure 5(b) corresponds to equal derivatives; now E and E' are on one surface, and D and D' on the other. With this labeling of points the following argument is valid for both cases. When we change the α's back to their values at the point Q, the graphs 6(b) and 6(c) collapse into 6(a). Now, if we continue to change the α's so as to reach the points D' and E', the pertaining graphs of f do not flip over into mirror versions of Fig. 6, because of the continuity of f under such changes. Therefore Lemma 2 applies to D' and E' exactly as to D and E, respectively. This is analogous if mirror versions of the graphs are associated with D and E at the outset. In any case, by Lemma 2, at the left points D and D' the graph of f has at the double root the same curvature, and at the right points E and E' the curvature is the opposite. Q.E.D.

Theorem 2 in conjunction with the corollary to Theorem 1 allows one to determine dynamical stability all around C if it has been determined for only half of one existence surface. Examples abound. A very simple one is found in the elastic pendulum; see STAB, Sec. V A. In this system, there is a Case (I) surface $\bar{p}_1 = 0$ which also marks the lower endpoint of the domain of $\bar{p}_1$. It describes pure suspension motion which remains orbitally stable up to a critical α value ($\alpha_2 = \epsilon^2/2\bar{\gamma}^2$ in the notation of STAB) where f has a triple root. Here a stable Case (II) (cup or cap motion) surface branches off and leaves the suspension oscillation unstable for all higher values of α_2.

In essence, the results of this section show that α bifurcations will group around intersections of I- and II-existence surfaces only in certain patterns.

B. Vanishing $\bar{p}_1$ derivatives

In an intersection C representing only third-order roots the existence surfaces cannot have tangents parallel to the $\bar{p}_1$ axis. Such tangents can occur outside C, however, and indicate α bifurcations with a characteristic signature.

Consider first a II-existence surface. It fulfills Eq. (3.1). We are now only interested in its parts which do not intersect with any I-existence sheets, and which therefore do not include the boundary of the domain of $\bar{p}_1$. In the interior of the domain, $\overline{F}$ is repeatedly differentiable as well as $\overline{P}$. At a point of any II-existence surface with a horizontal tangent, such as T in Fig. 7, the derivative Eq. (3.2) must be satisfied too; thus T is an intersection with the supplementary stability boundary STAB (3.19). The root of f corresponding to T, which satisfies $\overline{P} = \pm\overline{F} \neq 0$, is therefore of at least the third order.

Let us again assume the simplest case, that the root of f at T is exactly of the third order, i.e.,

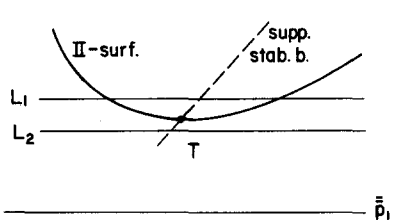

FIG. 7. Vanishing $\bar{p}_1$ derivative on a II-existence surface. Like Fig. 5, the figure is a projection into some plane containing the $\bar{p}_1$ axis. At the constant α values along the (amplitude modulation) line L_1, variation of c_1 yields two c-a motions, but along L_2 there are none.

$$\frac{\partial^3 \bar{P}}{\partial \bar{p}_1^3} \neq \pm \frac{\partial^3 \bar{F}}{\partial \bar{p}_1^3}, \quad \begin{matrix} \text{even} \\ \text{odd} \end{matrix} \tag{3.3}$$

Then the multiple roots of f in the vicinity of T, where Eq. (3.2) no longer holds, are of the second order. Moreover, the curvature of f at these roots changes sign as T is crossed by variation of the α's and c_1; this follows at once from the discussion in STAB, Sec. III D, together with (3.3). From this fact, together with Fig. 7, we conclude the following.

Theorem: A third-order definite-parity root of f marks a bifurcation in the sense that its dynamical neighborhood of α values contains one continuous part without any c-a motions, and a complementary part with pairs of one stable and one unstable Case (II) c-a motion which differ only in the value of c_1.

Second, consider a I-existence surface. Of $\bar{F} = 0$, only the sheet $\bar{Q} = 0$ could have a tangent with $\partial \bar{Q} / \partial \bar{p}_1 = 0$. Then $\partial \bar{F} / \partial \bar{p}_1 = 0$ holds, too, and since Eq. (3.1) must not be satisfied, so as to exclude an intersection with a II-existence surface, it follows that the pertaining root of f cannot be of order higher than the second. Moreover, it follows that $|\partial \bar{P} / \partial \bar{p}_1| \neq 0$, and hence, that the root is orbitally stable, by criterion STAB, Eq. (3.12). As in its dynamical vicinity there is nothing discontinuous, we are not now faced with a bifurcation. Indeed, we have here one of those "double skew root inside the domain" motions which are difficult even to recognize; cf. PAR, Sec. IV D.

IV. PROCEDURAL RULES

Cursory as the preceding survey is, it allows us to outline a general procedure for spotting all motion types in a given system.

First of all, locate the endpoints of the domain of $\bar{p}_1$. If the d.f.'s defining one or both of them can change, then the set of all physically possible values $\alpha_2, \ldots, \alpha_n$ should at once be subdivided into corresponding subsets.

Excluding confluences of exceptional low-amplitude conditions, if any, all α bifurcations are associated with change in stability of c-a motions, and occur at roots of f of order higher than the second, as we have shown above. Thus, locate these roots; determine by means of a stability diagram and arguments such as those developed above, which of them gives rise to an α bifurcation, and further subdivide the α's into subsets in accordance with the findings.

Then consider each α subset separately and vary c_1 through all possible values while keeping the α's constant. The remaining, distinct motion types are separated by c_1 bifurcations.

Lastly, take up the confluences of low-amplitude conditions, if any, and add details on conversion motions, if appropriate.

Parenthetically, we remark that in the course of sorting out α and c_1 intervals one obviously also comes across dynamically stable, multiple roots of f which move into or out of the domain of $\bar{p}_1$, or which appear or disappear inside the domain. The corresponding (dis)appearances of c-a motions deserve to be noted, of course, but because of the smooth nature of their phase space neighborhoods they cannot be called "bifurcations" in any contemporary sense.

In essence, this procedure amounts to a systematic reordering of all representative solutions into contiguous classes distinguished from each other by major features at the expense of less prominent ones. It thus leads a long way towards the goal first formulated in PAR, to obtain a qualitative description and classification of motions with variable amplitude.

V. AN EXAMPLE

To illustrate the procedure we choose a system of two d.f.'s with coupling $\gamma q_1^2 q_2$, but with m_2 and ω_2 negative so that the resonant condition is $2\omega_1 + \omega_2 = \epsilon$. This system has some importance in celestial mechanics.[7] We touched upon it in STAB, Sec. V A, and can now add detail. For brevity, we omit all algebraic manipulations. For definiteness, we assume $\gamma > 0$ and $\epsilon > 0$ throughout; if one of the two signs is changed, primarily "even" and "odd" change places.

A. Subsets of α values

The momentum integral is for this system

$$\bar{p}_2 = \bar{p}_2 - \tfrac{1}{2}\bar{p}_1 = \alpha, \tag{5.1}$$

and α has therefore no physical, lower bound. The domain of $\bar{p}_1 = \frac{1}{2}\bar{p}_1$ evidently has no upper bound, while its lower one lies at $\max(0, -\alpha)$; cf. STAB, Sec. III C. Thus the range of α values must be divided at $\alpha = 0$.

The integration constants E and

$$c_1 = E - \omega_2 \alpha \tag{5.2}$$

also have no physical bounds. Given that

$$\bar{F} = \bar{\gamma}\bar{p}_1[2(\bar{p}_1 + \alpha)]^{1/2},$$

where

$$\bar{\gamma} = \gamma(m_1^2\omega_1^2 m_2\omega_2)^{-1/2}, \tag{5.3}$$

the Case (I) existence line is simply $\bar{p}_1 = 0$; the other possibility $\bar{p}_1 = -\alpha$ means $\bar{p}_2 = 0$, which lies at the extreme of an exceptional low-amplitude region and would require special study, which we omit. Given also

$$\bar{P} = c_1 - \epsilon\bar{p}_1, \tag{5.4}$$

the Case (II) existence line (3.1) is calculated to be

$$\alpha = \tfrac{1}{2}(\tfrac{1}{2}\theta^2 - 3\bar{p}_1) \pm \tfrac{1}{2}[\theta^2(\tfrac{1}{4}\theta^2 - \bar{p}_1)]^{1/2},$$

where

$$\theta = \epsilon/\bar{\gamma}; \tag{5.5}$$

the c-a motion is odd or even according as $\theta > 0$ or $\theta < 0$, respectively. The supplementary stability boundary (3.2) is

$$\alpha = -\tfrac{3}{4}\bar{p}_1. \tag{5.6}$$

Since $f = \bar{F}^2 - \bar{P}^2$ is cubic, no roots of order higher than three exist.

The stability diagram from (5.3), (5.5), and (5.6) is shown in Fig. 8. The intersection at A, where $\alpha = \frac{1}{2}\theta^2$, and the horizontal tangent at B, where $\alpha = -\frac{1}{8}\theta^2$, mark α bifurcations of the types discussed in conjunction with Figs. 5(a) and 7. Since the slope of $\bar{F}$ clearly steepens with increasing α at $\bar{p}_1 = 0$, the Case (I) must at high α become unstable according to criterion STAB, Eq. (3.12), and the other stability as-

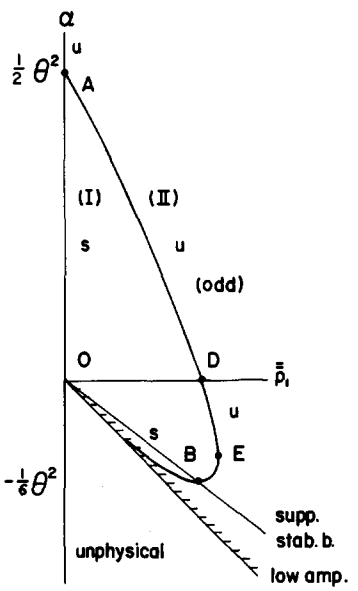

FIG. 8. Stability diagram for coupling $\gamma q_1^2 q_2$ in the resonance $2\omega_1 + \omega_2 = \epsilon$. This is an affine image of the right half of Fig. 2 from STAB. At the I–II intersection A $(0, \frac{1}{2}\theta^2)$ there is a skew triple root; at B $(\frac{1}{3}\theta^2, -\frac{1}{6}\theta^2)$ there is an odd triple root with a horizontal tangent; at both points the typical stability changes discussed in Sec. III occur. The drawing assumes $\theta = \epsilon/\bar{\gamma} > 0$; for $\theta < 0$ replace odd by even.

signments now follow at once from Sec. III. Thus the values $\alpha = -\frac{1}{6}\theta^2, \frac{1}{2}\theta^2$ further subdivide the α range.

B. The behavior of f

The Case (II) c-a motions of Fig. 8 require multiple roots of f in the interior of the domain of $\bar{p}_1$. If as usual we plot $\bar{P}$ and $\pm\bar{F}$ from (5.3) and (5.4) as in Fig. 9, we see at once that contacts between the lines are only possible inside the domain if the slope of $\bar{F}$ is not too steep, corresponding to $-\frac{1}{6}\theta^2 \leqslant \alpha \leqslant \frac{1}{2}\theta^2$.

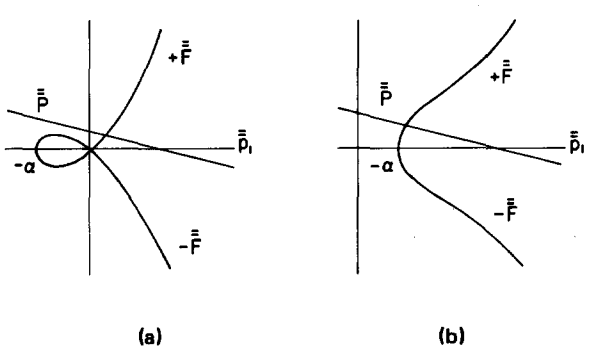

FIG. 9. Formation of the roots of f in different α ranges. The graph of $\bar{P}$ is always a straight line (5.4) with slope independent of α, and intercept still adjustable by choice of c_1; cf. (5.2). (a) $\alpha > 0$; the domain of $\bar{p}_1$ begins at the origin. For large α, the loop on the left is large, and no $\bar{P}$ line of the given slope can make more than one intercept in the domain. As α decreases, contact in the domain becomes possible when $\alpha < \frac{1}{2}\theta^2$; point A of Fig. 8 requires contact at the origin. (b) $\alpha < 0$; the domain begins at $-\alpha$. At large $|\alpha|$ the slope of $\pm\bar{F}$ is too steep for more than one intercept. Contact becomes possible at $\alpha > -\frac{1}{6}\theta^2$, corresponding to the Case (II) motions above point B in Fig. 8. The drawing assumes $\epsilon > 0$ and $\gamma > 0$.

It is also seen that at any given α, for every c_1 whatsoever there is *at least* one intercept between $\bar{P}$ and $\pm\bar{F}$, and beyond this intercept $|\bar{P}| < |\bar{F}|$ holds so that f remains positive out to infinity. Thus at any pair of values α, c_1 there exists a motion with unbounded $\bar{p}_1$. Bounded motion is possible only when there are two more intercepts, as can only happen for $-\frac{1}{6}\theta^2 < \alpha < \frac{1}{2}\theta^2$, and will require appropriate initial conditions.

C. The c_1 bifurcations

1. $\alpha \geqslant \frac{1}{2}\theta^2$

There can be only one intercept between $\bar{P}$ and $\pm\bar{F}$ in the domain of $\bar{p}_1$. If $c_1 = c_{1\Gamma} = 0$, the intercept lies at the lower endpoint of the domain and yields a Case (I) motion $\bar{p}_1 \equiv 0$. If $c_1 \neq 0$ the motion is necessarily unbounded. The value $c_{1\Gamma} = 0$ marks a bifurcation inasmuch as it divides motions with an even from motions with an odd, lower turning point according as $c_1 > 0$ or $c_1 < 0$, respectively [see Fig. 9(a)]. Point A of Fig. 8 is now readily seen to be unstable.

2. $0 \leqslant \alpha < \frac{1}{2}\theta^2$

Consider Fig. 9(a), flatten the loop to correspond to the reduced α, and shift the $\bar{P}$ line up from below. At negative c_1, only unbounded motion with an odd turning point is possible. At $c_{1\Gamma} = 0$ the $\bar{P}$ line passes through the origin; the resultant, new Case (I) is stable because at neighboring, positive values of c_1 there is now an even–odd pair of neighboring single roots which have moved into the domain from the left. This $c_{1\Gamma}$ marks a typical (dis)appearance of the kind briefly mentioned in Sec. IV.

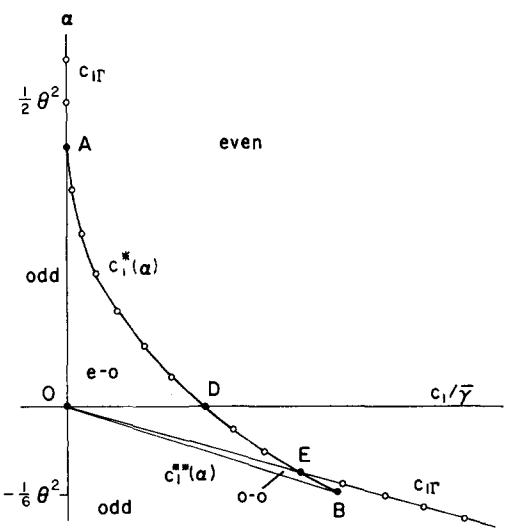

FIG. 10. The c_1 bifurcations. An infinite plane of α vs $c_1/\bar{\gamma}$ represents the unbounded motions; it is bifurcated by the chain-linked line into classes having even and odd amplitude modulation minima. Overlaid on the plane, and joined to it along the c_1^* arc $ADEB$, is the curved triangle AOB. It represents the bounded motions and is divided by its bifurcation line OE (which represents exceptional low amplitudes) into an even–odd range AOE and a narrow odd–odd range EOB. Its free edges AO and OB represent stable c-a motions. Points O, A, B, D, E correspond to Fig. 8. The drawing assumes $\epsilon > 0$ and $\gamma > 0$; if one of the two signs is changed, interchange even and odd and change the direction of the $c_1/\bar{\gamma}$ axis.

At a certain higher value $c_1 = c_1^*$ the $\bar{\bar{P}}$ line will make contact with the $-\bar{\bar{F}}$ curve, leading to the unstable Case (II) on the arc AD in Fig. 8, and to a c_1 bifurcation precisely like the one depicted in Fig. 1. To calculate the critical c_1^*, note that in Eq. (5.2) the constant E is the Hamiltonian SF (3.6), which for an odd Case (II) in our system yields $c_1^* = \epsilon\bar{\bar{p}}_1 - \bar{\bar{F}}$; here the required (constant) value of $\bar{\bar{p}}_1$ is determined by the existence condition (5.5), so that by elimination of $\bar{\bar{p}}_1$ we obtain c_1^* as a function of α. The result is plotted in Fig. 10. At still higher $c_1 > c_1^*$, only unbounded motion with an even turning point remains.

3. $-\frac{1}{6}\theta^2 \leqslant \alpha < 0$.

Proceed in the same way in Fig. 9(b). Only one, odd, single root exists for large, negative c_1. Then at a certain $c_1 = c_1^{**}$ the $\bar{\bar{P}}$ line will make contact with the $-\bar{\bar{F}}$ curve from *below*, resulting in the stable, odd Case (II) on the arc OB in Fig. 8; c_1^{**} can be calculated as a function of α like the c_1^* above, and is plotted in Fig. 10. This c_1^{**} marks another (dis)appearance.

At a certain, still higher value $c_1 = c_1^*$ the $\bar{\bar{P}}$ line will make contact with the $-\bar{\bar{F}}$ curve from *above*, yielding the odd Case (II) along the arc DEB in Fig. 8. This c_1^* is the continuation of the c_1^* for the arc AD, as follows from the elimination process described above. This Case (II) is now unstable and the corresponding c_1 bifurcation is again of the type of Fig. 1.

The $\bar{\bar{P}}$ line passes through the apex point $\bar{\bar{p}}_1 = -\alpha$ in Fig. 9(b) when $c_1 = c_{1\Gamma} = -\epsilon\alpha$; cf. Eq. (5.4). This value marks a c_1 bifurcation of the kind depicted in Fig. 4, where a single root of f changes parity. At smaller values of $|\alpha|$ this $c_{1\Gamma}$ lies *between* c_1^{**} and c_1^* so that the bifurcation separates odd–odd and even–odd *bounded* motions, but at larger $|\alpha|$ it lies beyond c_1^* so that the bifurcation separates *unbounded* motions with even and odd amplitude minima. See Fig. 10.

4. $\alpha < -\frac{1}{6}\theta^2$.

Again the $\pm\bar{\bar{F}}$ curves are too steep for more than one intercept. There are only unbounded motions, separated by a bifurcation at $c_{1\Gamma} = -\epsilon\alpha$ into an even and odd class.

D. The α bifurcations

It is now possible to return to the α bifurcations to study them in more detail throughout entire neighborhoods of the critical values $-\frac{1}{6}\theta^2$, 0, and $\frac{1}{2}\theta^2$. We prefer not to do this in words, but refer to Fig. 10 which fully exhibits the complexity of the situation, and can be read along verticals $c_1 = \text{const}$, always keeping in mind the important change at $\alpha = 0$ depicted in Fig. 9. Incidentally, a survey of more such verticals bears out the correctness of the rule "divide the α range first, then study the c_1 bifurcations," for it is the latter which cause the most interesting phenomena.

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Regular precession in Jacobi's decomposition theorem

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In this paper, Jacobi's decomposition theorem, which states that the motion of a heavy symmetrical top can be decomposed into the motions of two torque-free triaxial tops (free asymmetrical tops), is applied to the case of a regular precession (no nutation) of the heavy symmetrical top, and it is found that the heavy top motion can be expressed as a composite motion consisting of two torque-free symmetrical tops with no nutation. A top motion without nutation is an extremely simple motion since it consists of only spin and precession, which are merely constant rotations. The dynamical relations among the three symmetrical tops are obtained. Quantum analysis of a torque-free top is completely known. Since the Hamiltonian of the regular precession of a heavy symmetrical top has the same form as that of the Stark effect of a symmetrical molecule, our result indicates a possibility of quantum treatment of Jacobi's decomposition theorem.

I. INTRODUCTION

In the rigid body dynamics, there are three soluble cases which can be solved under general initial conditions: (1) Lagrange's case,[1-3] (2) Euler's case,[2-4] and (3) Kowalenski's case.

Lagrange's case is normally referred to as the heavy symmetrical top, which is the motion of a symmetrical top ($I_1 = I_2$) with one point fixed under the uniform gravitational field. This is a usual toy top.

Euler's case is the motion of an asymmetrical rigid body with its center of mass fixed and this is referred to as the torque-free triaxial top.

Jacobi discovered that the motion of a heavy symmetrical top can be expressed as a composite motion of two torque-free triaxial tops.[1] This is remarkable because the angular momentum of a heavy symmetrical top is not constant due to the gravity, and the angular momentum of a torque-free triaxial top is clearly constant. That is, the angular momenta of the composite motion are constant. This theorem discovered by Jacobi is generally known as Jacobi's decomposition theorem.

In either Lagrange's case or Euler's case, three motions are involved[2]: (a) nutation, (b) precession, and (c) spin. In this paper we will show that Jacobi's theorem still works even when no nutation is involved. In the case of a heavy symmetrical top, the motion without nutation is referred to as regular precession.[2] The question is that, in Jacobi's decomposition theorem, what kind of composite motion results when the heavy top undergoes a regular precession. In Sec. V, we show that the motion of a heavy symmetrical top without nutation can be decomposed into the motions of two torque-free symmetrical tops instead of triaxial tops.

Since there is no nutation in the motion of a torque-free symmetrical top, Jacobi's decomposition theorem in this case involves no nutation. That is, each of the three symmetrical tops involved in the decomposition theorem precesses around an axis while it is spinning with a fixed inclination of the axis of symmetry.

In general, the rigid body dynamics is nonlinear and, therefore, Jacobi's decomposition theorem is described in terms of transcendental functions, that is, elliptic functions and theta functions.[1,4] In Sec. V, however, we show that as the nutations approach zero, the whole dynamics approaches a linear dynamics, and the transcendental functions reduce to familiar trigonometric functions in the limit of zero nutations. This is discussed in the final section, the Appendix.

The total energy of a heavy symmetrical top undergoing a regular precession is expressed as a sum of the total energy of a torque-free symmetrical top and the gravitational interaction energy. Then, since the quantum-mechanical analysis of a torque-free symmetrical top is completely known,[5] we can quantize the regular precession of a heavy symmetrical top by diagonalizing the Hamiltonian of the heavy top.[5] This suggests that in the case of a regular precession, the whole decomposition theorem is possibly treated quantum-mechanically. Then one immediate application would be the molecular Stark effect.[5] This is discussed in Sec. VII.

II. SUMMARY OF THE DYNAMICS AND THE KINEMATICS OF TOP MOTIONS PERTAINING TO THE DECOMPOSITION THEOREM

An instantaneous orientation of a rotating rigid body with one point fixed with respect to some inertial frame of reference (x, y, z) can be expressed by specifying three Euler angles θ, ϕ, and ψ as explicit functions of time.[1-3] Angle θ describes the nutation or the oscillation of the body z axis with respect to the space z axis, angle ϕ describes the precession, and angle ψ describes the spin motion.[1]

A. A heavy symmetrical top[1-3]

For a given heavy symmetrical top, an initial condition determines several constants of motion: the total energy, constant components of the total angular momentum, and so on. Yamada and Shieh[6] introduced the physical constants

$$\alpha', \alpha, a, b, x_1, x_2, x_3, \tag{2.1}$$

and also introduced the transcendental constants

$$n, k, q_1, q_2. \tag{2.2}$$

But only three of the above eleven constants are independent. Although we can choose any three of them as indepen-

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dent constants, we choose the following three constants since their physical nature is very clear: $\alpha' =$ a quantity related to the total energy of the heavy top; $a =$ a quantity proportional to the angular momentum component along the axis of symmetry; and $b =$ a quantity proportional to the angular momentum component along the space z axis which is antiparallel to the gravity. Then all the remaining eight constants can be expressed in terms of α', a, and b.

Although Euler's equations are expressed in terms of the orthogonal angular velocity components (ω_x, ω_y, and ω_z) (Refs. 2 and 3), it is more convenient to solve the energy equation which is expressed in terms of Euler angles[2]

$$E = \tfrac{1}{2} I_2(\dot\theta^2 + \dot\phi^2 \sin^2\theta) + \tfrac{1}{2} I_3 \omega_{z_2}^2 + Mgl\cos\theta, \quad (2.3)$$

where E is the total energy, I_2 and I_3 are the moments of inertia, M is the total mass of the heavy symmetrical top, and l is the length between the center of mass and the fixed point.

By rearranging the above energy equation and using the three physical constants introduced above, we can set up the following three coupled first-order nonlinear differential equations[1,2,3]:

$$\dot x^2 = (1-x^2)(\alpha' - x) - (b - ax)^2, \quad (2.4)$$

$$\dot\phi = (b - ax)/(1 - x^2), \quad (2.5)$$

$$\dot\psi = ((I_2 - I_3)/I_3)a + (a - bx)/(1 - x^2), \quad (2.6)$$

where

$$x = \cos\theta. \quad (2.7)$$

Here we compare Eq. (2.4) with the energy equation of a simple harmonic oscillator which is given by

$$\dot x^2 = 2E/M - \omega^2 x^2,$$

and we see that the right-hand side is a quadratic equation in x and we know that the solution gives a linear oscillation. On the other hand, Eq. (2.4) is a cubic equation in x. Therefore, the solution to Eq. (2.4) will not give any linear oscillation, but it is expressed in terms of a transcendental function (an elliptic function). The detailed solutions of Eqs. (2.4)–(2.6) are given by Jacobi.[1] The final form of the solution of Eq. (2.4) is given by

$$\cos\theta(t) = x_3 + (x_2 - x_3)\mathrm{sn}^2(nt), \quad (2.8)$$

where $\mathrm{sn}(nt)$ is the elliptic function which is a periodic function. Thus we see that $\theta(t)$ oscillates about the fixed value x_3. This motion is called nutation.

The solutions of Eqs. (2.5) and (2.6) are, respectively, expressed as[1]

$$\phi(t) = \phi_p(t) + \phi_s(t), \quad (2.9)$$

$$\psi(t) = \psi_p(t) + \psi_s(t), \quad (2.10)$$

where $\phi_p(t)$ and $\psi_p(t)$ represent periodic functions which consist of Jacobian theta functions and are expressed in terms of the constants given by Eqs. (2.1) and (2.2). Further, $\phi_s(t)$ and $\psi_s(t)$ in Eqs. (2.9) and (2.10), respectively, represent secular terms; that is, the terms which are proportional to time t. Because of these secular terms, the angles ϕ and ψ increase indefinitely. It is very important to note that the two Euler angles ϕ and ψ consist of two separate parts; a periodic part and a secular term.

B. A torque-free triaxial top[3,4]

This is the motion of an asymmetrical top whose center of mass is fixed so that its total angular momentum is constant even under a uniform gravitational field. Yamada and Shieh[6] introduced the following four physical constants for the motion of a torque-free asymmetrical top:

$$s_0 = \frac{h_1}{l_1}, \quad s_1 = \frac{l_1}{C_1}, \quad s_2 = \frac{l_1}{A_1}, \quad s_3 = \frac{l_1}{B_1}, \quad (2.11)$$

where l_1 is the magnitude of the total angular momentum, h_1 is twice the total energy (kinetic energy), and A_1, B_1, and C_1 are the moments of inertia. In terms of these physical constants, we can define the following transcendental constants[6]:

$$n_1, k_1, p_1. \quad (2.12)$$

The Euler angles which specify the orientation of the free top with respect to an inertial frame of reference are denoted by θ_1, ϕ_1, and ψ_1. Then the angular velocity components are given by[7]

$$\dot\theta_1 = (s_2 - s_3)\sin\theta_1 \sin\psi_1 \cos\psi_1, \quad (2.13)$$

$$\dot\phi_1 = s_2 \sin^2\psi_1 + s_3 \cos^2\psi_1, \quad (2.14)$$

$$\dot\psi_1 = (\cos\theta_1/\sin^2\theta_1)(s_1 - s_0). \quad (2.15)$$

These are coupled nonlinear differential equations for the Euler angles θ_1, ϕ_1, and ψ_1.

As in the case of the motion of a heavy symmetrical top, we consider the energy equation which is given by

$$E_1 = \tfrac{1}{2}(A_1\omega_1^2 + B_1\omega_2^2 + C_1\omega_3^2), \quad (2.16)$$

where[8]

$$\begin{aligned}\omega_1 &= \dot\phi_1 \sin\theta \sin\psi + \dot\theta\cos\psi,\\ \omega_2 &= \dot\phi_1 \sin\theta\cos\psi - \dot\theta\sin\psi,\\ \omega_3 &= \dot\phi_1\cos\theta + \dot\psi_1.\end{aligned} \quad (2.17)$$

By properly combining these equations with Eqs. (2.13)–(2.15), we can obtain the Euler angles exactly[3,4]

$$\cos\theta_1(t) = ((s_0 - s_2)/(s_1 - s_2))^{1/2}\,\mathrm{dn}(n_1 t), \quad (2.18)$$

$$\phi_1(t) = \phi_{1p}(t) + \phi_{1s}(t), \quad (2.19)$$

$$\tan\psi_1(t) = \left(\frac{s_1 - s_3}{s_1 - s_2}\right)^{1/2} \frac{\mathrm{cn}(n_1 t)}{\mathrm{sn}(n_1 t)}, \quad (2.20)$$

where dn, cn, and sn represent the elliptic functions. The constant n_1 is one of the transcendental constants introduced in Eq. (2.12).

As shown in Eq. (2.19), in the case of the motion of a torque-free triaxial top, only the precession angle ϕ_1 can be expressed as a sum of a periodic part ϕ_{1p} and a secular term ϕ_{1s}, which is simply proportional to time.

III. JACOBI'S DECOMPOSITION THEOREM[1]

First we describe the motion of a heavy symmetrical top in matrix representation.

Let $\mathbf{X}$ represent a column matrix whose elements are x, y, and z, which are the Cartesian coordinates of a frame of reference fixed in space where a uniform gravitational field $\mathbf{g}$ exists in the direction of the negative z axis. Further, let $\mathbf{X}_2$ be a column matrix whose elements are x_2, y_2, and z_2, which are the principal axes of a heavy symmetrical top. Axis z_2 is

along the axis of symmetry of the heavy top. Now when the rotational motion of the frame $\mathbf{X}_2$ is observed from the frame of reference $\mathbf{X}$, the rotational motion can be expressed as[9]

$$\mathbf{X} = N(\theta,\phi,\psi)\mathbf{X}_2, \tag{3.1}$$

where $N(\theta,\phi,\psi)$ represents a 3×3 matrix whose nine elements are the direction cosines expressed in terms of the Euler angles θ, ϕ, and ψ, which are functions of time as shown in Eqs. (2.8), (2.9), and (2.10), respectively. Then, when Eq. (3.1) is inverted, we obtain the matrix representation of a heavy symmetrical top. Here we recall that precession angle ϕ and spin angle ψ are expressed as a sum of a periodic part and a secular term, as shown in Eqs. (2.9) and (2.10). Then the orthogonal matrix N can be written as[9]

$$N(\theta,\phi,\psi) = P(\phi_s)M(\theta,\phi_p,\psi_p)S(\psi_s), \tag{3.2}$$

where $P(\phi_s)$ is a 3×3 matrix consisting only of the precession secular term ϕ_s. The $S(\psi_s)$ is a 3×3 matrix consisting only of the spin secular term ψ_s. Matrix M in Eq. (3.2) consists of angle θ and pure periodic parts ϕ_p and ψ_p.

After expressing all the nine elements of matrix $M(\theta,\phi_p,\psi_p)$ in terms of the theta functions and changing them into appropriate forms, Jacobi employed the fundamental theorem of theta functions and the addition theorem of the elliptic functions to discover that matrix $M(\theta,\phi_p,\psi_p)$ can be written as a product of two orthogonal matrices M_1 and J_2,[1]

$$M(\theta,\phi_p,\psi_p) = M_1J_2. \tag{3.3}$$

Now, like the motion of a heavy symmetrical top, the motion of a torque-free triaxial top can also be expressed in matrix representation with the nine elements in terms of the theta functions. We observe that matrix M_1 in Eq. (3.3) has exactly the same structure as that of a torque-free triaxial top except that the precession angle includes only the periodic part[4]; that is, ϕ_{1p} of Eq. (2.19). Then we can write $M_1 = M_1(\theta_1,\phi_{1p},\psi_1)$.

Matrix J_2 in Eq. (3.3) turned out to be the transposed form of a matrix M_2 which describes the motion of another torque-free triaxial top

$$J_2 = \tilde{M}_2.$$

The nine elements of matrix M_2 are expressed in terms of three Euler angles: θ_2,ϕ_{2p}, and ψ_2. Note that the precession angle again consists only of the periodic part $\phi_{2p}(\phi_2 = \phi_{2s} + \phi_{2p})$. Thus we can write $J_2 = \tilde{M}_2(\theta_2,\phi_{2p},\psi_2)$. Consequently, Eq. (3.3) can be written

$$M(\theta,\phi_p,\psi_p) = M_1(\theta_1,\phi_{1p},\psi_1)\tilde{M}(\theta_2,\phi_{2p},\psi_2). \tag{3.4}$$

This is the furthest Jacobi pursued since this turned out to be his last work in his life and this paper appeared as his posthumous paper.[1]

After noting Jacobi's work, Darboux[10] approached this problem by strictly considering the dynamics of the rigid body motion and predicted the existence of the decomposition theorem. Darboux showed that the decomposition theorem exists even when all the secular terms ϕ_s, ψ_s, ϕ_{1s}, and ψ_{2s} are included.[10] Then, since

$$\phi = \phi_p + \phi_s, \quad \psi = \psi_p + \psi_s,$$

$$\phi_1 = \phi_{1p} + \phi_{1s}, \quad \phi_2 = \phi_{2p} + \phi_{2s},$$

that is, the secular terms are simply added to the periodic terms, when we modify Eq. (3.4) by adding the secular terms, the effect appears in the form[9]

$$P(\phi_s)M(\theta,\phi_p,\psi_p)S(\psi_s)$$
$$= P_1(\phi_{1s})M_1(\theta_1,\phi_{1p},\psi_1)\tilde{M}_2(\theta_2,\phi_{2p},\psi_2)\tilde{P}_2(\phi_{2s}). \tag{3.5}$$

The left-hand side of Eq. (3.5) comes from Eq. (3.2). The $P_1(\phi_{1s})$ is a 3×3 matrix consisting only of the secular precession angle of the first free top, and $P_2(\phi_{2s})$ is a 3×3 matrix including only the secular precession term of the second free top.

By writing

$$N_1(\theta_1,\phi_1,\psi_1) = P_1(\phi_{1s})M_1(\theta_1,\phi_{1p},\psi_1), \tag{3.6}$$

$$N_2(\theta_2,\phi_2,\psi_2) = P_2(\phi_{2s})M_2(\theta_2,\phi_{2p},\psi_2), \tag{3.7}$$

and using Eq. (3.2), Eq. (3.5) can now be written as

$$N(\theta,\phi,\psi) = N_1(\theta_1,\phi_1,\psi_1)\tilde{N}_2(\theta_2,\phi_2,\psi_2), \tag{3.8}$$

which includes all the angles. Each matrix in Eq. (3.8) can be interpreted as $N(\theta,\phi,\psi)$ = the matrix describing the motion of a heavy symmetrical top relative to a frame of reference fixed in space; $N_1(\theta_1,\phi_1,\psi_1)$ = the matrix describing the motion of a torque-free triaxial top relative to the same frame of reference; and $N_2(\theta_2,\phi_2,\psi_2)$ = the matrix describing the motion of another torque-free triaxial top observed from the frame of the heavy symmetrical top. Then clearly Eq. (3.8) tells us that the motion of a heavy symmetrical top can be decomposed into the motions of two torque-free triaxial tops.

IV. REGULAR PRECESSION OF A HEAVY SYMMETRICAL TOP

Most of the standard mechanics textbooks treat the regular precession.[2] In general, the equation of the motion of a rotating rigid body is given by[2]

$$\left(\frac{d\mathbf{L}}{dt}\right)_{\text{space}} = \left(\frac{d\mathbf{L}}{dt}\right)_{\text{body}} + \boldsymbol{\omega}\times\mathbf{L}, \tag{4.1}$$

where $\mathbf{L}$ is the total angular momentum and $\boldsymbol{\omega}$ stands for the angular velocity vector.

In terms of Euler angles, $\boldsymbol{\omega}$ can be written

$$\boldsymbol{\omega} = \dot{\boldsymbol{\theta}} + \dot{\boldsymbol{\phi}} + \dot{\boldsymbol{\psi}}. \tag{4.2}$$

When there is no nutation, we have $\dot{\theta} = 0$ or $\theta = \text{const}$, and this condition results in regular precession. Let us see this in more detail.

When $\dot{\theta} = 0$, Eq. (4.2) becomes

$$\boldsymbol{\omega} = \dot{\boldsymbol{\phi}} + \dot{\boldsymbol{\psi}}. \tag{4.3}$$

Now, in the case of a heavy symmetrical top, the angular momentum component along the body z_2 axis is always constant[2]

$$L_{z_2} = \text{const}. \tag{4.4}$$

With these two conditions expressed by Eqs. (4.3) and (4.4), it is easy to show

$$\left(\frac{d\mathbf{L}}{dt}\right)_{\text{body}} = \mathbf{L}\times\dot{\boldsymbol{\psi}}. \tag{4.5}$$

Substituting Eq. (4.5) into Eq. (4.1), we obtain

$$\left(\frac{d\mathbf{L}}{dt}\right)_{\text{space}} = \dot{\boldsymbol{\phi}}\times\mathbf{L}, \tag{4.6}$$

which represents an equation of precession. This equation clearly shows that the magnitude of the angular momentum **L** of a heavy symmetric top under a regular precession is constant, and the vector **L** merely precesses around the vector $\dot{\boldsymbol{\phi}}$.

V. THE DECOMPOSITION THEOREM IN THE LIMIT WHEN THE MODULI k's APPROACH ZERO

In general, a rigid body motion is described by transcendental functions: the elliptic functions and the theta functions.[1,4] Each of these functions is characterized by a constant called modulus.[6] This modulus also characterizes the nonlinearity of a rigid body motion. The moduli k, k_1, and k_2 of a heavy symmetrical top, the first torque-free triaxial top, and the second torque-free triaxial top are, respectively, defined as[6]

$$k^2 = (x_2 - x_3)/(x_1 - x_3), \tag{5.1}$$

$$k_1^2 = (s_3 - s_2)(s_1 - s_0)/(s_0 - s_2)(s_1 - s_3), \tag{5.2}$$

$$k_2^2 = (s_3' - s_2')(s_1' - s_0')/(s_0' - s_2')(s_1' - s_3'). \tag{5.3}$$

The modulus of a rigid body motion also determines the period of its motion. In the decomposition theorem, since the periods of all three top motions are the same, we have[6]

$$k = k_1 = k_2. \tag{5.4}$$

Now it is clear that when the moduli become zero, all the periodic motions disappear and it can be shown that all three tops undergo pure rotations with constant angular velocities.

A. A heavy symmetrical top

From Eq. (5.1), when $k = 0$, we have $x_2 = x_3$, and when we put this condition in Eq. (2.8), we obtain

$$x = \cos\theta = x_3 = \text{const},$$

which means $\theta = \text{const}$ and the nutation disappears. Further, when we put the condition $x = \text{const}$ in Eqs. (2.5) and (2.6), we obtain $\dot{\phi} = \text{const}$ and $\dot{\psi} = \text{const}$. Thus, the motion becomes a pure rotation without periodic motion. Clearly, Eqs. (2.4)–(2.6) are linear differential equations for $x = \text{const}$. Thus, in Eqs. (2.9) and (2.10), when $k = 0$, we can conclude

$$\phi_p = \psi_p = 0.$$

That is, $\phi = \phi_s$ and $\psi = \psi_s$.

B. A torque-free triaxial top

From the paper of Yamada and Shieh,[6] we have

$$s_1 - s_0 = \pm n_1[i\,\mathrm{dn}(ip_1)/\mathrm{sn}(ip_1)\mathrm{cn}(ip_1)], \tag{5.5}$$

$$s_2 - s_0 = \pm n_1[\mathrm{sn}(ip_1)\mathrm{dn}(ip_1)/i\,\mathrm{cn}(ip_1)], \tag{5.6}$$

$$s_3 - s_0 = \pm n_1[k_1'^2\,\mathrm{sn}(ip_1)/i\,\mathrm{cn}(ip_1)\mathrm{dn}(ip_1)], \tag{5.7}$$

where $k_1'^2 = 1 - k_1^2$.

Now we impose the condition $k_1 = 0$ in the above expressions. In the Appendix, we show that as k_1 approaches zero, we have

$$\mathrm{dn}(ip_1) = 1, \quad \mathrm{sn}(ip_1) = \sin(ip_1),$$

$$\mathrm{cn}(ip_1) = \cos(ip_1), \quad k_1'^2 = 1.$$

Then Eqs. (5.5), (5.6), and (5.7), respectively, become

$$s_1 - s_0 = \pm n_1[i/\sin(ip_1)\cos(ip_1)], \tag{5.8}$$

$$s_2 - s_0 = \pm n_1 \tan(ip_1), \tag{5.9}$$

$$s_3 - s_0 = \pm n_1 \tan(ip_1). \tag{5.10}$$

From Eqs. (5.9) and (5.10), we can conclude

$$s_2 = s_3. \tag{5.11}$$

Or by Eq. (2.11), we have

$$A_1 = B_1. \tag{5.12}$$

That is, the two moments of inertia of the torque-free triaxial top become equal (a symmetrical free top). Putting the condition of Eq. (5.11) in Eq. (2.13) immediately gives

$$\dot{\theta}_1 = 0, \quad \text{or } \theta_1 = \text{const}. \tag{5.13}$$

That is, the nutation disappears. With this condition, Eq. (2.15) becomes

$$\dot{\psi}_1 = \text{const}. \tag{5.14}$$

Then Eq. (2.14) gives

$$\dot{\phi}_1 = \text{const}. \tag{5.15}$$

Again the motion becomes pure rotations and the periodic motions disappear. We note that Eqs. (5.13), (5.14), and (5.15) are linear differential equations. Here we recall Eq. (2.19) and, since we have just seen that all the periodic motions vanish, we conclude that

$$\phi_{1p} = 0.$$

Now we can put a conclusion for the limiting case when the moduli approach zero: In the three top motions associated with the decomposition theorem, in those Euler angles which are expressed as a sum of a periodic term and a secular term, the periodic term vanishes in each top motion. That is,

$$\phi_p = \psi_p = \phi_{1p} = \phi_{2p} = 0,$$

and the matrix representation of Jacobi's decomposition theorem given by Eq. (3.4) becomes

$$M(\theta,0,0) = M_1(\theta_1,0,\psi_1)\tilde{M}_2(\theta_2,0,\psi_2). \tag{5.16}$$

In Jacobi's paper,[1] all the matrix elements of Eq. (3.4) are expressed in terms of the theta functions and each theta function is an infinite series as shown in the Appendix. However, when the moduli become zero, each theta function becomes a monomial (a single term). Under the condition $k = k_1 = k_2 = 0$, it can be shown that matrix equation (5.16) is still satisfied. Consequently, Eq. (3.8) is still valid. But since all the periodic terms vanish, only the secular terms survive. Thus, in the limit when the moduli are zero, Eq. (3.8) can be written

$$N(\theta,\phi_s,\psi_s) = N_1(\theta_1,\phi_{1s},\psi_1)\tilde{N}_2(\theta_2,\phi_{2s},\psi_2). \tag{5.17}$$

Further, it can be shown that in Eq. (5.17), matrix $N(\theta,\phi_s,\psi_s)$ describes the regular precession of a heavy symmetrical top, $N_1(\theta_1,\phi_{1s},\psi_1)$ describes the motion of a torque-free symmetrical top, and $N_2(\theta_2,\phi_{2s},\psi_2)$ describes the motion of another torque-free symmetrical top. Thus we can conclude that the regular precession of a heavy symmetrical top can be decomposed into the motions of two torque-free symmetrical tops and no asymmetric top (triaxial top) will appear.

VI. CONNECTION FORMULAS AMONG THE DYNAMICAL CONSTANTS OF THE THREE TOP MOTIONS WHEN THE HEAVY SYMMETRICAL TOP UNDERGOES A REGULAR PRECESSION

Yamada and Shieh obtained the connection formula for a general case.[6] In Sec. V, we showed that in the motion of a heavy symmetrical top, when the modulus k becomes zero, Eq. (5.1) gives $x_2 = x_3$ and this condition results in a regular precession. When the condition $x_2 = x_3$ is imposed on the connection formulas obtained by Yamada and Shieh,[6] we immediately obtain

$$l_1/A_1 = l_1/B_1 = (a - bx_2)/2(\alpha - x_2), \tag{6.1}$$

$$l_1/C_1 = (a - bx_1)/2(\alpha - x_1), \tag{6.2}$$

$$h_1/l_1 = b/2. \tag{6.3}$$

Clearly $A_1 = B_1$; that is, the first torque-free top is symmetrical. Also, we obtain

$$l_2/A_2 = l_2/B_2 = (b - ax_2)/2(\alpha' - x_2), \tag{6.4}$$

$$l_2/C_2 = (b - ax_1)/2(\alpha' - x_1), \tag{6.5}$$

$$h_2/l_2 = a/2. \tag{6.6}$$

Again we have $A_2 = B_2$; that is, the second torque-free top is also symmetrical.

The result of a free triaxial top becoming a symmetrical top was already obtained in Sec. V as shown in Eq. (5.12).

VII. FEASIBILITY OF QUANTUM TREATISE OF JACOBI'S DECOMPOSITION THEOREM

The total energy E of a heavy symmetrical top is given by

$$E = \frac{L^2}{2I_1} + \frac{1}{2}\left(\frac{1}{I_1} - \frac{1}{I_3}\right)L_3^2 + Mgl\cos\theta, \tag{7.1}$$

where $I_1 (= I_2)$ and I_3 are the principal moments of inertia and L^2 is the squared value of the total angular momentum. The L_3 is the angular momentum component along the axis of symmetry of the top and is constant in time. Therefore, the second term of Eq. (7.1) is always constant. Then, when there exists a nutation, since the last term $Mgl\cos\theta$ is not constant, the first term, or L^2, is not constant either because the total energy E is always constant. That is, the magnitude of the total angular momentum varies in time when there is a nutation.

However, when there is no nutation, or when the top undergoes a regular precession, since $Mgl\cos\theta$ is constant, we see that each term in Eq. (7.1) becomes constant. Under this condition, the first two terms of Eq. (7.1) can be identified as the total energy of a torque-free symmetrical top[5] in which the total angular momentum is constant. The fact that the magnitude of the total angular momentum of a heavy symmetrical top is constant is consistent with Eq. (4.6).

Thus, when a heavy symmetrical top undergoes a regular precession, its total energy can be written as a sum of the energy of a torque-free symmetrical top and the interaction energy $Mgl\cos\theta$. Then, since quantum-mechanical analysis of a torque-free symmetrical top is completely known,[5] we can evaluate the energies of the regular precession of a heavy symmetrical top by diagonalizing the Hamiltonian in the representation of the states of a torque-free symmetrical top.[5]

At this stage, however, the only way to check the validity of the connection formulas given by Eqs. (6.1)–(6.6) in the treatise of quantum mechanics is to check them numerically, since we can evaluate the dynamical constants of the regular precession of a heavy symmetrical top and those of the two torque-free symmetrical tops in terms of angular momentum quantum numbers. If the quantum treatise is established, one immediate application would be the molecular Stark effect, since its dynamical structure is the same as that of the regular precession of a heavy symmetrical top, i.e., the motion of a symmetric molecule possessing a permanent electric dipole moment along its symmetry axis placed in a uniform electric field.

APPENDIX[11]: PROPERTIES OF THE ELLIPTIC FUNCTIONS AND THE THETA FUNCTIONS

As we discussed in Sec. III, Jacobi discovered the decomposition theorem when he expressed each element (direction cosine) of the matrix which describes the motion of a heavy symmetrical top in terms of the theta functions. This is possible because the top motion is described by the elliptic functions, which can further be expressed by the theta functions. The elliptic functions $\mathrm{sn}(u)$ and $\mathrm{cn}(u)$ are expressed in terms of the four theta functions[11]

$$\mathrm{sn}(u) = [\Theta_1(0)/H_1(0)]\cdot[H(u)/\Theta(u)], \tag{A1}$$

$$\mathrm{cn}(u) = [\Theta(0)/H_1(0)]\cdot[H_1(u)/\Theta(u)], \tag{A2}$$

where H, Θ, H_1, and Θ_1 represent the theta functions and are expressed as infinite series similar to Fourier series[11]

$$H(u) = 2q^{1/4}\sin(\pi/2K)u - 2q^{9/4}\sin(3\pi/2K)u + 2q^{25/4}\sin(5\pi/2K)u - \cdots, \tag{A3}$$

$$\Theta(u) = 1 - 2q\cos(\pi/K)u + 2q^4\cos(2\pi/K)u - 2q^9\cos(3\pi/K)u + \cdots, \tag{A4}$$

$$H_1(u) = 2q^{1/4}\cos(\pi/2K)u + 2q^{9/4}\cos(3\pi/2K)u + 2q^{25/4}\cos(5\pi/2K)u + \cdots, \tag{A5}$$

$$\Theta_1(u) = 1 + 2q\cos(\pi/K)u + 2q^4\cos(2\pi/K)u + 2q^9\cos(3\pi/K)u + \cdots, \tag{A6}$$

where

$$q = \exp(-\pi(K'/K)), \tag{A7}$$

$$K = \int_0^{\pi/2} \frac{d\phi}{(1 - k^2\sin^2\phi)^{1/2}}, \tag{A8}$$

$$K' = \int_0^{\pi/2} \frac{d\phi}{(1 - k'^2\sin^2\phi)^{1/2}}, \tag{A9}$$

$$k'^2 = 1 - k^2. \tag{A10}$$

The factor k, as we already introduced in Sec. V, is the modulus.

Since the range of k is $0 \leqslant k \leqslant 1$, using Eqs. (A7)–(A9) we can easily prove that the range of q is also $0 \leqslant q \leqslant 1$. Then, from Eqs. (A3)–(A6), we observe that for $q < 1$, all the four theta functions rapidly converge. The relation between the modulus k and the value of q is given by[12]

$$q = Q + 2Q^5 + 15Q^9 + \cdots, \tag{A11}$$

where

$$Q = \tfrac{1}{2} \cdot \{[1 - (1 - k^2)^{1/4}]/[1 + (1 - k^2)^{1/4}]\} < 1. \tag{A12}$$

For example, we can obtain $q = 0.367\,8794$ for $k = 0.999\,5865$, and $q = 0.000\,6276$ for $k = 0.099\,958\,65$. Thus we see that Eq. (A11) shows that the value of q is extremely sensitive to the change of k, and q approaches zero much more rapidly than k does. Then it would be safe, for any value of k which is less than unity, to keep only the first term in Eqs. (A3) and (A5) and the first two terms in Eqs. (A4) and (A6). The elliptic functions can then be written

$$\mathrm{sn}(u) = 1(1 + 2q)\sin(\pi/2K)u/[1 - 2q\cos(\pi/K)u], \tag{A13}$$

$$\mathrm{cn}(u) = (1 - 2q)\cos(\pi/2K)u/[1 + 2q\cos(\pi/2)u]. \tag{A14}$$

Now in the limit $k = 0$, we have $q = 0$ from Eq. (A11) and $K = \pi/2$ from Eq. (A8). Then Eqs. (A13) and (A14) become

$$\mathrm{sn}(u) = \sin(u).$$

$$\mathrm{cn}(u) = \cos(u).$$

That is, the elliptic functions become trigonometric functions. Thus we can conclude that as the modulus k decreases, since the value of q decreases drastically, the elliptic functions rapidly approach the trigonometric functions. In the case of the motion of a heavy symmetrical top, as the value of k decreases, the motion rapidly approaches a regular precession.

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Elasticoviscous flow due to a plate which starts oscillating in the presence of a parallel stationary plate

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In this paper, the flow of a particular class of a non-Newtonian fluid between two parallel plates has been considered, employing a well-known transform technique, when one plate is stationary and the other plate suddenly starts oscillating. Both finite Fourier sine transform and Laplace transform techniques have been employed to solve the basic differential equations. The flow phenomenon has been characterized by the parameters S and ω. Expressions for the velocity have been calculated. Effects of the viscoelastic parameter and the frequency parameter on the fluid flow have been studied through several tables.

I. INTRODUCTION

The theoretical study of elasticoviscous liquids has been stimulated by the fact that many materials of industrial importance can be classified under this heading. It is required to formulate rheological equations of state to characterize the behavior of non-Newtonian liquids, and then to use these formulated equations, together with the familiar equations of motion and continuity, to predict the behavior of these materials. The non-Newtonian fluid considered is of Rivlin–Ericksen type.[1] Rayleigh[2] solved the viscous fluid problem of a semi-infinite space of fluid in contact with a plane wall initially at rest, the wall being suddenly accelerated to a constant velocity parallel to itself. Tanner[3] and Soundalgekar[4] solved the same problem replacing the viscous liquid by an elasticoviscous liquid. Viscous flow formation in Couetten motion has been discussed in the book by Schlichting.[5] Teipel[6] studied the flow near a wall suddenly set in motion for a particular class of non-Newtonian viscoelastic fluids (Rivlin–Ericksen type). The aim of this paper is to study the problem of flow of a viscoelastic liquid due to a plate which suddenly starts oscillating in the presence of another parallel stationary plate.

From Teipel[6] the flow field near a wall suddenly set in motion prescribes that the velocity component u along the wall is only a function of time and of the coordinate perpendicular to the wall. As a result one gets

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2} + \beta \frac{\partial^3 u}{\partial t\, \partial y^2}, \tag{1}$$

where ν is the kinematic coefficient of viscosity and β the kinematic coefficient of viscoelasticity.

The plate $y = 0$ suddenly starts oscillating from rest in its own plane while the plate $y = h$ is at rest. Since the plates are infinitely long, all physical quantities are independent of x. So the velocity field, consistent with the continuity equation is

$$u = u(y, t), \quad v = 0. \tag{2}$$

The nondimensional form of (1) is

$$\frac{\partial w}{\partial \tau} = \frac{\partial^2 w}{\partial \eta^2} + S \frac{\partial^3 w}{\partial \tau\, \partial \eta^2}, \tag{3}$$

where $\eta = y/h$, $\tau = \nu t/h^2$, $S = \beta/h^2$, and $w = u/U$. This equation (3) is to be solved with the initial and boundary conditions

$$\tau \leqslant 0, \quad w = 0, \quad \text{for } 0 \leqslant \eta \leqslant 1; \tag{4}$$

$$\tau \geqslant 0, \quad w = \begin{cases} \cos \omega \tau, & \text{for } \eta = 0, \\ 0, & \text{for } \eta = 1; \end{cases} \tag{5}$$

and further it is assumed that

$$\frac{\partial w}{\partial \tau} = 0, \quad \text{when } \tau = 0. \tag{6}$$

II. SOLUTION AND RESULTS

To solve Eq. (3) in exact form we first apply the finite Fourier sine transform. Following Sneddon[7] we define

$$w^*(m, \tau) = \int_0^1 w(\eta, \tau) \sin(m\pi\eta) d\eta,$$

so that

$$w(\eta, \tau) = 2 \sum_{m=1}^{\infty} w^* \sin(m\pi\eta). \tag{7}$$

Multiplying Eq. (3) throughout by $\sin m\pi\eta$ and integrating with respect to η within the limits 0 and 1, we get, using the conditions (5),

$$(1 + m^2\pi^2 S)\frac{\partial w^*}{\partial \tau} + m^2\pi^2 w^* = m\pi[\cos \omega\tau - S\omega \sin \omega\tau]. \tag{8}$$

The boundary conditions (4)–(6) yield

$$w^*(m,0) = \frac{\partial w^*(m,0)}{\partial \tau} = 0. \tag{9}$$

Let the Laplace transform of $w^*(m, \tau)$ be $\bar{w}^*(m, p)$ so that $\bar{w}^*(m, p) = \int_0^\infty e^{-p\tau} w^*(m, \tau) d\tau$. Taking a Laplace transform of both sides of Eq. (8) and using (9) we get

$$\bar{w}^*(m, p) = \alpha_1 (p - S\omega^2)/(p^2 + \omega^2)(p + \alpha_2), \tag{10}$$

where

$$\alpha_1 = m\pi/(1 + \pi^2 m^2 S) \tag{11}$$

and

$$\alpha_2 = \pi^2 m^2/(1 + \pi^2 m^2 s).$$

Taking the inverse Laplace transform of (10) we get

$$w^*(m; \tau) = \alpha_1 [A \cos \omega\tau + B \sin \omega\tau + C e^{-\alpha_2 \tau}], \tag{12}$$

where

$$A = (\alpha_2 + S\omega^2)/(\alpha_2^2 + \omega^2),$$

$$B = \omega(1 - \alpha_2^2 s)/(\alpha_2^2 + \omega^2),$$

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TABLE I. Effect of elastic element and frequency parameter on velocity and skin friction for $\tau = 0.1$.

η		Velocity profile			Skin friction		
		$\tau = 0.1$			$\tau = 0.1$		
		$\omega = 40$	$\omega = 60$	$\omega = 80$	$\omega = 40$	$\omega = 60$	$\omega = 80$
0.00	0.2	− 0.653 644	0.960 170	− 0.145 500	− 0.559 399	− 2.173 002	− 1.067 525
0.10		− 0.588 328	0.864 104	− 0.130 999	− 0.559 302	− 2.173 103	− 1.067 428
0.30		− 0.457 697	0.671 973	− 0.101 996	− 0.558 527	− 2.172 330	− 1.066 652
0.60		− 0.261 750	0.383 776	− 0.058 493	− 0.555 910	− 2.169 713	− 1.064 036
0.90		− 0.065 803	0.095 579	− 0.014 988	− 0.551 554	− 2.165 357	− 1.059 680
1.00		− 0.000 000	0.000 000	− 0.000 000	− 0.549 716	− 2.163 519	− 1.057 842
0.00	0.8	− 0.653 644	0.960 170	− 0.145 300	− 1.111 332	− 2.725 144	− 1.619 474
0.10		− 0.588 350	0.864 082	− 0.131 021	− 1.111 191	− 2.725 003	− 1.619 333
0.30		− 0.457 963	0.671 906	− 0.102 030	− 1.110 062	− 2.723 875	− 1.618 204
0.60		− 0.261 883	0.383 643	− 0.098 626	− 1.106 256	− 2.720 068	− 1.614 398
0.90		− 0.066 002	0.095 379	− 0.015 186	− 1.099 917	− 2.713 730	− 1.608 059
1.00		0.000 000	0.000 000	0.000 000	− 1.097 243	− 2.711 056	− 1.605 385
0.00	1.4	− 0.653 644	0.960 170	− 0.145 500	− 1.208 470	− 2.822 283	− 1.716 613
0.10		− 0.588 354	0.864 078	− 0.131 025	− 1.208 321	− 2.822 134	− 1.716 464
0.20		− 0.588 354	0.864 078	− 0.131 025	− 1.208 321	− 2.822 134	− 1.716 464
0.30		− 0.457 775	0.671 895	− 0.102 075	− 1.207 137	− 2.820 944	− 1.715 274
0.60		− 0.261 906	0.383 619	− 0.058 649	− 0.203 114	− 2.816 928	− 1.711 257
0.90		− 0.066 037	0.095 344	− 0.015 223	− 1.196 427	− 2.810 240	− 1.704 570
1.00		− 0.000 000	0.000 000	− 0.000 000	− 1.193 606	− 2.807 419	− 1.701 774

TABLE II. Effect of elastic element and frequency parameter on velocity and skin friction for $\tau = 0.3$.

η	S	Velocity profile			Skin friction		
		$\tau = 0.3$			$\tau = 0.3$		
		$\omega = 40$	$\omega = 60$	$\omega = 80$	$\omega = 40$	$\omega = 60$	$\omega = 80$
0.00	0.2	0.843 854	0.660 317	0.424 179	− 1.290 131	− 1.106 554	− 0.870 456
0.10		0.759 451	0.594 267	0.381 743	− 1.290 095	− 1.106 558	− 0.870 420
0.20		0.675 047	0.528 217	0.339 307	− 1.289 988	− 1.106 451	− 0.870 313
0.30		0.590 644	0.462 168	0.296 871	− 1.289 810	− 1.106 273	− 0.870 135
0.60		0.337 434	0.264 019	0.169 564	− 1.288 847	− 1.105 310	− 0.869 172
0.90		0.084 224	0.065 870	0.042 257	− 1.287 244	− 1.103 708	− 0.867 570
1.00		0.000 000	0.000 000	0.000 000	− 1.286 568	− 1.103 031	− 0.866 894
0.00	0.8	0.834 854	0.660 317	0.424 179	− 2.218 422	− 2.034 885	− 1.798 747
0.10		0.759 413	0.594 230	0.381 706	− 2.218 312	− 2.034 775	− 1.798 637
0.20		0.674 973	0.528 143	0.339 233	− 2.217 982	− 2.034 445	− 1.798 307
0.30		0.590 532	0.462 056	0.296 759	− 2.217 433	− 2.033 896	− 1.797 758
0.60		0.387 210	0.263 795	0.169 340	− 2.214 468	− 2.030 931	− 1.794 794
0.90		0.083 889	0.065 535	0.041 921	− 2.209 532	− 2.025 995	− 1.789 857
1.00		0.000 000	0.000 000	0.000 000	− 2.207 449	− 2.023 912	− 1.787 775
0.00	1.4	0.843 854	0.660 317	0.424 179	− 2.458 080	− 2.274 543	− 2.038 405
0.10		0.759 404	0.554 220	0.381 696	− 2.457 931	− 2.274 414	− 2.038 276
0.20		0.674 953	0.528 124	0.339 213	− 2.457 564	− 2.274 027	− 2.037 889
0.30		0.590 503	0.462 027	0.296 731	− 2.456 919	− 2.273 382	− 2.037 244
0.60		0.337 152	0.263 737	0.169 282	− 2.453 436	− 2.269.900	− 2.033 763
0.90		0.083 802	0.065 448	0.041 835	− 2.447 641	− 2.264 103	− 2.027 966
1.00		0.000 000	0.000 000	0.000 000	− 2.445 195	− 2.261 658	− 2.025 520

and

$$C = -A.$$

Using definition (7) and simplifying we get

$$w^*(\eta, \tau) = (1 - \eta)\cos\ \omega\tau + 2\sum_{m=1}^{\infty} \alpha_1[A_1 \cos\omega\tau + B \sin\omega\tau + C e^{-\alpha_2\tau}] \sin m\pi\eta, \quad (13)$$

where

$$A_1 = [\alpha_2(\alpha_2 + S\omega^2) - (\alpha_2^2 + \omega^2)]/\pi^2 m^2(\alpha_2^2 + \omega^2).$$

The shearing stress at the plate is given by

$$Txy = \frac{\partial w}{\partial \eta} + S\frac{\partial^2 w}{\partial \tau\, \partial \eta}. \quad (14)$$

Taking the Laplace transform of Eq. (14) and assuming that $Txy = 0$ when $\tau = 0$, we get

TABLE III. Effect of elastic element and frequency parameter on velocity and skin friction for $\tau = 0.5$.

η	S	Velocity profile			Skin friction		
		$\tau = 0.5$			$\tau = 0.5$		
		$\omega = 40$	$\omega = 60$	$\omega = 80$	$\omega = 40$	$\omega = 60$	$\omega = 80$
0.00	0.2	0.408 082	0.154 251	−0.686 938	−0.572 252	−0.318 442	0.502 759
0.10		0.367 267	0.138 820	−0.600 251	−0.572 243	−0.318 429	0.502 773
0.20		0.326 452	0.123 388	−0.533 504	−0.572 239	−0.318 390	0.502 812
0.30		0.285 638	0.107 556	−0.466 876	−0.572 200	−0.318 824	0.502 878
0.60		0.163 193	0.061 661	−0.266 815	−0.572 134	−0.317 970	0.503 232
0.90		0.040 749	0.015 386	−0.666 753	−0.571 780	−0.317 380	0.303 821
1.00		0.000 000	0.000 000	0.000 000	−0.571 196	−0.317 131	0.504 070
0.00	0.8	0.408 082	0.154 251	−0.666 938	−1.478 599	−1.224 770	−0.403 580
1.10		0.367 231	0.138 783	−0.600 287	−1.478 513	−1.224 684	−0.403 494
0.20		0.326 380	0.123 315	−0.553 637	−1.478 257	−1.224 497	−0.403 237
0.30		0.285 528	0.107 847	−0.466 986	−1.477 829	−1.224 000	−0.402 810
0.60		0.162 975	0.061 442	−0.267 033	−1.475 520	−1.221 691	−0.400 501
0.90		0.040 421	0.015 038	−0.067 081	−1.471 676	−1.217 846	−0.396 656
1.00		0.000 000	0.000 000	−0.000 000	−1.470 064	−1.216 225	−0.395 035
0.00	1.4	0.408 082	0.154 251	−0.666 938	−1.807 420	−1.553 590	−0.732 401
0.10		0.367 218	0.138 770	−0.600 301	−1.807 308	−1.553 478	−0.732 289
0.20		0.326 353	0.123 289	−0.553 663	−1.806 973	−1.883 143	−0.731 953
0.30		0.285 488	0.107 807	−0.467 025	−1.806 414	−1.852 584	−0.731 394
0.60		0.102 895	0.061 363	−0.367 113	−1.803 396	−1.549 566	−0.728 378
0.90		0.040 303	0.014 920	−0.067 129	−1.798 370	−1.544 540	−0.723 351
1.00		0.000 000	0.000 000	0.000 000	−1.796 250	−1.542 420	−0.721 231

$$\bar{T}xy = (1 + Sp)\frac{d\bar{w}}{d\eta}. \tag{15}$$

Taking the Laplace transform of Eq. (13) and then differentiating with respect to η, we get

$$\frac{d\bar{w}}{d\eta} = \frac{-p}{p^2+\omega^2} + 2\sum_{m=1}^{\infty} \pi m \alpha_1 \left[\frac{A_1 p}{p^2+\omega^2} + \frac{B\omega}{p^2+\omega^2} + \frac{C}{p+\alpha_2}\right] \cos m\pi\eta. \tag{16}$$

Substituting Eq. (16) into (15) and inverting we get

$$Txy = -\cos\omega\tau + 2\sum_{m=1}^{\infty} \pi m \alpha_1 [A_2 \cos\omega\tau + B_2 \sin\omega\tau + C_2 e^{-\alpha_2\tau}] \cos\pi m\eta, \tag{17}$$

where

$$A_2 = A_1 + BS, \quad B_2 = -A_1\omega S + B, \quad C_2 = C.$$

The skin friction S_1 and S_2 at the plates can be obtained by putting $\eta = 0$ and $\eta = 1$ in Eq. (17), respectively.

III. DISCUSSION

An examination of Tables I–III shows that for $\tau = 0.1$ the velocity at any point increases as the frequency parameter increases to a limit, but beyond this limit for frequency an opposite effect is observed. It is also observed that at $\eta = 0$, the velocity is not affected by the elastic parameter in each and every case. The same velocity is observed both for Newtonian and non-Newtonian fluid. The effect of the viscoelastic parameter is to decrease the velocity profile. For $\tau = 0.3$ and 0.5 the velocity at any point decreases as the frequency parameter increases.

The effect of elasticity is to decrease the velocity of the fluid particle. The value of η for which minimum values of velocity occur shifts towards the stationary plate normally. The velocity of the fluid increases as time increases to a limit for $\omega = 40$, 80, and beyond this limit for time an opposite effect is observed. For frequency $\omega = 60$ the velocity of the fluid decreases as time increases.

The skin friction of the fluid is decreased due to the elasticity of the fluid. The skin friction of the fluid is decreased at any point up to a limit but beyond this limit an opposite effect is observed for $\omega = 40$. For higher values of frequency (60, 80) the shearing stress increases as frequency increases and as time increases, too. Elasticity of the liquid decreases the shearing stress at the wall. For higher values of the frequency, the shearing stress always increases. For smaller values of frequency, the shearing stress first decreases for the viscoelastic parameter and then increases.

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On a new class of completely integrable nonlinear wave equations. I. Infinitely many conservation laws

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We point out a class of nonlinear wave equations which admit infinitely many conserved quantities. These equations are characterized by a pair of exact one-forms. The implication that they are closed gives rise to equations, the characteristics and Riemann invariants of which are readily obtained. The construction of the conservation laws requires the solution of a linear second-order equation which can be reduced to canonical form using the Riemann invariants. The hodograph transformation results in a similar linear equation. We discuss also the symplectic structure and Bäcklund transformations associated with these equations.

I. INTRODUCTION

Among the important successes of the inverse scattering method is the result that certain nonlinear wave equations admit infinitely many conserved quantities.[1,2] Indeed, the construction of these conserved quantities is immediate once a nonlinear evolution equation has been cast into the framework of the inverse scattering method.[3] However, there exist some nonlinear partial differential equations which do not fit into this general framework but nevertheless give rise to an infinite sequence of conservation laws. The equations governing long surface waves on shallow water are case in point. It is well known that they admit infinitely many conserved quantities[4,5] but in spite of the simplicity of these equations it has not been possible so far to formulate them as an inverse scattering problem. Thus we are led to the possibility that these equations may be a realization of a new general mathematical structure whereby a class of nonlinear partial differential equations can be shown to admit infinitely many conservation laws. In this paper we shall find that there is indeed such a structure and present an algorithm for constructing the conservation laws. The class of nonlinear wave equations which can be handled by this method turns out to be surprisingly large. It includes the nonlinear wave equations of Euler[6] and Poisson[7] describing the propagation of finite-amplitude waves in gases and fluids, large-amplitude string waves,[8] and Nambu's relativistic string and its massive version.[9] Our approach to these equations will be based on our earlier treatment of shallow water waves.[10]

II. GENERAL FORMALISM

We shall consider a class of nonlinear wave equations which can be written in the form of a continuity equation

$$f_t + g_x = 0, \tag{2.1}$$

where

$$f = f(\phi_t, \phi_x), \quad g = g(\phi_t, \phi_x) \tag{2.2}$$

are *arbitrary* differentiable functions of their arguments. These equations will be linear and homogeneous in the second derivatives

$$a(\phi_t, \phi_x)\phi_{tt} + 2h(\phi_t, \phi_x)\phi_{tx} + b(\phi_t, \phi_x)\phi_{xx} = 0, \tag{2.3}$$

with the nonlinearities entering through the coefficients a,b,h, which are obtained from f, g above. The variational principle $\delta I = 0$,

$$I = \int L(\phi_t, \phi_x)dx\,dt, \tag{2.4}$$

where the Lagrangian depends solely on the first derivatives of ϕ, provides an important, but by no means the only source of physically interesting equations of this type. Equations derivable from a variational principle must further satisfy

$$f_{\phi_x} = g_{\phi_t}, \tag{2.5}$$

which is not necessary for our purposes. Among the illustrative examples we shall discuss in this paper the Euler equation (3.1) satisfies Eq. (2.5), whereas the Poisson equation (4.1) does not.

A. First-order system

Our approach to Eq. (2.1) is based on the introduction of a new variable ψ so that we may express this second-order partial differential equation as the integrability condition of a pair of coupled first-order equations. Thus we consider the system

$$\psi_x = f(\phi_t, \phi_x), \quad \psi_t = -g(\phi_t, \phi_x), \tag{2.6}$$

and note that an arbitrary function of x and another one of t could have been included on the respective right-hand sides of Eqs. (2.6) consistent with the requirement that Eq. (2.1) should result as their integrability condition. But these functions can be removed by a redefinition of ψ and therefore it is not necessary to consider them except in the discussion of Bäcklund transformations in the sequel.

Equation (2.1) is not the only integrability condition of the first-order system. Provided Eqs. (2.6) can be inverted, we can write

$$\phi_x = p(\psi_t, \psi_x), \quad \phi_t = -q(\psi_t, \psi_x), \tag{2.7}$$

and this will result in another integrability condition

$$p_t + q_x = 0, \tag{2.8}$$

which is a second-order nonlinear partial differential equation for ψ.

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B. Exact one-forms α,ω

We were led to the first-order system because of our interest in its integrability conditions and now we shall consider a framework which *a priori* gives rise to such a system. For this purpose we first define

$$u = \phi_x, \quad v = \psi_x, \tag{2.9}$$

and suppose that the first-order equations (2.6) can be solved for the remaining variables

$$\begin{aligned} \phi_t &= U(u,v), \\ \psi_t &= V(u,v), \end{aligned} \tag{2.10}$$

in closed form. Alternatively, in Eqs. (2.9) and (2.10) we find four equations for two unknowns u,v which are consistent by virtue of Eqs. (2.6).

Now comes the key step in our approach: We introduce the one-forms

$$\begin{aligned} \alpha &= u\,dx + U\,dt, \\ \omega &= v\,dx + V\,dt, \end{aligned} \tag{2.11}$$

and note that the conditions for them to be exact,

$$\alpha = d\phi, \quad \omega = d\psi, \tag{2.12}$$

are simply Eqs. (2.9) and (2.10). Henceforth d will denote the exterior derivative and $\wedge$ the exterior product. Since α,ω are exact, they must also be closed

$$d\alpha = 0, \quad d\omega = 0, \tag{2.13}$$

and this results in the equations

$$\begin{aligned} u_t - U_u u_x - U_v v_x &= 0, \\ v_t - V_u u_x - V_v v_x &= 0, \end{aligned} \tag{2.14}$$

which are the integrability conditions of Eqs. (2.11). Having cast the problem into the form of Eqs. (2.14) we are now ready to consider the solution of Eq. (2.1). There is a formal symmetry of Eqs. (2.14) under the simultaneous interchange of u, U with v, V which will carry throughout the general formalism to be developed below. But this symmetry is only a formal one and disappears completely when we consider particular examples because U,V are, in general, different functions of u,v.

C. Characteristics and Riemann invariants

Equations (2.14) are partial differential equations which are linear and homogeneous in the first derivatives. We shall apply Riemann's method[11,12] of characteristics to this system of equations. The characteristics of Eqs. (2.14) are given by

$$x'^2 + (U_u + V_v)x't' + (U_u V_v - U_v V_u)t'^2 = 0, \tag{2.15}$$

where prime denotes differentiation with respect to a parameter running along the characteristics and

$$V_u u'^2 + (V_v - U_u)u'v' - U_v v'^2 = 0 \tag{2.16}$$

is the equation satisfied by the Riemann invariants. We can solve Eq. (2.15)

$$\frac{dx}{dt} = c(u,v;\epsilon),$$

where

$$c = -\tfrac{1}{2}(U_u + V_v) + \epsilon\left[\tfrac{1}{4}(U_u - V_v)^2 + U_v V_u\right]^{1/2}, \tag{2.17}$$

with

$$\epsilon = \pm 1, \tag{2.18}$$

and define the directional derivative

$$D^\epsilon = \frac{\partial}{\partial t} + c(u,v;\epsilon)\frac{\partial}{\partial x} \tag{2.19}$$

along the characteristics. Finally, Eqs. (2.16) are first-order ordinary differential equations

$$\frac{dv}{du} = \tfrac{1}{2}V_u^{-1}\{U_u - V_v + \epsilon[(U_u - V_v)^2 + 4U_v V_u]^{1/2}\}, \tag{2.20}$$

and we shall let

$$\begin{aligned} R^\epsilon(u,v) &= \text{const}, \\ \xi = R^+, &\quad \eta = R^- \end{aligned} \tag{2.21}$$

stand for its integrals. These are the Riemann invariants. Both of these invariants satisfy an equation which is equivalent to Eq. (2.16):

$$U_v \zeta_u^2 + (V_v - U_u)\zeta_u \zeta_v - V_u \zeta_v^2 = 0, \tag{2.22}$$

where ζ is either ξ or η depending on the choice of roots for this quadratic equation. Then Eqs. (2.14) are simply given by

$$D^\epsilon R^\epsilon = 0, \tag{2.23}$$

which is Reimann's canonical form.

D. Hodograph transformation

A qualitative picture of the solutions emerges from a knowledge of the characteristics and Riemann invariants. It is, however, possible to obtain the exact solution of Eqs. (2.14) with the help of the hodograph transformation

$$\{t,x\} \leftrightarrow \{u,v\},$$

interchanging the roles of dependent and independent variables. Using the standard hodograph relations

$$\begin{aligned} u_t &= -J^{-1}x_v, \quad u_x = J^{-1}t_v, \quad v_t = J^{-1}x_u, \\ v_x &= -J^{-1}t_u, \quad J = x_u t_v - x_v t_u \neq 0, \end{aligned} \tag{2.24}$$

we find that Eqs. (2.14) are transformed into the linear equations

$$\begin{aligned} x_v + U_u t_v - U_v t_u &= 0, \\ x_u - V_u t_v + V_v t_u &= 0, \end{aligned} \tag{2.25}$$

which can be decoupled to yield second-order equations for either x or t. These linear equations can be used to construct exact solutions. But we shall not discuss them any further here because they are similar to the equations we shall next obtain for the conservation laws and can be handled with similar techniques.

E. Conservation laws

We shall consider the conditions for Eqs. (2.14) to admit conservation laws of the form

$$F_t + G_x = 0, \tag{2.26}$$

where F,G are function of u,v but do not depend on x,t explicitly. Then from Eqs. (2.14), we find that Eqs. (2.26) results in the linear equations

$$G_u + U_u F_u + V_u F_v = 0\,,$$
$$G_v + U_v F_u + V_v F_v = 0\,, \tag{2.27}$$

which are to be compared to Eqs. (2.25). Decoupling these equations we find

$$V_u F_{vv} + (U_u - V_v)F_{uv} - U_v F_{uu} = 0\,, \tag{2.28}$$

and G satisfies an equation which is identical to this except for the presence of additional terms involving its first derivatives. The characteristics of Eqs. (2.27), (2.28), and (2.25) all satisfy Eq. (2.16) and therefore consist of the Riemann invariants (2.21) of Eqs. (2.14). With a transformation of the coordinates from u,v to ξ,η given by Eqs. (2.21), these equations can be brought to the canonical form

$$\mathscr{F}_{\xi\eta} + m(\xi,\eta)\mathscr{F}_{\xi} + n(\xi,\eta)\mathscr{F}_{\eta} = 0\,, \tag{2.29}$$

where $\mathscr{F}$ stands for an element of the set $\{F,G,t,x\}$ and the functions m,n are determined in each case. The reduction to canonical form suffices to construct the exact solution in particular examples. The solution of Eq. (2.29) will in general involve two arbitrary functions of two variables and therefore the conserved quantities

$$\mathscr{P} = \int F \quad dx \tag{2.30}$$

will be infinite in number.

F. Symplectic structure

Among the class of equations which can be written in the form of Eq. (2.1) there is a subclass which admits a symplectic structure. These equations will satisfy Hamilton's equations

$$u_t + [H,u] = 0, \quad v_t + [H,v] = 0\,, \tag{2.31}$$

where H is the Hamiltonian function and the square bracket stands for the Poisson bracket. The phase space will consist of infinitely differentiable functions of u,v and the Poisson bracket of two functions P,Q of these variables is defined by

$$[P,Q] = \int \nabla P J \nabla Q \, dx, \tag{2.32}$$

where ∇ is the gradient in function space

$$\nabla = \left(\frac{\partial}{\partial u}, \frac{\partial}{\partial v}\right),$$

and

$$J = -\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{\partial}{\partial x}$$

is the Hamiltonian operator. Equations (2.14) will be in the form of Eqs. (2.31) provided

$$H_u = -V, \quad H_v = -U\,, \tag{2.33}$$

which requires

$$U_u - V_v = 0\,, \tag{2.34}$$

and thereby the existence of the exact one-form

$$U\,dv + V\,du = -dH \tag{2.35}$$

is a necessary and sufficient condition for these equations to admit a symplectic structure.

G. Bäcklund transformations

We had earlier mentioned that the first-order system (2.6) can be regarded as a Bäcklund transformation between the second-order partial differential equations (2.1) and (2.8). More properly, these equations define a Bianchi transformation because they do not involve any arbitrary parameters. We can introduce such parameters by letting

$$\psi \to \psi + rx - st\,, \tag{2.36}$$

where r,s are arbitrary constants. This modification of Eqs. (2.6) is not significant for only a single set of transformations. However, it becomes meaningful when we consider the Bäcklund diagram in Fig. 1, which involves a succession of such transformations. In this diagram we have labeled the fields and accompanying parameters which enter into these transformations and it is important to note that not all the parameters r^1, r^2, s^1, s^2 can be eliminated by a redefinition of ψ.

Starting from a solution of Eq. (2.1) we can obtain another one by combining two transformations as in Fig. 1. Thus we can eliminate ψ and obtain relations of the form

$$\tilde{\phi}_t = \tilde{\phi}_t(\phi_t, \phi_x, r^1 - r^2, s^1 - s^2)\,,$$
$$\tilde{\phi}_x = \tilde{\phi}_x(\phi_t, \phi_x, r^1 - r^2, s^1 - s^2)\,, \tag{2.37}$$

where only the differences between the two pairs of parameters have proved to be significant. Equations (2.37) are the auto-Bäcklund transformations of Eqs. (2.1).

We have now presented the general formalism for dealing with equations of the type (2.1). In order to illustrate the usefulness of our approach we shall apply this formalism to the nonlinear wave equations of Euler and Poisson in the next two sections. We shall employ the same notation in discussing both of these equations as there is going to be no overlap between them.

III. EULER EQUATION

Euler's nonlinear wave equation for finite-amplitude wave propagation in an ideal gas is given by

$$\phi_{tt} - c^2(1 + \phi_x)^{-(1+\gamma)}\phi_{xx} = 0\,, \tag{3.1}$$

where ϕ is the particle displacement in a Lagrangian description of motion and γ,c are constants standing for the ratio of specific heats and the ordinary sound velocity, respectively. Of particular interest is the case $\gamma = 1$, which describes the propagation of sound waves in fluids and, as we shall find presently, sometimes requires separate treatment.

Euler's equation is the integrability condition of the first-order system

$$\phi_t + c^2\gamma^{-1}\psi_x = 0\,,$$
$$\psi_t - (1 + \phi_x)^{-\gamma} + 1 = 0\,, \tag{3.2}$$

where we have introduced a new field ψ as in Eqs. (2.6). Another integrability condition of Eqs. (3.2) is

$$\psi_{tt} - c^2(1 + \psi_t)^{1+1/\gamma}\psi_{xx} = 0\,, \tag{3.3}$$

which appears to be of physical interest as well.

The exact one-forms α,ω of Eqs. (2.11) are in this case

$$\phi \xrightarrow{r^1,\, s^1} \psi \xrightarrow{r^2,\, s^2} \tilde{\phi}$$

FIG. 1. Bäcklund diagram.

$$\alpha = u\,dx - c^2\gamma^{-1}v\,dt\,,$$
$$\omega = v\,dx + [(1+u)^{-\gamma} - 1]dt\,, \tag{3.4}$$

that is, from Eqs. (2.12)

$$u = \phi_x,\quad U = -c^2\gamma^{-1}v = \phi_t\,,$$
$$v = \psi_x,\quad V = (1+u)^{-\gamma} - 1 = \psi_t\,, \tag{3.5}$$

and Eqs. (3.2) follow from the elimination of u,v from these equations. The implication that α,ω are closed gives rise to

$$u_t + c^2\gamma^{-1}v_x = 0\,,$$
$$v_t + \gamma(1+u)^{-1-\gamma}u_x = 0\,, \tag{3.6}$$

which are the integrability conditions of Eqs. (3.5) and correspond to Eqs. (2.14). The characteristics of Eqs. (3.6) satisfy

$$x' = \epsilon c(1+u)^{-(1+\gamma)/2}t'\,, \tag{3.7}$$

and

$$D^\epsilon = \frac{\partial}{\partial t} + \frac{\epsilon c}{(1+u)^{(1+\gamma)/2}}\frac{\partial}{\partial x} \tag{3.8}$$

is the directional derivative (2.19) along the characteristics. Depending on the value of γ it is necessary to distinguish two cases for the Riemann invariants. We find

$$R^\epsilon = \epsilon cv + (2\gamma/(1-\gamma))(1+u)^{(1-\gamma)/2}\,,$$

for $\gamma \neq 1$ and

$$R_1^\epsilon = \epsilon cv + \ln|1+u|\,, \tag{3.9}$$

for the exceptional case $\gamma = 1$. Equations (3.6) are cast into Riemann's canonical form (2.23) through the use of Eq. (3.8) and either one of Eqs. (3.9) depending on the value of γ. These results are due to Riemann and Earnshaw who, however, did not base their discussion on the simple system (3.6) (cf. Rayleigh[13]).

From a knowledge of the characteristics and Riemann invariants we can obtain solutions, in particular Fubini's solution[14] of the Euler equation. However, exact solutions can be readily constructed using the hodograph transformation (2.24). The first-order equations (2.25) are now given by

$$c^2t_u + \gamma x_v = 0\,,$$
$$\gamma t_v + (1+u)^{1+\gamma}x_u = 0\,, \tag{3.10}$$

and they result in decoupled second-order linear equations.

On the other hand, the requirement that Eqs. (3.6) admit conservation laws of the form (2.26) leads to

$$c^2F_u - \gamma G_v = 0\,,$$
$$\gamma F_v - (1+u)^{1+\gamma}G_u = 0\,, \tag{3.11}$$

which are the same as Eqs. (3.10) with the identification $F = t$, $G = -x$. From these equations we obtain

$$F_{vv} - c^2\gamma^{-2}(1+u)^{1+\gamma}F_{uu} = 0\,,$$
$$G_{vv} - c^2\gamma^{-2}[(1+u)^{1+\gamma}G_u]_u = 0\,, \tag{3.12}$$

and we shall transform them to canonical form using the Riemann invariants.

Let us first consider the case $\gamma \neq 1$ and use the Riemann invariants as new coordinates. Then Eqs. (3.12) are transformed into the form

$$(\xi+\eta)F_{\xi\eta} - \nu(F_\xi + F_\eta) = 0\,,$$
$$(\xi+\eta)G_{\xi\eta} + \nu(G_\xi + G_\eta) = 0\,, \tag{3.13}$$
$$\nu = \tfrac{1}{2}(1+\gamma)/(1-\gamma)\,,$$

the familiar Euler–Darboux–Poisson equation. The Riemann–Green function for these equations is given by[12]

$$\mathcal{G}(\xi,\eta;\xi_0,\eta_0) = \frac{(\xi+\eta)^\nu}{(\xi_0+\eta_0)^\nu}P_{\pm\nu}\left(1 + 2\frac{(\xi-\xi_0)(\eta-\eta_0)}{(\xi+\eta)(\xi_0+\eta_0)}\right), \tag{3.14}$$

where P stands for the Legendre function. With the help of the Riemann–Green function we can construct solutions satisfying appropriate boundary conditions.

The case $\gamma = 1$ turns out to be even simpler because Eqs. (3.13) can then be transformed into the form of a two-dimensional Klein–Gordon equation with unit mass. The solution is given by

$$F = \int [A(\mu)(1+u)^{-\mu} + B(\mu)(1+u)^{\mu+1}] \times [C(\mu)e^{\lambda v} - D(\mu)e^{-\lambda v}]\lambda\,d\mu\,,$$
$$G = \int [-\mu A(\mu)(1+u)^{-\mu-1} + (\mu+1)B(\mu)(1+u)^{\mu}] \times [C(\mu)e^{\lambda v} + D(\mu)e^{-\lambda v}]c^2\,d\mu\,, \tag{3.15}$$
$$\lambda = c[\mu(\mu+1)]^{1/2}\,,$$

and A, B, C, D are arbitrary functions of μ which must be chosen to suit given boundary conditions. In particular, the specialization of these relations to the form

$$F = \int \lambda A(\mu)[(1+\phi_x)^{-\mu} - (1+\phi_x)^{\mu+1}] \times \sinh(\lambda\phi_t/c^2)d\mu\,,$$
$$G = c^2\int A(\mu)[\mu(1+\phi_x)^{-\mu-1} + (\mu+1)(1+\phi_x)^{\mu}] \times \cosh(\lambda\phi_t/c^2)d\mu \tag{3.16}$$

enables us to construct quantities which involve an arbitrary function $A(\mu)$ and vanish in the limit $\phi_x \to 0$, $\phi_t \to 0$. With these expressions for F,G it can be directly verified that the continuity equation (2.26) results in the Euler equation (3.1).

Euler's equation admits a symplectic structure. From Eqs. (3.4) we find that Eq. (2.34) is satisfied, and integrating Eq. (2.35) yields the Hamiltonian

$$H = (c^2/2\gamma)v^2 - [1/(1-\gamma)](1+u)^{1-\gamma} + u\,,$$

for $\gamma \neq 1$ and

$$H_1 = \tfrac{1}{2}c^2v^2 - \ln|1+u| + u\,, \tag{3.17}$$

in the remaining case $\gamma = 1$. It is also possible to formulate a variational principle for Euler's equation as Eq. (2.5) is fulfilled in this case. We find that the Lagrangian for Eq. (3.1) is given by

$$\mathcal{L} = \tfrac{1}{2}\phi_t^2 + [c^2/\gamma(1-\gamma)](1+\phi_x)^{1-\gamma},$$
$$\mathcal{L}_1 = \tfrac{1}{2}\phi_t^2 + c^2\ln|1+\phi_x|\,, \tag{3.18}$$

for $\gamma \neq 1$ and $\gamma = 1$, respectively, while for Eq. (3.3) the Lagrangian is

$$\mathcal{L}' = \tfrac{1}{2}c^2\psi_x^2 - [\gamma^2/(1-\gamma)](1+\psi_t)^{1-1/\gamma},$$
$$\mathcal{L}_1' = \tfrac{1}{2}c^2\psi_x^2 + \ln|1+\psi_t|\,, \tag{3.19}$$

where again we distinguish the cases $\gamma \neq 1$ and $\gamma = 1$. There is a variational principle underlying Eqs. (3.6) as well. The Lagrangian now involves both variables

$$\mathscr{L}'' = \phi_t \psi_x + \psi_t \phi_x + c^2 \gamma^{-1} \psi_x^2 - 2(1 + \phi_x)^{-\gamma}, \tag{3.20}$$

and this form is the most suitable one for passing to a Hamiltonian formalism via Dirac's theory of constraints.[10]

Bäcklund transformations of Euler's equation can be obtained after modifying the first-order system (3.2) according to Eq. (2.36). Then Eq. (3.3), which is the Bäcklund companion of Euler's equation, is changed by the addition of $s^{1,2}$ to the terms enclosed by parentheses there. The result of performing two such transformations is

$$\begin{aligned} \tilde{\phi}_t &= \phi_t - r, \\ \tilde{\phi}_x &= [(1 + \phi_x)^{-\gamma} + s]^{-1/\gamma} - 1, \end{aligned} \tag{3.21}$$

where $r = c^2 \gamma^{-1} (r^1 - r^2), s = s^1 - s^2$. In particular for $\gamma = 1$ the latter of Eqs. (3.21) becomes the linear fractional transformation

$$\tilde{\phi}_x = (-s + (1 - s)\phi_x)/(1 + s + s\phi_x).$$

The Euler equation (3.1) is invariant under the transformations (3.21).

IV. POISSON'S EQUATION

We shall now discuss the nonlinear wave equation of Poisson

$$\phi_{tt} + 2\phi_x \phi_{xt} - (1 - \phi_x^2)\phi_{xx} = 0, \tag{4.1}$$

which is derived from an Eulerian description of fluid motion, and ϕ denotes the velocity potential. Once again we shall introduce a new potential ψ whereby Poisson's equation can be obtained as the integrability condition of

$$\begin{aligned} &\phi_t - \psi_x + \phi_x^2 = 0, \\ &\psi_t - \phi_x + \frac{1}{3}\phi_x^3 = 0, \end{aligned} \tag{4.2}$$

which is the required first-order system. It is not possible to obtain a simple equation for ψ as the integrability condition of these equations since the latter of Eqs. (4.2) is cubic in ϕ_x. With the help of the continued fraction

$$T(z) = 1 - \frac{1}{3}\left[\frac{z}{1 - \frac{1}{3}(z/(1 - \cdots))^2}\right]^2,$$

we can write this equation in the form

$$3T(\psi_t)\psi_{tt} + 6\psi_t \psi_{tx} + [2\psi_t^2 - 3T^3(\psi_t)]\psi_{xx} = 0. \tag{4.3}$$

The first-order system of equations (4.2) are the conditions for the one-forms

$$\begin{aligned} \alpha &= u\,dx + (v - u^2)dt, \\ \omega &= v\,dx + (1 - \tfrac{1}{3}u^2)u\,dt, \end{aligned} \tag{4.4}$$

to be exact because they result as a consequence of the relations

$$\begin{aligned} &u = \phi_x, \quad U = v - u^2 = \phi_t, \\ &v = \psi_x, \quad V = u - \tfrac{1}{3}u^3 = \psi_t, \end{aligned} \tag{4.5}$$

which follow from Eqs. (4.3) and (2.12). The first part of Eqs. (4.5) is the definition of the fluid velocity u. Once again, α and ω are closed one-forms and we find

$$\begin{aligned} &u_t + 2uu_x - v_x = 0, \\ &v_t - (1 - u^2)u_x = 0, \end{aligned} \tag{4.6}$$

as the integrability conditions of Eqs. (4.5). These equations correspond to Eqs. (2.14) and they will form the basis of our discussion of the conservation laws and the solution of Poisson's equation.

The characteristics of Eqs. (4.6) are given by

$$x' = (u + \epsilon)t', \tag{4.7}$$

so that

$$D^\epsilon = (u + \epsilon)\frac{\partial}{\partial x} + \frac{\partial}{\partial t},$$

and the Riemann invariants are

$$R^\epsilon = \tfrac{1}{4}(v - \tfrac{1}{2}u^2 - \epsilon u). \tag{4.8}$$

With these expressions Eqs. (4.6) are cast into Riemann's canonical form (2.23).

The hodograph transformation leads to the linear equations

$$\begin{aligned} &x_u - (1 - u^2)t_v = 0, \\ &x_v - 2ut_v - t_u = 0, \end{aligned} \tag{4.9}$$

and

$$\begin{aligned} &t_{uu} + 2ut_{uv} - (1 - u^2)t_{vv} + 2t_v = 0, \\ &x_{uu} + 2ux_{uv} - (1 - u^2)x_{vv} + [2u/(1 - u^2)]x_u = 0, \end{aligned} \tag{4.10}$$

are the resulting decoupled second-order linear equations. Equations (2.27) for the conservation laws are now given by

$$G_u - 2uF_u + (1 - u^2)F_v = 0, \quad G_v + F_u = 0, \tag{4.11}$$

and they yield

$$\begin{aligned} &F_{uu} + 2uF_{uv} - (1 - u^2)F_{vv} = 0, \\ &G_{uu} + 2uG_{uv} - (1 - u^2)G_{vv} \\ &\quad + [2/(1 - u^2)][uG_u + (1 + u^2)G_v] = 0, \end{aligned} \tag{4.12}$$

which are no longer similar to Eqs. (4.10), unlike the situation in Euler's equation. The first one of Eqs. (4.12) reduces to a Klein–Gordon equation when we transform it to canonical form using Eqs. (4.8) as new coordinates, and its solution yields

$$\begin{aligned} F = \int &[A(\mu)e^{[\mu/(1-\mu^2)]u} + B(\mu)e^{-[\mu/(1-\mu^2)]u}] \\ &\times [C(\mu)e^{[\mu^2/(1-\mu^2)](v - u^2/2)} \\ &+ D(\mu)e^{-[1/(1-\mu^2)](v - u^2/2)}]d\mu, \end{aligned} \tag{4.13}$$

which through Eq. (2.30) gives the conserved quantities for Poisson's equation. Finally, the Bäcklund transformations for Eq. (4.1) are given by

$$\begin{aligned} &\phi_t - \tilde{\phi}_t + \phi_x^2 - \tilde{\phi}_x^2 = r, \\ &(\phi_x - \tilde{\phi}_x)[1 - \tfrac{1}{3}(\phi_x^2 + \phi_x \tilde{\phi}_x + \tilde{\phi}_x^2)] = s, \end{aligned} \tag{4.14}$$

where r,s are arbitrary parameters. Poisson's equation does not admit a symplectic structure as Eqs. (2.34) are not satisfied for the results of Eqs. (4.5).

V. CONCLUSION

We have considered a class of nonlinear partial differential equations in two dimensions. By introducing a new potential these equations were expressible as a first-order system which we have then formulated as the conditions for a pair of one-forms α,ω to be exact. The implication that these differential forms are closed gave rise to a set of homogeneous first-order partial differential equations ideally suited to an application of Riemann's method of characteristics. We have shown that with the help of the hodograph transformation these equations can be turned into linear equations and thereby solved exactly. Furthermore the requirement that these equations admit conservation laws led, once again, to linear second-order equations, the characteristics of which are the Riemann invariants. The solution of these linear equations has enabled us to construct infinitely many conserved quantities. We have obtained the necessary and sufficient conditions for a nonlinear wave equation which belongs to this class to admit a symplectic structure. Finally, we have discussed the interpretation of the first-order system as a Bäcklund transformation. We have illustrated this formalism using the equations of Euler and Poisson which play prominent roles in the theory of nonlinear acoustics.[15,16]

Immediate generalizations of this method which will enable us to handle a larger variety of nonlinear wave equations consist of the following: We shall consider a family of fields

$$\phi^i, \quad i = 1,2,...,n , \tag{5.1}$$

and given functions

$$\lambda^\iota(x,t), \quad \iota = 1,2,...,m , \tag{5.2}$$

the field equations for which will be in the form of continuity equations (2.1), where

$$f^i = f^i(\phi^k_t, \phi^k_x, \lambda^\kappa) ,$$
$$g^i = g^i(\phi^k_t, \phi^k_x, \lambda^\kappa) \tag{5.3}$$

are arbitrary differentiable functions of the indicated arguments. The examples of Refs. 8 and 9 are of this type and a discussion of these nonlinear wave equations will be presented later.

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Energy-momentum tensors and stress tensors in geometric field theories

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Lagrangian field theories of geometric objects are the most natural framework for investigating the notion of general covariance. We discuss here geometric theories of interacting fields, depending on Lagrangians of arbitrary order, and we give general definitions of energy flow, partial energy flows, energy-momentum tensors, and stress tensors. We also investigate the role which energy-momentum tensors and stress tensors play in formulating the natural conservation laws associated with the second theorem of Noether. Examples of application may be found elsewhere.

I. INTRODUCTION

One of the principal bases of any reasonable physical field theory consists of what physicists call the principle of general invariance (or also general covariance or relativistic invariance). Many formulations of this fundamental principle may be found in the literature, but all of them essentially amount to requiring that the differential equations governing the dynamics of fields (i.e., the field equations) have the same form for all observers, i.e., for all frames of reference in space-time. Differential calculus over manifolds tells us that this happens if and only if field equations have tensorial character, a property which was known since the formulation of Einstein's theory of general relativity. What seems to be relatively less understood is that general invariance does not require all fields to be tensor fields over space-time, but merely the much less stringent requirement that fields may be Lie-dragged along the flow of any vector field in space-time. Again, differential calculus over manifold tells us that this happens only if the fields are fields of geometric objects, which, roughly speaking, amounts to requiring that changes of coordinates in space-time define uniquely the transformation laws of the objects themselves. Lagrangian field theories depending on geometric objects and having generally invariant field equations will be called here geometric field theories; space-time will be generically denoted by M.

Geometric field theories are important for several reasons. To our understanding, the main feature of this class of theories consists in the fact that they are the natural framework for defining and investigating the physically fundamental concept of energy. In fact, for any generally invariant Lagrangian $\mathscr{L}$ and any vector field X on M we can uniquely define a vector density $E^i(\mathscr{L};X)$, called the energy flow of $\mathscr{L}$ along X, such that its divergence vanishes along all solutions to the relevant field equations (namely, the Euler–Lagrange equations of $\mathscr{L}$). According to this property, Stokes' theorem implies that the integral of $E^i(\mathscr{L};X)$ is zero over any closed (i.e., compact without boundary) hypersurface of M; this justifies the physical interpretation of E^i itself as the flux of energy associated with all fields. The vanishing of the divergence of E^i expresses then the conservation of energy.

As is well known, the physically most significant theories are those which describe the interaction of several fields, or, even better, the dynamics of a single field which unifies more than one elementary field. According to a standard viewpoint, when dealing with theories of interacting fields one tends to select some of the fields involved and to interpret them as the basic fields, considering the remaining ones as sources for the basic fields. Widely known examples are provided by the relativistic theories of gravitation (see, e.g., Ref. 1) and by gauge theories of elementary particles interacting with fundamental forces (see, e.g., Ref. 2). More generally, one may envisage situations in which the fields are split into more than two groups.

In all these cases, it is either assumed *a priori* or obtained by some trick (such as, e.g., partial Legendre transformation, spontaneous symmetry breaking, etc.), that the Lagrangian governing the theory splits into a suitable number of partial Lagrangians $\mathscr{L}_{(\alpha)}$. Each partial Lagrangian $\mathscr{L}_{(\alpha)}$ is then interpreted as the basic Lagrangian for one or more of the fields. Physically meaningful interpretations of these partial Lagrangians are in fact available only if some additional requirement is made on the splitting, like, for example, the so-called minimal coupling conditions.

When dealing with interacting fields, it is a classical procedure to describe the details of their interaction through suitable tensorial or pseudotensorial objects, called stress tensors or stress pseudotensors, which roughly speaking express the response of some of the fields when the remaining ones are subjected to deformations induced by changes of coordinates in space-time. Again we see, just from this naive definition, that geometric field theories constitute the natural framework for defining and discussing the notion of stress tensors. In this paper, we shall deal with geometric theories of interacting fields, with the aim of providing a general framework suited to investigate energy, conservation laws, and stress tensors for any Lagrangian theory of geometric fields, no matter how many fields are involved and how many of their derivatives enter the Lagrangian.

II. GENERALITIES

In this section we shall discuss some generalities concerning the global structure of higher-order calculus of variations. We shall assume that the reader is familiar with the main concepts from the theory of fibered manifolds, jet prolongations, and bundles of geometric objects. All manifolds, mappings, and objects considered here are assumed to be smooth (in the C^∞ sense). Further details and deeper discussions of these general concepts may be found, for example, in Refs. 3–5.

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A. Fibered manifolds and jet prolongations

Let M be a differentiable manifold, with $\dim(M)=m$. The following standard notation will be used throughout: $\mathrm{diff}(M)$ denotes the set of local diffeomorphisms of M into M; $T(M)$ denotes the tangent bundle of M; and $A^p_q(M)$ [resp. $S^p_q(M)$] is the vector bundle of p-contravariant and q-covariant skew-symmetric (resp. symmetric) tensors over M. In particular, the bundle $A^0_q(M)$ coincides with the qth exterior power $\wedge^q[T^*(M)]$ of the cotangent bundle of M.

Let then $B=(B,M,\beta)$ be a fibered manifold over the manifold M. We shall adopt the following notation: $\mathrm{aut}(B)$ is the set of all local automorphisms of the fibered manifold B; $C^\infty(B)$ is the set of local sections of class C^∞ of B; and $V(B)=(V(B),B,\nu_B)$ denotes the vertical bundle of B. As is well known, $V(B)$ is a vector bundle over B, whose sections are called vertical vector fields over B.

The k th-order jet prolongation of a fibered manifold B (where k is any positive integer) will be denoted by $J^k(B)=(J^k(B),M,\beta^k)$; we agree that the zeroth-order prolongation of B coincides with B itself. We recall also that for any $h\geqslant k$ there is a canonical projection β^h_k from $J^h(B)$ onto $J^k(B)$, such that $J^h_k(B)=(J^h(B),J^k(B),\beta^h_k)$ is a fiber bundle; in particular, we know that $J^{k+1}_k(B)$ is an affine bundle. Furthermore, if $Z=(Z,J^k(B),\zeta)$ is a fibered manifold and h is any integer larger than k, the pullback $(\beta^h_k)^*(Z)$ is a bundle over $J^h(B)$; accordingly, any fibered morphism $f:J^h(B)\to Z$ over the projection β^h_k may be canonically identified to a section of the pullback bundle $(\beta^h_k)^*(Z)$ over $J^h(B)$.

We consider now the following family of vector bundles over $J^k(B)$:

$$A^0_q(M)\otimes\wedge^p\{V^*[J^k(B)]\},$$

where (q,p,k) are three non-negative integers, which will often enter our next considerations on higher-order calculus of variations. Given any integer $h\geqslant k$, one can use the canonical projections β^h_k and β^h to identify, by pullback, the bundle above with a vector subbundle of $A^0_{p+q}[J^h(B)]$ which will be denoted by $\Phi^p_q(\beta^h_k)$. Accordingly, any fibered morphism $f:J^h(B)\to A^0_q(M)\otimes\wedge^p\{V^*[J^k(B)]\}$, over the projection β^h_k, may be canonically identified to a section of the bundle $\Phi^p_q(\beta^h_k)$, i.e., to a suitable $(p+q)$ form on $J^h(Q)$. Clearly, this applies also to local fibered morphisms, which give rise to local $(p+q)$ forms.

Let us now give some local coordinate notations. In any local chart $(U;x^i)$ of the manifold M, we define the following (local) forms:

$$ds(x)=dx^1\wedge dx^2\wedge\cdots\wedge dx^m,$$
$$ds_{h_1\cdots h_r}(x)=\frac{\partial}{\partial x^{h_r}}\rfloor\cdots\rfloor\frac{\partial}{\partial x^{h_1}}\rfloor ds(x). \tag{2.1}$$

The m form $ds(x)$ defines a basis of the vector bundle $A^0_m(U)$, while the $(m-1)$ forms $(ds_1(x),..,ds_m(x))$ constitute a basis for the vector bundle $A^0_{m-1}(U)$.

Now, let B be a fibered manifold over M. In the sequel, we agree to consider only charts $(W;z^\alpha)$ of B, with $\alpha=1,...,\dim(B)$, which are fibered over the charts of an atlas of M; these charts will be shortly called fibered charts of B. The corresponding coordinates, called fibered coordinates, will be generally denoted by (x^i,y^A), with $i=1,...,m$ and $A=1,...,\dim(B)-m$, where (x^i) stands for any system of local coordinates in the open subset $\beta(W)\subseteq M$.

For any fibered chart $(W;x^i,y^A)$ of B there exists an induced fibered chart $(V(W);x^i,y^A,v^A)$ of $V(B)$, where $V(W)=(\nu_B)^{-1}(W)$, which is called the natural fibered chart of $V(B)$ (induced by the fibered chart W of B). Moreover, any fibered chart $(W;x^i,y^A)$ of B induces (uniquely) natural fibered charts in each one of the bundles $J^k(B)$, $V[J^k(B)]$, and $J^s[T(M)]$. The domains of these charts will be denoted by $J^k(W)$, $V[J^k(W)]$, and $J^s[T(W)]$, respectively, while the corresponding local coordinates will be denoted, respectively, by

$$(x^i;y^A,y^A_{j_1},...,y^A_{j_1\cdots j_k}),$$
$$(x^i;y^A,y^A_{j_1},...,y^A_{j_1\cdots j_k};v^A,v^A_{j_1},...,v^A_{j_1\cdots j_k}),$$
$$(x^i;X^i,X^i_{j_1\cdots j_s}).$$

We finally recall that for any fibered manifold B and any integer k $(k\geqslant 0)$ there exists a canonical isomorphism $i^k:J^k[V(B)]\to V[J^k(B)]$. For any local differentiable function $f:J^k(W)\to R$, where $W\subseteq B$ is the domain of a fibered chart, we shall denote by $d_i(f):J^{k+1}(W)\to R$ the formal partial derivative of f with respect to the coordinate x^i.

B. Linear connections and tensorization procedures

We shall recall here the well-known procedure which allows us to replace the partial derivatives of the components of a vector field, having nontensorial character, with a suitable set of tensors constructed using the symmetrized covariant derivatives of these components with respect to an arbitrary (linear) connection.

Let C be any linear connection on a differentiable manifold M. As it is well known, the connection C induces a linear isomorphism

$$\psi_C:J^r[T(M)]\to\overset{r}{\underset{p=0}{\oplus}}S^1_p(M),$$

having the following local representation:

$$(x^h,X^h,X^h_{j_1},...,X^h_{j_1\cdots j_r})\to(x^h,X^h,\nabla_{j_1}X^h,...,\nabla_{(j_1}\cdots\nabla_{j_r)}X^h), \tag{2.2}$$

where ∇ denotes the covariant derivative with respect to C. Notice that we can also define a dual isomorphism for any pair of non-negative integers (q,r)

$$\bar\psi_C:[A^0_{m-q}(M)]\otimes\{J^r[T(M)]\}^*\to[A^0_{m-q}(M)]\otimes\left[\overset{r}{\underset{p=0}{\oplus}}S^p_1(M)\right],$$

by setting

$$\langle\zeta\,|j^r(X)\rangle=\langle\bar\psi_C(\zeta)|\psi_C[j^r(X)]\rangle, \tag{2.3}$$

for any point ζ in $[A^0_{m-q}(M)]\otimes\{J^r[T(M)]\}^*$ and any vector field X.

Let $(x^i,z^{h_1\cdots h_q}_i,z^{h_1\cdots h_q j_1}_i,...,z^{h_1\cdots h_q j_1\cdots j_r}_i)$ and $(x^i,Z^{h_1\cdots h_q}_i,Z^{h_1\cdots h_q j_1}_i,...,Z^{h_1\cdots h_q j_1\cdots j_r}_i)$ now, respectively, be natural fibered coordinates in the two vector bundles $[A^0_{m-q}(M)]\otimes\{J^r[T(M)]\}^*$ and $[A^0_{m-q}(M)]\otimes\left[\overset{r}{\underset{p=0}{\oplus}}S^p_1(M)\right]$. In these local coordinates we can describe as follows the action of the dual morphism $\bar\psi_C$. We first rep-

resent the point ζ and its image $\bar{\psi}_C(\zeta)$ as follows:

$$\langle \zeta \,|j^r(X)\rangle = \frac{1}{q!} ds_{h_1\cdots h_q}(x)\langle z^{h_1\cdots h_q}|j^r(X)\rangle,$$

$$\langle \bar{\psi}_C(\zeta)|\psi_C[j^r(X)]\rangle = \frac{1}{q!} ds_{h_1\cdots h_q}(x) < Z^{h_1\cdots h_q}|\psi_C[j^r(X)]\rangle,$$

we can describe as follows the action of the dual morphism $\bar{\psi}_C$. We first represent the point ζ and its image $\bar{\psi}_C(\zeta)$ as follows:

$$\langle \zeta \,|j^r(X)\rangle = \frac{1}{q!} ds_{h_1\cdots h_q}(x)\langle z^{h_1\cdots h_q}|j^r(X)\rangle,$$

$$\langle \bar{\psi}_C(\zeta)|\psi_C[j^r(X)]\rangle = \frac{1}{q!} ds_{h_1\cdots h_q}(x) \times \langle Z^{h_1\cdots h_q}|\psi_C[j^r(X)]\rangle,$$

where $\langle z^{h_1\cdots h_q}|j^r(X)\rangle$ and $\langle Z^{h_1\cdots h_q}|\psi_C[j^r(X)]\rangle$ are the (skew-symmetric) tensor densities defined by the following expansions:

$$\langle z^{h_1\cdots h_q}|j^r(X)\rangle = z_i^{h_1\cdots h_q}X^i + z_i^{h_1\cdots h_q j_1}X^i_{j_1} + \cdots + z_i^{h_1\cdots h_q j_1\cdots j_r}X^i_{j_1\cdots j_r}, \tag{2.4}$$

and

$$\langle Z^{h_1\cdots h_q}|\psi_C[j^r(X)]\rangle = Z_i^{h_1\cdots h_q}X^i + Z_i^{h_1\cdots h_q j_1}\nabla_{j_1}X^i + \cdots + Z_i^{h_1\cdots h_q j_1\cdots j_r}\nabla_{(j_1}\cdots\nabla_{j_r)}X^i. \tag{2.5}$$

The explicit relations between the coefficients z and Z may be thus obtained by applying (2.3), i.e., by equating the right-hand sides of expressions (2.4) and (2.5).

C. Bundles of geometric objects and Lie derivatives

As it was already remarked in the Introduction, the correct setting for dealing with generally invariant field theories is the framework of bundles of geometric objects (of finite order), also known as natural bundles. In fact, in the formulation of physical field theories it is unavoidable to introduce nontensorial entities, like, for example, jet prolongations of tensor fields and linear connections. We shall here assume that the reader is familiar with the notion of bundles of geometric objects and we shall limit ourselves to recall its role in the definition of Lie derivatives. Further details and references may be found in Refs. 5–7.

Let $B = (B,M,\beta)$ be a bundle of geometric objects (of finite order) over a manifold M. A functorial mapping is then defined as

$$(\ )_B : \mathrm{diff}(M) \to \mathrm{aut}(B),$$

which lifts any local diffeomorphism φ of the basis M into a (unique) local automorphism φ_B (over φ) of the bundle B; this automorphism is called the natural lift of φ. Well-known examples of bundles of geometric objects over a manifold M are the following: the tangent bundle $T(M)$, with the lift given by $\varphi \to T(\varphi)$; all tensor bundles over M, with the natural lift defined by the push forward of tensors; and the bundle $C(M)$ of linear connections over M, with the lift defined by the natural action of $\mathrm{diff}(M)$ on connections, etc. Recall also that for any bundle of geometric objects $B = (B,M,\beta)$ the tensor bundles $(T^r_s(B),M,\beta\circ\tau^r_s)$, the bundle $(V(B),M,\beta\circ\nu_B)$, and all the jet prolongations $(J^k(B),M,\beta^k)$ are bundles of geometric objects over M.

Let $X: M \to T(M)$ be a vector field on M. Using $(\ )_B$ we can associate to X a unique vector field $X_B: B \to T(B)$, which is called the natural lift of X to the bundle B. The vector field X_B is defined as follows: for any $b \in B$ one sets

$$X_B(b) = \frac{d}{dt}\,[(\varphi_t)_B(b)]\,|_{t=0},$$

where φ_t denotes the (local) flow in M generated by X. The mapping

$$(\ )_B : C^\infty[T(M)] \to C^\infty[T(B)],$$

defined by $X \to X_B$, is linear and satisfies the following properties: (i) for any vector field X over M one has $T(\beta)\circ X_B = X\circ\beta$; and (ii) for any pair (X,Y) of vector fields on M, one has $([X,Y])_B = [X_B,Y_B]$.

Now, let σ be a local section of B, i.e., $\sigma: U \to B$, and X be a vector field over U. We can define a local section $L_X(\sigma): U \to V(B)$ of the bundle $(V(B),M,\beta\circ\nu_B)$ by setting

$$L_X(\sigma) = T(\sigma)\circ X - X_B\circ\sigma. \tag{2.6}$$

The local section $L_X(\sigma)$ is called the Lie derivative of σ along the vector field X and it satisfies the following property: $\nu_B\circ L_X(\sigma) = \sigma$. We now recall that for any positive integer $k \geqslant 0$ there exists a canonical isomorphism from $V[J^k(B)]$ to $J^k[V(B)]$. It is then easy to show that the following holds:

$$L_X[j^k(\sigma)] = j^k[L_X(\sigma)],$$

for any (local) section σ of the bundle B and for any (local) vector field X over the basis manifold M. Moreover, the following properties hold.

(i) For any vector field X over M, the mapping $\sigma \to L_X(\sigma)$ is a first-order quasilinear differential operator.

(ii) For any local section σ of B, the mapping $X \to L_X(\sigma)$ is a linear differential operator, having as order the order s of B as a bundle of geometric objects.

From (i) and (ii) above it follows that the local representations of $L_X(\sigma)$ have necessarily the following form:

$$x^i\circ L_X(\sigma) = x^i\circ\sigma,\quad y^A\circ L_X(\sigma) = y^A\circ\sigma,$$

$$v^A\circ L_X(\sigma) = X^i y^A{}_i\circ[j^1(\sigma)] + b^A{}_i(x,y\circ\sigma)X^i + b^{Aj_1}{}_i(x,y\circ\sigma)X^i_{j_1} + \cdots + b^{Aj_1\cdots j_s}{}_i(x,y\circ\sigma)X^i_{j_1\cdots j_s},$$

where $(x^i,y^A,v^A,y^A{}_i)$ are natural fibered coordinates and the coefficients $b^A{}_i(x,y)$ and $b^{Aj_1\cdots j_p}{}_i(x,y)$ (with $1 \leqslant p \leqslant s$) are functions of (x^i,y^A) which depend on the choice of the fibered chart in B but do not depend on the particular section σ chosen.

We finally recall from Ref. 8 that a bundle of geometric objects is said to be of differential type if it admits (at least) one natural atlas whose fibered charts (x^i,y^A) are such that the coefficients $b^A{}_i(x,y)$ vanish identically, while the coefficients $b^{Aj_1\cdots j_p}{}_i(x,y)$ $(1 \leqslant p \leqslant s)$ depend only on the fiber coordinates y^A. We remark that, to our knowledge, all the bundles of geometric objects which enter the formulation of physical field theories are precisely of this type. Accordingly, in the following we shall restrict our attention only to this class of bundles.

D. Calculus of variations on fibered manifolds

We now have to recall some concepts we need from the geometric formulation of the calculus of variations on fibered manifolds, as it was developed in Refs. 9–11. In these papers the reader may find more details and further references, also concerning alternative viewpoints.

According to Ref. 9 a variational problem of order k is defined by assigning the following: (i) a fibered manifold $Q=(Q,M,\pi)$ over a differentiable manifold M of dimension m and (ii) a morphism $\mathscr{L}:J^k(Q)\to A^0_m(M)$ of fibered manifolds over M. The fibered manifold Q is called the configuration space and its local sections represent the physical fields. The fibered morphism $\mathscr{L}$ is called the Lagrangian density of the variational problem; it defines the action functionals $\mathscr{L}_D:C^\infty\to R$ by

$$\mathscr{L}_D(\sigma)=\int_D \mathscr{L}\circ j^k(\sigma),$$

where $D\subseteq M$ is any compact domain. Solving the variational problem consists thence in finding the critical sections of the action functionals, i.e., those (local) sections $\sigma\in C^\infty(Q)$ which make stationary all functionals above when D ranges through all compact domains of M.

We remark that there exists the following canonical isomorphism of vector bundles over $J^k(Q)$:

$$(\pi^k)^*[A^0_m(M)]\simeq A^0_m(M)\otimes\wedge^0\{V^*[J^kQ)]\}.$$

Therefore, according to the remarks of Sec. II A, the Lagrangian $\mathscr{L}$ can be canonically identified to a (global) section $\Phi(\mathscr{L})$ of the vector bundle $\Phi^0_m[J^k(Q)]$, i.e., to a (global) m form over $J^k(Q)$. The form $\Phi(\mathscr{L})$ is, in fact, a horizontal m form of $J^k(Q)$.

Then, let $\mathscr{L}:J^k(Q)\to A^0_m(M)$ be a Lagrangian (of order k) over the configuration space $Q=(Q,M,\pi)$ and let $\mathscr{L}=ds(x)\otimes L$ be its local representation with respect to any system of natural fibered coordinates. Restricting $T(\mathscr{L})$ to the vector subbundle $V[J^k(Q)]$ of $T[J^k(Q)]$ and taking into account the linearity of the tangent map, we may define uniquely a fibered morphism over the identity of M,

$$\hat{p}(\mathscr{L}):J^k(Q)\to A^0_m(M)\otimes V^*[J^k(Q)].$$

According to Sec. II A, the morphism $\hat{p}(\mathscr{L})$ can also be interpreted as a (global) section $\Phi[\hat{p}(\mathscr{L})]$ of the vector bundle $\Phi^1_m[J^k(B)]$ over $J^k(B)$, i.e., as a (global) $(m+1)$ form over $J^k(B)$. It is easily seen that the $(m+1)$ form $\Phi[\hat{p}(\mathscr{L})]$ so defined is in fact the exterior differential $d\Phi(\mathscr{L})$ of the m form $\Phi(\mathscr{L})$ which is canonically associated to the Lagrangian $\mathscr{L}$ itself. The action over $V[J^k(Q)]$ of the morphism $\hat{p}(\mathscr{L})$ may be represented as follows for any system of natural fibered coordinates:

$$\begin{aligned}\langle\hat{p}(\mathscr{L})|v\rangle &= ds(x)\langle p(L)|v\rangle\\ &= ds(x)\big[p_A(L)v^A+p_A{}^{j_1}(L)v^A{}_{j_1}\\ &\quad+\cdots+p_A{}^{j_1\cdots j_k}(L)v^A{}_{j_1\cdots j_k}\big],\end{aligned}\tag{2.7}$$

where we have set

$$\begin{aligned}p_A(L)&=\frac{\partial L}{\partial y^A},\\ p_A{}^{j_1\cdots j_h}(L)&=\frac{\partial L}{\partial y^A{}_{j_1\cdots j_h}}\quad(1\le h\le k).\end{aligned}\tag{2.8}$$

As is well known, the critical sections σ of our variational problem satisfy the Euler–Lagrange equations, which, although being generally written in coordinates, are globally and intrinsically well-defined over M (see, e.g., Ref. 12). In fact, these equations may be represented as follows:

$$\hat{e}(\mathscr{L})\circ j^{2k}(\sigma)=0,\tag{2.9}$$

where

$$\hat{e}(\mathscr{L}):J^{2k}(Q)\to A^0_m(M)\otimes V^*(Q)$$

is a (global) morphism of fibered manifolds over M. The action of $\hat{e}(\mathscr{L})$ over $V(Q)$ is defined, for any natural fibered chart, by the following local expressions:

$$\langle\hat{e}(\mathscr{L})|v\rangle=ds(x)\langle e(L)|v\rangle=ds(x)[e_A(L)v^A],\tag{2.10}$$

with

$$\begin{aligned}e_A(L)&=p_A(L)-d_{j_1}[p_A{}^{j_1}(L)]\\ &\quad+\cdots+(-1)^k d_{j_k}\cdots d_{j_1}[p_A{}^{j_1\cdots j_k}(L)].\end{aligned}\tag{2.11}$$

This morphism is commonly known as the Euler–Lagrange operator associated to the Lagrangian $\mathscr{L}$ (see, e.g., Refs. 10 and 12). We remark that it can be canonically identified to a (global) section $\Phi[\hat{e}(\mathscr{L})]$ of the vector bundle $\Phi^1_m[J^{2k}(Q)]$, i.e., to a (global) $(m+1)$ form over $J^{2k}(Q)$.

E. First variation formula and the Poincaré–Cartan forms

We conclude this section with a short discussion about the role which the so-called Poincaré–Cartan form plays in the formulation of the first variation formula in higher-order variational problems. The results developed here will be of great use for a precise definition of stress tensors and energy-momentum tensors, which will be investigated in Secs. III and IV.

Let $\mathscr{L}:J^k(Q)\to A^0_m(M)$ be a Lagrangian (of order k) over the configuration space $Q=(Q,M,\pi)$. It is possible to show that there exists (at least) one global morphism $\hat{f}(\mathscr{L})$ of fiber bundles over $J^{k-1}(Q)$

$$\hat{f}(\mathscr{L}):J^{2k-1}(Q)\to A^0_{m-1}(M)\otimes V^*[J^{k-1}(Q)],$$

such that the following holds:

$$\begin{aligned}\langle\hat{p}(\mathscr{L})\circ j^k(\sigma)|j^k(v)\rangle &= \langle\hat{e}(\mathscr{L})\circ j^{2k}(\sigma)|v\rangle\\ &\quad+d\langle\hat{f}(\mathscr{L})\circ j^{2k-1}(\sigma)|j^{k-1}(v)\rangle,\end{aligned}\tag{2.12}$$

where $v:U\to V(Q)$ is any (local) section and $\sigma:U\to Q$ is the (local) section of Q defined by $\sigma=\nu_Q\circ v$. Integrating (2.12) over any compact domain $D\subseteq U$, we recover the well-known first variation formula (over D) for the Lagrangian $\mathscr{L}$. According to Sec. II A, also in this case the global morphism $\hat{f}(\mathscr{L})$ can be canonically identified to a global section $\Phi[\hat{f}(\mathscr{L})]$ of the vector bundle $\Phi^1_{m-1}[J^{2k-1}(Q)]$, i.e., to a global m form on $J^{2k-1}(Q)$. The action of the global morphism $\hat{f}(\mathscr{L})$ on the vector bundle $V[J^{k-1}(Q)]$ is defined, in any natural fibered chart, by the following local expression:

$$\begin{aligned}\langle\hat{f}(\mathscr{L})|v\rangle &= ds_i(x)\langle f^i(L)|v\rangle\\ &= ds_i(x)\big[f^i{}_A(L)v^A+f^{ij_1}{}_A(L)v^A{}_{j_1}\\ &\quad+\cdots+f^{ij_1\cdots j_{k-1}}{}_A(L)v^A{}_{j_1\cdots j_{k-1}}\big].\end{aligned}\tag{2.13}$$

Moreover, rewriting (2.12) in a natural fibered chart we find the following local expression:

$$\langle p(L)\circ j^k(\sigma)|j^k(v)\rangle = \langle e(L)\circ j^{2k}(\sigma)|v\rangle + d_i\langle f^i(L)\circ j^{2k-1}(\sigma)|j^{k-1}(v)\rangle, \tag{2.14}$$

which is more significant than (2.12) itself, since, roughly speaking, it amounts to decomposing the first variation of $\mathscr{L}$ into field equations plus a (formal) total divergence. From the physical viewpoint, the divergence appearing in (2.14) will allow us to define the so-called Noether's conserved currents (see Sec. III).

As far as the uniqueness of the morphisms $\hat{e}(\mathscr{L})$ and $\hat{f}(\mathscr{L})$ is concerned, we remark the following.

(i) In general, there exists a whole family of (global) morphisms $\hat{f}(\mathscr{L})$ which satisfy the properties above. In any case, no matter which one of them is chosen, the morphism $\hat{e}(\mathscr{L})$ such that (2.12) holds is uniquely defined. This property is commonly known as the unicity of the Euler–Lagrange operator (see e.g., Ref. 12).

(ii) The morphism $\hat{f}(\mathscr{L})$ is uniquely defined if the order of the Lagrangian is 1, no matter which is the dimension m of the basis M (i.e., $m\geqslant 1, k=1$) (see Ref. 13). It is also uniquely defined if the basis manifold M is one dimensional, no matter which is the order k of the Lagrangian (i.e., $m=1, k\geqslant 1$) (see Ref. 14).

(iii) However, when $m\geqslant 2$ and also $k\geqslant 2$, the morphism $\hat{f}(\mathscr{L})$ is globally but not uniquely defined. In fact, let $\hat{f}_1(\mathscr{L})$ be a global morphism which satisfies the required properties; then, if we consider any (global) fibered morphism over $J^{k-2}(Q)$

$$\hat{h}: J^{2k-2}(Q)\to A^0_{m-2}(M)\otimes V^*[J^{k-2}(Q)],$$

and we denote by

$$\mathrm{div}(\hat{h}): J^{2k-1}(Q)\to A^0_{m-1}(M)\otimes V^*[J^{k-1}(Q)]$$

its formal divergence, we easily see that the (global) morphism

$$\hat{f}_2(\mathscr{L},\hat{h}) = \hat{f}_1(\mathscr{L}) + \mathrm{div}(\hat{h})$$

satisfies the required properties, too (see Ref. 10). For example, as was shown in Refs. 15 and 16, from any such morphism one can generate a whole family which depends on a couple of connections.

(iv) We finally remark that in the particular case $m\geqslant 2$ and $k=2$, there exists a canonical global morphism $\hat{f}(\mathscr{L})$ satisfying the required properties, which is defined, in any natural fibered chart, by the following local expressions:

$$f^i{}_A(L) = p^i{}_A(L) - d_j p^{ij}{}_A(L),\quad f^{ij}{}_A(L) = p^{ij}{}_A(L). \tag{2.15}$$

Let us now remark that, taking into account the methods discussed in Sec. II A, to any k th-order Lagrangian and to each global morphism $\hat{F}: J^{2k-1}(Q)\to A^0_{m-1}(M)\otimes V^*[J^{k-1}(Q)]$ there corresponds a global m form $\Theta(\mathscr{L},\hat{F})$ over $J^{2k-1}(Q)$, defined by the following prescription:

$$\Theta(\mathscr{L},\hat{F}) = (\pi^{2k-1}_k)^*\Phi(\mathscr{L}) + \Phi(\hat{F}). \tag{2.16}$$

According to the terminology used by Krupka,[10] when the morphism $\hat{F}$ is any one of the morphisms $\hat{f}(\mathscr{L})$ which satisfy Eq. (2.14), the corresponding m form $\Theta[\mathscr{L},\hat{f}(\mathscr{L})]$ is said to be a (global) Lepagean equivalent of the Lagrangian $\mathscr{L}$. Any such m form can be assumed as a Poincaré–Cartan form associated to the Lagrangian $\mathscr{L}$. According to our remarks above, we see thus that the following hold: (i) the Poincaré–Cartan form is uniquely defined if the order of the Lagrangian is one, no matter which is the dimension m of the basis M (i.e., $m\geqslant 1, k=1$), as well as if the basis manifold M is one dimensional, no matter which is the order k of the Lagrangian (i.e., $m=1$, $k\geqslant 1$); (ii) when $m\geqslant 2$ and also $k\geqslant 2$, there exists a whole family of (global) Poincaré–Cartan forms, which locally differ by a formal divergence (for example, one can generate a family of global Poincaré–Cartan forms which depend on a couple of connections); and (iii) in the particular case $m\geqslant 2$ and $k=2$, there exists however a canonical Poincaré–Cartan form.

III. GEOMETRIC FIELD THEORIES AND NATURAL CONSERVATION LAWS

As was already remarked in the Introduction, in this paper we are mainly concerned with Lagrangian field theories which are based on the jet prolongations of bundles of geometric objects. This, in fact, is the natural framework for introducing the concept of natural conservation laws, which will be discussed below.

A. General invariance, geometric field theories, and energy flow

As it is well known, one of the fundamental requirements of physical field theories over space-time is the invariance of their field equations with respect to any change of (local) coordinates in the space-time manifold itself; this requirement, which has been generally accepted since the early developments of Einstein's general relativity theory, is commonly known as general invariance (or relativistic invariance, or also as general covariance). However, when dealing with Lagrangian field theories one usually makes a stronger assumption; namely, one requires the general invariance of the Lagrangian itself. Requiring the general invariance of the Lagrangian allows us then to apply the so-called second theorem of Noether and to generate, as a consequence, a whole family of natural conservation laws, i.e., those conservation laws which are naturally associated with the dragging of physical fields along the flows generated by vector fields over the basis. We shall assume here that the reader is familiar with the fundamental concepts and ideas of this theory; for a detailed and comprehensive account of them we refer to Refs. 17–19 (and references quoted therein).

We are now in position to give the following definition: A k th-order Lagrangian theory is called a geometric field theory if the following two conditions are satisfied.

(i) The configuration space $Q=(Q,M,\pi)$ is a bundle of geometric objects of order s.

(ii) The Lagrangian $\mathscr{L}$ governing the dynamics of fields is generally invariant.[18] The order s of the bundle Q will be called the geometric order of the theory, while the sum $r=k+s-1$ will be called the differential degree of the theory. This terminology will be clarified later.

According to standard results,[18] requiring the general invariance of the Lagrangian $\mathscr{L}$ in a geometric field theory implies that $\mathscr{L}$ should satisfy the following relation:

$$T(\mathscr{L})\circ j^k[L_X(\sigma)] = L_X[\mathscr{L}\circ j^k(\sigma)], \tag{3.1}$$

where X is any vector field over the basis manifold M and σ is

any (local) section of the bundle Q. Since $\mathscr{L}\circ j^k(\sigma)$ is a scalar density, the following holds:

$$L_X[\mathscr{L}\circ j^k(\sigma)] = d_i\{X^i[L\circ j^k(\sigma)]\}ds(x).$$

As a consequence, relation (3.1) can be rewritten as follows:

$$T(L)\circ j^k[L_X(\sigma)] = d_i\{X^i[L\circ j^k(\sigma)]\}. \tag{3.2}$$

We can now apply the general relation (2.14) to obtain the following result: for any vector field X over M and any local section σ of Q we have

$$d_i[E^i(L;X,\sigma)] = -\langle e(L)\circ j^{2k}(\sigma)|L_X(\sigma)\rangle, \tag{3.3}$$

where the vector density $E^i(L;X,\sigma)$ is defined by

$$E^i(L;X,\sigma) = \langle f^i(L)\circ j^{2k-1}(\sigma)|j^{k-1}[L_X(\sigma)]\rangle - X^i[L\circ j^k(\sigma)]. \tag{3.4}$$

If we restrict the above relation (3.3) to any local section σ of Q which satisfies the Euler–Lagrange equations $e(L)\circ j^{2k}(\sigma)=0$, we find

$$d_i[E^i(L;X,\sigma)] = 0, \quad \forall X\in C^\infty[T(M)]. \tag{3.5}$$

Relations (3.5) express the so-called (weak) natural conservation laws associated with the Lagrangian $\mathscr{L}$ (see, e.g., Refs. 17 and 20).

Remarks. (i) We can also define a (local) $(m-1)$ form $E(\mathscr{L};X,\sigma)$ on the basis manifold M by setting

$$E(\mathscr{L};X,\sigma) = E^i(L;X,\sigma)ds_i(x).$$

This form is called the energy flow of the Lagrangian $\mathscr{L}$ along the vector field X and the (local) section σ of Q. Using the energy flow $E(\mathscr{L};X,\sigma)$, the natural conservation laws (3.5) are turned into the well-known equivalent expression

$$d[E(\mathscr{L};X,\sigma)] = 0. \tag{3.6}$$

Using the Stokes theorem, Eq. (3.6) implies in turn the following relation:

$$\int_{\partial D} E(\mathscr{L};X,\sigma) = 0,$$

where ∂D denotes the $(m-1)$-dimensional boundary of any regular domain $D\subseteq \mathrm{dom}(\sigma)\subseteq M$. This last relation expresses the natural conservation laws in their integral form.

(ii) If one eliminates the arbitrary vector field X and the arbitrary section σ from the relation (3.1) [or, equivalently, from (3.2)], one obtains a set of first-order partial differential equations in the unknown Lagrangian $\mathscr{L}$. These equations characterize the whole family of generally invariant k th-order Lagrangians over Q (i.e., depending on the given fields together with their derivatives up to the order k). See Refs. 19 or 21 for examples of application.

B. Energy momentum tensors associated to a generally invariant Lagrangian

In this section we shall investigate in detail the energy flow defined above. Recalling that the geometric order of the theory is s, from Eq. (3.4) we see that the energy flow $E(\mathscr{L};X,\sigma)$ satisfies the following properties.

(i) For any (local) section σ of the configuration space Q, the mapping $X\to E(\mathscr{L};X,\sigma)$ is a linear differential operator of order equal to the differential degree $r=k+s-1$.

(ii) For any vector field X on M, the mapping $\sigma\to E(\mathscr{L};X,\sigma)$ is a (generally nonlinear) differential operator of order $2k-1$. From these two properties we infer the existence of a morphism of fibered manifolds

$$\hat{E}(\mathscr{L}):J^{2k-1}(Q)\to[A^0_{m-1}(M)]\otimes\{J^r[T(M)]\}^*,$$

such that the following holds:

$$E^i(L;X,\sigma) = \langle E^i(L)\circ j^{2k-1}(\sigma)|j^r(X)\rangle = \langle E^i(L)|j^r(X)\rangle\circ j^{2k-1}(\sigma), \tag{3.7}$$

where σ is any (local) section of Q, X is any vector field over M and $E^i(L)$ denotes the ith component of $\hat{E}(\mathscr{L})$, i.e., $\hat{E}(\mathscr{L}) = ds_i(x)\otimes E^i(L)$. Representing the relation (3.7) in any natural fibered chart we obtain the following expansion:

$$E^i(L;X,\sigma) = [e^i{}_h(L)\circ j^{2k-1}(\sigma)]X^h + [e^{ij_1}{}_h(L)\circ j^{2k-1}(\sigma)]X^h{}_{j_1} + \cdots + [e^{ij_1\cdots j_r}{}_h(L)\circ j^{2k-1}(\sigma)]X^h{}_{j_1\cdots j_r}, \tag{3.8}$$

where $(x^h,X^h,X^h{}_{j_1},\ldots,X^h{}_{j_1\cdots j_r})$ and $(x^h,e^i{}_h,e^{ij_1}{}_h,\ldots,e^{ij_1\cdots j_r}{}_h)$ denote, respectively, the natural fibered coordinates in the vector bundles $J^r[T(M)]$ and $[A^0_{m-1}(M)]\otimes\{J^r[T(M)]\}^*$. Let us now remark that the sections of these vector bundles are fields of geometric objects over the basis manifold M, but in general they do not have tensorial character. Therefore, also the coefficients $(e^i{}_h(L),e^{ij_1}{}_h(L),\ldots,e^{ij_1\cdots j_r}{}_h(L))$, which are symmetric with respect to the upper indices j, are not tensors over M; they are called energy-momentum pseudotensors associated with the Lagrangian $\mathscr{L}$. This clarifies the meaning of the differential degree r: it is in fact the maximum order of derivatives of X which appear in the expansion above. In other words, for any theory of differential degree r there are exactly $r+1$ energy pseudotensors.

Using the general procedure described in Sec. II B, we can reexpand the energy flow $E(\mathscr{L};X,\sigma)$ by means of tensorial coefficients, rather than with the pseudotensors above. Let us then consider any linear connection C over the basis manifold M, together with the linear isomorphism

$$\psi_C:J^r[T(M)]\to\bigoplus_{p=0}^{r} S^1_p(M)$$

and the dual isomorphism

$$\bar{\psi}_C:[A^0_{m-1}(M)]\otimes\{J^r[T(M)]\}^* \to[A^0_{m-1}(M)]\otimes\left[\bigoplus_{p=0}^{r} S^p_1(M)\right]$$

(defined above). Equation (2.3) then gives

$$\langle\hat{E}(\mathscr{L})|j^r(X)\rangle = \langle\bar{\psi}_C[\hat{E}(\mathscr{L})]|\bar{\psi}_C[j^r(X)]\rangle, \tag{3.9}$$

from which follows immediately the equivalent expansion

$$\langle E^i(L)|j^r(X)\rangle = E^i{}_h(L;C)X^h + E^{ij_1}{}_h(L;C)\nabla_{j_1}X^h + \cdots + E^{ij_1\cdots j_r}{}_h(L;C)\,\nabla_{(j_1}\cdots\nabla_{j_r)}X^h. \tag{3.10}$$

The coefficients $(E^i{}_h(L;C),E^{ij_1}{}_h(L;C),\ldots,E^{ij_1\cdots j_r}{}_h(L;C))$, which appear in (3.10), are tensor densities, symmetric with respect to their upper indices j. They are called the energy-momentum tensors (of the Lagrangian $\mathscr{L}$) associated with the connection C.

We can now insert the explicit expansion (3.8) into the natural conservation laws (3.5) and eliminate the arbitrary vector field X from the resulting expression. Owing to the linearity of the differential operator $X\to E(\mathscr{L};X,\sigma)$ and to the

Leibniz rule for the formal derivative d_i, it turns out also that the quantity $d_i[E^i(L;X,\sigma)]$ may be expanded as a linear combination of the quantities X^h and $X^h{}_{j_1\cdots j_p}$, with $1\leqslant p\leqslant r+1=k+s$. Therefore, eliminating X amounts to setting all the coefficients in this expansion equal to zero, which gives rise to the following set of (first-order) linear differential equations in the pseudotensors $e^i{}_h(L)$ and $e^{ij_1\cdots j_p}{}_h(L)$:

$$\begin{aligned} &e^{(ij_1\cdots j_r)}{}_h(L)=0,\\ &e^{(ij_1j_2\cdots j_p)}{}_h(L)+d_i\left[e^{(ij_1j_2\cdots j_p)}{}_h(L)\right]=0\ (1\leqslant p\leqslant r), \qquad (3.11)\\ &d_i\left[e^i{}_h(L)\right]=0. \end{aligned}$$

These equations, which are completely equivalent to the single equation (3.5), take often the name of conservation laws for the energy-momentum pseudotensors.

It is clear that an equivalent set of natural conservation laws may be obtained also for the energy-momentum tensors (associated with any connection C). To obtain these equations, which are rather more complicated than Eq. (3.11) (and therefore will not be written here explicitly), there are at least two possible ways. A first method consists in inserting directly into Eq. (3.11) the explicit expressions of the energy-momentum pseudotensors $(e^i{}_h(L),e^{ij_1}{}_h(L),\ldots,e^{ij_1\cdots j_r}{}_h(L))$ in terms of the tensors $(E^i{}_h(L;C),E^{ij_1}{}_h(L;C),\ldots,E^{ij_1\cdots j_r}{}_h(L;C))$ and the appropriate jet prolongation of the connection C itself; the resulting equations may be further simplified by taking suitable linear combinations which are directly suggested by their very structure.

The second approach, on the contrary, does not require us to express explicitly the pseudotensors in terms of the corresponding tensors (which, as we said above, is not always a simple matter). The method consists first in reexpressing the natural conservation laws (3.5) by means of the formal covariant derivative with respect to the connection C chosen; one finds

$$d_i[E^i(L;X,\sigma)]=\nabla_i[E^i(L;X,\sigma)]+T^a{}_{ai}(C)E^i(L;X,\sigma)=0, \qquad (3.12)$$

where $T^a{}_{bi}(C)$ denotes the torsion of C. Then the expansion (3.10) should be inserted into Eq. (3.12) and the resulting expression should be rewritten as a linear combination of the components X^h and their symmetrized covariant derivatives $\nabla_{j_1}\cdots\nabla_{j_p}X^h$, with $1\leqslant p\leqslant r$ [this is, of course, possible, in virtue of the linearity of the differential operator $X\to E(\mathscr{L};X,\sigma)$ and of the bundle morphism ψ_C]. Finally, the appropriate set of first-order differential equations for the energy-momentum tensors $(E^i{}_h(L;C),E^{ij_1}{}_h(L;C),\ldots,E^{ij_1\cdots j_r}{}_h(L;C))$ is obtained by setting equal to zero all the coefficients of the resulting linear combination. We remark that, owing to the well-known commutation rules for iterated covariant derivatives, the equations so found will contain explicitly the Riemann curvature tensor and the torsion of the connection C, together with their covariant derivatives up to the order at most $r-2$. These equations may be further simplified by using Bianchi identities and all the existing symmetries of the Riemann tensor.

C. Interacting fields of geometric objects

As it was already remarked in the Introduction, physical field theories are mainly aimed to describe the dynamics of interacting elementary fields, both in the case of theories describing previously existing free fields which are allowed to interact, or in the case of already unified theories. In the first case, each one of the free fields is conveniently described as a section of an appropriate configuration space $\mathscr{Q}_{(\alpha)}$, and the total configuration space of the interaction theory is assumed to be the fibered product $\mathscr{Q}=\times_{\alpha=1}^n\mathscr{Q}_{(\alpha)}$. In the case of unified theories, on the contrary, it is assumed that a single field can be conveniently split to define a number of elementary interacting subfields in such a way that the free dynamics of the unified field is equivalent to the interaction dynamics of its subfields. In this case, a single configuration space $\mathscr{Q}'$ is assigned, and breaking the unified theory into the equivalent interaction theory will produce a new configuration space $\mathscr{Q}$ (possibly nonisomorphic to $\mathscr{Q}'$ itself), which is the fibered product of a number of spaces $\mathscr{Q}_{(\alpha)}$, which are interpreted as the configuration spaces of the elementary subfields themselves. According to this viewpoint, we shall limit ourselves to consider here only the case of interacting fields. We shall moreover assume that all fields are fields of geometric objects, in order to be able to define the energy flow.

Let $\mathscr{Q}_{(\alpha)}=(\mathscr{Q}_{(\alpha)},M,\pi_{(\alpha)})$, with $1\leqslant\alpha\leqslant n$, be bundles of geometric objects over the same basis M and let us denote by $\mathscr{Q}=\times_{\alpha=1}^n\mathscr{Q}_{(\alpha)}=\mathscr{Q}_{(1)}\times_M\cdots\times_M\mathscr{Q}_{(n)}$ their fibered product. In physical applications, M will be the space-time manifold (or possibly the real line or some other physically meaningful basis), each bundle $\mathscr{Q}_{(\alpha)}$ will be the configuration space of an elementary field $\sigma_{(\alpha)}:M\to\mathscr{Q}_{(\alpha)}$, and $\mathscr{Q}$ will be the total configuration space of the total field $\sigma:M\to\mathscr{Q}$ defined by

$$\sigma(x)=(\sigma_{(1)}(x),\ldots,\sigma_{(n)}(x)). \qquad (3.13)$$

Lagrangian theories of interacting fields of geometric objects assume that the dynamics is governed by the Euler–Lagrange equations of a suitable total Lagrangian $\mathscr{L}$, which is a generally invariant Lagrangian, depending on all the fields $\sigma_{(\alpha)}$ together with their partial derivatives

$$\mathscr{L}:J^k(\mathscr{Q})\to A^0_m(M). \qquad (3.14)$$

We remark that in all main physical applications the order k of the Lagrangian is either 1 or 2 and in $\mathscr{L}$ only geometric fields of order 1 or 2 appear; in any case, the theory will be developed here for all orders, since no conceptual simplification would occur in requiring those orders to be equal to 2.

We remark also that each field $\sigma_{(\alpha)}$ may enter the Lagrangian $\mathscr{L}$ through its derivatives of order at most $k_{(\alpha)}$, with $k_{(\alpha)}\leqslant k$ (possibly different from field to field) and $k=\max(k_{(1)},\ldots,k_{(n)})$; more precisely, this amounts to assuming that the Lagrangian $\mathscr{L}$ is the pullback to $J^k(\mathscr{Q})$ of a fibered morphism from the product $J^{k_1}[\mathscr{Q}_{(1)}]\times_M\cdots\times_M\times J^{k_n}[\mathscr{Q}_{(n)}]$ into $A^0_m(M)$. In this case, each integer $k_{(\alpha)}$ is called a partial order of $\mathscr{L}$ (relative to the field $\sigma_{(\alpha)}$) and k is called the total order of $\mathscr{L}$.

Moreover, in most cases it is assumed from the beginning that there exists some physically meaningful splitting of the Lagrangian $\mathscr{L}$ into the sum of n generally invariant Lagrangians $\mathscr{L}_{(\alpha)}$; the summands $\mathscr{L}_{(\alpha)}$ are called partial Lagrangians and their sum $\mathscr{L}$ is called the total Lagrangian of the theory. In this case, the αth Lagrangian $\mathscr{L}_{(\alpha)}$ is assumed to depend explicitly at least on the $k_{(\alpha)}$th-order jet of the

corresponding αth field $\sigma_{(\alpha)}$ and possibly also on all the remaining fields (while the remaining partial Lagrangians $\mathcal{L}_{(\beta)}$, with $\beta \neq \alpha$, may depend on lower-order derivatives of the αth field $\sigma_{(\alpha)}$). Such an assumption is dictated by the hope that each partial Lagrangian should represent the dynamics of the corresponding field; we stress, however, that under the most general assumptions above the dynamics of the various fields are highly interacting, because the physically relevant object is in fact the total Lagrangian itself. We finally recall that the so-called minimal coupling prescription amounts to requiring instead that the αth Lagrangian $\mathcal{L}_{(\alpha)}$ will not depend on the derivatives of the fields other than the αth one. In this case, each partial Lagrangian $\mathcal{L}_{(\alpha)}$ governs the dynamics of the corresponding field $\sigma_{(\alpha)}$ when the remaining $(n-1)$ fields are kept fixed. We remark that further splittings of the total Lagrangian may be prescribed (like, for instance, the usual decompositions in free Lagrangians plus interaction Lagrangians); in any case, these further splittings can always be reelaborated to fit into the scheme above.

As a final remark, we should mention that in some cases only the total Lagrangian is given and no splitting *a priori* is assigned (this is *a fortiori* true if one is dealing with a unified theory). We stress that in such cases it is always possible to perform suitable (partial) Legendre transformations which introduce momenta as new variables and allow us to split conveniently the transformed Lagrangian (which actually becomes a sort of Routh function).

D. Partial energy flows and work in geometric field theories

Let us consider a k th-order Lagrangian field theory over the bundle of geometric objects $Q = \times_{\alpha=1}^{n} Q_{(\alpha)} = Q_{(1)} \times_M \cdots \times_M Q_{(n)}$, governed by a total Lagrangian $\mathcal{L} = \mathcal{L}_{(1)} + \cdots + \mathcal{L}_{(n)}$, of partial orders $(k_{(1)},\ldots,k_{(n)})$, as in the previous section. If $\sigma(x) = (\sigma_{(1)}(x),\ldots,\sigma_{(n)}(x))$ is a (local) field over M, then we have the following:

$$\mathcal{L} \circ j^k(\sigma) = \mathcal{L}_{(1)} \circ (j^{k_{(1)}}(\sigma_{(1)}),\ldots,j^{k_{(n)}}(\sigma_{(n)})) + \cdots + \mathcal{L}_{(n)} \circ (j^{k_{(1)}}(\sigma_{(1)}),\ldots,j^{k_{(n)}}(\sigma_{(n)})). \quad (3.15)$$

From the assumption that the configuration space Q of the theory is a fibered product, it follows immediately that there exist partial fibered morphisms $\hat{p}_{(\alpha)}(\mathcal{L})$, $\hat{e}_{(\alpha)}(\mathcal{L})$, and $\hat{f}_{(\alpha)}(\mathcal{L})$,

$$\hat{p}_{(\alpha)}(\mathcal{L}): J^k(Q) \to A^0_m(M) \otimes V^*[J^{k_{(\alpha)}}(Q_{(\alpha)})],$$
$$\hat{e}_{(\alpha)}(\mathcal{L}): J^{2k}(Q) \to A^0_m(M) \otimes V^*(Q_{(\alpha)}),$$
$$\hat{f}_{(\alpha)}(\mathcal{L}): J^{2k-1}(Q) \to A^0_{m-1}(M) V^*[J^{k_{(\alpha)}-1}(Q_{(\alpha)})],$$

(with $\alpha = 1,\ldots,n$), such that we have $\hat{p}(\mathcal{L}) = \hat{p}_{(1)}(\mathcal{L}) + \cdots + \hat{p}_{(n)}(\mathcal{L})$, $\hat{e}(\mathcal{L}) = \hat{e}_{(1)}(\mathcal{L}) + \cdots + \hat{e}_{(n)}(\mathcal{L})$, and $\hat{f}(\mathcal{L}) = \hat{f}_{(1)}(\mathcal{L}) + \cdots + \hat{f}_{(n)}(\mathcal{L})$, and moreover the following holds:

$$\langle p_{(\alpha)}(L) \circ j^k(\sigma) | j^{k_\alpha}[L_X(\sigma_{(\alpha)})] \rangle = \langle e_{(\alpha)}(L) \circ j^{2k}(\sigma) | L_X(\sigma_{(\alpha)}) \rangle + d_i \langle f^i_{(\alpha)}(L) \circ j^{2k-1}(\sigma) | j^{k_{(\alpha)}-1}[L_X(\sigma_{(\alpha)})] \rangle, \quad (3.16)$$

for any vector field X over M and any (local) section σ of Q. In particular, the morphisms $\hat{e}_{(\alpha)}(\mathcal{L})$ are the partial Euler–Lagrange morphisms, which define the field equations of each single field, while the morphisms $\hat{f}_{(\alpha)}(\mathcal{L})$ define the partial Poincaré–Cartan forms.

Using the fact that the total Lagrangian $\mathcal{L}$ splits into the sum of n generally invariant Lagrangians $\mathcal{L}_{(\alpha)}$, we can now define the n partial energy flows $E^i_{(\alpha)}(\mathcal{L};X,\sigma)$ by setting

$$E^i_{(\alpha)}(L;X,\sigma) = \langle f^i_{(\alpha)}(L) \circ j^{2k-1}(\sigma) | j^{k_{(\alpha)}-1}[L_X(\sigma_{(\alpha)})] \rangle - X^i[L_{(\alpha)} \circ j^k(\sigma)]. \quad (3.17)$$

It then follows that

$$E^i(L;X,\sigma) = E^i_{(1)}(L;X,\sigma) + \cdots + E^i_{(n)}(L;X,\sigma). \quad (3.18)$$

Let us now define for each couple of indices (α,β) a horizontal n form $W_{(\alpha)(\beta)}(\mathcal{L};X,\sigma) = W_{(\alpha)(\beta)}(L;X,\sigma)\, ds(x)$ by setting

$$W_{(\alpha)(\beta)}(L;X,\sigma) = \langle p_{(\alpha)}(L_{(\beta)}) \circ j^k(\sigma) | j^{k_{(\alpha)}}[L_X(\sigma_{(\alpha)})] \rangle - \langle p_{(\beta)}(L_{(\alpha)}) \circ j^k(\sigma) | j^{k_{(\beta)}}[L_X(\sigma_{(\beta)})] \rangle. \quad (3.19)$$

The density $W_{(\alpha)(\beta)}(L;X,\sigma)$ measures the work which is performed over the αth field when the β th field is Lie-dragged along the flow of the vector field X. The sum

$$W_{(\alpha)}(L;X,\sigma) = W_{(\alpha)(1)}(L;X,\sigma) + \cdots + W_{(\alpha)(n)}(L;X,\sigma) \quad (3.20)$$

measures then the total work which is performed over the αth field. From the definition (3.19) it follows immediately that the sum of all the total work vanishes, i.e.,

$$W_{(1)}(L;X,\sigma) + \cdots + W_{(n)}(L;X,\sigma) = 0. \quad (3.21)$$

Calculating then the formal divergence of each partial energy flow, we find

$$d_i[E^i_{(\alpha)}(L;X,\sigma)] = -\langle e_{(\alpha)}(L) \circ j^{2k}(\sigma) | L_X(\sigma_{(\alpha)}) \rangle + W_{(\alpha)}(L;X,\sigma), \quad (3.22)$$

along any section σ of the bundle Q. In particular, along sections σ which make $e_{(\alpha)}(L)$ vanishing (i.e., along solutions of the αth field equations), the work performed is equal to the divergence of the corresponding energy flow. Accordingly, we have the following system of n partial natural conservation laws:

$$d_i[E^i_{(\alpha)}(L;X,\sigma)] = W_{(\alpha)}(L;X,\sigma), \quad \forall X \in C^\infty[T(M)], \quad (3.23)$$

where σ is any solution of the field equations of the theory. The system of conservation laws (3.23) follows from the total conservation law (3.5) when taking into account the splitting of the Lagrangian. In fact, from (3.18), (3.21), and (3.23) one obtains immediately

$$d_i[E^i_{(1)}(L;X,\sigma)] + \cdots + d_i[E^i_{(n)}(L;X,\sigma)] = 0, \quad (3.24)$$

which merely reasserts that the total energy flow is conserved along solutions of the field equations.

E. Energy momentum tensors and stress tensors for interacting fields of geometric objects

Our considerations of Sec. III B can now be extended to the case of total Lagrangians $\mathcal{L}$ of the form (3.15), describing the interaction of n fields of geometric objects $\sigma_{(\alpha)}$. Following the terminology of Sec. III A, we give first the follow-

ing definitions: the order $s_{(\alpha)}$ of the αth field will be called the αth partial geometric order of the theory; the sum $r_{(\alpha)} = k_{(\alpha)} + s_{(\alpha)} - 1$ will be called the αth partial differential degree of the theory; the supremum $s = \max(s_{(1)},\ldots,s_{(n)})$ is the total geometric order; and the supremum $r = \max(r_{(1)},\ldots,r_{(n)})$ is the total differential degree of the theory.

From strict analogy with Sec. III B also, the partial energy flows $E^{i}{}_{(\alpha)}(L;X,\sigma)$ may be expanded as linear combinations of partial derivatives of the components X^h. In fact, from Eq. (3.17) it turns out immediately that the assignment $X \to E^{i}{}_{(\alpha)}(L;X,\sigma)$ defines a linear differential operator, whose order equals the (α)th partial differential degree $r_{(\alpha)}$. Therefore, one finds expansions of the following kind:

$$E^{i}{}_{(\alpha)}(L;X,\sigma) = [e^{i}_{h}(L)\circ j^{2k-1}(\sigma)]X^{h} + [e^{ij_1}_{h}(L)\circ j^{2k-1}(\sigma)]X^{h}{}_{j_1} + \cdots + [e^{ij_1\cdots j_{r_{(\alpha)}}}_{h}(L)j^{2k-1}(\sigma)]X^{h}{}_{j_1\cdots j_{r_{(\alpha)}}}, \quad (3.25)$$

where the coefficients $(e^{i}_{h}(L), e^{ij_1}_{h}(L),\ldots, e^{ij_1\cdots j_{r_{(\alpha)}}}_{h}(L))$, which are symmetric with respect to the upper indices j, are called partial energy momentum pseudotensors of the αth field, associated with the Lagrangian $\mathscr{L}$. Equivalent sets of αth partial energy-momentum tensors, which are denoted by $(E^{i}{}_{h}(L;C), E^{ij_1}{}_{h}(L;C),\ldots, E^{ij_1\cdots j_{r_{(\alpha)}}}{}_{h}(L;C))$, can then be obtained by choosing any linear connection C and applying the standard tensorization procedures. We remark that all these partial (pseudo) tensors are uniquely defined by the total Lagrangian $\mathscr{L}$ itself, no matter which splitting (3.15) is chosen, apart from the first ones e^{i}_{h} and $E^{i}{}_{h}$: looking in fact to (3.17), one realizes immediately that the splitting chosen affects explicitly only the term in X^h.

An analogous expansion procedure can now be applied to the partial works $W_{(\alpha)(\beta)}(L;X,\sigma)$ and to the total works $W_{(\alpha)}(L;X,\sigma)$. Leaving aside the explicit expansions of the partial works, which have no interest here (but may have some interest in investigating the inner details of the energy exchange), we shall discuss here only the proper expansions of the total works $W_{(\alpha)}(L;X,\sigma)$.

From the definition (3.19) and the definition of partial geometric orders, we see first that the assignment $X \to W_{(\alpha)(\beta)}(L;X,\sigma)$ defines, for each couple (α,β), a linear differential operator of order $w_{(\alpha)(\beta)} = \max(r_{(\alpha)}, r_{(\beta)}) + 1$. Accordingly, representing the density $W_{(\alpha)}(L;X,\sigma)$ in natural fibered coordinates, we find an expansion of the following kind:

$$W_{(\alpha)}(L;X,\sigma) = [s_{h}(L)\circ j^{k}(\sigma)]X^{h} + [s^{j}_{h}(L)\circ j^{k}(\sigma)]X^{h}{}_{j} + \cdots + [s^{j_1\cdots j_{r+1}}_{h}(L)\circ j^{k}(\sigma)]X^{h}{}_{j_1\cdots j_{r+1}}, \quad (3.26)$$

where r is the total differential degree of the theory. We stress that it is the total degree r, rather than the partial one $r_{(\alpha)}$, which enters this expansion: this is in fact a direct consequence of the definition of the αth total work itself. Choosing any linear connection C over the basis manifold M, we can also expand as follows the total work as a linear combination of symmetrized covariant derivatives of X:

$$\langle W_{(\alpha)}(L)|j^{r}(X)\rangle = S_{h}(L;C)X^{h} + S^{j_1}_{h}(L;C)\nabla_{j_1}X^{h} + \cdots + S^{j_1\cdots j_{r+1}}_{h}(L;C)\nabla_{(j_1}\cdots\nabla_{j_{r+1})}X^{h}. \quad (3.27)$$

The coefficients $(s_{h}(L), s^{j_1}_{h}(L),\ldots, s^{j_1\cdots j_{r+1}}_{h}(L))$, which are symmetric with respect to the upper indices j, are called stress pseudotensors of the αth field, associated with the total Lagrangian $\mathscr{L}$ and with its splitting (3.15). The coefficients $(S_{h}(L;C), S^{j_1}_{h}(L;C),\ldots, S^{j_1\cdots j_{r+1}}_{h}(L;C))$ have the same symmetry properties; they are tensor densities and take the name of stress tensors of the αth field, associated with $\mathscr{L}$ and corresponding to the connection C. We remark that, contrary to the energy-momentum (pseudo) tensors, the stress (pseudo) tensors of $\mathscr{L}$ will depend explicitly on the splitting of $\mathscr{L}$ itself into the sum of n partial Lagrangians. This should not be surprising, because the stress tensors account explicitly for the way in which interaction dictates how one field acts as a source for the others (and vice versa).

To end this section, it is important to remark that field dynamics establishes explicit differential relations between the energy-momentum (pseudo) tensors and the stress (pseudo) tensors of an interaction theory. In fact, one can insert the (local) expansions (3.25) and (3.26) into the partial natural conservation laws (3.23) and eliminate the arbitrary vector field X from the resulting expressions. In this way, first-order linear partial differential equations are obtained, which express the stress pseudotensors in terms of the energy-momentum pseudotensors together with their first derivatives. Explicitly, one finds

$$\begin{aligned} &e^{(ij_1\cdots j_p)}_{h}(L) = s^{ij_1\cdots j_r}_{h}(L), \\ &e^{j_1 j_2\cdots j_p}_{h}(L) + d_i[e^{ij_1 j_2\cdots j_p}_{h}(L)] = s^{j_1 j_2\cdots j_p}_{h}(L), \\ &d_i[e^{i}_{h}(L)] = s_{h}(L), \end{aligned} \quad (3.28)$$

with $1 \leqslant p \leqslant r$. Clearly, analogous (but, owing to commutation relations, fairly more complicated) differential relations can be obtained between the corresponding tensors.

F. Conclusions

We have therefore shown that with each Lagrangian theory of free fields of geometric objects one can always associate, in a unique way, a whole set of energy-momentum (pseudo) tensors, which allow us to express in a convenient form the natural conservation laws associated with Noether's theorem. This result provides a unique and canonical way to define partial energy-momentum tensors for theories of geometric fields in interaction; the number of these objects grows with the order of the theory (i.e., the number of derivatives of fields it involves) and with the geometric order of the fields themselves (i.e., the number of derivatives of local diffeomorphisms which enter their transformation laws). Considering interaction as a way for some of the fields to act as sources for the others opens the possibility to define, again in a unique and canonical way, the concept of work. We have also shown that each preferred way to split the total Lagrangian into the sum of a suitable number of partial Lagrangians allows one to define uniquely and canonically a whole set of stress tensors, which express the response of fields under deformations of their sources. In addition, the number of these objects grows with the different orders of the theory and the geometric fields involved. We have finally shown that the natural conservation laws may be expressed as relations between those two families of ob-

jects, a fact which is often misunderstood in the physical literature. The machinery developed in this paper is applicable to all geometric theories, no matter how complicated they are.

Clearly, the long series of definitions and equations which have been discussed above would be meaningless without providing explicit examples of applications. We shall not give here any example: the reader will find some, concerning the theories of geometric fields interacting with a gravitational field, in Ref. 21, where the simpler case of two interacting fields was described in lesser details. A more thorough discussion of stress tensors in geometric theories of gravitation will be contained in a forthcoming monograph.[22]

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Cumulant expansions for thermal density matrices and ground state logarithmic perturbation series

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We express the logarithm of the thermal density matrix $\rho_{H,\beta}(X,X')\equiv\langle X|e^{-\beta H}|X'\rangle$, where $H=H_0+V$, as a cumulant expansion in powers of the perturbation V, by associating with $\{H_0,|X\rangle,|X'\rangle\}$ a stochastic process. If the ground state of H_0 is isolated, this stochastic process is of finite memory; it then follows from the properties of cumulants that the above expansion of $\ln\rho$ is nonsecular as $\beta\to\infty$ (all its terms $\sim\beta$), and is thus usable down to zero temperature, unlike the direct expansion of ρ in powers of V, whose nth term $\sim\beta^n$. To determine explicitly the low-temperature behavior, we apply an analysis familiar in the theory of relaxation, and obtain the form $\ln\rho_{H,\beta}(X,X')=h(X,X',\beta)+a(X)+a(X')^{\dagger}-b\beta$, where a,b,h are cumulant expansions in powers of V; $a(X)$, b are independent of β; and $h(X,X',\beta)\to 0$ as $\beta\to\infty$. Comparing with $\rho\to\langle X|\psi_0\rangle e^{-\beta E_0}\langle\psi_0|X'\rangle$ as $\beta\to\infty$, where ψ_0 and E_0 are the ground state and energy of H, we deduce $E_0=b$, $\ln\langle X|\psi_0\rangle=a(X)$, i.e., the Rayleigh–Schrödinger perturbation series for E_0 and $\ln\langle X|\psi_0\rangle$ (with $\langle\psi_0|\psi_0\rangle=1$) emerge as cumulant expansions. In the case of a many-body system, the properties of cumulants immediately imply linked cluster theorems for $\ln\rho$, as well as for E_0 and $\ln\langle X|\psi_0\rangle$.

I. INTRODUCTION

A fundamental quantity in equilibrium statistical mechanics is the density matrix

$$\rho_{H,\beta}(X,X')=\langle X|e^{-\beta H}|X'\rangle, \tag{1.1}$$

where β^{-1} is the temperature, H the Hamiltonian, and $|X\rangle,|X'\rangle$ are (arbitrary) quantum states of the system considered (these states are often taken as position eigenstates). Usually, ρ_H cannot be calculated exactly, and approximations must be found. In cases that

$$H=H_0+V, \tag{1.2}$$

where H_0 is such that ρ_{H_0} is known exactly, and V is small in some sense, the natural procedure is to expand

$$\rho_{H,\beta}(X,X')=\langle X|e^{-\beta(H_0+V)}|X'\rangle \tag{1.3}$$

in powers of the perturbation V. However, as may be guessed from inspecting (1.3), such an expansion is essentially in powers of βV, i.e., it is "secular" (nth term $\sim\beta^n$) as $\beta\to\infty$, hence useless as an approximation scheme at low temperatures.

The situation is similar to that met in the theory of relaxation,[1,2] where one usually finds that the direct expansion of the time correlation function considered, $C(t)$ say, in powers of some perturbation V, is secular, hence useless at large times. However, if instead one expands $\ln C(t)$ in powers of V, one obtains a cumulant expansion,[1,2] which, provided the stochastic processes causing the relaxation have a finite memory, is free of secularities (all terms $\sim t$) due to the special properties of cumulants[3]; one thereby gets a perturbation expansion which stays usable at large times.

We here apply a similar procedure to ρ_H: we first associate with $\{H_0,|X\rangle,|X'\rangle\}$ a stochastic process which has a finite memory, provided the ground state of H_0 is isolated (i.e., there is a finite energy gap between the ground and lowest excited states). By expanding $\ln\rho_H$ in powers of V, we obtain a cumulant expansion whose terms all increase linearly with β as $\beta\to\infty$, i.e., we get a perturbation expansion usable down to zero temperature.

In relaxation theory, analysis of the cumulant expansion of $\ln C(t)$ naturally leads to the decomposition[1,2]

$$\ln C(t)=a-bt+h(t), \tag{1.4}$$

where $h(t)\to 0$ as $t\to\infty$, and a,b are crucial (complex) constants which govern the large-time (exponential) decay of $C(t)$. In the present case, we similarly obtain

$$\ln\rho_{H,\beta}(X,X')=a(X)+a(X')^{\dagger}-b\beta+h(X,X',\beta), \tag{1.5}$$

where $h(X,X',\beta)\to 0$ as $\beta\to\infty$. On the other hand, we also have

$$\rho_{H,\beta}(X,X')=\sum_n\langle X|\Psi_n\rangle\, e^{-\beta E_n}\,\langle\Psi_n|X'\rangle \tag{1.6}$$

$$\to\langle X|\Psi_0\rangle\, e^{-\beta E_0}\,\langle\Psi_0|X'\rangle, \quad \text{as } \beta\to\infty, \tag{1.7}$$

i.e.,

$$\ln\rho_{H,\beta}(X,X')\to\ln\langle X|\Psi_0\rangle+\ln\langle\Psi_0|X'\rangle-\beta E_0 \quad \text{as } \beta\to\infty, \tag{1.7'}$$

where Ψ_n and E_n are the eigenstates and energies of H (the index 0 referring to the ground state). Comparing with (1.5), we deduce

$$E_0=b, \quad \ln\langle X|\psi_0\rangle=a(X). \tag{1.8}$$

Since b and $a(X)$ are cumulant expansions in powers of V, Eqs. (1.8) are just the Rayleigh–Schrödinger (RS) perturbation series for E_0 and $\ln\langle X|\psi_0\rangle$, *in cumulant form*. Note that ψ_0 in (1.8) is normalized, $\langle\psi_0|\psi_0\rangle=1$ (whereas the usual RS series is for $\bar{\psi}_0\equiv\psi_0/\langle\phi_0|\psi_0\rangle$, satisfying $\langle\phi_0|\bar{\psi}_0\rangle=1$, where ϕ_0 is the ground state of H_0).[4]

Conceptually, it is satisfying that the density matrix ρ_H, and the ground state energy and wave function, have structurally similar, closely interrelated, perturbation series. From a practical point of view, the cumulant form of the perturbation series may often be especially convenient, be-

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cause of the well-known statistical meaning and properties of cumulants. In particular, in the case of a many-body system, the basic property of cumulants (vanishing whenever their arguments separate into two or more statistically independent subsets) immediately implies linked cluster theorems[5] for $\ln\rho$, as well as for E_0 and $\ln\langle X|\psi_0\rangle$.

The above features seem to indicate that the perturbation series of $\ln\langle X|\Psi_0\rangle$ is more "primitive" than that of $\langle X|\Psi_0\rangle$. Let us mention in that respect that Aharonov and Au[6] have recently studied the perturbation expansion of $\ln\langle X|\Psi_0\rangle$ in the case where $|X\rangle$ are position eigenstates (calling it a "logarithmic perturbation expansion"), and found it to have attractive computational advantages.

In Sec. II, a stochastic process is associated with $\{H_0,|X\rangle,|X'\rangle\}$, and its properties studied. In Sec. III, the cumulant perturbation expansion of $\ln\rho_{H,\beta}(X,X')$ is constructed. The low-temperature (large-"time") behavior of that cumulant expansion is exposed in Sec. IV, leading to the logarithmic Rayleigh–Schrödinger perturbation series for the ground state of H, in Sec. V. In Sec. VI, the case of a many-body system is considered, and linked cluster theorems deduced. We conclude with a brief discussion in Sec. VII. Two appendices contain the more technical details.

Notation: The eigenstates and energies of H_0 are denoted ϕ_n,ϵ_n:

$$H_0|\phi_n\rangle=\epsilon_n|\phi_n\rangle.$$

Those of H are denoted ψ_n,E_n:

$$H|\psi_n\rangle=E_n|\psi_n\rangle.$$

II. STOCHASTIC PROCESS ASSOCIATED WITH H_0,X,X'

Multiplying and dividing by $\rho_{H_0,\beta}(X,X')$, we rewrite (1.3) as

$$\rho_{H,\beta}(X,X')=\rho_{H_0,\beta}(X,X')R(X,X',T), \tag{2.1}$$

$$R(X,X',T)={}^{X,0}\left\langle\exp\left(-\int_0^T dt\,v(t)\right)\right\rangle^{X',T}, \tag{2.2}$$

where we have set

$$v\equiv V/\hbar,$$

introduced the "time"

$$T\equiv\beta\hbar,$$

and denoted

$$A(t)\equiv e^{-tH_0/\hbar}Ae^{tH_0/\hbar} \tag{2.3}$$

for any operator A; the "stochastic average" ${}^{X,T}\langle(\cdots)\rangle^{X',T'}$ is defined by

$${}^{X,T}\langle(\cdots)\rangle^{X',T'}=\frac{\langle X|e^{TH_0/\hbar}T_{\rightarrow}(\cdots)e^{-T'H_0/\hbar}|X'\rangle}{\langle X|e^{-(T'-T)H_0/\hbar}|X'\rangle}, \tag{2.4}$$

where $T_{\rightarrow}$ orders operators such that their time arguments increase from left to right ($T_{\rightarrow}$ is part of the averaging operation). We used

$$e^{-\beta(H_0+V)}e^{\beta H_0}=T_{\rightarrow}\exp\left(-\int_0^T dt\,\frac{V(t)}{\hbar}\right). \tag{2.5}$$

The stochastic process defined by (2.4) is not stationary [no time translation invariance inside ${}^{X,T}\langle(\cdots)\rangle^{X',T'}$], because of the fixed times T and T' on which it depends. We have, however, for any t,

$${}^{X,T}\left\langle\prod_i A_i(t_i)\right\rangle^{X',T'}={}^{X,T+t}\left\langle\prod_i A_i(t_i+t)\right\rangle^{X',T'+t}. \tag{2.6}$$

Also, since (2.3) implies $A(t)^{\dagger}=A^{\dagger}(-t)$,

$$\left[{}^{X,T}\left\langle\prod_i A_i(t_i)\right\rangle^{X',T'}\right]^{\dagger}={}^{X',-T'}\left\langle\prod_i A_i^{\dagger}(-t_i)\right\rangle^{X,-T}. \tag{2.7}$$

We henceforth assume that the ground state of H_0 is isolated, i.e., that (see the end of Sec. I for notation)

$$\bar{\tau}\equiv\hbar/(\epsilon_1-\epsilon_0)\quad\text{is finite.} \tag{2.8}$$

We then have (dropping $\hbar$'s for simplicity)

$$e^{-tH_0}=\sum_n|\phi_n\rangle e^{-t\epsilon_n}\langle\phi_n|\rightarrow|\phi_0\rangle e^{-t\epsilon_0}\langle\phi_0|\quad\text{as } t\rightarrow\infty. \tag{2.9}$$

For discussion purposes, let us assume more specifically that the limit is essentially reached when t is larger than some time $\tau\gg\bar{\tau}$, i.e.,[7]

$$e^{-tH_0}\cong|\phi_0\rangle e^{-t\epsilon_0}\langle\phi_0|,\quad\text{if } t>\tau. \tag{2.10}$$

Consider now (assuming $T\leqslant t_1\leqslant t_2\cdots\leqslant t_n\leqslant T'$)

$${}^{X,T}\langle V(t_1)V(t_2)\cdots V(t_n)\rangle^{X',T'}=\frac{\langle X|e^{-(t_1-T)H_0}Ve^{-(t_2-t_1)H_0}\cdots Ve^{-(T'-t_n)H_0}|X'\rangle}{\langle X|e^{-(T'-T)H_0}|X'\rangle}. \tag{2.11}$$

If $t_1-T>\tau$, whence also $T'-T>\tau$, we have

$$\frac{\langle X|e^{-(t_1-T)H_0}}{\langle X|e^{-(T'-T)H_0}}\cong\frac{\langle X|\phi_0\rangle e^{-(t_1-T)\epsilon_0}\langle\phi_0|}{\langle X|\phi_0\rangle e^{-(T'-T)\epsilon_0}\langle\phi_0|}=\frac{\langle\phi_0|e^{-t_1H_0}}{\langle\phi_0|e^{-T'H_0}}. \tag{2.12}$$

A similar near equality holds if $T'-t_n>\tau$. Insertion into (2.11) yields

$${}^{X,T}\langle V(t_1)\cdots\cong{}^{-\infty}\langle V(t_1)\cdots,\quad\text{if } t_1-T>\tau, \tag{2.13}$$

$$\cdots V(t_n)\rangle^{X',T'}\cong\cdots V(t_n)\rangle^{\infty}\quad\text{if } T'-t_n>\tau,$$

where $\rangle^{\infty}$ and ${}^{-\infty}\langle$ are defined by

$$\lim_{T\rightarrow-\infty}{}^{X,T}\langle(\cdots)\rangle^{X',T'}=\frac{\langle\phi_0|T_{\rightarrow}(\cdots)e^{-T'H_0}|X'\rangle}{\langle\phi_0|e^{-T'H_0}|X'\rangle}\equiv{}^{-\infty}\langle(\cdots)\rangle^{X',T'}, \tag{2.14a}$$

$$\lim_{T'\rightarrow\infty}{}^{X,T}\langle(\cdots)\rangle^{X',T'}=\frac{\langle X|e^{TH_0}T_{\rightarrow}(\cdots)|\phi_0\rangle}{\langle X|e^{TH_0}|\phi_0\rangle}\equiv{}^{X,T}\langle(\cdots)\rangle^{\infty}, \tag{2.14b}$$

$$\lim_{\substack{T\rightarrow-\infty\\T'\rightarrow\infty}}{}^{X,T}\langle(\cdots)\rangle^{X',T'}=\langle\phi_0|T_{\rightarrow}(\cdots)|\phi_0\rangle\equiv{}^{-\infty}\langle(\cdots)\rangle^{\infty}. \tag{2.14c}$$

The near equalities (2.13) become exact as $T\rightarrow-\infty$ and/or $T'\rightarrow\infty$. Observe that the stochastic average ${}^{-\infty}\langle(\cdots)\rangle^{\infty}$ is

stationary, i.e., we have the time translation invariance[8]

$$ {}^{-\infty}\left\langle \prod_i A_i(t_i)\right\rangle^{\infty} = {}^{-\infty}\left\langle \prod_i A_i(t_i+t)\right\rangle^{\infty}. \tag{2.15}$$

Suppose now that $t_{j+1}-t_j>\tau$, whence also $T'-T>\tau$; inserting then Eq. (2.10) with $t=t_{j+1}-t_j$ in the numerator of (2.11), and with $t=T'-T$ in the denominator, we get

$$\begin{aligned} &{}^{X,T}\langle V(t_1)\cdots V(t_j)V(t_{j+1})\cdots V(t_n)\rangle^{X',T'} \\ &\quad\cong {}^{X,T}\langle V(t_1)\cdots V(t_j)\rangle^{\infty}\ {}^{-\infty}\langle V(t_{j+1})\cdots V(t_n)\rangle^{X',T'} \\ &\quad\cong \left({}^{X,T}\langle V(t_1)\cdots V(t_j)\rangle^{X',T'}\right)\left({}^{X,T}\langle V(t_{j+1})\cdots V(t_n)\rangle^{X',T'}\right), \end{aligned} \tag{2.16}$$

the last line in view of (2.13) and the fact that $t_{j+1}-t_j>\tau$ implies $t_{j+1}-T,T'-t_j>\tau$. The above near equalities become exact as $t_{j+1}-t_j\to\infty$. Equation (2.16), stating that interactions $V(t_i)$ become statistically independent when separated in time by more than τ, characterizes the stochastic process ${}^{X,T}\langle\ \ \rangle^{X',T'}$ as of finite memory $\cong\tau$.

The stochastic process introduced here, and the associated notion of a "quantum memory" τ, become very intuitive when $|X\rangle$ are position eigenstates, and the density matrices (1.1) are represented as path integrals.[9]

III. CUMULANT PERTURBATION EXPANSION OF THE DENSITY MATRIX

By expanding the exponential in (2.2), we obtain the (direct) perturbation expansion of $\rho_{H,\beta}(X,X')$ in powers of V:

$$\rho_{H,\beta}(X,X')=\rho_{H_0,\beta}(X,X')\left\{1-\hbar^{-1}\int_0^T dt\ {}^{X,0}\langle V(t)\rangle^{X',T} + \hbar^{-2}\int_0^T dt_2\int_0^{t_2} dt_1\ {}^{X,0}\langle V(t_1)V(t_2)\rangle^{X',T}+\cdots\right\}. \tag{3.1}$$

However, this expansion is useless as an approximation scheme at low temperatures (large T), because the term of nth order in V diverges like T^n as $T\to\infty$; this follows from the fact that when T is very large ($T\gg n\tau$), then

$${}^{X,0}\left\langle\prod_{i=1}^n V(t_i)\right\rangle^{X',T}\cong\prod_{i=1}^n {}^{X,0}\langle V(t_i)\rangle^{X',T}\cong\prod_{i=1}^n {}^{-\infty}\langle V(0)\rangle^{\infty} \tag{3.2}$$

within the bulk of the integration volume $\int_0^T d^n t$ not in the vicinity of hyperplanes with two or more t_i's equal, or near boundaries (one or more t_i near 0 or T) [the first equality in (3.2) holds if the t_i are all well separated from each other, by (2.16), and the second near equality follows from ${}^{X,0}\langle V(t)\rangle^{X,T}\cong {}^{-\infty}\langle V(t)\rangle^{\infty}={}^{-\infty}\langle V(0)\rangle^{\infty}$ except in the vicinity of $t=0$ and $t=T$, by (2.13) and (2.15)].

The situation here is quite similar to that met in the theory of relaxation,[1,2] and the same solution obtains, viz., expand $\ln\rho_H$ rather than ρ_H, i.e., perform the cumulant expansion[3] of (2.2). Doing so, we get

$$\rho_{H,\beta}(X,X')=\rho_{H_0,\beta}(X,X')e^{K(X,X',T)}, \tag{3.3}$$

where

$$\begin{aligned} K(X,X',T)=\ln R(X,X',T) &= {}^{X,0}\left\langle \exp\left(-\int_0^T dt\, v(t)\right)-1\right\rangle_c^{X',T} \\ &= -\int_0^T dt\ {}^{X,0}\langle v(t)\rangle^{X',T}+\int_0^T dt_2\int_0^{t_2} dt_1\ {}^{X,0}\langle v(t_1)v(t_2)\rangle_c^{X',T}+\cdots. \end{aligned} \tag{3.4}$$

The cumulants $\langle V_1V_2\cdots\rangle_c$, whose explicit expressions are[3]

$$\begin{aligned} &\langle V_1\rangle_c=\langle V_1\rangle,\quad \langle V_1V_2\rangle_c=\langle V_1V_2\rangle-\langle V_1\rangle\langle V_2\rangle, \\ &\langle V_1V_2V_3\rangle_c=\langle V_1V_2V_3\rangle-\langle V_1V_2\rangle\langle V_3\rangle-\langle V_1V_3\rangle\langle V_2\rangle-\langle V_2V_3\rangle\langle V_1\rangle+2\langle V_1\rangle\langle V_2\rangle\langle V_3\rangle,\cdots, \end{aligned} \tag{3.5}$$

have the fundamental property of vanishing whenever their arguments separate into two or more statistically independent subsets.[3] Thus, because of the finite memory property (2.16), ${}^{X,0}\langle\Pi_{j=1}^n v(t_j)\rangle_c^{X',T}$ vanishes if there is a gap $t_j-t_{j-1}>\tau$, i.e., the cumulants in (3.4) are nonzero only if the times in them are clustered together; this implies that all the terms in the expansion (3.4) grow like T as $T\to\infty$, so that this expansion stays a usable approximation scheme even as the temperature goes to zero.

IV. LOW-TEMPERATURE (LARGE-"TIME") BEHAVIOR

As just argued, $K(X,X',T)\sim T$ as $T\to\infty$; we want to determine more precisely this asymptotic behavior. For this purpose, we adapt a procedure used in the theory of relaxation[1,2] [the fact that here the averaging operation ${}^{X,0}\langle(\cdots)\rangle^{X',T}$ depends on T and is not stationary introduces a slight complication]. We first rewrite (3.4) as (see Appendix A)

$$K(X,X',T)=-\int_0^T dt\ {}^{X,0}\langle v(t)\rangle^{X',T} + \int_0^T dt_2\int_0^{t_2} dt_1\, C_{X,0}^{X',T}(t_1,t_2), \tag{4.1}$$

where

$$C_{X,T}^{X',T'}(t_1,t_2) \equiv {}^{X,T}\left\langle v(t_1)\exp\left(-\int_{t_1}^{t_2} dt\, v(t)\right)v(t_2)\right\rangle_c^{X',T'}. \tag{4.2}$$

The clustering property of cumulants implies that $C_{X,0}^{X',T}(t_1,t_2)$ vanishes as $t_2-t_1\to\infty$ (it being always understood that $0\le t_1\le t_2\le T$). For discussion purposes, let us assume more specifically that $C_{X,0}^{X',T}(t_1,t_2)$ is negligibly small when t_2-t_1 is larger than some time τ':

$$C_{X,0}^{X',T}(t_1,t_2)\cong 0,\quad \text{if } t_2-t_1>\tau'. \tag{4.3}$$

Note that if v is sufficiently small, then

$C^{X',T}_{X,0}(t_1,t_2) \cong {}^{X,0}\langle v(t_1)v(t_2)\rangle^{X',T}_c$,

so that $\tau' \cong \tau$ in view of (2.16); but in general, τ' can be quite different from the memory τ. We also have, on account of (2.13),

$$C^{X',T}_{X,0}(t_1,t_2) \cong C_\infty(t_2 - t_1), \quad \text{if } \tau < t_1 \leqslant t_2 < T - \tau, \tag{4.4}$$

where

$$C_\infty(\sigma) \equiv C^{\infty}_{-\infty}(0,\sigma) = {}^{-\infty}\left\langle v(0)\exp\left(-\int_0^\sigma dt\, v(t)\right)v(\sigma)\right\rangle^{\infty}_c \tag{4.5}$$

[because of (2.15), $C^{\infty}_{-\infty}(t_1,t_2) = C^{\infty}_{-\infty}(0,t_2 - t_1)$ depends only on $t_2 - t_1$]. The form of relations (4.3) and (4.4) suggests that we introduce relative variables

$$\left.\begin{aligned}\theta &= \tfrac{1}{2}(t_1 + t_2)\\ \sigma &= t_2 - t_1\end{aligned}\right\} \leftrightarrow \left\{\begin{aligned}t_1 &= \theta - \sigma/2\\ t_2 &= \theta + \sigma/2\end{aligned}\right., \tag{4.6}$$

whereby (4.3) and (4.4) become

$$C^{X',T}_{X,0}(\theta;\sigma) \cong \begin{cases}0, & \text{if } \sigma > \tau', \quad (4.3')\\ C_\infty(\sigma), & \text{if } \tau < \theta - \sigma/2 \leqslant \theta + \sigma/2 < T - \tau, \quad (4.4')\end{cases}$$

where we use the notation (note the semicolon)

$$C^{X',T'}_{X,T}(\theta;\sigma) \equiv C^{X',T'}_{X,T}(\theta - \sigma/2, \theta + \sigma/2). \tag{4.7}$$

When expressed in terms of θ, σ, the double integral in (4.1) naturally breaks up into two pieces (corresponding to the two integration regions R_1 and R_2 shown in Fig. 1), simply related to one another, and leading to the convenient decomposition (see Appendix B)

$$K(X,X',T) = \bar{K}(X,X',T) + \bar{K}(X',X,T)^\dagger, \tag{4.8}$$

where

$$\bar{K}(X,X',T) = -\int_0^{T/2} dt\, {}^{X,0}\langle v(t)\rangle^{X',T} + \int_0^{T/2} d\theta \int_0^{2\theta} d\sigma\, C^{X',T}_{X,0}(\theta;\sigma) \tag{4.9}$$

[the double integral in (4.9) is over the region R_1 in Fig. 1; the integral of $C^{X',T}_{X,0}$ over R_2 yields the similar term in $\bar{K}(X',X,T)^\dagger$]. When T is large, (4.3) and (4.4) imply that $C^{X',T}_{X,0}(\theta;\sigma)$ is essentially equal to $C_\infty(\sigma)$ within most of the region (inside R_1) wherein it is sizable (see Fig. 1); since the latter region is of area $\sim T/2$, we conclude that as $T \to \infty$, the second term of (4.9) grows like $(T/2)\int_0^\infty d\sigma C_\infty(\sigma)$. We also have

$${}^{X,0}\langle v(t)\rangle^{X',T} \cong {}^{-\infty}\langle v(t)\rangle^{\infty} \equiv {}^{-\infty}\langle v\rangle^{\infty}, \quad \text{if } \tau < t < T - \tau \tag{4.10}$$

[${}^{-\infty}\langle v(t)\rangle^{\infty}$ is independent of t, by (2.15)], implying that the first term of (4.9) grows like $-(T/2)\,{}^{-\infty}\langle v\rangle^{\infty}$ as $T \to \infty$. Hence, the dominant large-time behavior of (4.9) is

$$\bar{K}(X,X',T) \sim \tfrac{1}{2}\bar{b}T \quad \text{as } T \to \infty, \tag{4.11}$$

where

$$\bar{b} = -{}^{-\infty}\langle v\rangle^{\infty} + \int_0^\infty d\sigma\, C_\infty(\sigma) \tag{4.12}$$

$$= -{}^{-\infty}\left\langle v(0)\exp\left(-\int_0^\infty dt\, v(t)\right)\right\rangle^{\infty}_c \tag{4.12'}$$

[the second line from using (4.5) and performing the integration over σ].

Let us now examine the difference

$$K(X,X',T) - \tfrac{1}{2}\bar{b}T \equiv A + B + D, \tag{4.13}$$

where

$$A = -\int_0^{T/2} dt\, [{}^{X,0}\langle v(t)\rangle^{X',T} - {}^{-\infty}\langle v\rangle^{\infty}], \tag{4.14A}$$

$$B = \int_0^{T/2} d\theta \int_0^{2\theta} d\sigma [C^{X',T}_{X,0}(\theta;\sigma) - C_\infty(\sigma)], \tag{4.14B}$$

$$D = -\int_0^{T/2} d\theta \int_{2\theta}^\infty d\sigma\, C_\infty(\sigma). \tag{4.14D}$$

[We broke up the part $\int_0^{T/2} d\theta \int_0^\infty d\sigma\, C_\infty(\sigma)$ of $\frac{1}{2}\bar{b}T$ into two pieces by setting $\int_0^\infty d\sigma = \int_0^{2\theta} d\sigma + \int_{2\theta}^\infty d\sigma$, and included the first piece in B, D being the rest. Note that the integration region is R_1 in (4.14B), and R_1' in (4.14D), shown in Fig. 1(b).] We show that A, B, and D tend to finite limits as $T \to \infty$ (we denote $A_\infty \equiv \lim_{T\to\infty} A$, etc.): Let T be large ($T \gg \tau + \tau'$). Then, the integrand in (4.14A) is sizable only for $t < \tau$ [since ${}^{X,0}\langle v(t)\rangle^{X',T} \cong {}^{-\infty}\langle v\rangle^{\infty}$ if $\tau < t \leqslant T/2$ with $T > 2\tau$], and moreover ${}^{X,0}\langle v(t)\rangle^{X',T} \cong {}^{X,0}\langle v(t)\rangle^{\infty}$ there, by (2.13), whence

$$A_\infty = -\int_0^\infty dt\, [{}^{X,0}\langle v(t)\rangle^{\infty} - {}^{-\infty}\langle v\rangle^{\infty}]. \tag{4.15}$$

Also, in (4.14B), $C^{X',T}_{X,0} - C_\infty$ is sizable only for $\sigma < \tau'$ and $\theta < \tau + \tau'/2$ [see Fig. 1(b)], and moreover $C^{X',T}_{X,0} \cong C^{\infty}_{X,0}$ there, by (2.13), whence

$$B_\infty = \int_0^\infty d\theta \int_0^{2\theta} d\sigma [C^{\infty}_{X,0}(\theta;\sigma) - C_\infty(\sigma)]. \tag{4.16}$$

Finally, in (4.14D), $C_\infty(\sigma)$ is sizable only for $\sigma < \tau'$, whence

$$D_\infty = \mathcal{N}, \tag{4.17}$$

where

$$\mathcal{N} = -\int_0^\infty d\theta \int_{2\theta}^\infty d\sigma\, C_\infty(\sigma) = -\frac{1}{2}\int_0^\infty \sigma\, d\sigma\, C_\infty(\sigma) \tag{4.18}$$

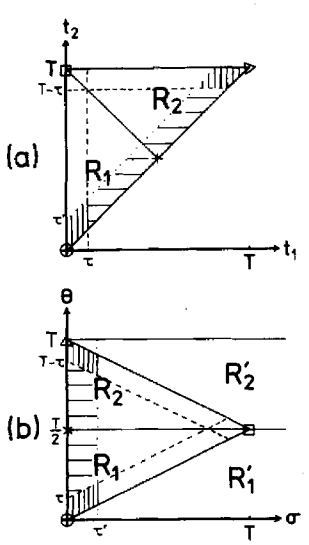

FIG. 1. The integration regions for the double integrals in Eqs. (4.1), (4.9), and (4.14D), in the (t_1,t_2) coordinates in (a), in the (θ,σ) coordinates in (b) (the small square, triangle, circle and cross serve to identify corresponding points in the two coordinate systems; the regions R_1 and R_2 are the triangles delimited by solid lines). The case $T \gg \tau + \tau'$ is depicted. The dashed lines are $t_1 = \theta - \sigma/2 = \tau$ and $t_2 = \theta + \sigma/2 = T - \tau$, the dotted line is $t_2 - t_1 = \sigma = \tau'$. In view of Eq. (4.3), $C^{X',T}_{X,0}$ is sizable only inside the hatched regions, and, on account of (2.13), essentially equal to C_∞ in the horizontally hatched part, to $C^{\infty}_{X,0}$ in the lower vertically hatched part, and to $C^{X',T}_{-\infty}$ in the upper vertically hatched part.

(we used $\int_0^\infty d\theta \int_{2\theta}^\infty d\sigma = \int_0^\infty d\sigma \int_0^{\sigma/2} d\theta$).

Combining (4.13)–(4.18), we get

$$\bar{K}(X,X',T) = \tfrac{1}{2}\bar{b}T + \alpha(X) + \mathcal{N} + \bar{k}(X,X',T), \quad (4.19)$$

or, in view of (4.8) [denoting $k(X,X',T) \equiv \bar{k}(X,X',T) + \bar{k}(X',X,T)^\dagger$],

$$K(X,X',T) = \bar{b}T + \alpha(X) + \alpha(X')^\dagger + 2\mathcal{N} + k(X,X',T), \quad (4.20)$$

where

$$\alpha(X) = A_\infty + B_\infty \quad (4.21)$$

and

$$\bar{k}(X,X',T) = \Delta A + \Delta B + \Delta D \to 0 \quad \text{as } T\to\infty, \quad (4.22)$$

where $\Delta A \equiv A - A_\infty$, etc., i.e., rearranging slightly,

$$\Delta A = -\int_0^{T/2} dt\,[{}^{X,0}\langle v(t)\rangle^{X',T} - {}^{X,0}\langle v(t)\rangle^{\infty}] + \int_{T/2}^{\infty} dt\,[{}^{X,0}\langle v(t)\rangle^{\infty} - {}^{-\infty}\langle v\rangle^{\infty}], \quad (4.23A)$$

$$\Delta B = \int_0^{T/2} d\theta \int_0^{2\theta} d\sigma [C_{X,0}^{X',T} - C_{X,0}^{\infty}] - \int_{T/2}^{\infty} d\theta \int_0^{2\theta} d\sigma [C_{X,0}^{\infty} - C_{-\infty}^{\infty}], \quad (4.23B)$$

$$\Delta D = \int_{T/2}^{\infty} d\theta \int_{2\theta}^{\infty} d\sigma\, C_\infty(\sigma) = \frac{1}{2}\int_0^\infty \sigma\, d\sigma\, C_\infty(T+\sigma) \quad (4.23D)$$

(in the last line, we used $\int_{T/2}^\infty d\theta \int_{2\theta}^\infty d\sigma = \int_T^\infty d\sigma \int_{T/2}^{\sigma/2} d\theta$).

The form (4.19) and (4.20) should be a convenient starting point for getting low-temperature approximations. In particular, it yields, in the limit $T\to\infty$, the perturbation expansions for the ground state of H, as we now see explicitly.

V. LOGARITHMIC RAYLEIGH–SCHRÖDINGER PERTURBATION SERIES

Observing, in view of (2.9), that

$$\rho_{H_0,\beta}(X,X') \to \langle X|\phi_0\rangle\, e^{-\beta\epsilon_0}\langle\phi_0|X'\rangle \quad \text{as } \beta\to\infty, \quad (5.1)$$

we may set

$$\ln \rho_{H_0,\beta}(X,X') = \ln\langle X|\phi_0\rangle + \ln\langle\phi_0|X'\rangle - \beta\epsilon_0 + h_0(X,X',\beta\hbar), \quad (5.2)$$

thereby defining $h_0(X,X',T)\to 0$ as $T\to\infty$. Combining (3.3), (4.20) and (5.2) we obtain Eqs. (1.5) and (1.8) with

$$h(X,X',T) = h_0(X,X',T) + k(X,X',T) \to 0 \quad \text{as } T\to\infty, \quad (5.3)$$

$$\ln\langle X|\psi_0\rangle = a(X) = \ln\langle X|\phi_0\rangle + \alpha(X) + \mathcal{N}, \quad (5.4)$$

$$E_0 = b = \epsilon_0 - \bar{b} = \epsilon_0 + {}^{-\infty}\left\langle v(0)\exp\left(-\int_0^\infty dt\, v(t)\right)\right\rangle_c^\infty, \quad (5.5)$$

with [in view of (4.21), (4.18), (4.5)]

$$\alpha(X) = \lim_{T\to\infty}\left[{}^{X,0}\left\langle \exp\left(-\int_0^T dt\, v(t)\right)\right\rangle_c^\infty - {}^{-\infty}\left\langle \exp\left(-\int_0^T dt\, v(t)\right)\right\rangle_c^\infty\right], \quad (5.6)$$

$$\mathcal{N} = -\frac{1}{2}\int_0^\infty \sigma\, d\sigma\, {}^{-\infty}\left\langle v(0)\exp\left(-\int_0^\sigma dt\, v(t)\right)v(\sigma)\right\rangle_c^\infty \quad (5.7)$$

[in going from (4.21) to (5.6), we reverted to the variables t_1, t_2 in (4.16), and performed the integrations; each term in (5.6) diverges as $T\to\infty$, but their difference stays finite].

Equations (5.4)–(5.7), which are, of course, to be understood as expanded out in powers of v, are the Rayleigh–Schrödinger perturbation series for the ground state of H. Note that ψ_0 given by (5.4) is normalized,

$$\langle\psi_0|\psi_0\rangle = 1, \quad (5.8)$$

as is clear from (1.7). By setting $|X\rangle = |\phi_0\rangle$ in (5.4) [in which case ${}^{X,0}\langle = {}^{-\infty}\langle$], we find[10]

$$\mathcal{N} = \ln\langle\phi_0|\psi_0\rangle. \quad (5.9)$$

Thus, the state $\bar{\psi}_0$ defined by

$$\langle X|\bar{\psi}_0\rangle \equiv \langle X|\psi_0\rangle / \langle\phi_0|\psi_0\rangle = \langle X|\phi_0\rangle\, e^{\alpha(X)} \quad (5.10)$$

is normalized to

$$\langle\phi_0|\bar{\psi}_0\rangle = 1. \quad (5.11)$$

It is usually the expansion of $\bar{\psi}_0$ in powers of V which is constructed, and referred to as Rayleigh–Schrödinger series.[4]

By expanding out the cumulants in (5.4)–(5.7), and inserting $1 = \Sigma_n |\phi_n\rangle\langle\phi_n|$ between every pair of operators $v(t_i)$, one easily recovers, in the first few orders, the standard textbook form of the RS expansions[4] [for $\ln\psi_0(X)$, or for $\bar{\psi}_0(X)$ if one further expands $e^{\alpha(X)}$ in (5.10)]. But the cumulant form has definite operational and conceptual advantages, in view of the properties and statistical meaning of cumulants. In particular, it immediately leads to linked cluster theorems[5] in the case of a many-body system, as shown in the next section.

VI. MANY-BODY CASE—LINKED CLUSTER THEOREM

Let the physical system considered consist of N (not necessarily identical) particles in a volume $\mathcal{V}$, and

$$H_0 = \sum_{j=1}^N h_j, \quad V = \sum_{i<j} V_{ij}. \quad (6.1)$$

We choose the states $|X\rangle$ as products of single particle states,

$$|X\rangle = \prod_{j=1}^N |x_j\rangle^{(j)}, \quad (6.2)$$

where $|\rangle^{(j)}$ belongs to the Hilbert space of the jth particle. Here, we do not take account of quantum statistics [i.e., (6.2) is not (anti)symmetrized with respect to identical particles].

Consider now Eq. (2.2), with V given by (6.1). Defining (Mayer trick[11])

$$f_{ij} = \exp\left(-\int_0^T dt\, v_{ij}(t)\right) - 1, \quad (6.3)$$

where

$$v_{ij}(t) = e^{-tH_0} v_{ij} e^{tH_0} = e^{-t(h_i+h_j)} v_{ij} e^{t(h_i+h_j)}, \quad (6.4)$$

we have

$$\exp\left(-\int_0^T dt\, v(t)\right) - 1 = \prod_{i<j}(1+f_{ij}) - 1 \quad (6.5)$$

$$= \sum_{i<j} f_{ij} + \sum_{i<j<k} f_{ij} f_{ik} + \cdots$$

$$= \sum_{\Gamma} \Gamma^f. \tag{6.6}$$

In the last line, the sum is over all Mayer graphs[11] consisting of 2,3,...,N vertices (i.e., black dots representing particles) with zero or one edge (representing f_{ij}) between every pair of vertices [see Fig. 2(a)], and we denote

$$\Gamma^f = \prod_{(i,j)\in\Gamma} f_{ij}, \tag{6.7}$$

the product being over all edges of Γ. Equation (2.2) thus becomes

$$R(X,X',T) = 1 + {}^{X,0}\left\langle \sum_{\Gamma} \Gamma^f \right\rangle^{X',T}. \tag{6.8}$$

Because the averaging operation $\langle\ \rangle$ contains the time-ordering operation, the f_{ij} in (6.8) are, of course, to be understood as ultimately expanded in powers of v_{ij}. One may therefore prefer to use alternative, more detailed, diagrammatic representations. Thus, if one expands the 1hs of (6.5) as

$$\exp\left(-\int_0^T dt\, v(t)\right) - 1$$
$$= -\int_0^T dt\, v(t) + \frac{1}{2}\int_0^T dt_2 \int_0^T dt_1\, v(t_2)v(t_1) + \cdots, \tag{6.9}$$

then, on substituting (6.1), one gets terms like

$$\int_0^T dt_3 \int_0^T dt_2 \int_0^T dt_1\, v_{12}(t_1)v_{23}(t_2)v_{12}(t_3), \tag{6.10}$$

which may be represented by multigraphs (i.e., graphs with possibly more than one edge between each pair of vertices), wherein each particle is again represented by a vertex, and each edge, drawn as a dashed line, represents an interaction v_{ij} [akin to Feynman diagrams,[12] see Fig. 2(b)]. Or, if instead one uses the explicitly time-ordered form

$$\exp\left(-\int_0^T dt\, v(t)\right) - 1$$
$$= -\int_0^T dt\, v(t) + \int_0^T dt_2 \int_0^{t_2} dt_1\, v(t_1)v(t_2) + \cdots, \tag{6.11}$$

then one will obtain terms like

$$\int_0^T dt_3 \int_0^{t_3} dt_2 \int_0^{t_2} dt_1\, v_{12}(t_1)v_{23}(t_2)v_{12}(t_3), \tag{6.12}$$

which may be represented by a time-ordered graph (akin to Goldstone diagrams[12]) wherein time flows upwards, each particle is represented by a vertical line (which may be called a "vertex"), and the interaction $v_{ij}(t_n)$ is drawn as a dashed horizontal line ("edge") at level t_n, connecting lines i and j [see Fig. 2(c)]. We then have, as more detailed versions of (6.8),

$$R(X,X',T) = 1 + {}^{X,0}\langle \text{sum of } v \text{ multigraphs}\rangle^{X',T} \tag{6.13}$$
$$= 1 + {}^{X,0}\langle \text{sum of time-ordered graphs}\rangle^{X',T}. \tag{6.13'}$$

Although they must be understood as ultimately expanded out in terms of time-ordered graphs, the Mayer f graphs in (6.8) are much more compact and convenient to work with (each f graph standing for an infinite number of v multigraphs or time-ordered graphs).

Let us now introduce (6.6) into the cumulant expansion (3.4), i.e.,

$$K(X,X',T) = {}^{X,0}\left\langle \sum_{\Gamma} \Gamma^f \right\rangle_{c\{v\}}^{X',T}, \tag{6.14}$$

where the argument $\{v\}$ is a reminder that the cumulants are built with the interactions v_{ij} (not with the f_{ij}).

A diagram is said to be connected if the set of its vertices (or "vertices") cannot be partitioned into two or more subsets such that there are no edges connecting vertices belonging to different subsets. The connected subdiagrams of a diagram are called its connected components. Let the graph Γ have $n \geqslant 2$ connected components $\Gamma_1, \Gamma_2, \ldots, \Gamma_n$; then, in view of (6.2) and (6.7),

$${}^{X,0}\langle \Gamma^f \rangle^{X',T} = {}^{X,0}\left\langle \prod_{i=1}^{n} \Gamma_i^f \right\rangle^{X',T} = \prod_{i=1}^{n} {}^{X,0}\langle \Gamma_i^f \rangle^{X',T}, \tag{6.15}$$

i.e., the different connected components (and the interactions they contain) are statistically independent. It then follows from the basic property of cumulants (vanishing if their arguments are independent) that

$${}^{X,0}\langle \Gamma^f \rangle_{c\{v\}}^{X',T} = 0, \quad \text{if } \Gamma \text{ is not connected.} \tag{6.16}$$

Hence, Eq. (6.14) reduces to

$$K(X,X',T)$$
$$= {}^{X,0}\Big\langle \sum_{\Gamma}^{\text{conn}} \Gamma^f \Big\rangle_{c\{v\}}^{X',T}$$
$$= {}^{X,0}\langle \text{sum of connected } v \text{ multigraphs}\rangle_{c\{v\}}^{X',T}$$
$$= {}^{X,0}\langle \text{sum of connected time-ordered graphs}\rangle_{c\{v\}}^{X',T}, \tag{6.17}$$

where $\Sigma_{\Gamma}^{\text{conn}}$ sums over only connected Mayer graphs. Thus, the cumulant expansion gets rid of both time secularities and disconnected diagrams.

Equation (6.17) is a "linked cluster theorem." It, of course, carries over to each individual term in the decomposition (4.20), in particular to the energy $E_0 = b$, implying that the latter is proportional to the number of particles N.[13] The linked cluster theorem for E_0 was first proven in the first few orders of perturbation theory by Brueckner,[5(a)] and in general by Goldstone,[5(b)] for particles obeying quantum statistics. The present general proof for the case of Boltzmann statistics seems to be new. Quantum statistics may also be incorporated in the present treatment by using the methods of Ref. 14; this shall be discussed elsewhere.

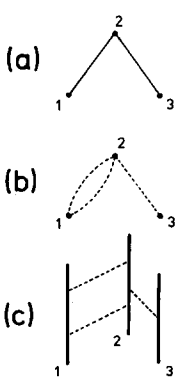

FIG. 2. The three kinds of diagrams used. The labeled fat dots and vertical lines (vertices) represent particles 1,2, and 3. In graph (a), representing $f_{12}f_{23}$, each edge (dark line) stands for a factor f_{ij}. In the multigraph (b), representing (6.10), and in the time-ordered graph (c), representing (6.12), each edge (dashed line) represents an interaction v_{ij}. In (c), time runs upwards, and the diagram is drawn three dimensionally; its projection onto the horizontal plane (defined by the three "feet") yields the multigraph (b).

VII. CONCLUSION

The cumulant expansion of $\ln \rho_{H_0+V,\beta}(X,X')$ in powers of the perturbation V was shown to provide an approximation scheme which stays usable even as the temperature goes to zero. In that limit, $\rho_{H,\beta}$ becomes expressible in terms of the ground state energy and wave function of H, whence emerge the Rayleigh–Schrödinger perturbation expansions of these quantities, in cumulant form.

It is conceptually pleasing to see a common, statistically meaningful structure, cumulants, underlie the perturbation treatments of such diverse objects as time correlation functions,[1,2] partition functions,[14] thermal density matrices, and quantum eigenstates and energies.

The cumulant forms of the RS perturbation expansions of E_0 and $\ln \psi_0(X)$ seem to be new. The way they were arrived at in the present paper is not the most direct (our principal object of interest here being ρ_H, not E_0 and ψ_0 *per se*); other, more natural derivations, also adaptable to the case of (nondegenerate) excited states, will be given in a separate paper dealing specifically with the cumulant perturbation expansions of E_0 and $\ln \psi_0(X)$ and their properties.

In dealing with the case of a many-body system, we used three types of diagrams, analogous to Mayer, Feynman, and Goldstone diagrams. Although they must be understood as ultimately expanded in "Goldstone" diagrams, the Mayer diagrams are the more compact and easier to work with; in particular, they prove to be by far the more convenient when one considers the ground state energy E_0 in the thermodynamic limit ($N,\mathcal{V}\to\infty$, keeping the density $N/\mathcal{V}$ fixed), and constructs its expansion in powers of the density, as will be discussed elsewhere.

APPENDIX A: PROOF OF EQ. (4.1)

Equation (4.1) follows from the identity

$$\frac{d^2}{dt\,dT}\exp\left(-\int_t^T ds\, v(s)\right) = -v(t)\exp\left(-\int_t^T ds\, v(s)\right)v(T) \tag{A1}$$

and the following lemma.

Lemma: For any function $F(t,T)$ of two time arguments,

$$F(t,T) = F(t,t) + \int_t^T dt_1\, F'(t_1,t_1) - \int_t^T dt_2 \int_t^{t_2} dt_1\, {}'F'(t_1,t_2), \tag{A2}$$

where

$$F'(t_1,t_2) \equiv \frac{d}{dt_2}F(t_1,t_2), \quad {}'F(t_1,t_2) \equiv \frac{d}{dt_1}F(t_1,t_2), \text{ etc.}$$

Proof: Denote by $G(t,T)$ the rhs of (A2). To prove that $F \equiv G$, it suffices to show that as functions of T (for any fixed t), F and G are equal at $T=t$ and have equal first derivatives. That $F(t,t) = G(t,t)$ is obvious; there remains to show that $F'(t,T) = G'(t,T)$, where

$$G'(t,T) = F'(T,T) - \int_t^T dt_1\, {}'F'(t_1,T). \tag{A3}$$

Considering F' and G' as functions of t (T fixed), we clearly have $F'(T,T) = G'(T,T)$ (equal initial values) and ${}'G'(t,T) = {}'F'(t,T)$ (equal first derivatives), whence $F' \equiv G'$. Q.E.D.

APPENDIX B: PROOF OF EQ. (4.8)

Under the change of variables (4.6), Eq. (4.1) becomes

$$K(X,X',T) = -\int_0^T dt\, {}^{X,0}\langle v(t)\rangle^{X',T} + \iint_{R_1+R_2} d\theta\, d\sigma\, C_{X,0}^{X',T}(\theta;\sigma), \tag{B1}$$

where the integration regions R_1 and R_2 are shown in Fig. 1, i.e.,

$$\iint_{R_1} d\theta\, d\sigma \equiv \int_0^{T/2} d\theta \int_0^{2\theta} d\sigma,$$

$$\iint_{R_2} d\theta\, d\sigma \equiv \int_{T/2}^{T} d\theta \int_0^{2(T-\theta)} d\sigma. \tag{B2}$$

We now note that

$$C_{X,0}^{X',T}(\theta;\sigma) = C_{X',-T}^{X,0}(-\theta;\sigma)^\dagger = C_{X',0}^{X,T}(T-\theta;\sigma)^\dagger, \tag{B3}$$

the first equality by (2.7) and the second one by (2.6). There follows

$$\int\int_{R_2} C_{X,0}^{X',T} = \int_{T/2}^{T} d\theta \int_0^{2(T-\theta)} d\sigma\, C_{X',0}^{X,T}(T-\theta;\sigma)^\dagger = \int_0^{T/2} d\theta' \int_0^{2\theta'} d\sigma\, C_{X',0}^{X,T}(\theta';\sigma)^\dagger = \left[\int\int_{R_1} C_{X',0}^{X,T}\right]^\dagger \tag{B4}$$

(we set $\theta' = T-\theta$). Likewise, we have

$${}^{X,0}\langle v(t)\rangle^{X',T} = [{}^{X',-T}\langle v(-t)\rangle^{X,0}]^\dagger = [{}^{X',0}\langle v(T-t)\rangle^{X,T}]^\dagger, \tag{B5}$$

again by (2.7) and (2.6). Then,

$$\int_{T/2}^{T} dt\, {}^{X,0}\langle v(t)\rangle^{X',T} = \int_{T/2}^{T} dt\, [{}^{X',0}\langle v(T-t)\rangle^{X,T}]^\dagger = \left[\int_0^{T/2} dt'\, {}^{X',0}\langle v(t')\rangle^{X,T}\right]^\dagger \tag{B6}$$

(we set $t' = T-t$). Equation (4.8) follows immediately from (B4) and (B6). Note that $K(X,X',T)^\dagger = K(X',X,T)$; but $\bar{K}(X,X',T)$ does not satisfy a like relation.

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[4] See any textbook on quantum mechanics, e.g., G. Baym, *Lectures on Quantum Mechanics* (Benjamin, Reading, MA, 1969), pp. 225–230.

[5](a) K. Brueckner, Phys. Rev. **100**, 36 (1953); (b) J. Goldstone, Proc. R. Soc. London Ser. A **239**, 267 (1957).

[6]Y. Aharonov and C. K. Au, Phys. Rev. Lett. **42**, 1582 (1979); Phys. Rev. A **20**, 2245 (1979).

[7]The time τ should be more precisely defined as $\tau \equiv \text{Max}\, \tau(\chi,\chi')$, where $\tau(\chi,\chi')$ is defined by

$$\langle\chi|e^{-iH_0}|\chi'\rangle \cong \langle\chi|\phi_0\rangle e^{-i\epsilon_0}\langle\phi_0|\chi'\rangle, \quad \text{for } t > \tau(\chi,\chi'),$$

and the maximum is taken with respect to a set of states relevant to the problem considered; thus, strictly speaking, τ depends on the states $|X\rangle$ and $|X'\rangle$, unless the particle (or particles) is (are) confined by sufficiently steep potential walls, in which case τ can be defined in an absolute manner (see Appendix E of Ref. 9 for a more detailed discussion). At any rate, the memory τ is introduced only to facilitate discussion and understanding, and is not essential for the validity of the final results.

[8]Note that inside ${}^{X,T}\langle(\cdots)\rangle^{X',T'}$, we can time translate freely to the extent that we keep away from the end times T and T', i.e., (for

$$T \leqslant t_1 \leqslant t_2 \leqslant \cdots \leqslant t_n \leqslant T'),$$

$${}^{X,T}\left\langle \prod_{i=1}^{n} V(t_i) \right\rangle^{X',T'} \cong {}^{X,T}\left\langle \prod_{i=1}^{n} V(t_i + t) \right\rangle^{X',T'},$$

provided $t_1 - T, (t_1 + t) - T, T' - t_n$, and $T' - (t_n + t)$ are all larger than τ.

[9]A Royer, "Cumulant approximations and renormalized Wigner–Kirkwood expansion for quantum Boltzmann densities," unpublished.

[10]If we set $|X\rangle = |X'\rangle = |\phi_0\rangle$, then $\Delta A = \Delta B = 0$ [see Eqs. (4.23)], whence

$$\begin{aligned}\ln\langle\phi_0|e^{-\beta H}|\phi_0\rangle e^{\beta\epsilon_0} &= \ln {}^{-\infty}\left\langle \exp\left(-\int_0^T dt\, v(t)\right)\right\rangle^{\infty} \\ &= \bar{b}T + 2\mathcal{N} + 2\Delta D. \qquad (*)\end{aligned}$$

This could also be obtained by applying directly to the cumulant expansion of the left hand side exactly the same analysis as in Sec. 3B of Ref. 2, since ${}^{-\infty}\langle(\cdots)\rangle^{\infty} = \langle\phi_0|(\cdots)|\phi_0\rangle$ is stationary. Equation (*) above, and the expressions of $\bar{b}, \mathcal{N}$, and ΔD [Eqs. (4.12), (4.18), and (4.23D)], are identical in form to Eqs. (3.27), (3.24), (3.28), and (3.29) of Ref. 2.

[11]J. E. Mayer, J. Chem. Phys. **5**, 67 (1937); J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (Wiley, New York, 1940); or K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).

[12]See, e.g., R. D. Mattuck, *A Guide to Feynman Diagrams in the Many-body Problem* (McGraw–Hill, New York, 1976).

[13]The energy E_0 is proportional to the number of particles N, because it involves [see Eq. (5.5)] the operation ${}^{-\infty}\langle(\cdots)\rangle^{\infty} = \langle\phi_0|(\cdots)|\phi_0\rangle$, which averages over a *uniform* distribution of the N particles throughout the volume $\mathcal{V}$, so that each particle interacts, on average, with only a small number of neighbors, whence a total interaction energy $\sim N$. This argument, however, does not apply to $\ln\langle X|\psi_0\rangle$ and $\ln\rho_H(X,X')$ (even though these contain only connected diagrams), because they involve the averages ${}^{X,0}\langle(\cdots)\rangle^{\infty}$ or ${}^{X,0}\langle(\cdots)\rangle^{X',T}$ where $|X\rangle$, $|X'\rangle$ are *arbitrary* (e.g., they may locate all the particles near each other, whence a total interaction energy $\sim N^2$). But if we let $|X\rangle = |X'\rangle = |\phi_0\rangle$, then the argument applies, i.e., $\ln\langle\phi_0|\psi_0\rangle$ and $\ln\langle\phi_0|e^{-\beta H}|\phi_0\rangle$ are proportional to N [as is clear from the fact that, like E_0, they are then expressible in terms of $C_\infty(\sigma)$, see Eqs. (4.12), (4.18), (4.23D) and (5.9), and Eq. (*) in Ref. 10].

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Quantum electrodynamic perturbation theory based on semiclassical representation

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A perturbation theory-based procedure for calculating mean values of quantum electrodynamic operators is proposed. Analytical solutions to similar electrodynamic problems are used as zero-order approximations for the above approach.

I. INTRODUCTION

Models relying on the interaction between a quantum system and an external field are widely used in quantum theory. In particular, this kind of external field approximation or, in other words, the semiclassical approach, proves to be extremely useful in laser physics,[1] laser spectroscopy,[2] relativistic particle radiation theory,[3] etc. Recently, great interest has been focused on optical effects that seem to require a more detailed quantum treatment. For example, it is generally assumed that strong fields satisfying the classical Maxwell equations represent the asymptotic case of the complete quantum description. However, the quantum theory calculation gives rise to insurmountable difficulties that do not allow the use of the higher-order perturbation theory.

The present paper reports a new perturbation theory based procedure for calculating mean values of Heisenberg operators in quantum electrodynamics. There exist a few analytical solutions to the problems of the quantum-system behavior in an external field. These solutions provide the basis for the zero-order approximation of the proposed perturbation theory. The required mean Heisenberg operators are obtained as a power series of the coupling constant.

For illustration purposes the operator properties defined in terms of the semiclassical representation[4] are briefly discussed in Sec. II. Further, the basic formula for calculating mean values of operators is derived. Finally, in Sec. IV the above calculation is illustrated by estimating the mean energy of the two-level atom interacting with the quantum field. It is shown that fairly good agreement with the complete quantum theory is achieved as low as the first-order perturbation theory.

II. SEMICLASSICAL REPRESENTATION METHOD

The semiclassical representation method has already been studied in sufficient detail.[4,5] Here we discuss only the algebraic aspects of the above approach.

Consider the creation $\hat{a}^+$ and annihilation $\hat{a}^-$ operators, which obey the following Bose commutation relation:

$$[\hat{a}^-,\hat{a}^+] = 1. \tag{1}$$

The operators $\hat{a}^\pm$ are defined in a Hilbert space H. Let the operator $\hat{a}^-$ be represented as the sum of the two operators a_0 and Δa as follows:

$$\hat{a}^- = a_0 + \Delta a. \tag{2}$$

However, this definition gives rise to numerous ambiguities which can be removed provided certain restrictions are imposed on the summands in Eq. (2), viz.,

$$[a_0,a_0^+] = [\Delta a,a_0] = 0; \quad [\Delta a,a_0^+] = [\Delta a^+,\Delta a] = 1. \tag{3}$$

Consider the interrelation between the operators $a_0^\pm$, $\Delta a^\pm$ and the operators $\hat{a}^\pm$. One can readily see the relationship between them in the case where $a_0^\pm$ and $\Delta a^\pm$ are defined in the Hilbert space $W = H \otimes H$, where $\otimes$ is the sign of the direct product.

It has been shown[4] that Eqs. (3) are fulfilled provided the operators $a_0^\pm$, $\Delta a^\pm$ satisfy the relations

$$\hat{a}_W^\pm = \hat{a}^\pm \otimes I, \quad \hat{a}_0^\pm = \hat{a}^\pm \otimes I + I \otimes \hat{a}^\mp,$$
$$\Delta a^\pm = -I \otimes \hat{a}^\mp, \tag{4}$$

where $I = 1$.

The density matrix R defined in the Hilbert space W is the direct product of the initial density matrix ρ and a vacuum state projector[6]

$$R = \rho \otimes |0\rangle\langle 0|. \tag{5}$$

There are two interesting features of the operator function $F(a_0^\pm,\Delta a^\pm)$. These are manifested in the fact that Eqs. (6) and (7) below are obtained using Eqs. (4) and (5) and a vacuum state vector property

$$\mathrm{Tr}\, RF(a_0^\pm) = \mathrm{Tr}\, \rho F^A(\hat{a}^\pm), \tag{6}$$

where $F^A(\hat{a}^\pm)$ is an antinormally ordered operator,

$$\mathrm{Tr}\, R\Delta aF(a_0^\pm,\Delta a^\pm) = \mathrm{Tr}\, RF(a_0^\pm,\Delta a^\pm)\Delta a^+ = 0. \tag{7}$$

These features permit the calculation procedure of the proposed perturbation theory to be simplified significantly.

III. PERTURBATION THEORY

Convergence of the perturbation theory series is known to depend on the proper choice of a zero-order approximation. It is proposed to choose analytical solutions to semiclassical electrodynamic problems as a zero-order approximation for solving similar quantum electrodynamic problems.

Using the semiclassical representation method, the Schrödinger evolution operator equation,

$$i\hbar \frac{\partial U}{\partial t} = H_{\mathrm{int}}(\hat{a}^\pm,x,t)\, U, \tag{8}$$

can be reduced to the coupled equations of the form

$$i\hbar \frac{\partial C}{\partial t} = H_{\mathrm{int}}(a_0^\pm,x,t)C, \tag{9}$$

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$$i\hbar\frac{\partial Q}{\partial t}=H_Q(a_0^{\pm},\Delta a^{\pm},x,t)Q. \tag{10}$$

Here the evolution operator $U=CQ$, $H_{\rm int}(\hat{a}^{\pm},x,t)$ is the interaction Hamiltonian in the interaction picture; x are quantum subsystem variables (e.g., atoms, particles, molecules, etc.).

Due to the commutativity of $a_0^{\pm}$, Eq. (9) is assumed to describe the quantum subsystem dynamics in the external field with amplitudes a_0^{*}. Therefore, its solution will be employed as a zero-order approximation or, in other words, as the basic formula for finding mean values of quantum electrodynamic quantities using the perturbation theory under consideration.

To calculate any operator in the Heisenberg picture, an integral equation may be used

$$F_H(t)=U^{+}FU$$
$$=C^{+}(t)FC(t)+\frac{1}{i\hbar}\int_0^t d\tau\, Q^{+}(\tau)$$
$$\times[C^{+}(t)FC(t),H_Q(\tau)]Q(\tau). \tag{11}$$

Without loss of generality, let us consider, e.g., the interaction Hamiltonian linear in the field amplitude. To simplify the calculation, the operator $F_H(t)$ in Eq. (11) can be ordered as follows:

$$F_H(t)=F^{0}(a_0^{\pm},x,t)+\Delta aF^{10}(a_0^{\pm},\Delta a^{\pm},x,t)$$
$$+F^{01}(a_0^{\pm},\Delta a^{\pm},x,t)\Delta a^{+}. \tag{12}$$

Using Eqs. (6), (7), and (12) yields the mean value of F_H to the second order in the coupling constant

$$\begin{aligned}\mathrm{Tr}\,R\,F_H(t)\simeq&\mathrm{Tr}\,R\left(F_0(a_0^{\pm},x,t)+\frac{1}{i\hbar}\int_0^t d\tau\,[F_0,H_Q(\tau)]+\frac{1}{(i\hbar)^2}\int_0^t d\tau\int_0^{\tau}d\tau'[[F_0,H_Q(\tau)],H_Q(\tau')]\right)\\
=&\mathrm{Tr}\,R\left\{F_0+\frac{1}{i\hbar}\int_0^t d\tau\,\overline{F(\tau,t)}+\frac{1}{(i\hbar)^2}\int_0^t d\tau\int_0^{\tau}d\tau'\Big[[\overline{F(\tau,t)},H_Q^{0}(\tau')]+[F_0,H_Q^{01}(\tau)]\,H_Q^{10}(\tau')\right.\\
&-H_Q^{01}(\tau')[F_0,H_Q^{10}(\tau)]+\frac{\partial}{\partial a_0}H_Q^{0}(\tau')[F_0,H_Q^{10}(\tau)]-[F_0,H_Q^{01}(\tau)]\frac{\partial}{\partial a_0}H_Q^{0}(\tau')+H_Q^{01}(\tau')\frac{\partial}{\partial a_0}\overline{F(\tau,t)}\\
&\left.-\frac{\partial}{\partial a_0^{+}}\overline{F(\tau,t)}\cdot H_Q^{10}(\tau')+\frac{\partial}{\partial a_0^{+}}[F_0,H_Q^{01}(\tau)]\frac{\partial}{\partial a_0}H_Q^{10}(\tau')-\frac{\partial}{\partial a_0^{+}}H_Q^{01}(\tau')\frac{\partial}{\partial a_0}[F_0,H_Q^{10}(\tau)]\Big]\right\}.\end{aligned} \tag{13}$$

Here $\overline{F(\tau,t)}$ is defined as

$$\overline{F(\tau,t)}=[F^{0}(t),H_Q^{0}(\tau)]+H_Q^{01}(\tau)\frac{\partial F^{0}(t)}{\partial a_0}-\frac{\partial F^{0}(t)}{\partial a_0^{+}}H_Q^{10}(\tau). \tag{14}$$

IV. EXAMPLE

To illustrate this method we estimate the mean energy of a two-level atom interacting with a quantized plane wave. This problem has been chosen for two reasons. First, it allows for analytical solutions to the evolution operator both for the case where the atom is subject to an external field[7] and that of its interaction with a quantized wave.[2] Second, it does not require any cumbersome analytical computations.

The dynamics of a two-level atom interaction with a plane monochromatic wave is determined by the relation

$$i\hbar\frac{\partial C}{\partial t}=\lambda\omega_0\hbar(a_0\sigma_{+}e^{i\epsilon t}+\text{c.c.}), \tag{15}$$

whose solution has the following form

$$\begin{aligned}C=&-\frac{i\omega_0\lambda}{\Omega}a_0\sin\Omega t\exp\left(\frac{i\epsilon t}{2}\right)\sigma_{+}\\
&-\frac{i\omega_0\lambda}{\Omega}a_0^{+}\sin\Omega t\exp\left(\frac{-i\epsilon t}{2}\right)\sigma_{-}+2i\left(\cos\Omega t\sin\frac{\epsilon t}{2}\right.\\
&\left.-\beta\sin\Omega t\cos\frac{\epsilon t}{2}\right)\sigma_z+\cos\Omega t\cos\frac{\epsilon t}{2}+\beta\sin\Omega t\sin\frac{\epsilon t}{2}.\end{aligned} \tag{16}$$

Here $\sigma_{\pm}$, σ_z are Pauli spin matrices for the atom of interest, $\beta=\epsilon/2\Omega$, $\epsilon=\omega_0-\omega$; $\Omega=\sqrt{\lambda^2\omega_0^2a_0^{*}a_0+\epsilon^2/4}$ is the Rabi frequency, λ is the coupling constant, and ω, ω_0 are the incident field and atomic frequencies, respectively. The operators $H_{\rm int}$ and H_Q in Eqs. (9) and (10) are defined as

$$H_{\rm int}(a_0^{\pm},\sigma_{\pm},t)=\lambda\hbar\omega_0(a_0\sigma_{+}e^{i\epsilon t}+\text{c.c.}), \tag{17}$$

$$H_Q(a_0^{\pm},\Delta a^{\pm},t)=\lambda\hbar\omega_0C^{+}(t)(\Delta a\sigma_{+}e^{i\epsilon t}+\text{c.c.})C(t).$$

Ordering H_Q as in Eq. (12) yields for its terms

$$H_Q^{0}(t)=-i\lambda^2\omega_0^2\hbar$$
$$\times\left[\int_0^t d\tau\,C^{+}(\tau)\sigma_{-}C(\tau)C^{+}(t)\sigma_{+}C(t)e^{i\epsilon(t-\tau)}-\text{c.c.}\right], \tag{18}$$

$$H_Q^{10}=(H_Q^{01})^{+}=\lambda\hbar\omega_0C^{+}(t)\sigma_{+}C(t).$$

The two-level mean energy is calculated under the assumptions that the initial atomic density matrix ρ has only diagonal nonzero elements and that the initial state of the field can be described by the n-photon wave function.

Thus using Eqs. (13) and (18), one obtains

$$\begin{aligned}\hbar\omega_0\,\mathrm{Tr}\,R\sigma_z=&\hbar\omega_0(\mathrm{Tr}\,\rho\sigma_z(1-(1-\beta^2)(1-\cos2\Omega t))\\
&-(\lambda^2\omega_0^2/2\Omega^2)(\beta^2(1-\cos2\Omega t)\\
&+(1-\beta^2)t\Omega\sin2\Omega t)(\mathrm{Tr}\,\rho\sigma_z+\tfrac{1}{2})).\end{aligned} \tag{19}$$

To eliminate the secular term which appears in Eq. (19), one can make use of the Lindschtedt procedure.[8] Thus the field amplitude a_0 can be renormalized as

$$\tilde{a}_0=a_0(1+\lambda^2A_2+\lambda^4A_4+\cdots). \tag{20}$$

Then, retaining the terms proportional to the square of the coupling constant λ^2, one can rewrite Eq. (17) and recalcu-

late the mean energy. In doing so, there appears another secular term

$$(2\lambda^2\omega_0^2 a_0^+ a_0/\Omega^2)\,[\tilde{\beta}(1-\cos 2\tilde{\Omega}t)+(1-\tilde{\beta}^2)t\tilde{\Omega}\sin 2\tilde{\Omega}t\,]A_2. \tag{21}$$

Let the constant A_2 satisfy the following relation:

$$A_2 = (\mathrm{Tr}\,\rho\sigma_z + \tfrac{1}{2})/4a_0^+ a_0\,\mathrm{Tr}\,\rho\sigma_z. \tag{22}$$

Then the factor immediately preceding the secular term vanishes. Hence, the expectation value of the mean energy is determined up to the square of the coupling constant λ^2 given by the relation

$$\hbar\omega_0\,\mathrm{Tr}\,R\sigma_z = \hbar\omega_0(1-(1-\tilde{\beta}^2)(1-\cos 2\tilde{\Omega}t))\,\mathrm{Tr}\,\rho\sigma_z, \tag{23}$$

where $\tilde{\beta}=\epsilon/2\tilde{\Omega}$, $\tilde{\Omega}=\sqrt{\lambda^2\omega_0^2(n+2a_0^+a_0A_2)+\epsilon^2/4}$ is the renormalized Rabi frequency. It should be noted that our result agrees fairly well with the one obtained by using the quantum field approach.[9]

V. CONCLUDING REMARKS

It has been shown that mean values of operators in quantum electrodynamics can be derived from the relevant data obtained in the semiclassical formalism. The above procedure is found to be conveniently performed in terms of the semiclassical representation. In this case the equation for the evolution operator may be separated into two coupled equations. One of the resultant relations describes the dynamics of a quantum system in an external field, while its analytical solution serves as a zero-order approximation for solving the other relation, where quantum properties of the electromagnetic field are taken into account. The reported perturbation theory suggests the feasibility of the calculation procedure under consideration for a wide spectrum of problems pertaining, e.g., to the intermolecular interaction and to the quantum theory of angular momentum.[5]

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C^*-algebraic scattering theory and explicitly solvable quantum field theories

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A general theoretical framework is developed for the treatment of a class of quantum field theories that are explicitly exactly solvable, but require the use of C^*-algebraic techniques because time-dependent scattering theory cannot be constructed in any one natural representation of the observable algebra. The purpose is to exhibit mechanisms by which inequivalent representations of the observable algebra can arise in quantum field theory, in a setting free of other complications commonly associated with the specification of dynamics. One of two major results is the development of necessary and sufficient conditions for the concurrent unitary implementation of two automorphism groups in a class of quasifree representations of the algebra of the canonical commutation relations (CCR). The automorphism groups considered are induced by one-parameter groups of symplectic transformations on the classical phase space over which the Weyl algebra of the CCR is built; each symplectic group is conjugate by a fixed symplectic transformation to a one-parameter unitary group. The second result, an analog to the Birman–Belopol'skii theorem in two-Hilbert-space scattering theory, gives sufficient conditions for the existence of Møller wave morphisms in theories with time-development automorphism groups of the above type. In a paper which follows, this framework is used to analyze a particular model system for which wave operators fail to exist in any natural representation of the observable algebra, but for which wave morphisms and an associated S matrix are easily constructed.

I. INTRODUCTION

This study treats simple model quantum field theories that illustrate mechanisms by which nonstandard representations of the algebra of observables arise in the solution of a field theory. The discussion deals with field-theoretic analogs to systems with finite numbers of degrees of freedom that are solvable by transformation to normal modes.

The point of view is different from that in other treatments of representation theory for quantum field theory, because the discussion is not concerned with the problem of how to specify a dynamical law. Rather, from the start, the dynamics is given by well-defined automorphism groups on a C^* algebra for a quantum field, and the analysis concerns the scattering of the associated particles. With this framework it is possible to study representation-theoretic questions involved in the formulation of scattering theory, in the absence of other problems commonly encountered in the specification of dynamics for general quantum field theories.

Even in this simple setting, a C^*-algebraic viewpoint is essential for time-dependent scattering theory, because usual (second-quantized) wave operators generally fail to exist in any natural representation of the observable algebra, while unitary S matrices with conventional physical interpretation can be constructed via a representation-independent framework. This class of model theories is thus of pedagogical value, and illustrates some aspects of the C^*-algebraic approach to quantum field theory.

The theories describe nonrelativistic systems involving the linear interaction of a quantum field with other systems, such as classical external potentials, other quantum mechanical systems, or other quantum fields. These theories are algebraically exactly solvable by a technique analogous to transformation to normal modes; their salient feature is that the "diagonalization" morphism need not be implementable in a given representation of the CCR algebra.

In each model, both the interacting and free time developments are given by prescribed one-parameter automorphism groups on the Weyl algebra of the CCR, so the proper dynamical law for the system is unambiguous. For each of the two automorphism groups, there is an explicit invariant state on the algebra determining a representation in which the automorphism group is implemented by a strongly continuous unitary group with positive generator.

Given this situation, several questions immediately arise. Are the two representations determined by the invariant states unitarily equivalent? If not, can the two automorphism groups be concurrently unitarily implemented in either representation? In any representation? Do Møller wave operators exist in a given representation? Can representation-independent Møller wave morphisms exist and define a scattering morphism? If a scattering morphism exists, in what representations is it implementable? What is the relationship among the states invariant under the two automorphism groups and the state(s) invariant under the scattering morphism?

To answer these and other questions for this class of models, we develop a general theoretical framework which is independent of any specific model. The framework is comprised of two sets of results which address two main issues. The first issue concerns the conventional approach to scattering theory, the construction of wave operators on the carrier space of a fixed representation. The results deal with automorphism groups of the CCR algebra which are induced by symplectic groups on the underlying classical phase space, and their unitary implementability in quasi-free representations. In particular, we develop necessary and sufficient conditions for a representation symplectically related to the Fock representation to admit concurrent unitary implementation of both free and interacting automorphism groups.

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The second issue concerns the alternative algebraic approach to scattering theory, the construction of wave morphisms on the CCR algebra. The results deal with morphisms which are induced by partial symplectic transformations (the real-linear analogs of complex-linear partial isometries) on the classical phase space. In particular, we establish conditions sufficient to ensure the existence of wave morphisms, and we introduce the notion of the partial-isometric implementation of a partial symplectic transformation, and determine necessary and sufficient conditions for such implementability. This algebraic framework allows the extension of the wave operator formalism to situations not previously treated.[1-9]

In a paper which follows,[10] henceforth referred to as [II], we illustrate the general results with a specific one-parameter family of model systems consisting of a quantum-mechanical oscillator interacting linearly with a massless scalar field, roughly modeling an atom interacting with light. It is found that for a range of physically reasonable couplings, the bare vacuum and interaction vacuum are inequivalent. This turns out to have the consequence that although the free and interacting time developments can be concurrently unitarily implemented in either representation determined by the two vacua, wave operators do not exist in these representations. Nevertheless, wave morphisms on the CCR algebra do exist and define a scattering morphism which is implementable in one of the representations.

More specifically, the topics discussed here are as follows. Section II establishes terminology.

In Sec. III, the class of models under study is characterized precisely. The idea that there exists a transformation to normal modes is embodied by the assumed form of the interacting dynamical automorphism group. This group is induced by a one-parameter symplectic group on the classical phase space over which the Weyl algebra is constructed. The symplectic group is conjugate by a fixed symplectic transformation (which induces the "diagonalization" morphism) to a one-parameter unitary group (which induces the "free" time development of the "normal modes"). Also in Sec. III, there is an outline of time-dependent scattering theory for this class of models.

In Sec. IV, the main mathematical results are summarized in Theorems 1 and 2. Theorem 1 gives necessary and sufficient conditions for a representation symplectically related to the Fock representation to admit continuous unitary implementation of an automorphism group of the above type. This theorem is a summary of the results established by Theorem 4 (Sec. VI) and Theorem 5 (Sec. VII). Theorem 2 establishes sufficient conditions for the existence and completeness of the Møller wave morphisms associated with the dynamical automorphism groups. It is analogous to the Birman–Belopol'skii theorem in two-Hilbert-space scattering theory[11]; in Theorem 2, however, the "identification map" is a (real-linear) symplectic transformation.

Section V relies on the work of Shale[12] to obtain the necessary and sufficient condition for the implementability of a single partial-symplectic morphism in a representation symplectically related to the Fock representation. The central result is presented in Theorem 3.

Section VI presents the core of the results in Theorem 1, Theorem 4, which can be roughly paraphrased in the following way. Let S be a self-real-adjoint invertible symplectic transformation, and let V_t be a one-parameter unitary group with positive self-adjoint generator H. Then $[S,V_t]$ is a Hilbert–Schmidt operator for all real t if and only if there exists an $m>0$ such that both $P_m(S-I)$ and $[S,i(I-P_m)H]$ are Hilbert–Schmidt operators, where P_m is the spectral projection for H onto spectral values larger than m. The importance of this theorem is that it translates information couched in terms of "all time" into specific readily verifiable conditions. Section VI also includes the application of Theorem 4 to the determination of the necessary and sufficient conditions for the unitary implementability of an automorphism group of the aforementioned type in a representation symplectically related to the Fock representation.

There is also a discussion in Sec. VI of the important special case when the generator H of the unitary group V_t has a spectrum bounded away from zero. This situation has the physical interpretation that there are no massless excitations in the theory, and it is shown that in this case the interacting dynamical automorphism group can be implemented unitarily only in the representations interchangeable with the representation induced by its invariant state. These facts lead later to the observation that the nontrivial behavior in the models studied here is an infrared-like phenomenon, predicated on the existence of massless particles in the theories.

Section VII presents Theorem 5, which asserts that whenever a symplectic automorphism group of the type specified has a unitary implementation in a representation symplectically related to the Fock representation, then the family of implementing unitary operators can be chosen to be a continuous unitary group. Thus there always exists a second-quantized Hamiltonian in the representations admitting unitary implementation of the time development.

Section VIII discusses the conditions a representation symplectically related to the Fock representation must satisfy if it is to admit concurrent unitary implementation of two automorphism groups, the free (uncoupled) time development, and the interacting time development.

Section IX compares the representation-dependent and the algebraic constructions of a scattering operator. It is indicated that even for the linear models treated here, the latter is essential.

Finally, Sec. X presents the proof of Theorem 2.

II. SYMPLECTIC MORPHISMS OF THE WEYL ALGEBRA AND THEIR IMPLEMENTATION

Before specifying the class of models under study more precisely, it is convenient to fix some terminology concerning the Weyl algebra of the CCR and its morphisms.

The representations of the CCR which occur naturally in the study of the systems in question are of the type known as quasifree representations.[13,14] The manifestation of the interesting features of the systems does not however depend on the use of completely general quasifree representations, and for simplicity the considerations here are restricted to the following framework.

Let $\mathscr{H}$ be a separable complex Hilbert space, also re-

garded as a real symplectic space with (nondegenerate) symplectic form equal to the imaginary part of the inner product. Let $\mathcal{F}(\mathcal{H})$ be the boson Fock space over the complex space $\mathcal{H}$, that is, $\mathcal{F}(\mathcal{H}) = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots$, where $\mathcal{H}_0 = \{c\Omega \mid c \in \mathbb{C}\}$ is one dimensional, $\mathcal{H}_1$ is isomorphic to $\mathcal{H}$, and $\mathcal{H}_n$ is the n-fold symmetrized tensor product of $\mathcal{H}_1$ with itself.

The Fock space $\mathcal{F}(\mathcal{H})$ carries the standard irreducible representation (by unitary operators) of the Weyl group $W:\mathcal{H} \to \mathcal{B}(\mathcal{F}(\mathcal{H}))$ over $\mathcal{H}$ in which

$$W(f)W(g) = \exp(-iB(f,g)/2)W(f+g),$$

where B is the symplectic form, and in which $\{W(f)\Omega \mid f \in \mathcal{H}\}$ is total in $\mathcal{F}(\mathcal{H})$. The abstract Weyl C^* algebra $\mathcal{W}$ generated by the Weyl group[15,16] is the algebra of the CCR under study. Throughout the following, the abstract Weyl algebra is identified with its standard faithful representation on Fock space.

Linear transformations on $\mathcal{H}$ which preserve the symplectic form B are of interest because they leave invariant the Weyl group structure. The following definition is well suited to the analysis here.

A *symplectic transformation* $S:\mathcal{H} \to \mathcal{H}$ is a bounded real-linear transformation such that $B(Sf,Sg) = B(f,g)$ for all $f,g \in \mathcal{H}$, and such that $S\mathcal{H}$ is a complex subspace of $\mathcal{H}$. Note that it is not assumed that S maps $\mathcal{H}$ *onto* $\mathcal{H}$; the models to be treated require that the range of S is not all of $\mathcal{H}$. In the models studied here, though, it is natural for the symplectic transformations which occur to have ranges which are complex subspaces of $\mathcal{H}$. Since much of the subsequent analysis simplifies in that case, the condition is incorporated into the definition from the start.

Denote by Λ the operation of multiplication by the complex number i on the Hilbert space $\mathcal{H}$. (Real-linear transformations do not, in general, commute with Λ.) For $Q:\mathcal{H} \to \mathcal{H}$ an arbitrary bounded real-linear transformation, the bounded real-linear transformation $Q^+:\mathcal{H} \to \mathcal{H}$ defined by $Q^+ \equiv \Lambda^* Q^* \Lambda$, with Q^* the real adjoint of Q, satisfies $B(Q^+ f,g) = B(f,Qg)$, for all $f,g \in \mathcal{H}$. From the fact that B is nondegenerate on $\mathcal{H}$, it follows that a bounded real-linear transformation S preserves B if and only if $S^+S = I$. It is furthermore easy to show that if $S\mathcal{H}$ is a complex subspace then SS^+ and $(I - SS^+)$ are complex-linear self-adjoint orthogonal projections, with $S\mathcal{H} = SS^+\mathcal{H}$.

Some of the following discussion requires consideration of transformations which are symplectic between proper subspaces of $\mathcal{H}$. Let $S:\mathcal{H} \to \mathcal{H}$ be a bounded real-linear transformation whose kernel and range are complex subspaces of $\mathcal{H}$. Then S will be said to be a *partial symplectic transformation* if $B(Sf,Sg) = B(f,g)$ for all f and g in the orthogonal complement $(\ker S)'$ of the kernel of S. If S is a partial symplectic transformation, it follows (see Appendix B) that S^+S and SS^+ are complex-linear self-adjoint projections onto the closed complex subspaces $(\ker S)'$ and $(\operatorname{ran} S)$, respectively.

A partial symplectic transformation S induces a morphism σ on the Weyl algebra by the action $\sigma(W(f)) \equiv W(Sf)$. Such a morphism σ (or, loosely speaking, the transformation S) is said to be *implementable by partial isometry* in a representation π of the Weyl algebra if there exists a partial isometry U on the carrier space of π such that $U\pi(W(f)) = \pi(\sigma(W(f)))U \equiv \pi(W(Sf))U$, for all $f \in \mathcal{H}$. If the transformation S is invertible (maps $\mathcal{H}$ onto $\mathcal{H}$), then $S^+ = S^{-1}$, and σ is an automorphism. Such an automorphism σ is said to be *unitarily implementable* in a representation π of the Weyl algebra if there exists a unitary operator on the carrrier space of π such that $U\pi(W(f))U^{-1} = \pi(\sigma(W(f))) \equiv \pi(W(Sf))$, for all $f \in \mathcal{H}$.

The representation π_R of $\mathcal{W}$ induced via the Gel'fand–Naimark–Segal construction by the state E_R on $\mathcal{W}$ given by

$$E_R(W(f)) \equiv E_I(W(Rf)),$$

where R is a symplectic transformation and $E_I(A) \equiv \langle \Omega \mid A\Omega \rangle$ is the Fock vacuum state, is said to be *symplectically related to* the Fock representation. Without loss of generality the Hilbert space carrying the representation π_R may be identified with the Fock space $\mathcal{F}(\mathcal{H})$. Then with the convention that the representation symbols are dropped for the Fock representation, $\pi_R(W(f)) = W(Rf)$. It is useful to classify representations according to their capacities for implementation of symplectic transformations. Let π_1 and π_2 be two representations of the Weyl algebra, and let σ_S be the automorphism of $\mathcal{W}$ induced by the invertible symplectic transformation $S:\mathcal{H} \to \mathcal{H}$. The representations π_1 and π_2 will be said to be *interchangeable* if for each invertible symplectic transformation S, σ_S is unitarily implementable in π_1 if and only if σ_S is unitarily implementable in π_2. Thus two representations are interchangeable if they both admit unitary implementation of exactly the same set of symplectic automorphisms.

It is convenient to introduce one further piece of terminology which is a natural generalization of the notion of unitary equivalence. Two representations π_1 and π_2 of $\mathcal{W}$ are said to be *isometrically equivalent* if there exists an isometric operator U from the carrier space of π_1 to the carrier space of π_2 such that $U\pi_1(A) = \pi_2(A)U$, for all $A \in \mathcal{W}$.

III. THE CLASS OF MODELS UNDER STUDY

The algebra $\mathcal{W}$ of the CCR is regarded as the algebra of observables for a system having the real symplectic space $\mathcal{H}$ as classical phase space. In the case of a scalar quantum field interacting with a quantum mechanical oscillator, for example, $\mathcal{H}$ is the direct sum of the "one-particle" Hilbert space (classical solutions of the wave equation), with the harmonic oscillator phase $\mathbb{C}$; the Weyl algebra has the corresponding product structure.

Scattering theory for the system is formulated in terms of two different one-parameter automorphism groups on $\mathcal{W}$, the uncoupled (free) time development β_t° and the interacting time development β_t.

The uncoupled dynamical automorphism $\beta_t^\circ:\mathcal{W} \to \mathcal{W}$ is induced by the free unitary time development on the phase space $\mathcal{H}$: $\beta_t^\circ(W(f)) \equiv W(V_t^\circ f)$, with V_t° a strongly continuous unitary group on $\mathcal{H}$. β_t° is implemented in the Fock representation of $\mathcal{W}$ by a strongly continuous group of unitary operators U_t° on $\mathcal{F}(\mathcal{H})$: $U_t^\circ W(f) U_t^{\circ *} = \beta_t^\circ(W(f))$.

The interacting dynamical automorphism $\beta_t:\mathcal{W} \to \mathcal{W}$ is, for the models under study, induced by the one-parameter group of invertible symplectic transformations T^+V_tT on

$\mathscr{H}$: $\beta_t(W(f)) \equiv W(T^+V_tTf)$, where $T:\mathscr{H}\to\mathscr{H}$ is a symplectic transformation and V_t is a continuous one-parameter unitary group on $T\mathscr{H}$. (In particular, V_t commutes for all t with the projection TT^+ onto $T\mathscr{H}$, insuring that T^+V_tT is an invertible symplectic transformation; see Appendix B. Without loss of generality V_t can be defined to be I on the orthogonal complement to the range of T.) This situation embodies the idea that there exist "normal-mode" variables $W'(f) \equiv W(T^+f)$ for f in $T\mathscr{H}$ which develop freely according to V_t, namely

$$\beta_t(W'(f)) = \beta_t(W(T^+f)) = W(T^+V_tTT^+f) = W'(V_tf).$$

The symplectic transformation T on $\mathscr{H}$ gives the "diagonalization" morphism on $\mathscr{W}$, and V_t specifies the time development of the normal modes. Note that V_t is, in general, different from V_t°, just as the normal mode frequencies of coupled oscillators are, in general, different from their uncoupled natural frequencies. It is assumed, though, that both generators H and H° of the strongly continuous unitary groups V_t and V_t° have nonnegative spectra. Note also that the complex structure on $\mathscr{H}$ plays a role in the specification of the "normal-mode variables"; the condition that V_t be unitary expresses the idea that the normal modes develop freely in time.

Now, β may very well not be unitarily implementable in the Fock representation, but there is always a representation symplectically related to the Fock representation in which β has a unitary implementation. This interaction-vacuum representation is simply the representation π_T. Since $\pi_T(\beta_t(W(f))) = \pi_T(W(T^+V_tTf)) = W(TT^+V_tTf)$ $= W(V_tTT^+Tf) = W(V_tTf)$, and since every unitary group V_t on $\mathscr{H}$ has a unitary implementation $U_tW(g)U_t^* = W(V_tg)$ in the Fock representation of $\mathscr{W}$, it follows that $\pi_T(\beta_t(W(f))) = U_tW(Tf)U_t^* = U_t\pi_T(W(f))U_t^*$. Thus β is unitarily implemented in π_T.

For a conventional quantum-mechanical system with free and interacting time developments given by unitary groups U_t° and U_t acting on a Hilbert space of state vectors, time-dependent scattering theory is formulated in terms of Møller wave operators $W_\pm \equiv \text{s-lim}_{t\to\pm\infty} U_{-t}U_t^\circ E_{\text{ac}}^\circ$, where E_{ac}° is the projection onto the absolutely continuous subspace of the generator of the group U_t°. For the systems described in the algebraic fashion here, it is not generally true that the time developments β_t° and β_t have a concurrent implementation in a given representation of $\mathscr{W}$, and it is natural to consider the algebraic analog of wave operators, Møller morphisms.

To motivate the signs in the following definition, suppose temporarily that the automorphisms β_t° and β_t each have a unitary implementation, by $\Gamma(\beta_t^\circ)$ and $\Gamma(\beta_t)$, respectively, in the Fock representation of $\mathscr{W}$. That is,

$$\Gamma(\beta_t^\circ)W(f)\Gamma(\beta_t^\circ)^* = \beta_t^\circ(W(f)) = W(V_t^\circ f),$$

with a similar formula for $\Gamma(\beta_t)$. The time developments β_t° and β_t are then represented on Fock space vectors by the unitary operators

$$U_t^\circ \equiv \Gamma(\beta_t^\circ)^* = \Gamma(\beta^\circ{}_{-t})$$

and

$$U_t \equiv \Gamma(\beta_t)^* = \Gamma(\beta_{-t}),$$

respectively. So the Møller wave operators on Fock space are partial isometries $W_\pm$ given by the limits

$$W_\pm\psi \equiv \lim_{t\to\pm\infty} U_{-t}U_t^\circ\psi = \lim_{t\to\pm\infty} \Gamma(\beta_t)\Gamma(\beta^\circ{}_{-t})\psi,$$

which we assume for purposes of illustration to exist for ψ in the subspace $E_{\text{ac}}^\circ\mathscr{F}(\mathscr{H})$. Thus for ψ_1 and ψ_2 in $E_{\text{ac}}^\circ\mathscr{F}(\mathscr{H})$, we have

$$\begin{aligned}\langle W_\pm\psi_1|W(f)W_\pm\psi_2\rangle &= \lim_{t\to\pm\infty}\langle\Gamma(\beta_t)\Gamma(\beta^\circ{}_{-t})\psi_1|W(f)\Gamma(\beta_t)\Gamma(\beta^\circ{}_{-t})\psi_2\rangle\\ &= \lim_{t\to\pm\infty}\langle\psi_1|\beta_t^\circ(\beta_{-t}(W(f)))\psi_2\rangle\\ &= \lim_{t\to\pm\infty}\langle\psi_1|W(V_t^\circ T^+V_{-t}Tf)\psi_2\rangle.\end{aligned}$$

These expressions suggest the definition

$$\Omega_\pm \equiv \text{s-lim}_{t\to\pm\infty} T^+V_tTV^\circ{}_{-t}P_{\text{ac}}^\circ,$$

where P_{ac}° is the projection onto the absolutely continuous subspace of the generator H° of the strongly continuous unitary group V_t°. If the indicated strong limits $\Omega_\pm$ exist and are partial symplectic transformations on $\mathscr{H}$, and if the morphisms $\tau_\pm$ induced by $(\Omega_\pm)^+$ are implemented by partial isometries $\Gamma(\tau_\pm)$ on $\mathscr{F}(\mathscr{H})$, then the partial isometries $\Gamma(\tau_\pm)^*$ are precisely the Møller wave operators, because then for ψ_1 and ψ_2 in $\Gamma(\tau_\pm)\mathscr{F}(\mathscr{H})$, we have

$$\begin{aligned}&\langle\Gamma(\tau_\pm)^*\psi_1|W(f)\Gamma(\tau_\pm)^*\psi_2\rangle\\ &\quad= \langle\psi_1|\tau_\pm(W(f))\Gamma(\tau_\pm)\Gamma(\tau_\pm)^*\psi_2\rangle\\ &\quad= \langle\psi_1|W((\Omega_\pm)^+f)\psi_2\rangle\\ &\quad= \lim_{t\to\pm\infty}\langle\psi_1|W(P_{\text{ac}}^\circ V_t^\circ T^+V_{-t}Tf)\psi_2\rangle.\end{aligned}$$

Henceforth we write $V_t \equiv e^{tAH}$ and $V_t^\circ \equiv e^{tAH^\circ}$, where H and H° are non-negative self-adjoint operators defined on domains dense in $\mathscr{H}$.

We are thus led to study the strong limits

$$\Omega_\pm \equiv \text{s-lim}_{t\to\pm\infty} T^+e^{tAH}Te^{-tAH^\circ}P_{\text{ac}}^\circ,$$

whose putative implementation in a representation of $\mathscr{H}$ are the usual Møller wave operators. Note that the convergence as $t\to\pm\infty$ of the automorphisms $\beta_t\,\beta^\circ{}_{-t}$ (on the Weyl algebra over $P_{\text{ac}}^\circ\mathscr{H}$) which is implied by the above strong limit on $\mathscr{H}$ is rather weak. We will see in [II] that requiring convergence of such limits in the C^* norm, for example, is too restrictive for even simple physical model theories.

Given this framework, two sets of questions arise. First, an alternative way to formulate time-dependent scattering theory would be to seek a representation of $\mathscr{H}$ in which the two automorphism groups β and β° were each implemented by unitary groups, and then to construct wave operators directly on the Hilbert space carrying the representation. With this in mind, we may ask whether the two representations determined by the states invariant under the two automorphism groups are isometrically equivalent. If they are, then either admits concurrent unitary implementation of both

groups, and the existence of the limits defining "second-quantized" wave operators can be studied. If they are not, can the two automorphism groups be unitarily implemented in either representation? In any representation?

These questions are answered by work which follows. In Sec. V, we establish the necessary and sufficient conditions for the isometric equivalence of the representations determined by the invariant states. In Sec. VIII, we establish the necessary and sufficient conditions for a representation π_R to admit concurrent unitary implementation of both automorphism groups. We find that it is possible for both β and β^o to have concurrent implementation despite the inequivalence of the representations determined by their invariant states. We will see in [II], however, that in this alternative "second-quantized" formulation, the expressions defining the wave operators may not converge, even though wave morphisms exist, induced by partial symplectic transformations $\Omega_\pm$.

The second set of questions has to do with the limits $\Omega_\pm$ on $\mathscr{H}$. We would like to know if these limits exist, and, if so, whether they are partial symplectic transformations. Can these transformations, moreover, be implemented in either of the natural representations of $\mathscr{W}$? In what representations can the resultant scattering morphism be implemented? What is the relationship among the states invariant under the two automorphism groups and the state(s) invariant under the scattering morphism?

Two of these questions are answered by Theorem 2, which gives sufficient conditions for the limits $\Omega_\pm$ to exist and to be partial symplectic transformations. The remaining questions are answered in [II] for the specific models discussed there.

IV. THE MAIN RESULTS

One central result used in the analysis of the model systems is the following theorem, which gives necessary and sufficient conditions for the unitary implementability of the automorphism group β_t induced by the one-parameter symplectic group T^+V_tT in a representation π_R symplectically related to the Fock representation.

Recall that Λ denotes multiplication by the complex number i.

Theorem 1: Let $\mathscr{H}$ be a separable complex Hilbert space, and let $\mathscr{W}$ be the Weyl C^* algebra over $\mathscr{H}$ regarded as a real Hilbert space with inner product equal to the real part of the complex inner product, and symplectic form equal to the imaginary part. Let π_R be the representation of $\mathscr{W}$ induced by the symplectic transformation $R:\mathscr{H}\to\mathscr{H}$, and let $T:\mathscr{H}\to\mathscr{H}$ be another symplectic transformation.

Let $H:D(H)\to T\mathscr{H}$ be a non-negative, self-adjoint, complex-linear transformation with domain $D(H)$ dense in $T\mathscr{H}$, and for $m>0$, let P_m be the spectral projection for H onto spectral values larger than m. Let $V_t\equiv e^{t\Lambda H}$ be the one-parameter group generated by H, and let $\beta_t:\mathscr{W}\to\mathscr{W}$ be the automorphism induced by (the invertible symplectic transformation) T^+V_tT:

$$\beta_t(W(f)) = W(T^+V_tTf), \quad \text{for all } f \text{ in } \mathscr{H}.$$

Then the automorphism β_t is unitarily implementable in the representation π_R of $\mathscr{W}$ for all real t if and only if for some $m>0$, both $P_m(|RT^+|^2-I)$ and $[|RT^+|^2, \Lambda(I-P_m)H]$ are Hilbert–Schmidt operators on $T\mathscr{H}$.

In particular, if H is bounded away from zero then β_t is unitarily implementable in π_R for all real t if and only if π_R is interchangeable with the representation π_T.

Furthermore, if β_t is unitarily implementable in π_R for all real t, then the one-parameter family of implementing unitary operators can be chosen to be a strongly continuous unitary group.

Remark: Here $|Q|^2\equiv Q^*Q$, with Q^* the real adjoint of Q, and the trace in the definition of the Hilbert–Schmidt norm is defined in terms of the real inner product on $\mathscr{H}$.

The proof of Theorem 1 follows directly from Theorems 4 and 5 to follow, and from the reasoning in Secs. V–VII. For a proof of Theorem 1 in the special case that $R=I$ and T is an invertible symplectic transformation, see Ref. 17.

The second central result is the following theorem, which establishes sufficient conditions for the existence and completeness of the Møller wave morphisms associated with the automorphism groups β and β^o. It is analogous to the Birman–Belopol'skii theorem in two-Hilbert-space scattering theory;[11] both the statement of this theorem and its proof are simple because here the "identification map" is a symplectic transformation.

Let $\mathscr{H}, \mathscr{W}, \Lambda, H$, and P_m be as in Theorem 1, and let P^o_m be the spectral projection for the self-adjoint operator H^o onto spectral values larger than m. Let P_{ac} and P^o_{ac} be the projections onto the absolutely continuous subspaces for H and H^o, respectively.

Theorem 2: Let H^o and H be non-negative complex-linear self-adjoint operators, and let $T:\mathscr{H}\to\mathscr{H}$ be a symplectic transformation such that $TD(H^o)=D(H)$. Suppose there exists an $M>0$ such that $(I-P_m)(\Lambda HT - T\Lambda H^o)(I-P^o_m)$ is a trace-class operator on $\mathscr{H}$ for all $m>M$. Then $\Omega_\pm \equiv \text{s-lim}_{t\to\pm\infty} T^+e^{t\Lambda H}Te^{-t\Lambda H^o}P^o_{ac}$ exist. If furthermore $e^{t\Lambda H}T\mathscr{H}\subset T\mathscr{H}$ for all t, then $\Omega_\pm$ are partial symplectic transformations with initial space $P^o_{ac}\mathscr{H}$ and final space $T^+P_{ac}T\mathscr{H}$.

Remark: The hypothesis that $TD(H^o)=D(H)$ can be weakened considerably. It is required only that H^o and H be mutually subordinate[11] with respect to the identification map T. The statement of the theorem here includes the more restrictive hypothesis for simplicity, and this form of the theorem suffices to treat the model theory discussed in [II].

The proof of Theorem 2 in Sec. X.

V. CRITERION FOR IMPLEMENTABILITY OF A PARTIAL-SYMPLECTIC MORPHISM

Consider the automorphism $\sigma:\mathscr{W}\to\mathscr{W}$ of the Weyl algebra induced by the invertible symplectic transformation $S:\mathscr{H}\to\mathscr{H}$ by $\sigma(W(f))\equiv W(Sf)$ for all f in $\mathscr{H}$, and consider the representation π_R of $\mathscr{W}$ induced by the symplectic transformation $R:\mathscr{H}\to\mathscr{H}$ as above.

What are the necessary and sufficient conditions for σ to be unitarily implementable in π_R?

Note first that σ implementable in π_R means that there exists a unitary operator U such that

$$U\pi_R(W(f))U^* = \pi_R(\sigma(W(f))), \quad \text{for all } f \text{ in } \mathscr{H},$$

that is,

$$U\,W(Rf)U^* = W(RSf), \quad \text{for all } f \text{ in } \mathscr{H},$$

that is,

$$U\,W(g)U^* = W(RSR^{+}g), \quad \text{for all } g \text{ in } R\mathscr{H}.$$

Thus the implementability in π_R of σ is equivalent to the implementability in the Fock representation (of the Weyl algebra over the Hilbert space $R\mathscr{H}$) of the automorphism induced by the transformation RSR^{+} which is an invertible symplectic transformation on $R\mathscr{H}$ (see Appendix B).

The following criterion for the unitary implementability in the Fock representation of the Weyl algebra of a given invertible symplectic transformation Q was found by Shale[12]:

There exists a unitary operator $U:\mathscr{F}(\mathscr{H})\to\mathscr{F}(\mathscr{H})$ such that

$U\,W(f)U^* = W(Qf)$ for all f in $\mathscr{H}$ if and only if $(|Q| - I)$ is a Hilbert–Schmidt operator.

Here $|Q| \equiv (Q^*Q)^{1/2}$, with Q^* the real adjoint of Q, and the trace in the definition of the Hilbert–Schmidt norm is taken over a real basis for $\mathscr{H}$.

Note that for a bounded real-linear transformation Y, $(|Y| - I)$ is a Hilbert–Schmidt operator if and only if $(|Y|^2 - I)$ is a Hilbert–Schmidt operator, because the set $B_{2r}(\mathscr{H})$ of real-linear operators of Hilbert–Schmidt type is a $*$ ideal, the operator $(|Y| + I)$ has a bounded inverse, and $(|Y|^2 - I) = (|Y| + I)(|Y| - I)$. Shale's criterion $(|Q| - I) \in B_{2r}(\mathscr{H})$ is thus equivalent to $(|Q|^2 - I) \in B_{2r}(\mathscr{H})$.

If we apply this criterion to the question of whether an invertible symplectic transformation S is unitarily implementable in the representation π_R of $\mathscr{W}$ induced by the symplectic transformation R, we find that

S is implementable in π_R iff $|RSR^{+}|^2 - I$ is a Hilbert–Schmidt operator on the space $R\mathscr{H}$.

Now we consider the more general question of the implementation of the morphism induced by a partial symplectic transformation Q.

We first restrict our attention to establishing a necessary and sufficient condition for the partial-isometric implementability of a partial symplectic transformation Q in the Fock representation of $\mathscr{W}$. Later we consider the implementation of a partial symplectic transformation in certain representations symplectically related to the Fock representation.

To establish the criterion, we first recall the well-known fact that if $\mathscr{H}$ is decomposed as the direct sum $\mathscr{H}_a \oplus \mathscr{H}_b$ of subspaces $\mathscr{H}_a$ and $\mathscr{H}_b$, then the Fock space $\mathscr{F}(\mathscr{H})$ over $\mathscr{H}$ is isomorphic to the tensor product $\mathscr{F}(\mathscr{H}_a) \otimes \mathscr{F}(\mathscr{H}_b)$ of the Fock spaces $\mathscr{F}(\mathscr{H}_a)$ and $\mathscr{F}(\mathscr{H}_b)$ over $\mathscr{H}_a$ and $\mathscr{H}_b$, respectively. Furthermore, $\mathscr{F}(\mathscr{H}_a)$ and $\mathscr{F}(\mathscr{H}_b)$ are naturally isomorphic to the subspaces $\mathscr{F}(\mathscr{H}_a) \otimes \{\Omega_b\} \subset \mathscr{F}(\mathscr{H})$ and $\{\Omega_a\} \otimes \mathscr{F}(\mathscr{H}_b) \subset \mathscr{F}(\mathscr{H})$, respectively, where Ω_a and Ω_b are the vacua of $\mathscr{F}(\mathscr{H}_a)$ and $\mathscr{F}(\mathscr{H}_b)$. In the following we omit mention of these isomorphisms and speak of $\mathscr{F}(\mathscr{H}_a)$ and $\mathscr{F}(\mathscr{H}_b)$ as subspaces of $\mathscr{F}(\mathscr{H})$. Neither do we distinguish between the usual action of Weyl operators on $\mathscr{F}(\mathscr{H})$, and their tensor product action on $\mathscr{F}(\mathscr{H}_a) \otimes \mathscr{F}(\mathscr{H}_b)$.

Second, we note that a complex-linear partial isometry $Z:\mathscr{H}\to\mathscr{H}$ always has an implementation on Fock space by a partial isometry U_Z which is defined as follows. Set $U_Z\Omega \equiv \Omega$ and

$$U_Z a^*[f_1]\cdots a^*[f_n]\Omega \equiv a^*[Zf_1]\cdots a^*[Zf_n]\Omega,$$

where $f_1,\ldots, f_n \in \mathscr{H}$. Because Z is a partial isometry, this definition extends by linearity to the entire Fock space $\mathscr{F}(\mathscr{H})$, and U_Z is bounded. It is, furthermore, easy to check that $U_Z^*\,\Omega = \Omega$ and that

$$U_Z^*\, a^*[f_1]\cdots a^*[f_n]\Omega = a^*[Z^*f_1]\cdots a^*[Z^*f_n]\Omega.$$

It follows from the decompositions

$$\mathscr{H} = Z^*Z\,\mathscr{H} \oplus (I - Z^*Z)\mathscr{H} = ZZ^*\,\mathscr{H} \oplus (I - ZZ^*)\mathscr{H}$$

that

$$\mathscr{F}(\mathscr{H}) \cong \mathscr{F}(Z^*Z\mathscr{H}) \otimes \mathscr{F}((I - Z^*Z)\mathscr{H})$$
$$\cong \mathscr{F}(ZZ^*\mathscr{H}) \otimes \mathscr{F}((I - ZZ^*)\mathscr{H}),$$

and that $U_Z^*\,U_Z$ is the projection onto $\mathscr{F}(Z^*Z\mathscr{H}) \otimes \{\Omega'\}$, while $U_ZU_Z^*$ is the projection onto $\mathscr{F}(ZZ^*\mathscr{H}) \otimes \{\Omega''\}$. The operator U_Z is therefore a partial isometry with initial space $\mathscr{F}(Z^*Z\mathscr{H}) \otimes \{\Omega'\}$ and final space $\mathscr{F}(ZZ^*\mathscr{H}) \otimes \{\Omega''\}$, and $U_Z W(f) = W(Zf)U_Z$, for all $f \in \mathscr{H}$, that is, U_Z implements Z.

We make use of these two observations in the proof of the following theorem, which establishes the analog of Shale's criterion for partial symplectic transformations.

Theorem 3: Let $Q:\mathscr{H}\to\mathscr{H}$ be a partial symplectic transformation. Then there exists a partial isometry $U:\mathscr{F}(\mathscr{H})\to\mathscr{F}(\mathscr{H})$ with initial space $\mathscr{F}(Q^{+}Q\mathscr{H})$ and final space $\mathscr{F}(QQ^{+}\mathscr{H})$ such that $UW(f) = W(Qf)U$ for all $f \in \mathscr{H}$ if and only if $(|Q|^2 - I)$ is a Hilbert–Schmidt operator on $Q^{+}Q\mathscr{H}$.

Remark: $(|Q|^2 - I)$ being a Hilbert–Schmidt operator on $Q^{+}Q\mathscr{H}$ is equivalent to $(|Q|^2 - Q^{+}Q)$ being a Hilbert–Schmidt operator on $\mathscr{H}$.

Proof: Suppose first that $(|Q|^2 - I) \in B_{2r}(Q^{+}Q\mathscr{H})$. By results in Appendix B we know that $|Q|$ is a partial symplectic transformation with initial and final spaces equal to $Q^{+}Q\mathscr{H}$. Since $|Q|$ is thus an invertible symplectic transformation on $Q^{+}Q\mathscr{H}$ which satisfies Shale's criterion, there exists a unitary operator

$$U_{|Q|}:\mathscr{F}(Q^{+}Q\mathscr{H})\to\mathscr{F}(Q^{+}Q\mathscr{H})$$

such that $U_{|Q|}\,W(g) = W(|Q|g)U_{|Q|}$, for all $g \in Q^{+}Q\mathscr{H}$.

Now regard $\mathscr{F}(Q^{+}Q\mathscr{H})$ as the subspace

$$\mathscr{F}(Q^{+}Q\mathscr{H}) \otimes \{\Omega'\}$$
$$\subset \mathscr{F}(\mathscr{H}) = \mathscr{F}(Q^{+}Q\mathscr{H}) \otimes \mathscr{F}((I - Q^{+}Q)\mathscr{H}),$$

and define a unitary extension U of $U_{|Q|}$ to all of $\mathscr{F}(\mathscr{H})$ by $U \equiv U_{|Q|} \otimes I$. Then $UW(f) = W(|Q|f + (I - Q^{+}Q)f)U$, for all $f \in \mathscr{H}$.

Next let Z be the complex-linear partial isometry in the polar decomposition $Q = Z|Q|$. By results in Appendix B we know that $Z^*Z = Q^{+}Q$ and $ZZ^* = QQ^{+}$. We also know from the reasoning earlier that Z has an implementation by the partial isometry $U_Z:\mathscr{F}(\mathscr{H})\to\mathscr{F}(\mathscr{H})$ with initial space $\mathscr{F}(Q^{+}Q\mathscr{H}) \otimes \{\Omega'\}$ and final space $\mathscr{F}(QQ^{+}\mathscr{H}) \otimes \{\Omega''\}$.

The operator $U_Q:\mathscr{F}(\mathscr{H})\to\mathscr{F}(\mathscr{H})$ defined by

$U_Q \equiv U_Z U$ is a partial isometry with initial space $\mathcal{F}(Q^+Q\mathcal{H}) \otimes \{\Omega'\}$ and final space $\mathcal{F}(QQ^+\mathcal{H}) \otimes \{\Omega''\}$, because $U_Q U_Q^* = U_Z U U^* U_Z^* = U_Z U_Z^*$ and $U_Q^* U_Q = U^*(U_Z^* U_Z)\, U = U^* U(U_Z^* U_Z) = U_Z^* U_Z$ by virtue of the fact that the projection $U_Z^* U_Z$ onto the subspace $\mathcal{F}(Q^+Q\mathcal{H}) \otimes \{\Omega'\}$ commutes with U. Furthermore it is easy to check that

$$\begin{aligned} U_Q W(f) &= U_Z W(|Q|f + (I - Q^+Q)f)U \\ &= W(Z|Q|f + Z(I - Q^+Q)f)U_Z U \\ &= W(Qf)U_Q, \end{aligned}$$

that is, U_Q implements Q.

For the converse, suppose that the partial symplectic transformation $Q:\mathcal{H} \to \mathcal{H}$ is implemented by a partial isometry $U_Q:\mathcal{F}(\mathcal{H}) \to \mathcal{F}(\mathcal{H})$ with initial space $\mathcal{F}(Q^+Q\mathcal{H}) \otimes \{\Omega'\}$ and final space $\mathcal{F}(QQ^+\mathcal{H}) \otimes \{\Omega''\}$. Thus $U_Q W(f) = W(Qf)U_Q$, for all $f \in \mathcal{H}$. We proceed by showing that the partial symplectic transformation $|Q|$ is *unitarily* implemented on $\mathcal{F}(Q^+Q\mathcal{H})$ and then appealing to Shale's results to conclude that $|Q|^2 - I \in B_{2r}(Q^+Q\mathcal{H})$.

Again let $Z:\mathcal{H} \to \mathcal{H}$ be the complex-linear partial isometry occurring in the polar decomposition $Q = Z|Q|$, and let $U_Z:\mathcal{F}(\mathcal{H}) \to \mathcal{F}(\mathcal{H})$ be the partial isometry implementing Z, as above. We know that U_Z has the same initial and final spaces as does U_Q, and that $U_Z^* U_Z = U_Q^* U_Q$, respectively $U_Z U_Z^* = U_Q U_Q^*$, are the projections onto those subspaces of $\mathcal{F}(\mathcal{H})$. Taking the adjoint of $U_Z W(f) = W(Zf)U_Z$ and using $W(h)^* = W(-h)$, we obtain

$$U_Z^* W(Zf) = W(f)\, U_Z^* \quad \text{for all} \quad f \in \mathcal{H}.$$

Therefore if we set $U_{|Q|} \equiv U_Z^* U_Q$ we have

$$\begin{aligned} U_{|Q|} W(f) &= U_Z^* W(Qf)U_Q = U_Z^* W(Z|Q|f)U_Q \\ &= W(|Q|f)\, U_Z^* U_Q \\ &= W(|Q|f)U_{|Q|}, \quad \text{for all} \quad f \in \mathcal{H}, \end{aligned}$$

that is, $U_{|Q|}$ implements $|Q|$. Furthermore,

$$U_{|Q|}^* U_{|Q|} = U_Q^*(U_Z U_Z^*) U_Q = U_Q^* U_Q,$$

and

$$U_{|Q|} U_{|Q|}^* = U_Z^*(U_Q U_Q^*) U_Z = U_Z^* U_Z = U_Q^* U_Q,$$

so $U_{|Q|}$ is a partial isometry with initial and final subspaces equal to $U_Q^* U_Q \mathcal{F}(\mathcal{H}) = \mathcal{F}(Q^+Q\mathcal{H}) \otimes \{\Omega'\}$. Thus $U_{|Q|}$ is a unitary operator on $\mathcal{F}(Q^+Q\mathcal{H}) \otimes \{\Omega'\}$, and we may regard $U_{|Q|}$ as the unitary implementation on $\mathcal{F}(Q^+Q\mathcal{H})$ of the invertible symplectic transformation $|Q|:(Q^+Q\mathcal{H}) \to (Q^+Q\mathcal{H})$. Thus $|Q|$ must satisfy Shale's criterion $|Q|^2 - I \in B_{2r}(Q^+Q\mathcal{H})$. This completes the proof of the theorem. ///

There are three straightforward applications of Theorem 3, to representations isometrically equivalent to, and interchangeable with, the Fock representation, and to the implementation of (suitable) partial symplectic transformations in a representation symplectically related to the Fock representation.

(A) We first apply Theorem 3 to answer the question of which representations π_R symplectically related to the Fock representation are isometrically equivalent to the Fock representation. Let $R:\mathcal{H} \to \mathcal{H}$ be a symplectic transformation. By definition, the representation π_R of $\mathcal{W}$ induced by R is isometrically equivalent to the Fock representation if and only if there exists an isometry $U:\mathcal{F}(\mathcal{H}) \to \mathcal{F}(\mathcal{H})$ such that $UW(f) = \pi_R(W(f))U$, for all $f \in \mathcal{H}$, that is, $UW(f) = W(Rf)U$, for all $f \in \mathcal{H}$. So π_R is isometrically equivalent to the Fock representation if and only if (the morphism induced by) R is isometrically implementable in the Fock representation, which is the case if and only if $(|R|^2 - I) \in B_{2r}(\mathcal{H})$.

(B) The relationship between two arbitrary representations of the Weyl algebra which are interchangeable is, in general, quite complicated. It is clear that if two representations are unitarily equivalent then they are interchangeable, but the converse is not true. The situation simplifies, however, if we consider the relationship between a representation of $\mathcal{W}$ induced by a symplectic transformation, and the Fock representation.

Lemma: Let $Q:\mathcal{H} \to \mathcal{H}$ be a symplectic transformation, and let π_Q be the representation of the Weyl algebra induced by Q, that is, $\pi_Q(W(f)) = W(Qf)$. Then π_Q is interchangeable with the Fock representation π_I if and only if π_Q is isometrically equivalent to the Fock representation.

Proof: We know that π_Q is isometrically equivalent to the Fock representation iff $(|Q|^2 - I) \in B_{2r}(\mathcal{H})$. We also know that π_Q is interchangeable with the Fock representation π_I if and only if for each invertible symplectic transformation $S:\mathcal{H} \to \mathcal{H}$, $|QS|^2 - |Q|^2 \in B_{2r}(\mathcal{H})$ iff $|S|^2 - I \in B_{2r}(\mathcal{H})$. (See Appendix C.)

(1) Suppose first that π_Q is isometrically equivalent to π_I; then $|Q|^2 - I \in B_{2r}(\mathcal{H})$. Because $|QS|^2 - |Q|^2 = S^*(|Q|^2 - I)S + (|S|^2 - I)$, it follows that $|QS|^2 - |Q|^2 \in B_{2r}(\mathcal{H})$ iff $|S|^2 - I \in B_{2r}(\mathcal{H})$.

(2) Suppose conversely that π_Q is interchangeable with π_I, and consider the invertible symplectic transformation $S \equiv \Lambda$. Because $|\Lambda|^2 = I$, $|\Lambda|^2 - I \in B_{2r}(\mathcal{H})$, so by assumption $|Q\Lambda|^2 - |Q|^2 \in B_{2r}(\mathcal{H})$. Now, $|Q\Lambda|^2 = \Lambda^*|Q|^2\Lambda = |Q|^{-2}$, because $|Q|^2$ is an invertible symplectic transformation on $\mathcal{H}$. Thus

$$|Q|^{-2}(I - |Q|^4) = |Q|^{-2}(I + |Q|^2)(I - |Q|^2) \in B_{2r}(\mathcal{H}).$$

By the ideal property of $B_{2r}(\mathcal{H})$, this implies $|Q|^2 - I \in B_{2r}(\mathcal{H})$, that is, π_Q is isometrically equivalent to the Fock representation. ///

(C) To apply Theorem 3 to the implementation of a partial symplectic transformation in a representation symplectically related to the Fock representation, consider a symplectic transformation $R:\mathcal{H} \to \mathcal{H}$, and let π_R be the induced representation of $\mathcal{W}$. It is easy to see as earlier that (the morphism induced by) a partial symplectic transformation $Q:\mathcal{H} \to \mathcal{H}$ is implementable by partial isometry in π_R if and only if RQR^+ is implementable by partial isometry in the Fock representation over $R\mathcal{H}$. It is possible, however, that RQR^+ may fail to be a partial symplectic transformation due to mismatch of the complex structures of the kernels and ranges of R and Q. But it is not difficult to see that RQR^+ is a partial symplectic transformation if and only if both $R(\ker Q)$ and $R(\operatorname{ran} Q)$ are complex subspaces of $\mathcal{H}$. If these

are in fact complex subspaces, we can apply the criterion developed above to conclude that Q is implementable by partial isometry in π_R if and only if $(|RQR^+|^2 - I)$ is a Hilbert–Schmidt operator on $RQ^+\mathscr{H}$, that is (by virtue of the results in Appendix C), if and only if $|RQ|^2 - |R|^2 \in B_{2r}(Q^+\mathscr{H})$.

VI. CRITERIA FOR IMPLEMENTATION OF AUTOMORPHISM GROUPS

The necessary and sufficient conditions given in Theorem 1 relating R,T, and the self-adjoint generator H of the continuous unitary group $V_t = e^{t\Lambda H}$ follow directly from Theorem 4 below, which is the crux of the matter. This theorem establishes the necessary and sufficient conditions for a symplectic transformation to commute modulo Hilbert–Schmidt operators with all elements of a one-parameter unitary group.

It is clear that if a positive symplectic operator S satisfies Shale's criterion $(S - I) \in B_{2r}(\mathscr{K})$ then $[S, V_t] \in B_{2r}(\mathscr{K})$, for all real t. But the converse is obviously not true. The properties of S which embody the fact that $[S, V_t] \in B_{2r}(\mathscr{K})$ for all t depend on the relationship between S and the Hamiltonian H; Theorem 4 states these properties in terms of the spectral projection P_m for H onto energies larger than $m > 0$.

Theorem 4: Let H be a non-negative, self-adjoint, complex-linear transformation with domain $D(H)$ dense in the separable Hilbert space $\mathscr{K}$. Let $V:\mathbb{R}\to B(\mathscr{K})$ be the (strongly continuous) unitary group generated by H, $V_t \equiv e^{t\Lambda H}$, and consider an open interval $\tau \subset \mathbb{R}$ with $0 \in \tau$. Let P_m be the spectral projection for H onto spectral values larger than m. Let S be an invertible symplectic transformation on $\mathscr{K}$ regarded as a real Hilbert space with inner product equal to the real part of the complex inner product on $\mathscr{K}$, and symplectic form equal to the imaginary part. Suppose S is self-real-adjoint. Then the following three statements are equivalent.

(I) $[S, V_t]$ is of Hilbert–Schmidt type for all $t \in \tau$.

(II) There exists an $m > 0$ such that (A) $P_m(S - I)$ is a Hilbert–Schmidt operator, and (B) $[S, \Lambda(I - P_m)H]$ is a Hilbert–Schmidt operator.

(III) Statements (A) and (B) hold for all $m > 0$.

The proof of this theorem appears in Ref. 17.

To make our discussion of the implications of this theorem concise, we introduce the following notation.

Definition: Denote by $\mathscr{R}_H(\mathscr{K})$ the set of all symplectic transformations $Q:\mathscr{K}\to\mathscr{K}$ satisfying $P_m(|Q| - I) \in B_{2r}(\mathscr{K})$ and $[|Q|, \Lambda(I - P_m)H] \in B_{2r}(\mathscr{K})$, for some $m > 0$.

The situation in which H is bounded away from zero is a special case of particular interest. If H is bounded away from zero, that is, there exists a $c > 0$ such that $\langle f|Hf\rangle \geq c\|f\|^2$ for all $f \in D(H)$, then choosing $0 < m < c$ gives $P_m = I$, and then as a result $Q \in \mathscr{R}_H(\mathscr{K})$ if and only if $(|Q| - I) \in B_{2r}(\mathscr{K})$. So for any H bounded away from the origin, $\mathscr{R}_H(\mathscr{K})$ is just the set of symplectic transformations Q which satisfy Shale's criterion $(|Q| - I) \in B_{2r}(\mathscr{K})$. Henceforth for consistency of notation we denote this set of symplectic transformations by $\mathscr{R}_I(\mathscr{K})$.

A mathematically simple example is given in Ref. 17 which shows that the set $\mathscr{R}_H(\mathscr{K})$ is properly larger than $\mathscr{R}_I(\mathscr{K})$ when the spectrum of H reaches zero. The example given in [II] provides a physically motivated demonstration of the same fact.

To apply this theorem to establish the necessary and sufficient conditions given in Theorem 1, we demonstrate that the unitary implementability of β in π_R is equivalent to the condition (I) of Theorem 4 that $[|RT^+|^2, V_t] \in B_{2r}(T\mathscr{H})$ for all t, as follows.

First note that by the hypotheses of Theorem 1, the unitary operator V_t commutes (for all t) with the projection TT^+ onto the range of the "diagonalization" symplectic transformation T, so the operator (T^+V_tT) is, by the results in Appendix B, an invertible symplectic transformation on all of $\mathscr{H}$ for all real t.

Second, according to the criterion developed in the preceding section, the automorphism group β_t induced by T^+V_tT is unitarily implementable in π_R if and only if $|RT^+V_tTR^+|^2 - I \in B_{2r}(R\mathscr{H})$.

Third, making use of the facts that $I = Q^+Q = Q^*Q^{*+}$ and $(QQ^+)^* = QQ^+$ for any symplectic Q, we can write

$$|RT^+V_tTR^+|^2 - I = R^{*+}T^*V_t^*(|RT^+|^2V_t - V_t|RT^+|^2)TR^+ + (RR^+ - I).$$

Now, in Appendix C it is shown that

$$R^{*+}XR^+ \in B_{2r}(R\mathscr{H}) \text{ iff } X \in B_{2r}(\mathscr{H}),$$

and that

$$T^*YT \in B_{2r}(\mathscr{H}) \text{ iff } Y \in B_{2r}(T\mathscr{H}).$$

Thus because $(RR^+ - I)$ vanishes on $R\mathscr{H}$, and because V_t^* has a bounded inverse, we have

$$|RT^+V_tTR^+|^2 - I \in B_{2r}(R\mathscr{H}) \text{ iff } [|RT^+|^2, V_t] \in B_{2r}(T\mathscr{H}).$$

Note that because R and T are symplectic, it follows from results in Appendix B that RT^+ is a partial symplectic transformation and hence that $S \equiv |RT^+|^2$ is an invertible symplectic transformation on the separable complex Hilbert space $TT^+\mathscr{H} = T\mathscr{H}$. Thus Theorem 4 above is applicable to $S \equiv |RT^+|^2$, with $\mathscr{K} = T\mathscr{H}$, and we conclude that the statements (A) and (B) are the necessary and sufficient conditions on $S \equiv |RT^+|^2$ for β to be unitarily implementable in π_R, as asserted in Theorem 1. Thus

β is unitarily implementable in π_R if and only if $|RT^+|^2 \in \mathscr{R}_H(T\mathscr{H})$.

We now consider the assertion in Theorem 1 about the situation in which H is bounded away from zero. In this case, the automorphism group β_t induced by T^+V_tT is implementable in the representation π_R if and only if $|RT^+|^2 \in \mathscr{R}_I(T\mathscr{H})$. This implies that β is unitarily implementable only in the representations π_R interchangeable with the representation π_T which naturally accommodates implementation of β, for the following reasons.

Suppose that β is implementable in π_R, that is, $(|RT^+|^2 - I) \in B_{2r}(T\mathscr{H})$. Since TT^+ is the complex-linear self-adjoint projection onto $T\mathscr{H}$, the quantity

$$|RT^+|^2 - I = T^{*+}R^*RT^+ - |TT^+|^2 + (TT^+ - I) = T^{*+}(R^*R - T^*T)T^+ + (TT^+ - I)$$

is in $B_{2r}(T\mathscr{H})$ if and only if $T^{*+}(|R|^2-|T|^2)T^+ \in B_{2r}(T\mathscr{H})$, and this is the case if and only if $(|R|^2-|T|^2) \in B_{2r}(\mathscr{H})$, by the results in Appendix C. Thus $(|RT^+|^2-I) \in B_{2r}(T\mathscr{H})$ if and only if $(|R|^2-|T|^2) \in B_{2r}(\mathscr{H})$. But it is shown in Appendix C that $(|R|^2-|T|^2) \in B_{2r}(\mathscr{H})$ implies that π_R and π_T are interchangeable. Therefore $|RT^+|^2 \in R_I(T\mathscr{H})$ implies that π_R is interchangeable with π_T.

There is physical content to the fact that H bounded away from zero implies β is unitarily implementable only in the representations π_R interchangeable with the natural representation π_T associated with β. If V_t is regarded as a time-development transformation generated by the Hamiltonian H for normal mode variables, then H is bounded away from zero only if there are no zero-mass normal-mode excitations. Thus only in theories with massless excitation can the interesting situation occur that β is unitarily implementable in representations not interchangeable with its natural associated representation π_T.

The example presented in [II] shows that the class of representations π_R which admit implementation of β does in fact contain representations inequivalent to π_T when massless particles are present.

VII. CONTINUITY OF THE IMPLEMENTATION

Suppose that the one-parameter group of invertible symplectic transformations $T^+V_tT = T^+(e^{t\Lambda H})T$ is in fact unitarily implementable in π_R. The assertion of Theorem 1 which does not follow directly from Theorem 4 is that the one-parameter family of implementing unitary operators can be chosen to be a strongly continuous unitary group. This implies in particular that, when V_t is regarded as a time development, there always exists a "second-quantized" Hamiltonian in representations where the dynamical automorphism β is unitarily implemented. As the following considerations show, the validity of this assertion follows from (the somewhat technical) Theorem 5 below.

Shale[12] showed that if Y_t is a one-parameter group of implementable symplectic transformations which is continuous in a certain topology, then there exists a strongly continuous unitary group implementing Y_t in the Fock representation. Specifically, let $\mathrm{rSp}(\mathscr{K})$ be the group of invertible symplectic transformations on the Hilbert space $\mathscr{K}$ satisfying Shale's criterion; the topology on $\mathrm{rSp}(\mathscr{K})$ is defined as follows. Polar decomposition (with respect to the real adjoint) of a transformation $T \in \mathrm{rSp}(\mathscr{K})$ gives $T = Z|T|$, where Z is complex unitary and $|T|$ is a (real $-$) positive invertible symplectic transformation. The topology on $\mathrm{rSp}(\mathscr{K})$ is the product topology obtained when $\mathrm{rSp}(\mathscr{K})$ is regarded as the Cartesian product of the space of unitary operators under the weak operator topology, with the space of positive invertible symplectic operators under the topology induced by the Hilbert–Schmidt norm [well defined because $(|T|-I) \in B_{2r}(\mathscr{K})$, for $T \in \mathrm{rSp}(\mathscr{K})$].

Shale furthermore showed that group multiplication is continuous in this topology, so that if Y_t is a one-parameter group of invertible symplectics, continuity of Y_t at $t=0$ implies continuity everywhere. Thus to show the existence of a continuous unitary implementation of Y_t in the Fock representation, it is sufficient to show that $Y:\mathbb{R}\to\mathrm{rSp}(\mathscr{K})$ is continuous at the origin.

To apply this criterion to the implementation of T^+V_tT in π_R, note that, as earlier, continuous implementation of T^+V_tT in π_R is equivalent to continuous implementation of the one-parameter group $Y_t \equiv RT^+V_tTR^+$ of symplectic transformations invertible on $\mathscr{K} \equiv R\mathscr{H}$ in the Fock representation of the Weyl algebra over $\mathscr{K}$. We may then make use of the following general theorem.

Theorem 5: Let $\mathscr{H}$ be a separable complex Hilbert space, also regarded as a real Hilbert space with inner product equal to the real part of the complex inner product on $\mathscr{H}$, and symplectic form equal to the imaginary part. Let $Q:\mathscr{H}\to\mathscr{H}$ be a partial symplectic transformation (whose range $Q\mathscr{H}$ is thus a separable complex Hilbert space). Let $H:D(H)\to Q\mathscr{H}$ be a nonnegative self-adjoint complex-linear transformation with domain $D(H)$ dense in $Q\mathscr{H}$, and set $V_t \equiv e^{t\Lambda H}$. Define $Y_t \equiv Q^+V_tQ$ (which is thus an invertible symplectic transformation on $Q^+Q\mathscr{H}$). If $(|Y_t|-I)$ is a Hilbert–Schmidt operator on $Q^+Q\mathscr{H}$ for all real t, then $Y:\mathbb{R}\to\mathrm{rSp}(Q^+Q\mathscr{H})$ is continuous for all t in Shale's topology. Hence Y has a strongly continuous unitary representation in the Fock representation of $\mathscr{W}$ over $Q^+Q\mathscr{H}$.

In view of the remarks above, to prove this theorem it suffices to show that Y_t is continuous at the origin in Shale's topology. The demonstration of this fact is a straightforward generalization of the proof of Theorem 3 in Ref. 17 to the partial symplectic transformations discussed here.[18] This theorem can, of course, be applied to the implementation of T^+V_tT in π_R by setting $Q \equiv TR^+$. The initial space of this partial symplectic transformation Q is $Q^+Q\mathscr{H} = R\mathscr{H}$ and the range of Q is $T\mathscr{H}$. By the earlier hypotheses on V_t, the group $Y_t \equiv RT^+V_tTR^+$ is of exactly the type described in the theorem. Since the hypothesis here that $(|Y_t|-I)$ be in the Hilbert–Schmidt class is equivalent to the unitary implementability of Y_t, it follows that if β is unitarily implementable in π_R then the implementing unitary family can always be chosen to be a strongly continuous unitary group.

VIII. CONCURRENT IMPLEMENTATION

Suppose that as in Sec. III the free time-development automorphism group β_t^o of $\mathscr{W}$ is induced by the unitary group $V_t^o = e^{t\Lambda H^o}$ and that the interacting automorphism β_t is induced by the one-parameter group $T^+V_tT = T^+(e^{t\Lambda H})T$. The criteria developed in the preceding sections imply that if there exists a representation π_R of $\mathscr{W}$ symplectically related to the Fock representation which admits concurrent unitary implementation of both automorphism groups β^o and β, then R satisfies

$$|R|^2 \in \mathscr{R}_{H^o}(\mathscr{H}) \quad \text{and} \quad |RT^+|^2 \in \mathscr{R}_H(T\mathscr{H}).$$

The situation simplifies considerably if either Hamiltonian H^o or H has spectrum bounded away from zero.

Suppose first that $|R|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$, where H^o is bounded away from the origin. Then $\mathscr{R}_{H^o}(\mathscr{H}) = \mathscr{R}_I(\mathscr{H})$ and so $(|R|^2-I) \in B_{2r}(\mathscr{H})$. This implies that π_R is isometrically equivalent to the Fock representation π_I. So in this case both automorphism groups must be implementable in the Fock representation if they are to be concurrently implemented in any representation π_R. Furthermore, since $|RT^+|^2$

$= T^{*+}(|R|^2 - I)T^+ + |T^+|^2$, the fact that $(|R|^2 - I) \in B_{2r}(\mathscr{H}) \subset B_{2r}(T\mathscr{H})$ implies that $|RT^+|^2 \in \mathscr{R}_H(T\mathscr{H})$ if and only if $|T^+|^2 \in \mathscr{R}_H(T\mathscr{H})$. Thus if H^o is bounded away from zero, the only automorphism groups β (induced by T^+V_tT) which can be unitarily implemented concurrently with β^o are those for which $|T^+|^2 \in \mathscr{R}_H(T\mathscr{H})$, and the implementation of the automorphism groups can be done only in the representations isometrically equivalent to the Fock representation.

Suppose instead that H is bounded away from zero, and $|RT^+|^2 \in \mathscr{R}_H(T\mathscr{H})$. Then since $\mathscr{R}_H(T\mathscr{H}) = \mathscr{R}_I(T\mathscr{H})$ for such an H, we have $|RT^+|^2 - I \in B_{2r}(T\mathscr{H})$, that is (as in Sec. VI), $|R|^2 - |T|^2 \in B_{2r}(\mathscr{H})$. This implies that π_R is interchangeable with the representation π_T which naturally implements β. So in this case both automorphism groups must be implementable in the representation π_T if they are to be concurrently implemented in any representation π_R. Furthermore, since $|R|^2 = |T|^2 + (|R|^2 - |T|^2)$, the fact that $|R|^2 - |T|^2 \in B_{2r}(\mathscr{H})$ implies that $|R|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$ if and only if $|T|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$. Thus if H is bounded away from zero, the only automorphism groups β^o (induced by V_t^o) which can be unitarily implemented concurrently with β are those for which H^o satisfies $|T|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$, and the implementation of the automorphism groups can only be done in the representations interchangeable with π_T.

In the case where both generators H^o and H have spectra bounded away from zero, the criteria $|R|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$ and $|RT^+|^2 \in \mathscr{R}_H(T\mathscr{H})$ for the concurrent unitary implementation of β and β^o in π_R reduce, by the preceding observations, to

$$|R|^2 - I \in B_{2r}(\mathscr{H}) \quad \text{and} \quad |T^+|^2 \in \mathscr{R}_H(T\mathscr{H}),$$
$$|R|^2 - |T|^2 \in B_{2r}(\mathscr{H}) \quad \text{and} \quad |T|^2 \in \mathscr{R}_{H^o}(\mathscr{H}).$$

The left-hand conditions immediately imply $|T|^2 - I \in B_{2r}(\mathscr{H})$, so T then automatically satisfies $|T|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$. Then, since $|T^+|^2 - I = T^{*+}(I - |T|^2)T^+ + (TT^+ - I)$, and since $(TT^+ - I)$ vanishes on $T\mathscr{H}$, it follows that $|T^+|^2 \in \mathscr{R}_H(T\mathscr{H})$ is satisfied also.

In this situation β^o and β must be implementable in the Fock representation if they are to be implementable in any representation π_R. Furthermore, for that to be possible, T must be isometrically implementable in the Fock representation. In this case, when no massless excitations occur in the theory, all objects of a well-formulated second-quantized theory are accomodated by the Fock space.

The situation is much less restrictive when massless particles occur in the theory. Then the spectra of the Hamiltonians extend to zero, and the sets $\mathscr{R}_H(\mathscr{H})$ can be much larger than $\mathscr{R}_I(\mathscr{H})$. This circumstance allows the framework to accommodate models with interactions that are more than small perturbations of the uncoupled dynamics, as is demonstrated by the example in [II].

IX. ALGEBRAIC VERSUS REPRESENTATION-DEPENDENT CONSTRUCTION OF A SCATTERING OPERATOR

In Sec. III we contemplated two formulations of scattering theory for the models studied here. We now review the two in light of the information established above.

Consider first the possibility of constructing wave operators directly on the Hilbert space which carries a representation π_R of $\mathscr{W}$. We have seen that concurrent implementation of the two automorphism groups β^o and β in π_R requires that $|R|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$ and $|RT^+|^2 \in \mathscr{R}_H(T\mathscr{H})$, where the set $\mathscr{R}_H(\mathscr{K})$ is defined in Sec. VI. We have also seen that the representations π_I and π_T determined by the states invariant under β^o and β, resepectively, are isometrically equivalent if and only if $|T|^2 - I \in B_{2r}(\mathscr{H})$. Therefore, if the diagonalization transformation T is so mild that π_I and π_T are isometrically equivalent, we may choose $R = I$ (choose π_R to be the Fock representation) or $R = T$ (choose π_R to be the interaction-vacuum representation) to obtain a representation π_R in which the automorphism groups have concurrent implementation. If π_I and π_T are inequivalent, we have seen that because $\mathscr{R}_H(\mathscr{K})$ is properly larger than $\mathscr{R}_I(\mathscr{K})$, there may still exist a representation π_R admitting implementation of both automorphism groups. Such a situation occurs in [II].

Whether the limit expressions for the wave operators converge in such a representation is a different question. For the particular model analyzed in [II], we find that these "second-quantized" expressions do not converge, although symplectic transformation which induce wave morphisms do exist. This fact shows that the idea of constructing a scattering operator in a fixed representation that carries concurrent unitary implementation of the automorphism groups is not sufficiently general to treat all theories of physical interest.

We therefore consider second the more algebraic construction of wave morphisms indicated earlier. We have seen that in order for the strong limits $\Omega_\pm$ to be partial symplectic transformations, it is sufficient that $(I - P_m) \times (\Lambda HT - T\Lambda H^o)(I - P_m^o)$ be in the trace class for all m larger than some fixed $M > 0$. That is, if for finite energies T intertwines ΛH and ΛH^o modulo the trace class, then $\Omega_\pm$ exist and induce wave morphisms on $\mathscr{W}$. Note that this construction is representation independent; whether $\Omega_\pm$ are implementable in a given representation is another (largely irrelevant) question. Now, because $\Omega_\pm$ are partial symplectic transformations with the same final space, the operator $S \equiv (\Omega_+)^+\Omega_-$ is an invertible symplectic transformation on the initial space $P_{ac}^o\mathscr{H}$ of $\Omega_\pm$. The transformation S induces the scattering morphism σ; the implementability of σ in a given representation is of interest, and varies from model to model.

In [II] we apply this framework to study a model theory which, despite its extreme simplicity, displays many of the nontrivial representation-theoretic phenomena discussed here.

X. EXISTENCE AND COMPLETENESS OF MØLLER WAVE MORPHISMS

This section is devoted to a proof of Theorem 2. This proof is similar to the presentation of the Birman–Belopol'skii Theorem in Ref. 11, but differs in two major respects. Since here the identification map T is only real-linear, some extra complications arise. On the other hand,

the fact that T is a symplectic transformation allows some simplifications.

The proof of Theorem 2 relies on the following real-linear analog to Pearson's Theorem for two-Hilbert-space scattering.[11]

Theorem 6: Let H and H^o be complex-linear self-adjoint operators on $\mathscr{H}$. Let J be a bounded real-linear operator such that $(\Lambda HJ - J\Lambda H^o)$ is of trace class, in the sense that there exists $C \in B_{1r}(\mathscr{H})$ such that $\langle f|Cg\rangle = \langle Hf|\Lambda Jg\rangle - \langle f|J\Lambda H^o g\rangle$ for all $f \in D(H)$ and all $g \in D(H^o)$. Then

$$\Psi_{\pm}(H,H^o;J) \equiv \text{s-lim}_{t\to\pm\infty} e^{t\Lambda H} J e^{-t\Lambda H^o} P^o_{\text{ac}}$$

exist.

The proof of this theorem is the same as the proof of Pearson's Theorem in Ref. 11, but with $C = \Lambda HJ - J\Lambda H^o$ and attention to the fact that Λ does not commute with J. ///

Proof of Theorem 2: We first establish the existence of the indicated strong limits. Let

$$\Psi(t) \equiv e^{t\Lambda H} T e^{-t\Lambda H^o} P^o_{\text{ac}}$$

and

$$\Phi(t) \equiv e^{t\Lambda H^o} T^+ e^{-t\Lambda H} P_{\text{ac}}.$$

Then the existence of

$$\Omega_{\pm} \equiv \text{s-lim}_{t\to\pm\infty} T^+ e^{t\Lambda H} T e^{-t\Lambda H^o} P^o_{\text{ac}}$$

is guaranteed by the existence of

$$\Psi_{\pm} \equiv \text{s-lim}_{t\to\pm\infty} \Psi(t);$$

we prove the latter.

For $m > 0$, define $J_m \equiv (I - P_m)T(I - P^o_m)$. By hypothesis, $(\Lambda HJ_m - J_m\Lambda H^o) \in B_{1r}(\mathscr{H})$, for all $m > M$. By the analog to Pearson's Theorem above, it follows that for $m > M$,

$$\Psi_{\pm}(H,H^o;J_m) \equiv \text{s-lim}_{t\to\pm\infty} e^{t\Lambda H} J_m e^{-t\Lambda H^o} P^o_{\text{ac}}$$

exist.

Now fix $\mu > M$, and consider $g \in (I - P^o_\mu)\mathscr{H}$. Then for $m > \mu$, $(I - P^o_m)g = g$, so that the norm limit

$$\lim_{t\to\pm\infty} e^{t\Lambda H}(I - P_m) T e^{-t\Lambda H^o} P^o_{\text{ac}} g = \Psi_{\pm}(H,H^o;J_m)g$$

exists. To demonstrate the existence of

$$\lim_{t\to\pm\infty} \Psi(t)g = \lim_{t\to\pm\infty} e^{t\Lambda H} T e^{-t\Lambda H^o} P^o_{\text{ac}} g,$$

it therefore suffices to show that

$$\lim_{m\to\infty} \sup_{t\in\mathbf{R}} \|P_m T e^{-t\Lambda H^o} P^o_{\text{ac}} g\| = 0.$$

To do this, we make use of the fact that H and H^o are mutually subordinate with respect to the identification map T, which follows from the condition $TD(H^o) = D(H)$.

Note first that, by virtue of the non-negativity of H and H^o and the condition $TD(H^o) = D(H)$, the operator

$$(I + H)T(I + H^o)^{-1}$$

has in its domain all $f \in \mathscr{H}$, and hence is bounded.

Next note that because $g \in (I - P^o_\mu)\mathscr{H}$, $g \in D(I + H^o)$. Thus

$$\begin{aligned}
&\|P_m T e^{-t\Lambda H^o} P^o_{\text{ac}} g\| \\
&\quad = \|P_m T(I + H^o)^{-1}(I + H^o) e^{-t\Lambda H^o} P^o_{\text{ac}} g\| \\
&\quad = \|(I + H)^{-1} P_m (I + H) T (I + H^o)^{-1} \\
&\qquad \times (I + H^o) e^{-t\Lambda H^o} P^o_{\text{ac}} g\| \\
&\quad \leqslant [1/(1 + m)]\|(I + H)T(I + H^o)^{-1}\| \cdot \|(I + H^o)g\| \\
&\quad \leqslant [(1 + \mu)/(1 + m)]\|(I + H)T(I + H^o)^{-1}\| \|g\|.
\end{aligned}$$

Therefore,

$$\lim_{m\to\infty} \sup_{t\in\mathbf{R}} \|P_m T e^{-t\Lambda H^o} P^o_{\text{ac}} g\| = 0,$$

for $g \in (I - P^o_\mu)\mathscr{H}$, as desired.

It follows that $\lim_{t\to\pm\infty} \Psi(t)g$ exists for $g \in (I - P^o_\mu)\mathscr{H}$. Since $\text{s-lim}_{\mu\to\infty}(I - P^o_\mu) = I$ and since $\|\Psi(t)\|$ is bounded in t, we have $\Psi_{\pm} \equiv \text{s-lim}_{t\to\pm\infty} \Psi(t)$ exists.

It is convenient to establish the existence of the limit $\Phi_{\pm} \equiv \text{s-lim}_{t\to\pm\infty} \Phi(t)$ as well. To do this, we simply note that the hypothesis $D(H) = TD(H^o)$ implies $T^+D(H) = T^+TD(H^o) = D(H^o)$, and that taking the adjoint with respect to B of the other hypothesis gives

$$(I - P^o_m)(\Lambda H^o T^+ - T^+\Lambda H)(I - P_m) \in B_{1r}(\mathscr{H}).$$

Then by interchanging H^o with H, and T^+ with T, in the preceding argument, we immediately conclude that $\Phi_{\pm} \equiv \text{s-lim}_{t\to\pm\infty} \Phi(t)$ exists.

We next establish that if $e^{t\Lambda H}$ preserves $T\mathscr{H}$ then the real-linear operator $\Omega_- = T^+\Psi_-$ satisfies the conditions $\Omega^{\pm}_-\Omega_- = P^o_{\text{ac}}$ and $\Omega_-\Omega^{\pm}_- = T^+P_{\text{ac}}T$, and that $\Omega_+ = T^+\Psi_+$ satisfies the corresponding conditions; these facts will complete the proof.

Because TT^+ is the complex-linear projection onto $T\mathscr{H}$, the hypothesis $e^{t\Lambda H}T\mathscr{H} \subset T\mathscr{H}$ means that TT^+ commutes on $T\mathscr{H}$ with $e^{t\Lambda H}$, and with P_{ac} as well. Thus $TT^+\Psi(t) = \Psi(t)$ for all t, and it follows that $TT^+\Psi_{\pm} = \Psi_{\pm}$.

Because $\Psi(t)^+\Psi(t) = P^o_{\text{ac}}$ and because $\Psi(t)$ is uniformly bounded in norm, it is not difficult to show that $\Psi^{\pm}_-\Psi_- = \Psi^{\pm}_+\Psi_+ = P^o_{\text{ac}}$. Therefore $\Omega^{\pm}_-\Omega_- = \Psi^{\pm}_-TT^+\Psi_- = \Psi^{\pm}_-\Psi_- = P^o_{\text{ac}}$, and similarly $\Omega^{\pm}_+\Omega_+ = P^o_{\text{ac}}$, as claimed.

To show that $\Omega_{\pm}\Omega^{\pm}_{\pm} = T^+P_{\text{ac}}T$, we will show that $\text{ran}\,\Psi_{\pm} = P_{\text{ac}}T\mathscr{H}$. It then follows that $\Psi_{\pm}$ are partial symplectic transformations with initial space $P^o_{\text{ac}}\mathscr{H}$ and final space $P_{\text{ac}}T\mathscr{H}$, whence

$$\begin{aligned}
&\Omega_{\pm}\Omega^{\pm}_{\pm} \\
&\quad = T^+\Psi_{\pm}\Psi^{\pm}_{\pm}T = T^+(P_{\text{ac}}TT^+)T = T^+P_{\text{ac}}T,
\end{aligned}$$

as claimed.

The demonstration that $\text{ran}\,\Psi_{\pm} = P_{\text{ac}}T\mathscr{H}$, which completes the proof, proceeds in two steps. First we show that $\text{ran}\,\Psi_{\pm} \subset P_{\text{ac}}T\mathscr{H}$, then, second, we make use of the properties of $\Phi_{\pm}$ to show that $P_{\text{ac}}T\mathscr{H} \subset \text{ran}\,\Psi_{\pm}$.

By virtue of the fact that $\Psi^{\pm}_{\pm}\Psi_{\pm} = P^o_{\text{ac}}$ and $\Psi_{\pm}P^o_{\text{ac}} = \Psi_{\pm}$, we have $\ker\Psi_{\pm} = (I - P^o_{\text{ac}})\mathscr{H}$. It follows easily that (see Appendix B)

$$(\mathrm{ran}|\Psi_\pm|)' = (\mathrm{ran}|\Psi_\pm|)_\perp = \ker\ \Psi_\pm ,$$

whence $\overline{(\mathrm{ran}|\Psi_\pm|)} = P^o_{\mathrm{ac}}\mathscr{H}$.

Now let $\Psi_\pm = Z_\pm|\Psi_\pm|$ be the real polar decomposition of $\Psi_\pm$. We know that $Z_\pm$ are partial real isometries with $\ker Z_\pm = \ker \Psi_\pm = (I - P^o_{\mathrm{ac}})\mathscr{H}$ and $\mathrm{ran}\, Z_\pm = \overline{\mathrm{ran}\, \Psi_\pm}$. Now, from the definition of $\Psi_\pm$, it is clear that $e^{-tAH}\Psi_\pm\, e^{tAH^o} = \Psi_\pm$. Using this and its adjoint, we conclude that $[|\Psi_\pm|, e^{-tAH^o}] = 0$. Therefore, $e^{-tAH}\Psi_\pm = \Psi_\pm\, e^{-tAH^o}$ (*) implies $e^{-tAH}Z_\pm|\Psi_\pm| = Z_\pm|\Psi_\pm| \times e^{-tAH^o} = Z_\pm\, e^{-tAH^o}|\Psi_\pm|$. So $e^{-tAH}Z_\pm = Z_\pm\, e^{-tAH^o}$ on $\overline{(\mathrm{ran}|\Psi_\pm|)} = P^o_{\mathrm{ac}}\mathscr{H}$. Furthermore, (*) implies that e^{-tAH^o} leaves $\ker\Psi_\pm = \ker Z_\pm = (I - P^o_{\mathrm{ac}})\mathscr{H}$ invariant, so that

$$e^{-tAH}Z_\pm = Z_\pm\, e^{-tAH^o} = 0$$

on $(I - P^o_{\mathrm{ac}})\mathscr{H}$. Therefore $e^{-tAH}Z_\pm = Z_\pm\, e^{-tAH^o}$ on all of $\mathscr{H}$, and since $H^o \restriction_{(\ker Z_\pm)'} = H^o \restriction_{P^o_{\mathrm{ac}}\mathscr{H}}$ is purely absolutely continuous, and since $Z_\pm$ is isometric, it follows that $H \restriction_{(\mathrm{ran}\, Z_\pm)} = H \restriction_{\overline{\mathrm{ran}\, \Psi_\pm}}$ is purely absolutely continuous. Thus $P_{\mathrm{ac}}\Psi_\pm = \Psi_\pm$, and since furthermore $TT^+\Psi_\pm = \Psi_\pm$, we have

$$\mathrm{ran}\ \Psi_\pm \subset P_{\mathrm{ac}}T\mathscr{H},$$

as desired.

To demonstrate the reverse inclusion, we repeat the argument above for $\Phi_\pm$ in place of $\Psi_\pm$. The same statements, with T interchanged with T^+, H^o interchanged with H, and P^o_{ac} interchanged with $P_{\mathrm{ac}}TT^+$, show that

$$\mathrm{ran}\ \Phi_\pm \subset P^o_{\mathrm{ac}}\mathscr{H}.$$

If we now write

$$\Psi(t)\Phi(t) = TT^+P_{\mathrm{ac}} - e^{tAH}\,Te^{-tAH^o}(I - P^o_{\mathrm{ac}})\Phi(t)$$

and take the strong limit, using the uniform boundedness of $\Psi(t)$ and $\Phi(t)$, we obtain

$$\Psi_+\Phi_+ = \Psi_-\Phi_- = TT^+P_{\mathrm{ac}} = P_{\mathrm{ac}}TT^+.$$

Therefore $P_{\mathrm{ac}}T\mathscr{H} \subset \mathrm{ran}\ \Psi_\pm$, as desired. It follows that $\mathrm{ran}\ \Psi_\pm = P_{\mathrm{ac}}T\mathscr{H}$, which completes the proof. ///

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APPENDIX A: REAL-LINEAR TRANSFORMATIONS

The framework in the text involves the reinterpretation of a complex Hilbert space as a real Hilbert space, with the real inner product being given by the real part of the complex inner product. Here the complex Hilbert space is *not* a complexification of the real Hilbert space, nor is the real Hilbert space the real linear span of a basis for the complex space. Rather, the same set $\mathscr{H}$ of vectors is regarded as being a Hilbert space under two (related) inner products, as follows.

Let $(\mathscr{H},\langle|\rangle)$ be a separable complex Hilbert space with (complex-valued) inner product $\langle|\rangle$. It is easy to see that the set $\mathscr{H}$ is also an inner product space (over the scalars $\mathbb{R}$) under the real-valued inner product $\mathrm{Re}\,\langle|\rangle$ induced by $\langle\ |\ \rangle$. Because furthermore $\langle f|f\rangle = \mathrm{Re}\langle f|f\rangle$, the norm induced by the real inner product is identical to the (usual) norm induced by $\langle|\rangle$. Thus $(\mathscr{H},\mathrm{Re}\langle|\rangle)$ is a real Hilbert space.

Most of the results for complex Hilbert spaces also hold for their reinterpretations as real Hilbert spaces. [A notable exception is the recovery of (the matrix elements of) a bounded operator from its expectation values alone.] This appendix is a review of those results needed for the analysis in the text which are real-linear analogs of standard results for complex Hilbert spaces and complex-linear operators. The complex-linear versions can all be found in the book by Reed and Simon;[19] most of the proofs can easily be adapted to the real-linear situation.

To begin on firm ground, note that if $\{h_n|n = 1,...,\infty\}$ is an orthonormal basis for the complex Hilbert space $(\mathscr{H},\langle|\rangle)$ then the set $\{h_n, ih_n|n = 1,...,\infty\}$ is an orthonormal basis for the real Hilbert space $(\mathscr{H},\mathrm{Re}\langle|\rangle)$. It is easy to see that the Bessel and Schwarz inequalities, the parallelogram law, and the Pythagorean theorem all hold for the real Hilbert space. Furthermore, if M is any real-linear manifold of the real Hilbert space $\mathscr{H}$, then its real-orthogonal complement

$$M_\perp \equiv \{f \in \mathscr{H} | \mathrm{Re}\langle f|g\rangle = 0,\ \text{for all}\ g \in M\}$$

is easily shown to be a closed real-linear subspace of $\mathscr{H}$. Real-linear versions of the projection theorem and the Riesz lemma are also easy to prove.

Definition: A bounded *real-linear transformation* is a map $T:\mathscr{H}\to\mathscr{H}$ such that $T(af + bg) = aT(f) + bT(g)$ for all $f,g \in \mathscr{H}$ and all $a,b, \in \mathbb{R}$, and such that for some $c \geq 0$, $\|T(f)\| \leq c\|f\|$ for all $f \in \mathscr{H}$.

Denote by Λ the operation of multiplication by the complex number i on the Hilbert space $\mathscr{H}$; Λ is a real-linear transformation. Real-linear transformations do not in general commute with Λ; those that do are called complex linear. Clearly Λ is a complex-linear transformation, and $\Lambda^{-1} = -\Lambda$. Note that the complex inner product can be expressed in terms of the real inner product by the use of Λ: $\langle f|g\rangle = \mathrm{Re}\langle f|g\rangle + i\,\mathrm{Re}\,\langle \Lambda f|g\rangle = \mathrm{Re}\langle f|g\rangle - i\,\mathrm{Re}\langle f|\Lambda g\rangle$. Note also that a real-linear transformation is uniquely decomposed into complex-linear and complex-antilinear parts by

$$Q_l \equiv (Q + \Lambda^{-1}Q\Lambda)/2,$$

$$Q_a \equiv (Q - \Lambda^{-1}Q\Lambda)/2,$$

so that $Q_l\Lambda = \Lambda Q_l$ and $Q_a\Lambda = -\Lambda Q_a$.

It is easy to verify that if $T:\mathscr{H}\to\mathscr{H}$ is a bounded real-linear transformation, there exists a unique bounded real-linear transformation $T^*:\mathscr{H}\to\mathscr{H}$ such that $\mathrm{Re}\langle T^*f|g\rangle = \mathrm{Re}\langle f|Tg\rangle$, for all $f,g \in \mathscr{H}$. The transformation T^* is called the *real adjoint* of T. If T is complex linear then T^* is the usual adjoint of T with respect to $\langle|\rangle$, because then $\langle h|g\rangle = \mathrm{Re}\langle h|g\rangle - i\,\mathrm{Re}\langle h|\Lambda g\rangle$ implies

$$\begin{aligned}\langle T^*f|g\rangle &= \mathrm{Re}\langle T^*f|g\rangle - i\,\mathrm{Re}\langle T^*f|\Lambda g\rangle \\ &= \mathrm{Re}\langle f|Tg\rangle - i\mathrm{Re}\langle f|T\Lambda g\rangle \\ &= \mathrm{Re}\langle f|Tg\rangle - i\,\mathrm{Re}\langle f|\Lambda Tg\rangle = \langle f|Tg\rangle.\end{aligned}$$

Also, if T is purely antilinear then

$$\begin{aligned}\langle T^*f|g\rangle &= \mathrm{Re}\langle f|Tg\rangle - i\,\mathrm{Re}\langle f|T\Lambda g\rangle \\ &= \mathrm{Re}\langle f|Tg\rangle + i\,\mathrm{Re}\langle f|\Lambda Tg\rangle \\ &= \mathrm{Re}\langle Tg|f\rangle + i\,\mathrm{Re}\langle \Lambda Tg|f\rangle = \mathrm{Re}\langle Tg|f\rangle \\ &\quad - i\,\mathrm{Re}\langle Tg|\Lambda f\rangle = \langle Tg|f\rangle,\end{aligned}$$

so the real adjoint gives the usual adjoint of an antilinear operator.

It is furthermore clear that $T^{**} = T$ and $(ST)^* = T^*S^*$, and that if T has a bounded inverse then $(T^*)^{-1} = (T^{-1})^*$.

An important result for real-linear operators is the polar decomposition theorem, for which we need the notion of a positive real-linear operator. In contrast to the complex-linear situation, the condition $\mathrm{Re}\langle f|Qf\rangle \geq 0$ for all f in $\mathscr{H}$ does not alone imply that Q is self-real-adjoint, so here the latter is incorporated into the definition of positivity of a real-linear transformation.

Definition: A bounded real-linear transformation $Q:\mathscr{H}\to\mathscr{H}$ is said to be *positive* if Q is self-real-adjoint and $\mathrm{Re}\langle f|Qf\rangle \geq 0$, for all $f\in\mathscr{H}$.

Note that if $T:\mathscr{H}\to\mathscr{H}$ is a bounded real-linear transformation then T^*T is self-real-adjoint and also clearly positive. This circumstance allows the definition of $|T|$.

Square Root Lemma: Let $Q:\mathscr{H}\to\mathscr{H}$ be a positive bounded real-linear transformation. Then there is a unique positive bounded real-linear transformation $R:\mathscr{H}\to\mathscr{H}$ such that $R^2 = Q$. Furthermore, R commutes with every bounded real-linear operator which commutes with Q.

The proof of this lemma rests on the norm convergence of the power series in the operator $(I - Q)$ for the square root. The fact that Q is self-real adjoint is used in the conclusion that $\|I - Q\| \leq 1$ whenever $\|Q\| \leq 1$, which follows from the observation that

$$\|Q\| = \sup_{f\in\mathscr{H}} |\langle f|Qf\rangle|/\|f\|^2, \quad \text{for self-real-adjoint } Q.$$

The operator R in the lemma is, of course, denoted $Q^{1/2}$.

Since $Q = T^*T$ satisfies the hypotheses of the theorem, we can define the (self-real-adjoint) positive operator $|T| \equiv (T^*T)^{1/2}$.

Definition: A real-linear transformation $Z:\mathscr{H}\to\mathscr{H}$ is said to be a *real-isometry* if $\|Zf\| = \|f\|$ for all $f\in\mathscr{H}$. We say Z is a *partial real-isometry* if Z is an isometry when restricted to the real-orthogonal complement $(\ker Z)_\perp$ of its kernel.

The proof of the following theorem proceeds exactly as in the complex-linear case.

Polar Decomposition Theorem: Let $T:\mathscr{H}\to\mathscr{H}$ be a bounded real-linear transformation. Then there is a partial real isometry $Z:\mathscr{H}\to\mathscr{H}$ such that $T = Z|T|$. The operator Z is uniquely determined by the condition $\ker Z = \ker T$. Furthermore, the range of Z is the norm closure of the range of T in $\mathscr{H}$.

To discuss real-linear transformations of Hilbert–Schmidt type, we need to define the notion of the real trace of real-linear operators. It is not difficult to verify the following.

Trace Theorem: Let $\{f_n | n = 1,\ldots,\infty\}$ be a real-orthonormal basis for the separable real Hilbert space $(\mathscr{H},\mathrm{Re}\langle|\rangle)$. Let Q be a bounded positive real-linear transformation, and define the *trace* $\mathrm{tr}_r\, Q$ of Q by $\mathrm{tr}_r\, Q \equiv \Sigma_n \mathrm{Re}\langle f_n|Qf_n\rangle$. Then $\mathrm{tr}_r\, Q$ is independent of the real-orthonormal basis chosen.

The trace of an operator can of course be equal to infinity.

Definition: A bounded real-linear transformation $T:\mathscr{H}\to\mathscr{H}$ is said to be a *Hilbert–Schmidt operator* if $\mathrm{tr}_r(T^*T) < \infty$. The set of all real-linear Hilbert–Schmidt operators on $\mathscr{H}$ is denoted $B_{2r}(\mathscr{H})$. The subset of complex-linear operators in $B_{2r}(\mathscr{H})$ is denoted by $B_{2c}(\mathscr{H})$.

Since $\{h_n, \Lambda h_n\}$ is a real-orthonormal basis for $(\mathscr{H},\mathrm{Re}\langle|\rangle)$ whenever $\{h_n\}$ is a complex-orthonormal basis for $(\mathscr{H},\langle|\rangle)$, if T is a complex-linear operator then $\mathrm{tr}_r(T^*T) = \Sigma_n \mathrm{Re}\langle f_n|T^*Tf_n\rangle = \Sigma_n \mathrm{Re}\langle Tf_n|Tf_n\rangle = \Sigma_n \|Tf_n\|^2 = \Sigma_n(\|Th_n\|^2 + \|T(\Lambda h_n)\|^2) = 2\Sigma_n\|Th_n\|^2 = 2\,\mathrm{tr}_c(T^*T)$, where tr_c denotes the (usual) complex trace. So $B_{2c}(\mathscr{H})$ is the class of complex-linear Hilbert–Schmidt operators. Note furthermore that if T is either complex-linear or purely complex-antilinear then $\mathrm{tr}_r(T^*T) = \Sigma_n\|Tf_n\|^2 = \Sigma_n(\|Th_n\|^2 + \|T(\Lambda h_n\|^2) = 2\Sigma_n\|Th_n\|^2 = 2\Sigma_{n,m}|\langle h_m|Th_n\rangle|^2$, with $\{h_n\}$ a complex-orthonormal basis.

Just as in the complex-linear case, the set $B_{2r}(\mathscr{H})$ is a $*$ ideal in the bounded real-linear operators. This property of $B_{2r}(\mathscr{H})$ is of great utility in the computations in the text.

Theorem: $B_{2r}(\mathscr{H})$ is a $*$ ideal in the bounded real-linear transformations, that is, (a) $B_{2r}(\mathscr{H})$ is a real vector space, (b) if $Q\in B_{2r}(\mathscr{H})$ then $Q^*\in B_{2r}(\mathscr{H})$, and (c) if $Q\in B_{2r}(\mathscr{H})$ and $R:\mathscr{H}\to\mathscr{H}$ is a bounded real-linear transformation, then QR and RQ are both in $B_{2r}(\mathscr{H})$.

Also, just as in the complex-linear situation, the set $B_{2r}(\mathscr{H})$ of real-linear transformations forms a Banach space over $\mathbb{R}$ with the norm $\|T\|_{2r} \equiv (\mathrm{tr}_r(T^*T))^{1/2}$, and the finite-rank real-linear operators are $\|\cdot\|_{2r}$ dense in $B_{2r}(\mathscr{H})$. Furthermore, if $Q\in B_{2r}(\mathscr{H})$ and R is a bounded real-linear transformation, then $\|Q^*\|_{2r} = \|Q\|_{2r}, \|QR\|_{2r} \leq \|R\|\|Q\|_{2r}$, and $\|RQ\|_{2r} \leq \|R\|\|Q\|_{2r}$, just as in the complex-linear theory.

Since $B_{2r}(\mathscr{H})$ is an ideal, it follows immediately that the linear and antilinear parts Q_l and Q_a of Q are elements of $B_{2r}(\mathscr{H})$ if and only if $Q\in B_{2r}(\mathscr{H})$. Furthermore, because $\{\Lambda f_j\}$ is a real-orthonormal basis for $\mathscr{H}$ whenever $\{f_j\}$ is a real-orthonormal basis for $\mathscr{H}$, if $Q\in B_{2r}(\mathscr{H})$ then $\mathrm{tr}_r(Q^*Q) = \mathrm{tr}_r(\Lambda^* Q^* Q\Lambda)$. It then follows, by the linearity of the trace over positive operators, that $\mathrm{tr}_r(Q^*Q) = \mathrm{tr}_r(Q_l^*Q_l) + \mathrm{tr}_r(Q_a^*Q_a)$.

APPENDIX B: SYMPLECTIC TRANSFORMATIONS

A symplectic space is a real linear space L with a nondegenerate skew-symmetric bilinear form $B:L\times L\to\mathbb{R}$. Real-linear transformations taking (domains in) L into L which preserve the symplectic form B are called symplectic transformations.

Here we take L to be the real Hilbert space $(\mathscr{H},\mathrm{Re}\langle|\rangle)$ introduced in Appendix A, and we let B be the nondegenerate skew form given by $B(f,g) \equiv \mathrm{Im}\langle f|g\rangle$ for f and g in the set $\mathscr{H}$. This special relationship between the complex and the symplectic structures on $\mathscr{H}$ is natural for the treatment of the model field theories under study.

Denote by Λ the operation of multiplication by the complex number i on $\mathscr{H}$. Then $B(f,g) \equiv \mathrm{Im}\langle f|g\rangle = \mathrm{Re}\langle \Lambda f|g\rangle$ and $\mathrm{Re}\langle f|g\rangle = B(f,\Lambda g) = \mathrm{Im}\langle f|\Lambda g\rangle$. If $Q:\mathscr{H}\to\mathscr{H}$ is an arbitrary bounded real-linear transformation, its real adjoint Q^* is also a bounded real-linear transformation. We define another bounded real-linear transformation $Q^+:\mathscr{H}\to\mathscr{H}$ by $Q^+ \equiv \Lambda^{-1}Q^*\Lambda$. Note that

$$B(Q^+f,g) = B(\Lambda^{-1}Q^*\Lambda f,g) = \mathrm{Re}\langle \Lambda(\Lambda^{-1}Q^*\Lambda f)|g\rangle$$
$$= \mathrm{Re}\langle Q^*\Lambda f|g\rangle = \mathrm{Re}\langle \Lambda f|Qg\rangle = B(f,Qg).$$

The transformation Q^+ is thus called the *adjoint* of Q *with respect to* B. It follows from the nondegeneracy of B that the transformation Q^+ satisfying $B(Q^+f,g) = B(f,Qg)$ is unique. Note that $\Lambda^+ = \Lambda^* = \Lambda^{-1} = -\Lambda$.

In the following, a real linear manifold in $\mathscr{H}$ will be called a *subspace*; here a subspace is not necessarily closed. For any subspace M of $\mathscr{H}$, define

$$M' \equiv \{f\in\mathscr{H} | B(f,g) = 0, \text{ for all } g\in M\}.$$

It is easy to show that if M is a complex subspace of $\mathscr{H}$ (that is, $\Lambda M = M$) then $M' = M_\perp$, and henceforth if M is complex, $M_\perp$ will be written M'.

Lemma: Let $Q:\mathscr{H}\to\mathscr{H}$ be a bounded real-linear transformation. Then $(\mathrm{ran}|Q|)_\perp = \ker Q$. If furthermore $(\ker Q)$ is a complex subspace of $\mathscr{H}$, then $\overline{\mathrm{ran}|Q|}$ is also a complex subspace.

Proof: To show that $(\mathrm{ran}|Q|)_\perp = \ker Q$, note that if $f\in\ker Q$, then for all $g\in\mathscr{H}$, $\mathrm{Re}\langle f||Q|g\rangle = \mathrm{Re}\langle |Q|f|g\rangle = 0$. Thus $(\ker Q)\subset(\mathrm{ran}|Q|)_\perp$. Conversely, if $f\in(\mathrm{ran}|Q|)_\perp$ then for all $g\in\mathscr{H}$, $0 = \mathrm{Re}\langle f||Q|g\rangle$. Choose $g\equiv|Q|f$ to get $0 = \mathrm{Re}\langle f||Q|^2f\rangle = \mathrm{Re}\langle Qf|Qf\rangle = \|Qf\|^2$, whence $f\in\ker Q$, that is, $(\ker Q)\supset(\mathrm{ran}|Q|)_\perp$.

For the second assertion, suppose $(\ker Q)$ is complex, and let $f\in\overline{(\mathrm{ran}|Q|)} = (\ker Q)_\perp$. Then for all $g\in\ker Q$ we have $\mathrm{Re}\langle \Lambda f|g\rangle = \mathrm{Re}\langle f|\Lambda^*g\rangle = 0$ because $\Lambda^*g\in\ker Q$. Thus $\Lambda f\in(\ker Q)_\perp = \overline{\mathrm{ran}|Q|}$ whenever $f\in\overline{\mathrm{ran}|Q|}$, that is, $\overline{\mathrm{ran}|Q|}$ is a complex subspace. ///

If M is a subspace of $\mathscr{H}$, then the form B is said to be *nondegenerate* on M if $f\in M$ and $B(f,g) = 0$ for all $g\in M$ imply $f = 0$. Note that if M is any complex subspace of $\mathscr{H}$ then B (defined as the imaginary part of the inner product) is nondegenerate on M, because

$$f\in M \text{ and } B(f,g) = 0, \quad \text{for all } g\in M$$
$$\text{iff } f\in M \text{ and } \mathrm{Re}\langle \Lambda f|g\rangle = 0, \quad \text{for all } g\in M,$$

which implies $\mathrm{Re}\langle \Lambda f|\Lambda f\rangle = 0$, that is, $f = 0$.

Definition: A bounded real-linear transformation $S:\mathscr{H}\to\mathscr{H}$ will be called a *partial symplectic transformation* if $(\ker S)$ and $(\mathrm{ran}\,S)$ are complex subspaces of $\mathscr{H}$ and $B(Sf,Sg) = B(f,g)$ for all f and g in $(\ker S)'$.

Remark: If $Q:\mathscr{H}\to\mathscr{H}$ is any bounded (hence continuous) real-linear transformation, then $(\ker Q)$ is closed because it is the inverse image of the closed set $\{0\}$, and both $(\ker Q)'$ and $(\mathrm{ran}\,Q)'$ are closed because the orthogonal complement of any subspace is closed. Although $(\mathrm{ran}\,Q)$ is a subspace, it is not *a priori* closed. It will turn out, however, that $(\mathrm{ran}\,S)$ is, in fact, closed if S is partially symplectic.

Definition: A bounded real-linear transformation $S:\mathscr{H}\to\mathscr{H}$ will be called a *symplectic transformation* if S is a partial symplectic transformation and $(\ker S) = \{0\}$, that is, $B(Sf,Sg) = B(f,g)$ for all f and g in $\mathscr{H}$.

Remark: This definition is somewhat different from those usually made in the literature. On one hand, it is less general because it requires $(\mathrm{ran}\,S)$ to be a complex subspace. On the other hand, it is more general because it allows S to have range smaller than the entire space.

Definition: A bounded real-linear transformation $S:\mathscr{H}\to\mathscr{H}$ will be called an *invertible symplectic transformation* if S is a symplectic transformation and $(\mathrm{ran}\,S) = \mathscr{H}$.

Definition: Let $M\subset\mathscr{H}$ be a closed complex subspace. A partial symplectic transformation $S:\mathscr{H}\to\mathscr{H}$ will be said to be an *invertible symplectic transformation on* M if $M\subset(\ker S)'$ and $SM = M$.

The relationship between the complex and symplectic structures on $\mathscr{H}$ induces several nice properties of partial symplectic transformations which are listed below.

Theorem: Let $S:\mathscr{H}\to\mathscr{H}$ be a partial symplectic transformation. Then we have the following.

(1) Each of $(\ker S)$, $(\ker S)'$, $(\mathrm{ran}\,S)$, and $(\mathrm{ran}\,S)'$ is a closed complex subspace of $\mathscr{H}$.

(2) Both S^+S and SS^+ are complex-linear self-adjoint projections, and

$$\text{(Initial subspace of } S) \equiv (\ker S)' = (\mathrm{ran}\,S^+) = S^+S\mathscr{H} = S^+\mathscr{H}$$
$$\equiv \text{(Final subspace of } S^+),$$
$$(\ker S) = (\mathrm{ran}\,S^+)' = (I - S^+S)\mathscr{H},$$
$$\text{(Final subspace of } S) \equiv (\mathrm{ran}\,S) = (\ker S^+)' = SS^+\mathscr{H}$$
$$= S\mathscr{H} \equiv \text{(Initial subspace of } S^+),$$
$$(\mathrm{ran}\,S)' = (\ker S^+) = (I - SS^+)\mathscr{H}.$$

(3) $S = SS^+S$ and $S^+ = S^+SS^+$.

(4) S^+ is a partial symplectic transformation whenever S is a partial symplectic transformation.

The proof of this theorem involves the straightforward verification of several assertions. Although there are many steps, none is difficult, and we omit the details.

With the basic facts in the above theorem, we can develop several results used in the text.

Lemma: Let $R:\mathscr{H}\to\mathscr{H}$ and $S:\mathscr{H}\to\mathscr{H}$ be symplectic transformations. Then $RS^+:\mathscr{H}\to\mathscr{H}$ is a partial symplectic transformation.

Proof: By virtue of the facts that R and S are partially symplectic and $\ker R = \ker S = \{0\}$, it follows that $S^+S = R^+R = I$. Because $\ker R = \{0\}$, $\ker RS^+ = \ker S^+$. Furthermore, $RS^+\mathscr{H} = RS^+S\mathscr{H} = R\mathscr{H}$, so that $\mathrm{ran}\,RS^+ = \mathrm{ran}\,R$. Thus $\ker RS^+$ and $\mathrm{ran}\,RS^+$ are complex subspaces. Now suppose $f,g\in(\ker RS^+)' = (\ker S^+)'$, and consider $B(RS^+f,RS^+g)$. Because $(\ker R)' = \mathscr{H}$, S^+f and S^+g are in $(\ker R)'$, so $B(RS^+f,RS^+g) = B(S^+f,S^+g) = B(f,g)$ because $f,g\in(\ker S^+)'$. Thus RS^+ is a partial symplectic transformation, as claimed. ///

Lemma: Let $T:\mathscr{H}\to\mathscr{H}$ be a partial symplectic transformation and let $S\equiv|T|^2\equiv T^*T$. Then S is an invertible symplectic transformation on $T^+T\mathscr{H}$, with $S^+S = SS^+ = T^+T$.

Proof: First we find ker S and ran S. Because $T^*Tf=0$ if and only if $Tf=0$, we have ker $S=$ ker $T=(I-T^+T)\mathscr{H}$ and $(\ker S)'=(\ker T)'=T^+T\mathscr{H}$. Next,

$$\text{ran } S=S\mathscr{H}=T^*T\mathscr{H}=\Lambda T^+\Lambda^*T\mathscr{H}=\Lambda T^+T\mathscr{H}$$
$$=\Lambda(\ker T)'=(\ker T)',$$

that is, ran $S=(\ker T)'=T^+T\mathscr{H}$.

Now we establish the preservation of B on $T^+T\mathscr{H}$. Let $f,g\in(\ker S)'=T^+T\mathscr{H}$. Then

$$B(Sf,Sg)=B(T^*Tf,T^*Tg)$$
$$=B(\Lambda T^+\Lambda^*Tf,\Lambda T^+\Lambda^*Tg)$$
$$=B(T^+\Lambda^*Tf,T^+\Lambda^*Tg).$$

Now, because ran $T=(\ker T^+)'$ is a complex subspace, $\Lambda^*Tf\in(\ker T^+)'$. Thus $B(Sf,Sg)=B(\Lambda^*Tf,\Lambda^*Tg)=B(Tf,Tg)=B(f,g)$ because $f,g\in T^+T\mathscr{H}=(\ker T)'$. So S preserves B on $T^+T\mathscr{H}$, ker $S=(T^+T\mathscr{H})'$, and ran $S=T^+T\mathscr{H}$.

Furthermore, $S^+S=T^+T^{*+}T^*T=T^+(TT^+)^*T=T^+TT^+T=T^+T$, and $SS^+=T^*TT^+T^{*+}=(T^+T^{*+}T^*T)^*=(T^+T)^*=T^+T$, as asserted.

Finally, $S(T^+T\mathscr{H})=SS^+S\mathscr{H}=S\mathscr{H}=T^+T\mathscr{H}$, so S is invertible on $T^+T\mathscr{H}$. ///

Corollary: If $T:\mathscr{H}\to\mathscr{H}$ is a symplectic transformation, then $|T|^2\equiv T^*T$ is an invertible symplectic transformation on all of $\mathscr{H}$.

Lemma: Let $S:\mathscr{H}\to\mathscr{H}$ be an invertible symplectic transformation on $K\subset\mathscr{H}$, and let P be the projection onto K. Then $S^+SP=SS^+P=P$.

Proof: By definition, $K\subset(\ker S)'$, $SK=K$, and $S:\mathscr{H}\to\mathscr{H}$ is partially symplectic. So for all $f,g\in K$, $B(Sf,Sg)=B(f,g)$, that is, $B(f,S^+Sg)=B(f,g)$ for all $f,g\in K$. Because K is a complex subspace, B is nondegenerate on K and so the above implies $S^+Sg=g$ for all $g\in K$, that is, $S^+SP=P$. This furthermore implies $SS^+Sg=Sg$ for all $g\in K$, that is, $SS^+f=f$ for all $f\in SK=K$. Thus $SS^+P=P$. ///

Lemma: Let $Q:\mathscr{H}\to\mathscr{H}$ be a partial symplectic transformation and let V be an invertible symplectic transformation on ran Q. Then $Y\equiv Q^+VQ$ is an invertible symplectic transformation on $Q^+Q\mathscr{H}$.

Proof: Because V is an invertible symplectic transformation on ran $Q=QQ^+\mathscr{H}=Q\mathscr{H}$,

$$V^+V(QQ^+)=VV^+(QQ^+)=QQ^+.$$

First we find ker Y:

ker Y

$$=\ker(Q^+(VQ))=(\ker VQ)\cup(VQ)^{-1}(\ker Q^+)$$
$$=(\ker Q)\cup(VQ)^{-1}((\text{ran } Q)').$$

Now, because $VQ\mathscr{H}=Q\mathscr{H}$, $VQ=QQ^+VQ$ so $(VQ)^{-1}((\text{ran } Q)')=\{0\}$ and ker $Y=$ ker Q. Thus $(\ker Y)'=(\ker Q)'=Q^+Q\mathscr{H}$.

Next we find ran Y: ran $Y=Y\mathscr{H}=Q^+VQ\mathscr{H}=Q^+Q\mathscr{H}$, and so ran $Y=$ ran $Q^+=(\ker Q)'$. Furthermore, $Y(Q^+Q\mathscr{H})=Q^+VQQ^+Q\mathscr{H}=Q^+VQ\mathscr{H}$, so that $Y(Q^+Q\mathscr{H})=Q^+Q\mathscr{H}$.

Finally, let $f,g\in(\ker Y)'=(\ker Q)'$. Then because $VQf\in\text{ran } Q=(\ker Q^+)'$, we have

$$B(Yf,Yg)=B(Q^+VQf,Q^+VQg)$$
$$=B(VQf,VQg)=B(Qf,Qg)=B(f,g).$$

Thus ker $Y=(Q^+Q\mathscr{H})'$ and ran $Y=Q^+Q\mathscr{H}$ are complex subspaces, $Y(Q^+Q\mathscr{H})=Q^+Q\mathscr{H}$, and Y preserves B on $Q^+Q\mathscr{H}$. ///

Recall that a positive real-linear transformation is, by the definition in Appendix A, also self-real-adjoint.

Lemma: If $T:\mathscr{H}\to\mathscr{H}$ is a partial symplectic transformation then T has the real polar decomposition $T=Z|T|$, where $|T|\equiv(T^*T)^{1/2}$ is a positive partial symplectic transformation, invertible on $T^+T\mathscr{H}$, with $|T|^+|T|=|T||T|^+=T^+T$, and where Z is a complex-linear partial isometry with $Z^+Z=Z^*Z=T^+T$ and $ZZ^+=ZZ^*=TT^+$.

Proof: From an earlier result we know $S\equiv|T|^2$ is an invertible symplectic on $T^+T\mathscr{H}$, with $S^+S=SS^+=T^+T$. Since S is positive, it has a unique positive square root $S^{1/2}$. Since $S^+\equiv\Lambda^*S^*\Lambda=\Lambda^*S\Lambda$ is also positive, it is not difficult to see that

$$(S^+)^{1/2}S^{1/2}=S^{1/2}(S^+)^{1/2}=T^+T.$$

[Consider the commuting operators $S^{1/4}$ and $(S^+)^{1/4}$, and recall that T^+T is a complex-linear self-adjoint projection.]

Because furthermore $(\Lambda^*S^{1/2}\Lambda)^2=\Lambda^*S\Lambda=S^+$, we have by the uniqueness of the positive square root that

$$(S^+)^{1/2}=\Lambda^*S^{1/2}\Lambda=(S^{1/2})^+=|T|^+.$$

Thus $|T|^+|T|=|T||T|^+=T^+T$ as claimed.

Now set $Z\equiv T|T|^+$. Then $Z|T|=T|T|^+|T|=TT^+T=T$, and

$$Z^+Z=|T|T^+T|T|^+=|T||T|^+|T||T|^+$$
$$=(T^+T)(T^+T)=T^+T,$$
$$Z^*Z=|T|^+T^*T|T|^+$$
$$=|T|^+|T|^2|T|^+=(T^+T)(T^+T)=T^+T,$$
$$ZZ^+=T|T|^+|T|T^+=TT^+TT^+=TT^+,$$
$$ZZ^*=T|T|^+|T|^+T^*=T\Lambda^*|T|^2\Lambda T^*$$
$$=T(\Lambda^*T^*\Lambda)(\Lambda^*T\Lambda)T^*$$
$$=TT^+T^{*+}T^*=(TT^+)(TT^+)^*=TT^+.$$

Finally, to show Z is complex-linear, we note that $|T||T|^+|T|=|T|$, because $|T|$ is a partial symplectic transformation. Thus

$$\Lambda^*Z\Lambda=\Lambda^*T|T|^+\Lambda=T^{*+}|T|=T^{*+}|T||T|^+|T|$$
$$=T^{*+}|T|^2|T|^+=(TT^+)^*T|T|^+$$
$$=TT^+T|T|^+=T|T|^+=Z,$$

so Z is complex linear. ///

APPENDIX C: TRACE-NORM PROPERTIES OF SYMPLECTIC TRANSFORMATIONS

In this appendix are a few observations used in the discussion in the text which involve Hilbert–Schmidt norms and symplectic transformations.

Lemma: Let $S:\mathscr{H}\to\mathscr{H}$ be a symplectic transformation. Then $S^{*+}XS^+\in B_{2r}(S\mathscr{H})$ if and only if $X\in B_{2r}(\mathscr{H})$.

Proof: Because $S\mathscr{H}$ and $(S\mathscr{H})'$ are orthogonal, we may choose a real-orthonormal basis for $\mathscr{H}$ each element of which is either in $S\mathscr{H}$ or in $(S\mathscr{H})'$. Since the trace in the

definition of the Hilbert–Schmidt norm is independent of the basis, we may evaluate traces in such a real-orthonormal basis $\{f_n\}$, and $\mathrm{tr}_r(Q^*Q) = \Sigma_{n,m}(\mathrm{Re}\langle f_n | Qf_m\rangle)^2$, Suppose first that $S^{*+}XS^+ \in B_{2r}(S\mathscr{H})$. Because $S^+(S\mathscr{H})' = \{0\}$, it follows that $S^{*+}XS^+ \in B_{2r}(\mathscr{H})$. Making use of the fact that $B_{2r}(\mathscr{H})$ is an ideal gives $S^*(S^{*+}XS^+)S \in B_{2r}(\mathscr{H})$. Since $I = S^+S = S^*S^{*+}$, this implies that $X \in B_{2r}(\mathscr{H})$. If, conversely, $X \in B_{2r}(\mathscr{H})$, then by the ideal property $S^{*+}XS^+ \in B_{2r}(\mathscr{H}) \subset B_{2r}(S\mathscr{H})$. ///

Lemma: Let $T:\mathscr{H}\to\mathscr{H}$ be a symplectic transformation. Then $T^*XT \in B_{2r}(\mathscr{H})$ if and only if $X \in B_{2r}(T\mathscr{H})$.

Proof: Again take traces in a real-orthonormal basis for $\mathscr{H}$ each element of which is either in $T\mathscr{H}$ or in $(T\mathscr{H})'$. Suppose first that $T^*XT \in B_{2r}(\mathscr{H})$. Then by the ideal property, $(TT^+)^*XTT^+ = T^{*+}(T^*XT)T^+ \in B_{2r}(\mathscr{H})$. Since $B_{2r}(\mathscr{H}) \subset B_{2r}(T\mathscr{H})$, and since TT^+ is the projection onto $T\mathscr{H}$, we have $X \in B_{2r}(T\mathscr{H})$. Conversely, suppose $X \in B_{2r}(T\mathscr{H})$. Then $T^{*+}T^*XTT^+ \in B_{2r}(T\mathscr{H})$, and since $TT^+(T\mathscr{H})' = \{0\}$, $T^{*+}T^*XTT^+ \in B_{2r}(\mathscr{H})$. Using the facts that $B_{2r}(\mathscr{H})$ is an ideal and that $I = T^+T = T^*T^{*+}$, we have $T^*(T^{*+}T^*XTT^+)T \in B_{2r}(\mathscr{H})$, hence $T^*XT \in B_{2r}(\mathscr{H})$. ///

Remark: If $Q:\mathscr{H}\to\mathscr{H}$ is a partial symplectic transformation then $Q \in B_{2r}(\mathscr{H})$ if and only if $Q \in B_{2r}(Q^+Q\mathscr{H})$, and the notation $\|Q\|_{2r}$ for the Hilbert–Schmidt norm of Q is unambiguous. This is because $(\ker Q)' = Q^+Q\mathscr{H}$ and $(\ker Q)$ are orthogonal subspaces of $\mathscr{H}$. Since the trace is basis independent we may choose a basis each element of which is either in $(\ker Q)$ or in $(\ker Q)'$ to compute the trace of $|Q|^2 : Q^+Q\mathscr{H} \to Q^+Q\mathscr{H}$; there is no contribution from the terms involving basis vectors in $(\ker Q)$.

Lemma: Let $T:\mathscr{H}\to\mathscr{H}$ be a symplectic transformation. Then $(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$ if and only if $(|T|^2 - I) \in B_{2r}(\mathscr{H})$. Furthermore, if $\dim(\ker T^+) = \mathrm{codim}(\mathrm{ran}\, T)$ is *finite*, then $(|T|^2 - I) \in B_{2r}(\mathscr{H})$ if and only if $(|T^+|^2 - I) \in B_{2r}(\mathscr{H})$.

Proof: Since $I = T^+T = T^*T^{*+}$, we have $(|T|^2 - I) = -T^*(|T^+|^2 - I)T$. It thus follows from the second lemma above that $(|T|^2 - I) \in B_{2r}(\mathscr{H})$ if and only if $(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$. For the second assertion, note that $(|T^+|^2 - I) = (|T^+|^2 - I)TT^+ - (I - TT^+)$. With the additional assumption that the subspace $(\ker T^+) = (I - TT^+)\mathscr{H}$ is finite dimensional, it follows that $(|T^+|^2 - I) \in B_{2r}(\mathscr{H})$ if and only if $(|T^+|^2 - I)TT^+ \in B_{2r}(\mathscr{H})$, which is the case if and only if $(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$. ///

Recall that two representations of the Weyl algebra are said to be interchangeable if they both admit unitary implementation of exactly the same set of symplectic automorphisms.

Lemma: Let $R:\mathscr{H}\to\mathscr{H}$ and $T:\mathscr{H}\to\mathscr{H}$ be symplectic transformations, and let π_R and π_T be the associated representations of the Weyl algebra, that is, with the conventions of Sec. II of the text, $\pi_R(W(f)) = W(Rf)$ and $\pi_T(W(f)) = W(Tf)$ for all $f \in \mathscr{H}$. If $(|R|^2 - |T|^2) \in B_{2r}(\mathscr{H})$, then the representations π_R and π_T are interchangeable.

Proof: Let $S:\mathscr{H}\to\mathscr{H}$ be an arbitrary invertible symplectic transformation and let σ_S be the automorphism of the Weyl algebra induced by S. We must show that σ_S is unitarily implementable in π_R if and only if σ_S is unitarily implementable in π_T, assuming $(|R|^2 - |T|^2) \in B_{2r}(\mathscr{H})$. Now, as in Sec. V, σ_S is unitarily implementable in π_R if and only if $(|RSR^+|^2 - I) \in B_{2r}(R\mathscr{H})$. Since RR^+ is the complex-linear self-adjoint projection onto $R\mathscr{H}$, the operator

$$(|RSR^+|^2 - I) = R^{*+}|RS|^2R^+ - |RR^+|^2 + (RR^+ - I)$$
$$= R^{*+}(|RS|^2 - |R|^2)R^+ + (RR^+ - I)$$

is in $B_{2r}(R\mathscr{H})$ if and only if $R^{*+}(|RS|^2 - |R|^2)R^+ \in B_{2r}(R\mathscr{H})$. By an earlier result in this Appendix, this latter condition is true if and only if $(|RS|^2 - |R|^2) \in B_{2r}(\mathscr{H})$. Thus σ_S is unitarily implementable in π_R if and only if $(|RS|^2 - |R|^2) \in B_{2r}(\mathscr{H})$. By hypothesis, $(|R|^2 - |T|^2) \in B_{2r}(\mathscr{H})$, so that $(|RS|^2 - |R|^2) = S^*(|R|^2 - |T|^2)S - (|R|^2 - |T|^2) + (|TS|^2 - |T|^2)$ is a Hilbert–Schmidt operator iff $(|TS|^2 - |T|^2) \in B_{2r}(\mathscr{H})$, that is, if and only if S is unitarily implementable in π_T. Thus π_R and π_T are interchangeable. ///

The proof of this lemma established the following fact which is worth recording separately.

Corollary: Let $R:\mathscr{H}\to\mathscr{H}$ be a symplectic transformation, and let $S:\mathscr{H}\to\mathscr{H}$ be an invertible sympletic transformation. The automorphism σ_S induced by S is unitarily implementable in the representation π_R induced by R if and only if $(|RS|^2 - |R|^2) \in B_{2r}(\mathscr{H})$.

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Simple physical models entailing inequivalent representations of the CCR

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This paper analyzes a family of model quantum field theories for which a C^*-algebraic viewpoint is essential because time-dependent scattering theory cannot be constructed in any one natural representation of the observable algebra. The models demonstrate, in an uncomplicated setting, mechanisms by which nonstandard representations of the canonical commutation relations (CCR) arise in the solution of the field theory. It is shown explicitly how sufficiently strong low-energy coupling between a massless quantum field and a quantum oscillator can result in the inequivalence of the free and interacting vacua, and in the failure of Møller wave operators to exist. It is also shown explicitly how an algebraic framework can be used to circumvent these representation-dependent difficulties and to easily construct an S matrix. The treatment relies on and illustrates the general theory developed in a preceding paper for scattering in models which are field-theoretic analogs to systems with finite numbers of degrees of freedom that are solvable by transformation to normal modes.

I. INTRODUCTION

This paper presents a family of model quantum field theories which illustrate the general framework developed in a preceeding paper,[1] henceforth referred to as [I]. These models demonstrate, in an uncomplicated setting, mechanisms by which nonstandard representations of the algebra of observables arise in the solution of a field theory.

The models are field-theoretic analogs of systems with finite numbers of degrees of freedom that are solvable by transformation to normal modes. They are of interest because a C^*-algebraic viewpoint is essential for their treatment in terms of time-dependent scattering theory; for these models, wave operators fail to exist in any natural representation of the Weyl algebra of the canonical commutation relations, while a conventional S matrix can be constructed using an algebraic framework.

The system under study consists of a quantum-mechanical oscillator interacting linearly with a massless scalar field, roughly modeling an atom interacting with light. It is a variant of a model proposed by Schwabl and Thirring[2] in their discussion of laser theory, and later treated by Arai[3] in a series of papers about the Lamb shift in quantum electrodynamics. The linear coupling studied by Arai and Schwabl and Thirring is "electrostatic" in nature, while the coupling studied here is a "spring force." The mathematical difference is manifest in the fact that the analyticity of a certain resolvent [$D(z)^{-1}$ in the following] does not depend too sensitively on the low-energy strength of the coupling in the model studied here.

There are significant differences in viewpoint and technique between the analysis here and that which Arai employs to treat the model of Schwabl and Thirring. Here there is no need to prove the existence and self-adjointness of a second-quantized Hamiltonian, because the interacting dynamical automorphism group of the Weyl C^* algebra is induced by a one-parameter group of symplectic transformations on the classical phase space. Thus a knowledge of the theory of free quantized fields and Shale's criterion for the implementability of symplectic morphisms [I] is sufficient to establish all the results needed about the second-quantized theory. Furthermore, the C^*-algebraic framework used here allows the treatment of a large class of coupling functions which cannot be handled by Arai's methods, and which give rise to interesting exactly solvable theories having "infrared problems."

The analysis proceeds as follows. In Sec. II we write formal equations for the system with linear coupling involving an unspecified coupling function. We then employ heuristic calculations to obtain a formal solution to the field equations, which suggests the formal "diagonalizing" transformation to "normal mode variables." This formal linear canonical transformation on the "quantized" field and oscillator variables is then seen to be induced by a certain map on the classical phase space.

This map T is the starting point for the analysis of the system. It is shown in Sec. III A that with certain mild restrictions on the coupling function, T is a bounded real-linear transformation. In Sec. III B we show that T is in fact a symplectic transformation.

In Secs. III C–III E, we examine the way the properties of T depend on the coupling function. Having introduced a specific one-parameter family of coupling functions with small-momentum behavior proportional to $|\mathbf{p}|^{-\alpha}$, we show in Sec. III C that for $0<\alpha\leqslant\frac{1}{2}$, the transformation T is isometrically implementable in the Fock representation of the CCR, but that for $\frac{1}{2}<\alpha<1$, T is not isometrically implementable in the Fock representation. In Sec. III D, we show that the interacting dynamical automorphism group is unitarily implementable in the Fock representation for all $\alpha\in(0,1)$, and in Sec. III E, we show that the free dynamical automorphism group is unitarily implementable for all $\alpha\in(0,1)$ in the representation π_T determined by the interaction-vacuum state.

In Sections III F–III H, we formulate time-dependent scattering theory in the algebraic framework presented in [I]. We show in Sec. III F that the model here satisfies the general hypotheses guaranteeing the existence of Møller wave morphisms. In Sec. III G, we calculate the wave morphisms explicitly; these are seen to be nonimplementable in each of the two natural representations. In Sec. III H we show that the scattering morphism which results is implementable in the bare-vacuum (Fock) representation, but not in the interaction-vacuum representation π_T.

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The results of the analysis in Sec. III and their immediate implications are summarized in Sec. IV. The reader who wishes to skip the detailed calculations of Sec. III may turn directly to Sec. IV after reading Sec. II.

Section V contains the physical interpretation of the preceding analysis. It is pointed out that the inequivalence of the bare vacuum and the interaction vacuum is an "infrared problem" which precludes the existence of second-quantized wave operators, but that an S matrix is easily calculated within the algebraic framework for time-dependent scattering theory.

II. PHYSICAL MODEL AND HEURISTIC ANALYSIS

The analysis in this section is not meant to be rigorous, but rather to illustrate the connection between traditional field equations and the symplectic transformation which is the starting point of our rigorous treatment. We work primarily with the momentum-space versions of field variables, elements of classical phase space, etc., which are Fourier transforms of the corresponding coordinate-space objects. In the following equations, the independent variables are the Hermitian scalar field $\phi(t,\mathbf{p})$ and the position coordinate $q(t)$ of a one-dimensional harmonic oscillator. The "uncoupled" field is supposed to be massless, and the ("uncoupled") harmonic oscillator has a natural frequency ω_0.

The equations of motion are

$$(\partial_t^2+\mathbf{p}^2)\phi(t,\mathbf{p}) = -\lambda\rho(\mathbf{p})\left(\int d^3k\ \overline{\rho(\mathbf{k})}\phi(t,\mathbf{k}) - q(t)\right),$$

$$(\partial_t^2+\omega_0^2)q(t) = -\lambda\left(q(t) - \int d^3k\ \overline{\rho(\mathbf{k})}\phi(t,\mathbf{k})\right),$$

where $\rho:\mathbb{R}^3\to\mathbb{C}$ is a coupling function and the real number $\lambda\geqslant 0$ gives the coupling strength. We make an assumption about the coupling function $\rho(\mathbf{p})$ which simplifies the analysis but does not affect the essential features of the model. Henceforth we assume that the coordinate-space Fourier transform $\tilde{\rho}(\mathbf{x})$ of ρ is a spherically symmetric real-valued function. It immediately follows that $\rho(\mathbf{p})$ is a spherically symmetric real-valued function of $\mathbf{p}$.

We can picture this system as an oscillator of mass m and natural frequency ω_0 coupled by a spring with spring constant $k=\lambda m$ to a string (in one spatial dimension) or a membrane (in two spatial dimensions) with the coupling smeared out by a function $\tilde{\rho}(\mathbf{x})$. If the coupling were to a point on the string or the membrane, $\tilde{\rho}$ would be proportional to a delta function.

We can formally solve these linear equations.[4] Introducing the "free (in) field" and "uncoupled oscillator" solutions

$$\phi^0(t,\mathbf{p}) \equiv (2\omega_p)^{-1/2}(b^*(\mathbf{p})e^{i\omega_p t} + b(-\mathbf{p})e^{-i\omega_p t}),$$

$$q^0(t) \equiv (2\omega_0)^{-1/2}(B^*e^{i\omega_0 t} + Be^{-i\omega_0 t}),$$

treating the right-hand sides of the equations of motion as source terms in the Yang–Feldman equations, and doing some algebra with the time-variable Fourier transforms of the various quantities, we obtain

$$\phi(t,\mathbf{p}) = (2\omega_p)^{-1/2}\int d^3k\,(\overline{L}^*(\mathbf{p},\mathbf{k})\,b^*(\mathbf{k})e^{i\omega_k t} + L^*(\mathbf{p},\mathbf{k})\,b(-\mathbf{k})e^{-i\omega_k t}),$$

$$q(t) = \int d^3k\,(2\omega_k)^{-1/2}(Q(\mathbf{k})\,b^*(\mathbf{k})e^{i\omega_k t} + \overline{Q}(\mathbf{k})\,b(-\mathbf{k})e^{-i\omega_k t}),$$

where we have defined the kernel

$$L(\mathbf{p},\mathbf{q}) \equiv \delta^3(\mathbf{p}-\mathbf{q}) + \frac{\lambda\rho(\mathbf{p})(\omega_0^2-\omega_p^2)\omega_q^{1/2}\rho(\mathbf{q})}{\omega_p^{1/2}D_+(\omega_p^2)(\omega_p^2-\omega_q^2+i0)}$$

and the function $Q(\mathbf{p}) \equiv \lambda\rho(\mathbf{p})/D_+(\omega_p^2)$. In these formulas $\omega_p \equiv |\mathbf{p}|$, and the function D_+ is given by $D_\pm(x) \equiv \lim_{\epsilon\to+0} D(x\pm i\epsilon)$ with

$$D(z) \equiv \lambda+\omega_0^2-z+\lambda(\omega_0^2-z)\int d^3p\,|\rho(\mathbf{p})|^2(\omega_p^2-z)^{-1}.$$

Note that the fixed number ω_0 is not to be mistaken for ω_p at $\mathbf{p}=0$. We denote by $\overline{L}(\mathbf{p},\mathbf{q})$ the complex conjugate of the quantity $L(\mathbf{p},\mathbf{q})$, and we set $L^*(\mathbf{p},\mathbf{q}) \equiv \overline{L}(\mathbf{q},\mathbf{p})$. For future convenience we also define

$$M(\mathbf{p},\mathbf{q}) \equiv \omega_p L(\mathbf{p},\mathbf{q})\omega_q^{-1}.$$

We will show in the next section that there are well-defined bounded operators L and M whose symbolic kernels are the expressions given here.

This model is in fact a field-theoretic analog of a system with finite number of degrees of freedom having a transformation to normal modes. To make the analogy explicit, we now rewrite the formal solutions above in terms of a (linear, canonical) "diagonalization" transformation.

To find this transformation, we introduce the time-zero decompositions of the field variables ϕ and the oscillator variable q in terms of amplitudes $a(\mathbf{p})$ and A, that is, we define a^*, a, A^*, and A by

$$\phi(0,\mathbf{p}) \equiv (2\omega_p)^{-1/2}(a^*(\mathbf{p}) + a(-\mathbf{p})),$$

$$\dot{\phi}(0,\mathbf{p}) \equiv i(\omega_p/2)^{1/2}(a^*(\mathbf{p}) - a(-\mathbf{p})),$$

$$q(0) \equiv (2\omega_0)^{-1/2}(A^*+A),$$

$$\dot{q}(0) \equiv i(\omega_0/2)^{1/2}(A^*-A).$$

Substituting these decompositions into the formal solutions and solving for a^*, a, A^*, and A, we find

$$a(\mathbf{p}) = \int d^3k\,\tfrac{1}{2}\{(\overline{L}^*-\overline{M}^*)(\mathbf{p},\mathbf{k})\,b^*(\mathbf{k}) + (L^*+M^*)(\mathbf{p},\mathbf{k})\,b(\mathbf{k})\},$$

$$a^*(\mathbf{p}) = \int d^3k\,\tfrac{1}{2}\{(\overline{L}^*+\overline{M}^*)(\mathbf{p},\mathbf{k})\,b^*(\mathbf{k}) + (L^*-M^*)(\mathbf{p},\mathbf{k})\,b^*(\mathbf{k})\},$$

and

$$A = \int d^3k\,\tfrac{1}{2}\{(\omega_0^{1/2}\omega_k^{-1/2} - \omega_0^{-1/2}\omega_k^{1/2})Q(\mathbf{k})b^*(\mathbf{k}) + (\omega_0^{1/2}\omega_k^{-1/2} + \omega_0^{-1/2}\omega_k^{1/2})\overline{Q}(\mathbf{k})b(\mathbf{k})\},$$

$$A^* = \int d^3k\,\tfrac{1}{2}\{(\omega_0^{1/2}\omega_k^{-1/2} + \omega_0^{-1/2}\omega_k^{1/2})Q(\mathbf{k})b^*(\mathbf{k}) + (\omega_0^{1/2}\omega_k^{-1/2} - \omega_0^{-1/2}\omega_k^{1/2})\overline{Q}(\mathbf{k})b^*(\mathbf{k})\}.$$

To arrive at the above, we have made use of the spherical symmetry of $(L-I)$, $(M-I)$, and Q to eliminate minus signs in the arguments.

These amplitudes A and a of course "satisfy the CCR" in a formal sense, and the symbolic expressions

$$W\begin{pmatrix}h\\u\end{pmatrix}\equiv\exp(i(a^*[h]+a[h]+A^*u+A\bar{u})/\sqrt{2}),$$

where $h\in L_2(\mathbb{R}^3)$, $u\in\mathbb{C}$, and $a[h]\equiv\int d^3p\,\overline{h(\mathbf{p})}a(\mathbf{p})$, $a^*[h]=(a[h])^*$, satisfy the Weyl relations

$$W\begin{pmatrix}h_1\\u_1\end{pmatrix}W\begin{pmatrix}h_2\\u_2\end{pmatrix}=W\begin{pmatrix}h_1+h_2\\u_1+u_2\end{pmatrix}\exp\left(-iB\left(\begin{pmatrix}h_1\\u_1\end{pmatrix},\begin{pmatrix}h_2\\u_2\end{pmatrix}\right)/2\right)$$

with symplectic form B given by

$$B\left(\begin{pmatrix}h_1\\u_1\end{pmatrix},\begin{pmatrix}h_2\\u_2\end{pmatrix}\right)\equiv\mathrm{Im}\langle h_1|h_1\rangle+\mathrm{Im}(\bar{u}_1u_2).$$

These heuristic manipulations serve to motivate the following considerations. The space $\mathscr{H}\equiv L_2(\mathbb{R}^3)\oplus\mathbb{C}$ with the symplectic form B defined as above is the classical phase space for a system consisting of an (uncoupled) scalar field and a harmonic oscillator. The abstract Weyl C^* algebra $\mathscr{W}$ over $\mathscr{H}$ has unitary elements $W\binom{h}{u}$ satisfying the Weyl relations above (see [I]). The "normal-mode" amplitudes b introduced for the free field (that is, the "in" field solution of the homogeneous wave equation) also satisfy the CCR and are related to the amplitudes A and a by the formulas above. These formulas can be combined to give $(a^*[h]+a[h]+A^*u+A\bar{u})=(b^*[h']+b[h'])$, where $h'\in L_2(\mathbb{R}^3)$ is related to h and u by a linear formula given below.

To make these observations precise, we can consider the "change of variables" from the symbols A and a to the symbols b as a map on the (abstract) Weyl algebra given by

$$\tau\left(W\begin{pmatrix}h\\u\end{pmatrix}\right)\equiv W\begin{pmatrix}h'\\0\end{pmatrix}.$$

It will turn out that τ is a morphism of $\mathscr{W}$ induced by a symplectic transformation T.

We can get a formal expression for the action of T as follows. Let $C:L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$ be the antilinear conjugation given by $(Ch)(\mathbf{p})\equiv\overline{h(-\mathbf{p})}$; here, of course, complex conjugation of the function h refers to the fixed complex structure on $L_2(\mathbb{R}^3)$. Decompose the function h as $h=f+ig$, where $f,g\in L_2(\mathbb{R}^3)$ are invariant under C, and let $u=v+iw$ with $v,w\in\mathbb{R}$. It is then straightforward to compute that $a^*[f+ig]+a[f+ig]+A^*(v+iw)+A(v-iw)=b^*[h']+b[h']$, where

$$h'(\mathbf{k})\equiv(Lf+iMg+\omega_0^{1/2}\omega^{-1/2}Qv+i\omega_0^{-1/2}\omega^{1/2}Qw)(\mathbf{k})$$
$$=f'(\mathbf{k})+ig'(\mathbf{k}),$$

with f' and g' the C-invariant functions

$$f'=\tfrac{1}{2}(L+\overline{L})f+\tfrac{1}{2}i(M-\overline{M})g+\tfrac{1}{2}\omega_0^{1/2}\omega^{-1/2}(Q+\overline{Q})v$$
$$+\tfrac{1}{2}i\omega_0^{-1/2}\omega^{1/2}(Q-\overline{Q})w,$$
$$g'=-\tfrac{1}{2}i(L-\overline{L})f+\tfrac{1}{2}(M+\overline{M})g-\tfrac{1}{2}i\omega_0^{1/2}\omega^{-1/2}(Q-\overline{Q})v$$
$$+\tfrac{1}{2}\omega_0^{-1/2}\omega^{1/2}(Q+\overline{Q})w.$$

Here we have made use of a self-explanatory symbolic operator notation. Henceforth we also represent elements of $\mathscr{H}=L_2(\mathbb{R}^3)\oplus\mathbb{C}$ as quadruples in $L_2(\mathbb{R}^3)_C\oplus L_2(\mathbb{R}^3)_C\oplus\mathbb{R}\oplus\mathbb{R}$:

$$\begin{pmatrix}f\\g\\v\\w\end{pmatrix},\quad\text{with } f,g\in L_2(\mathbb{R}^3)_C\equiv\{h\in L_2(\mathbb{R}^3)|Ch=h\}$$
$$\text{and } v,w\in\mathbb{R}.$$

With this notation, $\mathscr{H}$ is a real-linear space with symplectic form B the same as before but now written in terms of four-tuples as

$$B\left(\begin{pmatrix}f_1\\g_1\\v_1\\w_1\end{pmatrix},\begin{pmatrix}f_2\\g_2\\v_2\\w_2\end{pmatrix}\right)=\langle f_1|g_2\rangle-\langle g_1|f_2\rangle+v_1w_2-w_1v_2,$$

where for f and $g\in L_2(\mathbb{R}^3)_C$, $\langle f|g\rangle=\langle g|f\rangle=\overline{\langle f|g\rangle}$ by virtue of the C invariance of f and g. In this notation, the linear transformation $\Lambda:\mathscr{H}\to\mathscr{H}$ representing multiplication by the complex number i on $\mathscr{H}$ is given by

$$\Lambda=\begin{pmatrix}0&-I&0&0\\I&0&0&0\\0&0&0&-1\\0&0&1&0\end{pmatrix},$$

and the morphism τ, defined as above by

$$\tau(W\begin{pmatrix}f\\g\\v\\w\end{pmatrix})\equiv W\begin{pmatrix}f'\\g'\\0\\0\end{pmatrix}=W(T\begin{pmatrix}f\\g\\v\\w\end{pmatrix}),$$

is induced by the transformation T given by

$$2T=\begin{bmatrix}(L+\overline{L})&i(M-\overline{M})&|\omega_0^{1/2}\omega^{-1/2}(Q+\overline{Q})\rangle&i|\omega_0^{-1/2}\omega^{1/2}(Q-\overline{Q})\rangle\\-i(L-\overline{L})&(M+\overline{M})&-i|\omega_0^{1/2}\omega^{-1/2}(Q-\overline{Q})\rangle&|\omega_0^{-1/2}\omega^{1/2}(Q+\overline{Q})\rangle\\0&0&0&0\\0&0&0&0\end{bmatrix}.$$

The ket notation is employed to call attention to the fact that, for example, the operator $|\omega_0^{1/2}\omega^{-1/2}(Q+\overline{Q})\rangle:\mathbb{R}\to L_2(\mathbb{R}^3)_C$ acts on $\mathbb{R}$ by multiplication with the function $\omega_0^{1/2}\omega_p^{-1/2}(Q(\mathbf{p})+\overline{Q(\mathbf{p})})$.

III. CALCULATIONS

In this section we establish that the model discussed heuristically in the preceding section does in fact furnish an example of the general framework presented in [I], and we

analyze its properties. In Sec. III A and III B we define the symplectic transformation T precisely. In Sec. III C–III E we investigate the properties of T related to the implementation of T itself and to the implementation of the time development automorphism groups. In Sec. III F–III H we investigate the Møller wave morphisms and S matrix arising in the time-dependent scattering theory for this system.

Since the purpose is to provide an illustrative example rather than to analyze the most general case of the model at hand, we make specific assumptions about the coupling function $\rho(\mathbf{p})$ which streamline the discussion but preserve all the features of interest. In particular, we consider coupling functions $\rho(\mathbf{p})$ which are members of the family

$$\rho(\alpha;\mathbf{p}) \equiv |\mathbf{p}|^{-\alpha}(1+|\mathbf{p}|^2)^{-1/2}, \quad \text{where } 0<\alpha<1.$$

Note that every function in this family is a strictly positive spherically symmetric function which is continuously differentiable on $\mathbb{R}^3\setminus\{0\}$. The important feature of such a function ρ is its behavior near the origin. The factor $(1+|\mathbf{p}|^2)^{-1/2}$ is included to make ρ fall off quickly enough for large $|\mathbf{p}|$ to insure the convergence of various integrals; the precise form of this convergence factor is unimportant.

A. Rigorous definition of the transformation T

Much of the analysis depends on the properties of the function $D(z)$ introduced earlier. For a fixed coupling function $\rho(\alpha;\mathbf{p})$, we define

$$D(\alpha;z) \equiv \lambda+\omega_0^2-z + \lambda(\omega_0^2-z)\int d^3p|\rho(\alpha;\mathbf{p})|^2(\omega_p^2-z)^{-1},$$

for all z in the cut complex plane $\mathbb{C}\setminus[0,\infty)$. This function $D(\alpha;z)$ is analytic on $\mathbb{C}\setminus[0,\infty)$, and in fact we have

$$D(\alpha;z) = \lambda+\omega_0^2-z+2\pi^2\lambda(\sin\pi(\alpha-\tfrac{1}{2}))^{-1} \times((\omega_0^2-z)/(1+z))((-z)^{-\alpha+1/2}-1).$$

Here the function $w\mapsto w^{-\alpha+1/2}$ has a branch cut along the negative real axis and is real for positive w.

Furthermore, for $t>0$ the limits

$$D_{\pm}(\alpha;t) \equiv \lim_{\epsilon\to+0} D(\alpha;t\pm i\epsilon)$$

exist and are given by

$$D_+(\alpha;t) = \lambda+\omega_0^2-t + \frac{2\pi^2\lambda}{\sin\pi(\alpha-\frac{1}{2})}\frac{\omega_0^2-t}{1+t}\left(\frac{e^{i\pi(\alpha-1/2)}}{t^{\alpha-1/2}}-1\right),$$

with $D_-(\alpha;t)=\overline{D_+(\alpha;t)}$. [At $\alpha=\frac{1}{2}$, we have

$$D_+(\tfrac{1}{2};t) = \lambda+\omega_0^2-t+2\pi\lambda(\omega_0^2-t)(1+t)^{-1} \times(i\pi-\ln t).]$$

It is not difficult to see that $D_+(\alpha;t)$ is bounded away from zero for all t, and that $\lim_{t\to\infty} D_+(\alpha;t)/t=-1$. Furthermore, as $t\to+0$,

$$D_+(\alpha;t) = \begin{cases} \lambda+\omega_0^2+C+O(t^{1/2-\alpha}), & \text{if } 0<\alpha<\frac{1}{2}, \\ \lambda+\omega_0^2-2\pi\lambda\omega_0^2(\ln(t)-i\pi)+O(t\ln(t)), & \text{if } \alpha=\frac{1}{2}, \\ \lambda+\omega_0^2+C((\exp i\pi(\alpha-\frac{1}{2}))t^{-(\alpha-1/2)}-1) & \\ \quad +O(t^{3/2-\alpha}), & \text{if } \frac{1}{2}<\alpha<1, \end{cases}$$

where $C\equiv 2\pi^2\lambda\omega_0^2|\sin\pi(\alpha-\frac{1}{2})|^{-1}$ is a positive constant.

Now define the function $Q(\alpha;\mathbf{k})\equiv\lambda\rho(\alpha;\mathbf{k})/D_+(\alpha;\omega_k^2)$. Using the properties of D_+ above, it is easy to see that all of the functions $|\mathbf{k}|^{\gamma}Q(\alpha;\mathbf{k})$ are in $L_2(\mathbb{R}^3)$, for $0<\alpha<1$ and $-\frac{1}{2}\leqslant\gamma\leqslant\frac{3}{2}$.

In this subsection we make sense of the symbolic kernels $L(\mathbf{p},\mathbf{q})$ and $M(\mathbf{p},\mathbf{q})$ occurring in the transformation T. To this end, we define for $0<\alpha<1$ and $\epsilon>0$, the functions

$$(L_\alpha(\epsilon)-I)(\mathbf{p},\mathbf{q}) \equiv \frac{\lambda\rho(\alpha;\mathbf{p})(\omega_0^2-\omega_p^2)\omega_q^{1/2}\rho(\alpha;\mathbf{q})}{\omega_p^{1/2}D_+(\alpha;\omega_p^2)(\omega_p^2-\omega_q^2+i\epsilon)}$$

and

$$(M_\alpha(\epsilon)-I)(\mathbf{p},\mathbf{q}) \equiv \frac{\lambda\rho(\alpha;\mathbf{p})\omega_p^{1/2}(\omega_0^2-\omega_p^2)\rho(\alpha;\mathbf{q})}{D_+(\alpha;\omega_p^2)(\omega_p^2-\omega_q^2+i\epsilon)\omega_q^{1/2}},$$

which are reminiscent of the symbolic kernels in the last section.

The remainder of this subsection is devoted to showing that these two functions are kernels for bounded operators $L_\alpha(\epsilon)-I$ and $M_\alpha(\epsilon)-I$ whose strong limits as $\epsilon\to+0$ exist and are bounded operators denoted by $L_\alpha-I$ and $M_\alpha-I$, respectively. The transformation T is then defined in terms of L_α and M_α by exactly the same formula as in the last section.

To demonstrate these assertions, it is convenient to decompose the functions above, as follows:

$$(L_\alpha(\epsilon)-I)(\mathbf{p},\mathbf{q}) = R(\alpha;\mathbf{p})(G(\epsilon)(\mathbf{p},\mathbf{q})-\Delta_{1-\alpha}(\epsilon)(\mathbf{p},\mathbf{q}))(1+\omega_q^2)^{-1/2},$$

$$(M_\alpha(\epsilon)-I)(\mathbf{p},\mathbf{q}) = R(\alpha;\mathbf{p})(G(\epsilon)(\mathbf{p},\mathbf{q})-\Delta_\alpha^*(\epsilon)(\mathbf{p},\mathbf{q}))(1+\omega_q^2)^{-1/2},$$

where

$$R(\alpha;\mathbf{p}) \equiv (\omega_0^2-\omega_p^2)\omega_p^{1-2\alpha}Q(\alpha;\mathbf{p}) = \frac{\lambda(\omega_0^2-\omega_p^2)\omega_p^{1-2\alpha}}{D_+(\alpha;\omega_p^2)(1+\omega_p^2)^{1/2}}$$

and

$$G(\epsilon)(\mathbf{p},\mathbf{q}) \equiv (\omega_p\omega_q)^{-1/2}(\omega_p^2-\omega_q^2+i\epsilon)^{-1}$$

and, for $0<\gamma<1$,

$$\Delta_\gamma(\epsilon)(\mathbf{p},\mathbf{q}) \equiv \omega_p^{-\gamma}(\omega_p^\gamma-\omega_q^\gamma)G(\epsilon)(\mathbf{p},\mathbf{q}),$$

with

$$\Delta_\gamma^*(\epsilon)(\mathbf{p},\mathbf{q}) \equiv \overline{\Delta_\gamma(\epsilon)(\mathbf{q},\mathbf{p})}.$$

In view of the properties of D_+, it is easily established that the continuous function $R(\alpha;\mathbf{p})$ is bounded on $\mathbb{R}^3$ for all $\alpha\in(0,1)$.

The function $G(\epsilon)(\mathbf{p},\mathbf{q})$ was introduced by Arai[1] in the analysis of his model; it is the kernel for a bounded operator $G(\epsilon):L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$. The family $G(\epsilon)$ is norm-bounded uniformly in ϵ, and the strong limit s-$\lim_{\epsilon\to+0} G(\epsilon)$ exists and converges to a bounded operator $G:L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$, which is related to the Hilbert transform.

Entirely analogous statements are true of the function $\Delta_\gamma(\epsilon)(\mathbf{p},\mathbf{q})$ for $0<\gamma<1$, and are easy to prove by virtue of the fact that $\Delta_\gamma(0)(\mathbf{p},\mathbf{q})$ is itself the integral kernel for a bounded operator Δ_γ. It is shown in Appendix A that $\Delta_\gamma(\epsilon)(\mathbf{p},\mathbf{q})$ is the integral kernel for a bounded operator $\Delta_\gamma(\epsilon):L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$,

that the family $\Delta_\gamma(\epsilon)$ is for fixed γ norm-bounded uniformly in ϵ, and that $\underset{\epsilon\to+0}{\text{s-lim}}\,\Delta_\gamma(\epsilon)=\Delta_\gamma$ and $\underset{\epsilon\to+0}{\text{s-lim}}\,\Delta_\gamma(\epsilon)^*=\Delta_\gamma^*$, where the operator Δ_γ is induced by the integral kernel

$$\Delta_\gamma(0)(\mathbf{p},\mathbf{q})\equiv\omega_q^{-1/2}\omega_p^{-\gamma-1/2}(\omega_p^\gamma-\omega_q^\gamma)/(\omega_p^2-\omega_q^2).$$

Combining the properties of the operators $G(\epsilon)$ and $\Delta_\gamma(\epsilon)$ with the previous decompositions, we see that for $0<\alpha<1$, the functions $(L_\alpha(\epsilon)-I)(\mathbf{p},\mathbf{q})$ and $(M_\alpha(\epsilon)-\mathrm{I})(\mathbf{p},\mathbf{q})$ are integral kernels for the bounded operators

$$L_\alpha(\epsilon)-I\equiv R(\alpha;\mathbf{p})(G(\epsilon)-\Delta_{1-\alpha}(\epsilon))(1+\omega^2)^{-1/2}$$

and

$$M_\alpha(\epsilon)-I\equiv R(\alpha;\mathbf{p})(G(\epsilon)-\Delta_\alpha^*(\epsilon))(1+\omega^2)^{-1/2},$$

where here $R(\alpha;\mathbf{p})$ and $(1+\omega^2)^{-1/2}$ denote the operations of multiplication by the corresponding bounded functions. It also follows that the families $L_\alpha(\epsilon)$ and $M_\alpha(\epsilon)$ are uniformly bounded in norm for $\epsilon>0$, and that furthermore, the strong limits as $\epsilon\to+0$ of these operators exist.

We denote these bounded limit operators by L_α and M_α, respectively, and we have

$$L_\alpha=I+R(\alpha;\mathbf{p})(G-\Delta_{1-\alpha})(1+\omega^2)^{-1/2}$$

and

$$M_\alpha=I+R(\alpha;\mathbf{p})(G+\Delta_\alpha^*)(1+\omega^2)^{-1/2}.$$

Note that with these definitions, both $(L_\alpha-I)$ and $(M_\alpha-I)$ vanish on the subspace $(I-\Psi)L_2(\mathbb{R}^3)$, where Ψ is the spherical average introduced in Appendix A. This spherical symmetry of $(L_\alpha-I)$ and $(M_\alpha-I)$ implies that the operators $(L_\alpha+\overline{L_\alpha})$, $-i(L_\alpha-\overline{L_\alpha})$, $(M_\alpha+\overline{M_\alpha})$, and $i(M_\alpha-\overline{M_\alpha})$ all preserve the C-invariant subspace $L_2(\mathbb{R}^3)_C$. Furthermore, the spherical symmetry of the function $Q(\alpha;\mathbf{p})$ implies that the functions $\omega_p^{\pm1/2}(Q(\alpha;\mathbf{p})+\overline{Q(\alpha;\mathbf{p})})$ and $i\omega_p^{\pm1/2}(Q(\alpha;\mathbf{p})-\overline{Q(\alpha;\mathbf{p})})$ are all elements of $L_2(\mathbb{R}^3)_C$.

We have therefore shown that the expression for the transformation T given in Sec. II with L, M, and Q replaced by L_α, M_α, and $Q(\alpha;\mathbf{p})$ respectively, defines a bounded real-linear transformation $T_\alpha:\mathscr{H}\to\mathscr{H}$, where $\mathscr{H}$ is the classical phase space $\mathscr{H}\equiv L_2(\mathbb{R}^3)_C\oplus L_2(\mathbb{R}^3)_C\oplus\mathbb{R}\oplus\mathbb{R}$.

B. Verification that T is symplectic

The preceding discussion shows that T_α is a bounded real-linear transformation for $0<\alpha<1$. It is clear from the forms of Λ and of T that the range of T is a complex subspace of $\mathscr{H}=L_2(\mathbb{R}^3)_C\oplus L_2(\mathbb{R}^3)_C\oplus\mathbb{R}\oplus\mathbb{R}$. To complete the verification that T is symplectic, we need only show that $T^+T=I$. To do this, we require identities from the following list.

(1) $\|Q\|=1$.

(2) $L^*|\omega^{1/2}Q\rangle=0$ and $M^*|\omega^{-1/2}Q\rangle=0$.

(3) $L^*M=I$ and $M^*L=I$.

(4) $ML^*=I-|\omega^{1/2}Q\rangle\langle\omega^{-1/2}Q|$ and $LM^*=I-|\omega^{-1/2}Q\rangle\langle\omega^{1/2}Q|$.

(5) $\overline{L}=\eta L+(1-\eta)(I-\Psi)$ and $\overline{M}=\eta M+(1-\eta)(I-\Psi)$, where $\eta:\mathbb{R}^3\to C$ is given by $\eta(\mathbf{p})\equiv D_+(\omega_p^2)(D_-(\omega_p^2))^{-1}$, and where $\Psi:L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$ is the spherical average.

(6) $\overline{L}^*|h\overline{Q}\rangle=L^*|hQ\rangle$ and $\overline{M}^*|h\overline{Q}\rangle=M^*|hQ\rangle$ for any $h:\mathbb{R}^3\to\mathbb{C}$ that is spherically symmetric and such that $hQ\in L_2(\mathbb{R}^3)$.

(7) $\overline{L}^*h\overline{L}=L^*hL$ and $\overline{L}^*h\overline{M}=L^*hM$ and $\overline{M}^*h\overline{M}=M^*hM$ and $\overline{M}^*h\overline{L}=M^*hL$ for any $h:\mathbb{R}^3\to\mathbb{C}$ that is spherically symmetric and such that the indicated operators are well defined and bounded.

Statements (1)–(5) are verified by calculations which involve the explicit kernel functions for $L(\epsilon)$ and $M(\epsilon)$, while statements (6) and (7) follow directly from the others. These calculations are similar to those in Lemmas 4.6 and 4.9 of Ref. 3, and we omit them here.

Note that the following abuses of notation are routinely made here. If a function $h:\mathbb{R}^3\to C$ is spherically symmetric, we often write $h(p)$ when $p\equiv|\mathbf{p}|$ instead of $h(\mathbf{p})$. Furthermore, the argument α in $\rho(\alpha;\mathbf{p})$, $R(\alpha;\mathbf{p})$, $D_+(\alpha;\omega^2)$, etc. is often dropped for brevity. Thus, for example, $\rho(y^{1/2})$ means $\rho(\alpha;y^{1/2}\mathbf{e})$ for some fixed unit vector $\mathbf{e}$, or equivalently, $\rho(y^{1/2})=y^{-\alpha/2}(1+y)^{-1/2}$.

In the proof of these identities and in calculations to follow, use is made of the identity

$$D_-(t)-D_+(t)=4\pi^2i\lambda t^{1/2}(t-\omega_0^2)|\rho(t^{1/2})|^2\quad\text{for } t>0,$$

which holds for general spherically symmetric coupling functions ρ (under mild restrictions) as well as for those of the form $\rho(\alpha;\mathbf{p})$. Also used is the fact that $D(z)$ is an analytic function on the cut plane $\mathbb{C}\setminus[0,\infty)$ which is bounded in modulus away from zero, and which satisfies $\mathrm{Re}(D(z))>\lambda+\omega_0^2>0$ for $\mathrm{Re}(z)<0$, as well as $\lim_{|z|\to\infty}D(z)/z=-1$.

Now, the real-linear transformation T^+ is given by

$$2T^+=\begin{bmatrix}(M^*+\overline{M}^*) & i(M^*-\overline{M}^*) & 0 & 0\\ -i(L^*-\overline{L}^*) & (L^*+\overline{L}^*) & 0 & 0\\ \langle\omega^{1/2}\omega_0^{-1/2}(Q+\overline{Q})| & i\langle\omega^{1/2}\omega_0^{-1/2}(Q-\overline{Q})| & 0 & 0\\ -i\langle\omega_0^{1/2}\omega^{-1/2}(Q-\overline{Q})| & \langle\omega_0^{1/2}\omega^{-1/2}(Q+\overline{Q})| & 0 & 0\end{bmatrix}.$$

Straightforward matrix multiplication and use of the identities listed above establish that $T^+T=I$, as claimed. Thus T_α is a symplectic transformation for $0<\alpha<1$.

It is also instructive to compute the projection TT^+ onto the range of T. From identities (4) and (5) above, we easily obtain

$$\overline{L}M^*=-|\omega^{-1/2}\overline{Q}\rangle\langle\omega^{1/2}Q|+(I-\Psi)+\eta\Psi,\quad\overline{M}L^*=-|\omega^{1/2}\overline{Q}\rangle\langle\omega^{-1/2}Q|+(I-\Psi)+\eta\Psi.$$

Using these relationships and their complex conjugates, it is straightforward to show that

$$T_\alpha T_\alpha^+ = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Thus the kernel of the transformation T_α^+ is a two-real-dimensional complex subspace of $\mathscr{H}$. Note in particular that codim(ran T_α) is finite.

C. Implementability of T in π_I

The results in [I] show that the symplectic transformations T and T^+ are isometrically implementable in the Fock representation π_I if and only if $(|T|^2 - I) \in B_{2r}(\mathscr{H})$, or equivalently, if and only if $(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$. In this subsection we examine the operator $(|T^+|^2 - I)$ to determine whether or not it is of Hilbert–Schmidt type.

We analyze T^+ instead of T because the subsection which follows requires many of the results for T^+ which we establish here. The discussion in both subsections is simplified somewhat by the following few preliminary observations.

Note that if f and g are elements of L_2, then the dyadic $E \equiv |f\rangle\langle g|$ is a Hilbert–Schmidt operator, and furthermore, if A is any bounded operator, then EA and AE are both Hilbert–Schmidt operators. Thus terms in the expression for an operator which are dyadics do not influence the Hilbert–Schmidt character of the operator. So for the purposes of this subsection we may ignore dyadic terms in the expression for $(|T^+|^2 - I)$.

The real-linear transformation T^{+*} is given by

$$2T^{+*} = \begin{bmatrix} (M + \overline{M}) & i(L - \overline{L}) & |\omega^{1/2}\omega_0^{-1/2}(Q + \overline{Q})\rangle & i|\omega_0^{1/2}\omega^{-1/2}(Q - \overline{Q})\rangle \\ -i(M - \overline{M}) & (L + \overline{L}) & -i|\omega^{1/2}\omega_0^{-1/2}(Q - \overline{Q})\rangle & |\omega_0^{1/2}\omega^{-1/2}(Q + \overline{Q})\rangle \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Straightforward matrix multiplication shows that $|T^+|^2$ is of the form

$$|T^+|^2 = \begin{bmatrix} A & B & 0 & 0 \\ C & D & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + F,$$

with each of A, B, C and D mapping $L_2(\mathbb{R}^3)_C$ to $L_2(\mathbb{R}^3)_C$, and where the entries of the matrix F are dyadics from the vector entries in T^+. Using the formulas developed above for $\overline{L}$ and $\overline{M}$ in terms of L, M, η, and Ψ, it is straightforward to show that

$$4A = (1 - \eta)LL^*(1 - \overline{\eta}) + (1 + \eta)MM^*(1 + \overline{\eta}),$$

$$4B = -i(1 + \eta)LL^*(1 - \overline{\eta}) - i(1 - \eta)MM^*(1 + \overline{\eta}),$$

$$C = B^*,$$

$$4D = (1 + \eta)LL^*(1 + \overline{\eta}) + (1 - \eta)MM^*(1 - \overline{\eta}).$$

We now make use of these observations to determine the range of α for which $(|T_\alpha^+|^2 - I)$ is a Hilbert–Schmidt operator. In view of the above,

$$\mathrm{tr}_r((|T^+|^2 - I)^2) = 2 + \mathrm{tr}((A - I)^2 + BB^* + B^*B + (D - I)^2),$$

modulo addition of finite contributions from the matrix F. Here the latter trace is taken over a basis for $L_2(\mathbb{R}^3)_C$. It is straightforward, although tedious, to verify that

$$2((A - I)^2 + BB^* + B^*B + (D - I)^2) = (LL^* - I)^2 + \eta(LL^* - I)^2\overline{\eta} + (MM^* - I)^2 + \eta(MM^* - I)^2\overline{\eta}.$$

The conjugation $C: L_2(\mathbb{R}^3) \to L_2(\mathbb{R}^3)$, defined earlier by $(Cf)(\mathbf{p}) = \overline{f(-\mathbf{p})}$, has the property that $CLL^*C = \overline{LL^*} = \eta LL^*\overline{\eta}$, hence $C(LL^* - I)^2C = \eta(LL^* - I)^2\overline{\eta}$. Thus the operator $Z \equiv (LL^* - I)^2 + \eta(LL^* - I)^2\overline{\eta}$ commutes with C and hence preserves both $L_2(\mathbb{R}^3)_C = \frac{1}{2}(I + C)L_2(\mathbb{R}^3)$ and $L_2(\mathbb{R}^3)_C' = \frac{1}{2}(I - C)L_2(\mathbb{R}^3)$. Now, if $\{h_n\}$ is an orthonormal basis for $L_2(\mathbb{R}^3)_C$, then $\{ih_n\}$ is an orthonormal basis for $L_2(\mathbb{R}^3)_C'$. Since L commutes with multiplication by i, the trace of Z over the basis $\{h_n, ih_n\}$ for $L_2(\mathbb{R}^3)$ is just twice the trace of Z over the basis $\{h_n\}$ for $L_2(\mathbb{R}^3)_C$. We conclude that Z has finite trace over $L_2(\mathbb{R}^3)_C$ if and only if Z has finite trace over $L_2(\mathbb{R}^3)$.

Remark: This last observation is a complexification for the sake of calculational convenience, so that we may take traces later in bases for $L_2(\mathbb{R}^3)$ instead of $L_2(\mathbb{R}^3)_C$. This new $L_2(\mathbb{R}^3)$ is certainly *not* the original test function space which was decomposed as $L_2(\mathbb{R}^3) = L_2(\mathbb{R}^3)_C \oplus L_2(\mathbb{R}^3)_C$.

Identical reasoning holds for the terms in M, and it follows that $(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$ if and only if

$$(LL^* - I)^2 + \eta(LL^* - I)^2\overline{\eta} + (MM^* - I)^2 + \eta(MM^* - I)^2\overline{\eta}$$

has finite trace over $L_2(\mathbb{R}^3)$. Since each term in the above expression is the absolute square of an operator, the entire expression is in the trace class if and only if each term is in the trace class. Because η has modulus 1, $A\overline{\eta}$ is Hilbert–Schmidt if and only if A is Hilbert–Schmidt. We thus conclude that $(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$ if and only if both $(LL^* - I)$ and $(MM^* - I)$ are elements of $B_2(L_2(\mathbb{R}^3))$.

To carry the calculations further, it is convenient to introduce the operators

$$F_L \equiv LL^* - I + |\omega_0^{1/2}\omega^{-1/2}Q\rangle\langle\omega_0^{1/2}\omega^{-1/2}Q|$$

and

$$F_M \equiv MM^* - I + |\omega_0^{-1/2}\omega^{1/2}Q\rangle\langle\omega_0^{-1/2}\omega^{1/2}Q|.$$

Because the dyadics do not influence the Hilbert–Schmidt character of the expressions, we then have

$(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$ iff both F_L and F_M are in $B_2(L_2(\mathbb{R}^3))$.

The advantage gained by introducing these particular operators $F_{\frac{L}{M}}$ is that there are relatively simple functions $F_{\frac{L}{M}}(0)(\mathbf{p},\mathbf{q})$ such that $F_{\frac{L}{M}}$ is an element of $B_2(L_2(\mathbb{R}^3))$ if and only if $F_{\frac{L}{M}}(0)(\mathbf{p},\mathbf{q})$ is an element of $L_2(\mathbb{R}^6)$. (These functions are actually Carleman kernels for F_L and F_M, but this knowledge is not necessary here.)

In Appendix A we construct these functions as limits as $\epsilon \to 0$ of functions $F_{\frac{L}{M}}(\epsilon)$ which arise from the explicit integral kernels for the operators $L(\epsilon)$ and $M(\epsilon)$. The results are that $F_{\frac{L}{M}}(0)(\mathbf{p},\mathbf{q}) = K_{\frac{L}{M}}(0)(\omega_p^2,\omega_q^2)$, where

$$K_{\frac{L}{M}}(0)(s,t) \equiv \pm\left(\frac{-\lambda}{\pi}\right)\frac{(\omega_0^2 - s)}{D_+(s)}\frac{(\omega_0^2 - t)}{D_-(t)}\frac{\rho(s^{1/2})\rho(t^{1/2})}{(st)^{\pm 1/4}}Y_{\frac{L}{M}}(s,t),$$

with

$$Y_{\frac{L}{M}}(s,t) \equiv \int_0^\infty dy \frac{y^{\pm 1/2}D(-y)}{(y+\omega_0^2)(y+s)(y+t)}.$$

So the demonstration that $(|T_\alpha^+|^2 - I) \in B_{2r}(T_\alpha\mathscr{H})$ for $0 < \alpha < \frac{1}{2}$ now reduces to showing that $F_L(0)$ and $F_M(0)$ are in $L_2(\mathbb{R}^6)$ for $0 < \alpha < \frac{1}{2}$, and the demonstration that $(|T_\alpha^+|^2 - I) \notin B_{2r}(T_\alpha\mathscr{H})$ for $\frac{1}{2} < \alpha < 1$ now reduces to showing that $F_L(0)$, say, is not in $L_2(\mathbb{R}^6)$ for $\frac{1}{2} < \alpha < 1$. These demonstrations are a straightforward application of the estimates in Appendix B.

Suppose first that $0 < \alpha < \frac{1}{2}$. Then

$$\tau_{\frac{L}{M}}(0) \equiv \int d^3p\, d^3q |F_{\frac{L}{M}}(0)(\mathbf{p},\mathbf{q})|^2$$

$$= (2\pi)^2 \int_0^\infty ds\, dt\, (st)^{1/2} |K_{\frac{L}{M}}(0)(s,t)|^2,$$

and the estimates in Appendix B then give

$$\tau_{\frac{L}{M}}(0) < (2\pi d_1)^2 \int_0^\infty ds\, dt\, (1+s)^{-1}(1+t)^{-1}(st)^{-\alpha}(s+t)^{-1},$$

and this last integral is easily seen to be convergent for $0 < \alpha < \frac{1}{2}$. Thus $(|T_\alpha^+|^2 - I) \in B_{2r}(T_\alpha\mathscr{H})$ for $0 < \alpha < \frac{1}{2}$.

Now suppose that $\frac{1}{2} < \alpha < 1$. We have the decomposition $F_{\frac{L}{M}}(0)(\mathbf{p},\mathbf{q}) = F_{\frac{L}{M}}^{(1)}(0)(\mathbf{p},\mathbf{q}) + F_{\frac{L}{M}}^{(2)}(0)(\mathbf{p},\mathbf{q})$ made in Appendix B; to show that $F_L(0) \notin L_2(\mathbb{R}^6)$, we show that $F_L^{(1)}(0) \in L_2(\mathbb{R}^6)$ whereas $F_L^{(2)}(0) \notin L_2(\mathbb{R}^6)$. Let

$$\tau_L^{(j)}(0) \equiv \int d^3p\, d^3q |F_L^{(j)}(0)(\mathbf{p},\mathbf{q})|^2.$$

As above, the considerations in Appendix B show that for $\frac{1}{2} < \alpha < 1$, $\tau_L^{(1)}(0)$ is less than the convergent integral

$$(2\pi d_2)^2 \int_0^\infty ds\, dt\, (1+s)^{-1}(1+t)^{-1}(st)^{-(1-\alpha)}(s+t)^{-1}$$

so that $F_L^{(1)}(0) \in L_2(\mathbb{R}^6)$, as claimed. For future reference we note that in an identical fashion we find $F_M^{(1)}(0) \in L_2(\mathbb{R}^6)$ also.

The lower bound for $K_L^{(2)}(0)$ developed in Appendix B yields the lower bound

$$\tau_L^{(2)}(0) \geq (2\pi(1-\alpha)2^\alpha h_2(a))^2 \times \int_0^\nu ds\, dt\, (1+s)^{-1}(1+t)^{-1}(st)^{-(1-\alpha)}(s+t)^{-2\alpha},$$

where $\nu \equiv \omega_0^2/2$.

It is not difficult to verify that this last integral is divergent, for example, by making the change of variables $s = r\theta$ and $t = r(1-\theta)$. Thus $F_L^{(2)}(0) \notin L_2(\mathbb{R}^6)$, as asserted.

For brevity we have omitted the case $\alpha = \frac{1}{2}$; it can be shown that $(|T_{1/2}^+|^2 - I) \in B_{2r}(T_{1/2}\mathscr{H})$. We, therefore, have finally

$$(|T_\alpha^+|^2 - I) \in B_{2r}(T_\alpha\mathscr{H}), \quad \text{for } 0 < \alpha \leq \tfrac{1}{2},$$

but

$$(|T_\alpha^+|^2 - I) \notin B_{2r}(T_\alpha\mathscr{H}), \quad \text{for } \tfrac{1}{2} < \alpha < 1.$$

D. Implementability of β in π_I

The results of [I] guarantee that the time-development automorphism group β can be unitarily implemented in the Fock representation if and only if both $P_m(|T_\alpha^+|^2 - I) \in B_{2r}(T_\alpha\mathscr{H})$ and $[|T_\alpha^+|^2, \Lambda(I - P_m)H] \in B_{2r}(T_\alpha\mathscr{H})$. In this subsection we examine these two operators to determine whether or not they are of Hilbert–Schmidt type.

Because $(|T_\alpha^+|^2 - I) \in B_{2r}(T_\alpha\mathscr{H})$ for $\alpha < \frac{1}{2}$, it follows that both of $P_m(|T_\alpha^+|^2 - I)$ and $[(|T_\alpha^+|^2 - I), \Lambda(I - P_m)H]$ are Hilbert–Schmidt operators for $\alpha < \frac{1}{2}$. The remainder of this subsection analyzes these operators for the case $\frac{1}{2} < \alpha < 1$.

The Hamiltonian H which generates the time development operator $V_t = e^{t\Lambda H}$ for the normal modes is given by

$$H = \begin{bmatrix} \omega & 0 & 0 & 0 \\ 0 & \omega & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

and the spectral projection P_m for H onto energies larger than m is given by

$$P_m = \begin{bmatrix} \theta(|\mathbf{p}| - m) & 0 & 0 & 0 \\ 0 & \theta(|\mathbf{p}| - m) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

where $\theta: \mathbb{R} \to \mathbb{R}$ is the usual step function which vanishes for negative argument and has value 1 for positive argument.

The Hilbert–Schmidt nature of $P_m(|T^+|^2 - I)$ is easy to ascertain. Note first that because $(|T^+|^2 - I)P_m$ is its adjoint, $P_m(|T^+|^2 - I)$ is a Hilbert–Schmidt operator if and only if $(|T^+|^2 - I)P_m$ is a Hilbert–Schmidt operator. Note also that $P_m = \theta(|\mathbf{p}| - m)TT^+$, and that multiplication by $\theta(|\mathbf{p}| - m)$ commutes with the conjugation C. Then it is easy to see, by arguments parallel to those in Sec. III C, that $P_m(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$ if and only if both $(LL^* - I) \times \theta(|\mathbf{p}| - m)$ and $(MM^* - I)\theta(|\mathbf{p}| - m)$ are elements of $B_2(L_2(\mathbb{R}^3))$. With arguments identical to those used earlier, it

is easy to show that $(LL^* - I)\theta(|\mathbf{p}| - m)$ and $(MM^* - I)\theta(|\mathbf{p}| - m)$ are in $B_2(L_2(\mathbb{R}^3))$ if and only if $F_L(0)$ and $F_M(0)$ are elements of $L_2(\mathbb{R}^3 \times \{\mathbf{q} \in \mathbb{R}^3 | |\mathbf{q}| > m\})$.

To verify these latter conditions, we need only inspect the integrals

$$\sigma_{\substack{L \\ M}}^{(2)}(m) \equiv \int d^3p \int_{|\mathbf{q}|>m} d^3q |F_{\substack{L \\ M}}^{(2)}(0)(\mathbf{p},\mathbf{q})|^2,$$

because we already know that $F_{\substack{L \\ M}}^{(1)}(0) \in L_2(\mathbb{R}^6)$. Now, the estimates in Appendix B imply

$$\sigma_L^{(2)}(m) \leqslant (2\pi k_2(\alpha) m^{-2\alpha})^2 \int_0^\infty ds \int_{m^2}^\infty dt \times (1+s)^{-1}(1+t)^{-1}(st)^{-(1-\alpha)},$$

and

$$\sigma_M^{(2)}(m) \leqslant (2\pi k_2(\alpha) m^{-2\alpha(1-\alpha)})^2 \int_0^\infty ds \int_{m^2}^\infty dt \times (1+s)^{-1}(1+t)^{-1}(st)^{-\alpha}.$$

Since these last integrals are convergent, we see that the low-momentum cutoff has improved the integrals enough to make $\sigma_L^{(2)}(m)$ finite. Thus $(LL^* - I)\theta(|\mathbf{p}| - m)$ and $(MM^* - I)\theta(|\mathbf{p}| - m)$ are elements of $B_2(L_2(\mathbb{R}^3))$, hence $P_m(|T_\alpha^+|^2 - I) \in B_{2r}(T_\alpha \mathscr{H})$ for $\frac{1}{2} < \alpha < 1$.

The Hilbert–Schmidt nature of $[|T^+|^2, \Lambda(I - P_m)H]$ is determined by the following considerations. Let

$$\xi(\mathbf{p}) \equiv \begin{cases} |\mathbf{p}|, & \text{for } |\mathbf{p}| \leqslant m, \\ 0, & \text{for } |\mathbf{p}| > m. \end{cases}$$

Then $\Lambda(I - P_m)H$ is the bounded operator

$$\Lambda(I - P_m)H = \begin{bmatrix} 0 & -\xi & 0 & 0 \\ \xi & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

So we find

$$[|T^+|^2, \Lambda(I - P_m)H] = \begin{bmatrix} B\xi + \xi B^* & \xi D - A\xi & 0 & 0 \\ D\xi - \xi A & -\xi B - B^*\xi & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

and hence

$$\mathrm{tr}_r(|[|T^+|^2, \Lambda(I - P_m)H]|^2) = \mathrm{tr}(|D\xi - \xi A|^2 + |\xi D - A\xi|^2 + |B\xi + \xi B^*|^2 + |B^*\xi + \xi B|^2),$$

where the latter trace is taken over a basis for $L_2(\mathbb{R}^3)_C$.

It is again straightforward, although tedious, to verify that

$$2(|D\xi - \xi A|^2 + |\xi D - A\xi|^2 + |B\xi + \xi B^*|^2 + |B^*\xi + \xi B|^2) = |\xi MM^* - LL^*\xi|^2 + \eta|\xi MM^* - LL^*\xi|^2\overline{\eta} + |MM^*\xi - \xi LL^*|^2 + \eta|MM^*\xi - \xi LL^*|^2\overline{\eta}.$$

Again, the sum of the first two terms commutes with the conjugation C and with multiplication by i, and hence has finite $L_2(\mathbb{R}^3)_C$ trace if and only if it has finite $L_2(\mathbb{R}^3)$ trace. Since the third and fourth operators are adjoints of the first and second, respectively, the same reasoning as before leads to the conclusion

$$[|T^+|^2, \Lambda(I - P_m)H] \in B_{2r}(T\mathscr{H}) \quad \text{iff } \xi MM^* - LL^*\xi \in B_2(L_2(\mathbb{R}^3)).$$

To demonstrate that $(\xi M_\alpha M_\alpha^* - L_\alpha L_\alpha^* \xi) \in B_2(L_2(\mathbb{R}^3))$ for $\alpha > \frac{1}{2}$, we first observe that because the multiplicative operator ξ is bounded, we may employ the same arguments as before to establish that

$$(\xi MM^* - LL^*\xi) \in B_2(L_2(\mathbb{R}^3)) \quad \text{iff } \xi(\mathbf{p})F_M(0)(\mathbf{p},\mathbf{q}) - F_L(0)(\mathbf{p},\mathbf{q})\xi(\mathbf{q}) \in L_2(\mathbb{R}^6).$$

Next, because we already know that $F_{\substack{L \\ M}}^{(1)}(0) \in L_2(\mathbb{R}^6)$, we need only examine the function $\xi(\mathbf{p})F_M^{(2)}(0)(\mathbf{p},\mathbf{q}) - F_L^{(2)}(0)(\mathbf{p},\mathbf{q})\xi(\mathbf{q})$. Now note that

$$\sigma^{(2)} \equiv \int d^3p\, d^3q |\xi(\mathbf{p})F_M^{(2)}(0)(\mathbf{p},\mathbf{q}) - F_L^{(2)}(0)(\mathbf{p},\mathbf{q})\xi(\mathbf{q})|^2$$
$$= (2\pi)^2 \int_0^\infty ds\, dt\, (st)^{1/2} |\xi(s^{1/2}) \times K_M^{(2)}(0)(s,t) - K_L^{(2)}(0)(s,t)\xi(t^{1/2})|^2$$
$$\leqslant 2(2\pi)^2 \int_0^{m^2} s\, ds \int_0^\infty dt\, (st)^{1/2} \times (|K_M^{(2)}(0)(s,t)|^2 + |K_L^{(2)}(0)(t,s)|^2),$$

where we have interchanged the integration variable names in the second term in order to get the last expression. From the estimates in Appendix B we then find

$$\sigma^{(2)} \leqslant 2(2\pi k_2(\alpha))^2 \int_0^{m^2} ds \int_0^\infty dt\, (1+s)^{-1}(1+t)^{-1} \times \{s^{-(1-\alpha)}t^{-\alpha} + s^{-\alpha}t^{-(1-\alpha)}\}.$$

Since these last integrals are convergent it follows that

$$(\xi(\mathbf{p})F_M(0)(\mathbf{p},\mathbf{q}) - F_L(0)(\mathbf{p},\mathbf{q})\xi(\mathbf{q})) \in L_2(\mathbb{R}^6),$$

whence

$$[|T_\alpha^+|^2, \Lambda(I - P_m)H] \in B_{2r}(T_\alpha \mathscr{H}) \text{ for } \tfrac{1}{2} < \alpha < 1,$$

as asserted.

E. Implementability of β^o in π_T

According to the general theory developed in [I], the automorphism group β^o (which specifies the time development of the uncoupled system) is implementable in the representation π_T (which is induced by the state on $\mathscr{W}$ invariant under the interacting time-development automorphism β_t) if and only if $|T|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$. That is, β^o is implementable in π_T if and only if both $P_m^o(|T|^2 - I) \in B_{2r}(\mathscr{H})$ and $[|T|^2, \Lambda(I - P_m^o)H^o] \in B_{2r}(\mathscr{H})$.

Because we have shown above that $(|T|^2 - I) \in B_{2r}(\mathscr{H})$ for $\alpha < \frac{1}{2}$, it follows that both of the above operators are in the Hilbert–Schmidt class for $\alpha < \frac{1}{2}$. The remainder of this section analyzes these operators for the case $\frac{1}{2} < \alpha < 1$.

The Hamiltonian H^o, which generates the time development operator V_t^o for the uncoupled system, is given by

$$H^o = \begin{bmatrix} \omega & 0 & 0 & 0 \\ 0 & \omega & 0 & 0 \\ 0 & 0 & \omega_0 & 0 \\ 0 & 0 & 0 & \omega_0 \end{bmatrix},$$

and the spectral projection P_m^o for H^o onto energies larger than m is given by

$$P_m^o = \begin{bmatrix} \theta(\omega - m) & 0 & 0 & 0 \\ 0 & \theta(\omega - m) & 0 & 0 \\ 0 & 0 & \theta(\omega_0 - m) & 0 \\ 0 & 0 & 0 & \theta(\omega_0 - m) \end{bmatrix}.$$

The transformation $|T|^2$ is computed in a straightforward fashion, making use of the identities involving L, M, and Q given earlier, and is given by

$$|T|^2 = \begin{bmatrix} L^*L & 0 & |L^*\omega_0^{1/2}\omega^{-1/2}Q\rangle & 0 \\ 0 & M^*M & 0 & |M^*\omega^{1/2}\omega_0^{-1/2}Q\rangle \\ \langle L^*\omega_0^{1/2}\omega^{-1/2}Q| & 0 & \|\omega_0^{1/2}\omega^{-1/2}Q\|^2 & 0 \\ 0 & \langle M^*\omega^{1/2}\omega_0^{-1/2}Q| & 0 & \|\omega^{1/2}\omega_0^{-1/2}Q\|^2 \end{bmatrix}.$$

is easy to show that $(LL^* - I)\theta(|\mathbf{p}| - m)$ and $(MM^* - I)\theta(|\mathbf{p}| - m)$ are in $B_2(L_2(\mathbb{R}^3))$ if and only if $F_L(0)$ and $F_M(0)$ are elements of $L_2(\mathbb{R}^3 \times \{\mathbf{q} \in \mathbb{R}^3 | |\mathbf{q}| > m\})$.

To carry the calculations further, we once again reduce the investigation of the Hilbert–Schmidt character of these operators on $L_2(\mathbb{R}^3)$ to the investigation of the square integrability of associated functions on $\mathbb{R}^6$. This reduction is parallel to, and somewhat simpler than, the corresponding reduction developed earlier for the expressions involving LL^* and MM^* in place of L^*L and M^*M. For brevity, we merely outline the procedure here.

As in Appendix A, consideration of the kernal for the operator $(L(\epsilon)^* - I)(L(\epsilon) - I)$ leads, via contour integration (with one less residue term this time), to the conclusion that the operator $\tilde{F}_L \equiv L^*L - I$ is in the Hilbert–Schmidt class if and only if the function $\tilde{F}_L(0)(\mathbf{p},\mathbf{q})$ is in $L_2(\mathbb{R}^6)$. Similarly, $\tilde{F}_M \equiv M^*M - I$ is a Hilbert–Schmidt operator if and only if the function $\tilde{F}_M(0)(\mathbf{p},\mathbf{q})$ is in $L_2(\mathbb{R}^6)$. Here $\tilde{F}_L(\epsilon) \equiv \underset{M}{\tilde{K}}_L(\epsilon)(\omega_p^2,\omega_q^2)$, with $\underset{M}{\tilde{K}}_L(\epsilon)(s,t) \equiv \pm(-\lambda/\pi)(st)^{\pm 1/4}\rho(s^{1/2})\rho(t^{1/2})\underset{M}{\tilde{Y}}_L(s + i\epsilon, t - i\epsilon)$ and

$$\underset{M}{\tilde{Y}}_L(z,w) \equiv \int_0^\infty dy \frac{(y + \omega_0^2)}{y^{\pm 1/2}(y + z)(y + w)D(-y)}.$$

The demonstration that $(L^*L - I)\theta(\omega - m) \in B_2(L_2(\mathbb{R}^3))$ then reduces to showing that the function $\tilde{F}_L(0)(\mathbf{p},\mathbf{q}) \times \theta(|\mathbf{q}| - m)$ is in $L_2(\mathbb{R}^6)$. Similarly, we find that $(M^*M - I) \times \theta(\omega - m) \in B_2(L_2(\mathbb{R}^3))$ if and only if $\tilde{F}_M(0)(\mathbf{p},\mathbf{q}) \times \theta(|\mathbf{q}| - m) \in L_2(\mathbb{R}^6)$.

To show that the functions $F_L(0)$ and $F_M(0)$ are elements of $L_2(\mathbb{R}^3 \times \{\mathbf{q} \in \mathbb{R}^3 | |\mathbf{q}| > m\})$, we simply inspect the integrals

$$\underset{M}{\tilde{\sigma}}_L(m) \equiv \int d^3p \int_{|\mathbf{q}| > m} d^3q |\underset{M}{\tilde{F}}_L(0)(\mathbf{p},\mathbf{q})|^2.$$

The estimates in Appendix B show that these integrals are convergent for $\frac{1}{2} < \alpha < 1$. We therefore conclude that

$$P_m^o(|T|^2 - I) \in B_{2r}(\mathscr{H}), \quad \text{for all } \alpha \in (0,1).$$

We next consider the operator $[|T|^2, \Lambda(I - P_m^o)H^o]$. With ξ representing multiplication by the function $\xi(\mathbf{p})$ introduced earlier, and with $\xi_0 \equiv \omega_0\theta(m - \omega_0)$, we have

$$\Lambda(I - P_m^o)H^o = \begin{pmatrix} 0 & -\xi & 0 & 0 \\ \xi & 0 & 0 & 0 \\ 0 & 0 & 0 & -\xi_0 \\ 0 & 0 & \xi_0 & 0 \end{pmatrix}.$$

The same reasoning as for the analogous expression with T^+ and H leads to the conclusion

$$[|T|^2, \Lambda(I - P_m^o)H^o] \in B_{2r}(\mathscr{H}) \text{ iff } \xi M^*M - L^*L\xi \in B_2(L_2(\mathbb{R}^3)),$$

which is in turn equivalent to

$$\xi(\mathbf{p})\tilde{F}_M(0)(\mathbf{p},\mathbf{q}) - \tilde{F}_L(0)(\mathbf{p},\mathbf{q})\xi(\mathbf{q}) \in L_2(\mathbb{R}^6).$$

To verify this last condition, we can make use of the estimates in Appendix B to obtain

$$\begin{aligned} \tilde{\sigma} &\equiv \int d^3p\, d^3q |\xi(\mathbf{p})\tilde{F}_M(0)(\mathbf{p},\mathbf{q}) - \tilde{F}_L(0)(\mathbf{p},\mathbf{q})\xi(\mathbf{q})|^2 \\ &\leqslant 2(2\pi)^2 \int_0^{m^2} s\, ds \int_0^\infty dt\, (st)^{1/2} \\ &\quad \times (|\underset{M}{\tilde{K}}_M(0)(s,t)|^2 + |\underset{M}{\tilde{K}}_L(0)(t,s)|^2) \\ &\leqslant 16\pi^2\lambda^2 \int_0^{m^2} ds \int_0^\infty dt \frac{s}{(1 + s)(1 + t)(st)^\alpha(s + t)}. \end{aligned}$$

Since this last integral is convergent, it follows that $[|T|^2, \Lambda(I - P_m^o)H^o] \in B_{2r}(\mathscr{H})$ for $\frac{1}{2} < \alpha < 1$.

We have thus shown that both $P_m^o(|T|^2 - I)$ and $[|T|^2, \Lambda(I - P_m^o)H^o]$ are Hilbert–Schmidt operators for $\alpha \in (0,1)$, that is, $|T|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$. Thus β^o is implementable in π_T for all values of α.

F. Existence of wave morphisms

According to Theorem 2 of [I], the limits $\Omega_\pm \equiv \text{s-lim}_{t \to \pm\infty} T^+ e^{t\Lambda H} T e^{-t\Lambda H^o} P_{ac}^o$ exist on $\mathscr{H}$ if $TD(H^o) = D(H)$ and if $(I - P_m)(\Lambda HT - T\Lambda H^o)(I - P_m^o)$ is a trace-class operator on $\mathscr{H}$ for all sufficiently large m. In this section we illustrate the application of this theorem by verifying these conditions for the model under study. (Note that the

additional hypothesis of Theorem 2, that $e^{tAH}T\mathscr{H}\subset T\mathscr{H}$ for all t, is satisfied automatically in the model.)

It is easy to see that the condition $TD(H^o)=D(H)$ is equivalent to the conditions

$$LD(\omega)=D(\omega) \quad \text{and} \quad MD(\omega)=D(\omega),$$

where as before ω is the operation of multiplication by $\omega_p \equiv|\mathbf{p}|$ on $L_2(\mathbb{R}^3)$.

From the formulas for $L(\epsilon)$ and $M(\epsilon)$, it follows that for $f\in D(\omega)$ we have $M\omega f=\omega Lf$. Because L and M are bounded, and because $L^*M=I$, it follows immediately that $Lf\in D(\omega)$ if and only if $f\in D(\omega)$, that is, $LD(\omega)=D(\omega)$.

To show that $MD(\omega)=D(\omega)$, it is helpful to establish that the operator $Z\equiv\omega M-M\omega$ is a bounded operator on $L_2(\mathbb{R}^3)$. To do this, we simply examine the explicit integral kernel for $Z(\epsilon)\equiv\omega M(\epsilon)-M(\epsilon)\omega$:

$$Z(\epsilon)(\mathbf{p},\mathbf{q})=\omega_p^{1/2}Q(\mathbf{p})(\omega_0^2-\omega_p^2)\times\frac{\omega_p-\omega_q}{\omega_p^2-\omega_q^2+i\epsilon}\omega_q^{-1/2}\rho(\mathbf{q}).$$

It is not difficult to see that the integral operator is bounded uniformly in ϵ, hence that Z is bounded.

From the facts that $\omega Mf=M\omega f+Zf$ for $f\in D(\omega)$ and $L^*M=I$, it follows immediately that $MD(\omega)=D(\omega)$. Thus $TD(H^o)=D(H)$.

We next consider the operator $X\equiv(I-P_m)\times(\Lambda HT-T\Lambda H^o)(I-P_m^o)$. It is straightforward to show that

$$X^*X=\begin{pmatrix}|\theta M\xi-\xi L\theta|^2 & 0 & 0 & 0\\ 0 & |\xi M\theta-\theta L\xi|^2 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix},$$

modulo dyadic and constant terms which do not influence the finiteness of the trace norm. Here the symbol θ is a shorthand for the operation of multiplication by $\theta(m-\omega)$. Thus X belongs to the trace class if and only if both $|\theta M\xi-\xi L\theta|$ and $|\xi M\theta-\theta L\xi|$ have finite traces over $L_2(\mathbb{R}^3)$.

Now, $\xi=\omega\theta$, and $M\omega f=\omega Lf$ for $f\in D(\omega)$. Thus $(\theta M\xi-\xi L\theta)g=\theta(M\omega-\omega L)\theta g=0$ for all $g\in L_2(\mathbb{R}^3)$. That is, $\theta M\xi-\xi L\theta=0$. So we need consider only $\xi M\theta-\theta L\xi$.

By using the explicit kernels for $L(\epsilon)$ and $M(\epsilon)$, it is straightforward to calculate that

$$\xi M\theta-\theta L\xi=|\theta(m-\omega)\omega^{-1/2}(\omega_0^2-\omega^2)Q\rangle\times\langle\omega^{-1/2}\rho(\omega)\theta(m-\omega)|,$$

where each entry of the dyadic is in $L_2(\mathbb{R}^3)$. Thus we trivially have that $(\xi M\theta-\theta L\xi)$ is a trace-class operator as well. We have therefore shown that $X\in B_{1r}(\mathscr{H})$, and the hypotheses of Theorem 2 in [I] are thereby verified.

G. Explicit calculation of wave morphisms

The existence of the limits

$$\Omega_\pm\equiv\text{s-lim}_{t\to\pm\infty}\ T^+e^{tAH}Te^{-tAH^o}P_{\text{ac}}^o$$

is guaranteed by the fact T, H, and H^o satisfy the hypotheses of Theorem 2 in [I]. For the particular transformations at hand, however, we can obtain much more information by calculating these limits explicitly. The results are instructive and have implications for the choice of method used to construct the S matrix, as we will see later.

Let $\Phi(t)\equiv e^{tAH}Te^{-tAH^o}P_{\text{ac}}^o$. The projection P_{ac}^o onto the absolutely continuous subspace of H^o is given by

$$P_{\text{ac}}^o=\begin{pmatrix}I & 0 & 0 & 0\\ 0 & I & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}.$$

We note that in this model $P_{\text{ac}}^o=TT^+$.

With the temporary abbreviations

$$\sigma\equiv\sin\omega t,\quad \tau\equiv\cos\omega t,$$

$$\sigma_0\equiv\sin\omega_0 t,\quad \tau_0\equiv\cos\omega_0 t,$$

it is straightforward to compute that

$$\Phi(t)=\begin{pmatrix}\Phi_{11}(t) & \Phi_{12}(t) & 0 & 0\\ \Phi_{21}(t) & \Phi_{22}(t) & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix},$$

where

$$\begin{aligned}2\Phi_{11}(t)&=\tau(L+\bar{L})\tau+\sigma(M+\bar{M})\sigma\\&\quad+i\sigma(L-\bar{L})\tau-i\tau(M-\bar{M})\sigma,\\ 2\Phi_{12}(t)&=\tau(L+\bar{L})\sigma-\sigma(M+\bar{M})\tau\\&\quad+i\sigma(L-\bar{L})\sigma+i\tau(M-\bar{M})\tau,\\ 2\Phi_{21}(t)&=\sigma(L+\bar{L})\tau-\tau(M+\bar{M})\sigma\\&\quad-i\tau(L-\bar{L})\tau-i\sigma(M-\bar{M})\sigma,\\ 2\Phi_{22}(t)&=\sigma(L+\bar{L})\sigma+\tau(M+\bar{M})\tau\\&\quad+i\sigma(M-\bar{M})\tau-i\tau(L-\bar{L})\sigma.\end{aligned}$$

To evaluate the large $|t|$ limits of these expressions, we make use of the following lemma. Recall that Ψ: $L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$ is the spherical average, and that the function $\eta(\mathbf{p})\equiv D_+(\omega_p^2)/D_-(\omega_p^2)$ takes complex values with modulus 1.

Lemma: The operators L and M have the properties

$$\begin{aligned}&\text{s-lim}_{t\to+\infty}\ e^{-it\omega}(L-I)e^{it\omega}\\&\quad=\text{s-lim}_{t\to+\infty}\ e^{-it\omega}(M-I)e^{it\omega}=(\bar{\eta}-1)\Psi,\\&\text{s-lim}_{t\to-\infty}\ e^{-it\omega}(L-I)e^{it\omega}\\&\quad=\text{s-lim}_{t\to-\infty}\ e^{-it\omega}(M-I)e^{it\omega}=0.\end{aligned}$$

Proof: Let D be the dense subspace of $L_2(\mathbb{R}^3)$ consisting of continuously differentiable functions of compact support not including the origin. Let $A_t\equiv e^{-it\omega}(L-I)e^{it\omega}$. We will show that

$$\lim_{t\to+\infty}\|(A_t-(\bar{\eta}-1)\Psi)f\|=0 \quad\text{and}\quad \lim_{t\to-\infty}\|A_tf\|=0,$$

for $f\in D$. Because A_t is uniformly bounded, it then follows that $\text{s-lim}_{t\to+\infty}A_t=(\bar{\eta}-1)\Psi$ and $\text{s-lim}_{t\to-\infty}A_t=0$.

To establish these assertions, let $f\in D$. Then using the explicit formula for $L(\epsilon)$ and integrating over the angular variables, we find

$$(A_t f)(\mathbf{p}) = \lim_{\epsilon \to +0} \frac{-4\pi\lambda\rho(\mathbf{p})(\omega_0^2 - \omega_p^2)}{\omega_p^{1/2} D_+(\omega_p^2)} \times \int_0^\infty dq \frac{e^{it(q-\omega_p)} q^{5/2}\rho(q)}{q^2 - \omega_p^2 - i\epsilon} (\Psi f)(q).$$

Note that $h(q) \equiv q^{5/2}\rho(q)(\Psi f)(q)$ is a continuously differentiable function with compact support on the positive half-line. The remaining integral can now be written

$$\int_0^\infty dq \frac{e^{it(q-\omega_p)} h(q)}{q^2 - \omega_p^2 - i\epsilon} = \pi i \int_0^\infty dq \frac{(\epsilon/\pi) h(q) e^{it(q-\omega_p)}}{(q^2-\omega_p^2)^2 + \epsilon^2} + \int_0^\infty dq \frac{h(q) - h(\omega_p)}{q - \omega_p} \frac{e^{it(q-\omega_p)}}{q + \omega_p} \frac{(q^2-\omega_p^2)^2}{(q^2-\omega_p^2)^2 + \epsilon^2} + h(\omega_p) \int_0^\infty dq \frac{q^2 - \omega_p^2}{(q^2-\omega_p^2)^2 + \epsilon^2} e^{it(q-\omega_p)}.$$

Because $q^{-1}h(q)e^{it(q-\omega_p)}$ is a continuous integrable function of q, the first integral term on the right-hand side becomes, in the limit $\epsilon \to +0$, simply $(\pi i/2\omega_p)h(\omega_p)$. The second integral term becomes, in the limit $\epsilon \to +0$,

$$\int_0^\infty dq \frac{h(q) - h(\omega_p)}{q - \omega_p} \frac{e^{it(q-\omega_p)}}{q + \omega_p},$$

and has, by virtue of the nice properties of h, an absolutely integrable integrand. The third integral term becomes, in the limit $\epsilon \to +0$, the principal-value integral

$$h(\omega_p) P \int_0^\infty \frac{e^{it(q-\omega_p)}}{q^2 - \omega_p^2} dq = \frac{h(\omega_p)}{2\omega_p} \{ i\,\mathrm{Si}(t\omega_p)(1 + e^{-2it\omega_p}) - \pi(\sin|t\omega_p|)e^{-it\omega_p} + \mathrm{Ci}(t\omega_p)(e^{-2it\omega_p} - 1)\},$$

where Si and Ci are the sine and cosine integrals

$$\mathrm{Si}(x) \equiv \int_0^x \frac{\sin t}{t} dt \quad \text{and} \quad \mathrm{Ci}(x) \equiv -\int_x^\infty \frac{\cos t}{t} dt.$$

We now consider the limits as $t \to \pm\infty$ of these three terms. The first expression is independent of t. The second integral term vanishes as $|t| \to \infty$ by virtue of the Riemann–Lebesgue Lemma. Because $\lim_{|x|\to\infty} \mathrm{Ci}(x) = 0$ and $\lim_{x \to \pm\infty} \mathrm{Si}(x) = \pm\pi/2$, the third expression has the limit $\pm(\pi i/2\omega_p)h(\omega_p)$ as $t \to \pm\infty$. So we have

$$\lim_{t\to\pm\infty} \lim_{\epsilon\to+0} \int_0^\infty dq \frac{e^{it(q-\omega_p)} h(q)}{q^2 - \omega_p^2 - i\epsilon} = \frac{1 \pm 1}{2} \frac{\pi i}{\omega_p} h(\omega_p).$$

Upon substitution of this result into the formula for $A_t f$, and use of the identity

$$D_+(\omega_p^2) - D_-(\omega_p^2) = -4\pi^2 i\lambda\omega_p(\omega_p^2 - \omega_0^2)(\rho(p))^2,$$

we find

$$\lim_{t\to\pm\infty} (A_t f)(\mathbf{p}) = [(1 \pm 1)/2]((\bar{\eta} - 1)\Psi f)(\mathbf{p}),$$

as asserted.

The proof for M in place of L is the same. ///

Applying this lemma to the expressions above for $\Phi(t)$, we find

$$\lim_{t\to+\infty} \Phi(t) = P^o_{\mathrm{ac}} \quad \text{and} \quad \lim_{t\to-\infty} \Phi(t) = S,$$

where S is the partial isometry given by

$$S \equiv \begin{pmatrix} (I-\Psi) + (\mathrm{Re}\,\eta)\Psi & (\mathrm{Im}\,\eta)\Psi & 0 & 0 \\ -(\mathrm{Im}\,\eta)\Psi & (I-\Psi) + (\mathrm{Re}\,\eta)\Psi & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Thus, since $T^+ P^o_{\mathrm{ac}} = T^+$, we have

$$\Omega_+ = T^+ \quad \text{and} \quad \Omega_- = T^+ S.$$

Note that the partial isometry S induces the scattering morphism, because $(\Omega_+)^+\Omega_- = S$.

H. Nonimplementability of S in π_T

The partial isometry S which induces the scattering morphism is, of course, implementable in the Fock representation. It is natural to ask whether S is also implementable in the interaction-vacuum representation π_T. The answer is no for $\frac{1}{2} < \alpha < 1$, as the following analysis shows.

The theory developed in Sec. V of [I] shows that, if $T(\ker S)$ and $T(\mathrm{ran}\,S)$ are complex subspaces of $\mathscr{H}$, then the partial symplectic transformation S is implementable by partial isometry in π_T if and only if $(|TS|^2 - |T|^2) \in B_{2r}(S^+\mathscr{H})$. From the fact that S is a partial isometry with initial and final spaces equal to $T\mathscr{H}$, it is clear that $T(\ker S)$ and $T(\mathrm{ran}\,S)$ are complex subspaces. Because S is unitary on $T\mathscr{H}$, it follows that S is implementable in π_T if and only if $[S, |T|^2] \in B_{2r}(T\mathscr{H})$.

By straightforward calculation, making use of the identity $L\Psi = L - (I - \Psi)$ and the corresponding formula for M, it is not difficult to establish that $[S, |T|^2] \in B_{2r}(T\mathscr{H})$ if and only if all three of $[(\mathrm{Re}\,\eta), L^*, L]$, $[(\mathrm{Re}\,\eta), M^*M]$, and $((\mathrm{Im}\,\eta)L^*L - M^*M(\mathrm{Im}\,\eta))$ are elements of $B_2(L_2(\mathbb{R}^3))$. We now demonstrate that the third operator is not in fact of the Hilbert–Schmidt class.

As earlier, $((\mathrm{Im}\,\eta)L^*L - M^*M(\mathrm{Im}\,\eta)) \in B_2(L_2(\mathbb{R}^3))$ if and only if the function

$$X(\mathbf{p},\mathbf{q}) \equiv [(\mathrm{Im}\,\eta(\mathbf{p}))\tilde{F}_L(0)(\mathbf{p},\mathbf{q}) - \tilde{F}_M(0)(\mathbf{p},\mathbf{q})(\mathrm{Im}\,\eta(\mathbf{q}))]$$

is an element of $L_2(\mathbb{R}^6)$. It is easy to see from the formula for D_+ that for $\frac{1}{2} < \alpha < 1$,

$$\lim_{t\to0} \eta(t^{1/2}) = e^{i\pi(2\alpha-1)}.$$

There thus exists $\nu > 0$ such that

$$\mathrm{Im}\,\eta(t^{1/2}) > \delta \equiv \tfrac{1}{2}\sin\pi(2\alpha - 1) > 0, \quad \text{for all } t \in (0,\nu).$$

Now,

$$\int d^3p\, d^3q |X(\mathbf{p},\mathbf{q})|^2 = 4\lambda^2 \int_0^\infty ds\, dt \frac{(st)^{-(\alpha-1/2)}}{(1+s)(1+t)} \times |(\mathrm{Im}\,\eta(s^{1/2}))(st)^{1/4}\tilde{Y}_L(s,t) + (\mathrm{Im}\,\eta(t^{1/2}))(st)^{-1/4}\tilde{Y}_M(s,t)|^2.$$

To show that this integral is divergent, we note first that it is greater than the same expression with upper limits of integration equal to ν instead of ∞. We then use the estimate

Im $\eta(t^{1/2}) > \delta$ for $t \in (0,\nu)$ along with the lower bounds for $\tilde{Y}_{L_M}$ in Appendix B to show that $\int d^3p\, d^3q |X(\mathbf{p},\mathbf{q})|^2$ is bounded below by an integral which is positive and divergent.

Therefore, we have demonstrated that for $\frac{1}{2} < \alpha < 1$, $[S, |T|^2] \notin B_{2r}(T\mathscr{H})$. Thus for this range of α, S is not isometrically implementable in π_T.

IV. SUMMARY OF CALCULATIONS

In this section we summarize the results of the preceding calculations and indicate their immediate implications. In the section which follows, we draw some conclusions.

The model consists mathematically of the two one-parameter symplectic groups V_t^0 and $T^+ V_t T$ on the classical phase space $\mathscr{H}$ which is decomposed as $\mathscr{H} = L_2(\mathbf{R}^3)_C \oplus L_2(\mathbf{R}^3)_C \oplus \mathbf{R} \oplus \mathbf{R}$, with $V_t^0 \equiv e^{t\Lambda H^o}$ and $V_t \equiv e^{t\Lambda H}$. These two symplectic groups induce the one-parameter automorphism groups β_t^o and β_t on the Weyl C^* algebra $\mathscr{W}$ of the CCR over $\mathscr{H}$, with β^o giving the time development of the uncoupled system, and β giving the time development of the interacting system. The fixed symplectic transformation T is parametrized by the low-energy coupling power α, as is the automorphism group β_t. The natural state on the Weyl algebra invariant under β^o is the Fock vacuum state E_I, and the natural state invariant under β is the state E_T which induces the representation π_T.

After establishing that the heuristic formulas for the diagonalization transformation do indeed define a bounded operator T_α that is a symplectic transformation for $0 < \alpha < 1$, we proceeded to analyze the properties of T_α which determine the implementability of the various morphisms under consideration.

(1) Isometric implementability of the diagonalizing transformation T: According to the general theory developed in [I], the diagonalizing transformation T_α is isometrically implementable in the Fock representation of $\mathscr{W}$ if and only if $|T_\alpha|^2 - I \in B_{2r}(\mathscr{H})$, or equivalently, $|T_\alpha^+|^2 - I \in B_{2r}(T_\alpha \mathscr{H})$. The above calculations using the explicit formula for T_α show that for α in the interval $(0,\frac{1}{2}]$, $|T_\alpha|^2 - I \in B_{2r}(\mathscr{H})$, whereas for α in $(\frac{1}{2},1)$, $|T_\alpha|^2 - I \notin B_{2r}(\mathscr{H})$. Thus the diagonalizing transformation is isometrically implementable in the Fock representation only for α in the range $(0,\frac{1}{2}]$. This is equivalent to the statement that the representation π_T (induced by the invariant state for the interacting automorphism group β) is isometrically equivalent to the Fock representation for α in $(0,\frac{1}{2}]$, but not for α in $(\frac{1}{2},1)$.

Note also that T is isometrically implementable in π_T if and only if $|TTT^+|^2 - I \in B_{2r}(T\mathscr{H})$; because TT^+ is the projection onto the range of T, this is equivalent to $|T|^2 - I \in B_{2r}(T\mathscr{H})$. Because the range of T has finite codimension, this is in turn equivalent to $|T|^2 - I \in B_{2r}(\mathscr{H})$, so that we conclude T_α is isometrically implementable in π_T for α in $(0,\frac{1}{2}]$, but not for α in $(\frac{1}{2},1)$.

(2) Unitary implementability of the automorphism groups: We know that the automorphism group β^o trivially has unitary implementation in the representation π_I, for all values of α. The general results in [I] establish that β has a unitary implementation in the Fock representation if and only if $|T^+|^2 \in \mathscr{R}_H(T\mathscr{H})$, that is, if and only if for some $m > 0$, $P_m(|T^+|^2 - I) \in B_{2r}(T\mathscr{H})$ and $[|T^+|^2, \Lambda(I - P_m)H] \in B_{2r}(T\mathscr{H})$. Similarly, the group β^o has a unitary implementation in π_T if and only if $|T|^2 \in \mathscr{R}_{H^o}(\mathscr{H})$. The calculations above show that for all α in $(0,1)$, both automorphism groups are unitarily implementable in each of the representations π_I and π_T. (It should be noted that this situation is a peculiarity of the model under study; there are examples of such automorphism groups β^o and β which are concurrently unitarily implementable in only one, or in neither, of the representations induced by the corresponding invariant states.) From the general theory in [I], we know that in either representation π_I or π_T we may choose the unitary families which implement β^o and β to be strongly continuous unitary groups. Thus in either representation, for all values of α, there exist self-adjoint ("second-quantized") generators for each of the free and interacting time developments.

The second half of the analysis concerned the properties of T_α which govern the existence of the wave morphisms and scattering morphism.

(3) Wave morphisms: According to Theorem 2 in [I], the limits

$$\Omega_\pm \equiv \text{s-lim}_{t \to \pm\infty} T^+ e^{t\Lambda H} T e^{-t\Lambda H^o} P_{\text{ac}}^o$$

on $\mathscr{H}$ exist and are symplectic transformations if $TD(H^o) = D(H)$ and

$$(I - P_m)(\Lambda H T - T\Lambda H^o)(I - P_m^o) \in B_{1r}(\mathscr{H}).$$

To illustrate the application of this theorem to the model under study, we have in the above calculations verified these conditions for all α in $(0,1)$. The symplectic transformations $\Omega_\pm$ which induce the wave morphisms thus exist for all values of the coupling strength.

We were able, however, to obtain much more information by calculating $\Omega_\pm$ explicitly. We found that $\Omega_+ = T^+$ and $\Omega_- = T^+ S$, where S is the partial isometry given earlier, with initial and final spaces equal to the finite-codimension "field" subspace $T\mathscr{H} = P_{\text{ac}}^o \mathscr{H}$ in $\mathscr{H}$. Note that these results for $\Omega_\pm$ reveal the important fact that for α in $(\frac{1}{2},1)$, *the wave morphisms are implementable in neither π_I nor π_T.* To see this, recall that $(I - TT^+)$ is a finite-dimensional projection, and that $S^*S = SS^* = TT^+$. Thus from the general theory in [I], we have the following.

(a) Ω_+ implementable in π_I
$\Leftrightarrow |\Omega_+|^2 - I \in B_{2r}(\Omega_+^+ \Omega_+ \mathscr{H})$
$\Leftrightarrow |T^+|^2 - I \in B_{2r}(T\mathscr{H})$.

(b) Ω_- implementable in π_I
$\Leftrightarrow |\Omega_-|^2 - I \in B_{2r}(\Omega_-^+ \Omega_- \mathscr{H})$
$\Leftrightarrow |T^+ S|^2 - I \in B_{2r}(T\mathscr{H})$
$\Leftrightarrow S^*(|T^+|^2 - I)S + (S^*S - I) \in B_{2r}(T\mathscr{H})$
$\Leftrightarrow |T^+|^2 - I \in B_{2r}(T\mathscr{H})$.

(c) Ω_+ implementable in π_T
$\Leftrightarrow |T\Omega_+ T^+|^2 - I \in B_{2r}(T\Omega_+^+ \mathscr{H})$
$\Leftrightarrow |T^+|^2 - I - T^{*+}(I - TT^+)T^+ \in B_{2r}(T\mathscr{H})$
$\Leftrightarrow |T^+|^2 - I \in B_{2r}(T\mathscr{H})$.

(d) Ω_- implementable in π_T

$$\Leftrightarrow |T\Omega_- T^+|^2 - I \in B_{2r}(T\Omega_\pm^+ \mathscr{H})$$
$$\Leftrightarrow |TT^+ST^+|^2 - I \in B_{2r}(T\mathscr{H})$$
$$\Leftrightarrow |ST^+|^2 - I \in B_{2r}(T\mathscr{H})$$
$$\Leftrightarrow |T^+|^2 - I - T^{*+}(I - TT^+)T^+ \in B_{2r}(T\mathscr{H})$$
$$\Leftrightarrow |T^+|^2 - I \in B_{2r}(T\mathscr{H}).$$

So in this model, $\Omega_\pm$ are implementable in π_I and in π_T if and only if T is implementable in the Fock representation. We therefore conclude from our earlier results that for α in $(\frac{1}{2},1)$, the wave morphisms are not implementable in either of the representations π_I or π_T.

(4) Scattering morphism: The scattering morphism is induced by the partial isometry $S = (\Omega_+)^+\Omega_-$, which of course has a partial-isometric implementation in the Fock representation. On the other hand, S is implementable in π_T if and only if $|TST^+|^2 - I \in B_{2r}(TS^+ \mathscr{H})$, or equivalently, $S|T|^2 - |T|^2 S \in B_{2r}(T\mathscr{H})$. The calculations above show that for $\alpha \in (\frac{1}{2},1)$, $S_\alpha |T_\alpha|^2 - |T_\alpha|^2 S_\alpha \notin B_{2r}(T_\alpha \mathscr{H})$, that is, the scattering morphism is not implementable in the representation π_T induced by the state invariant under the interacting dynamical automorphism group.

V. PHYSICAL INTERPRETATION

The model system we have analyzed furnishes a simple situation in which a single representation of the observable algebra does not accommodate the computation of all physically interesting quantities. We have found that for the weak low-energy-coupling range $0 < \alpha \leqslant \frac{1}{2}$, the diagonalizing transformation T can be isometrically implemented in the Fock representation, or equivalently, the representation π_T is isometrically equivalent to the Fock representation. This is the standard situation envisioned in scattering theory in which the state invariant under the interacting dynamics is a vector state in the (Fock) representation carrying the unitary implementation of the free dynamics. If $\Gamma(T)$ is the isometric operator implementing T, the state invariant under the automorphism group β is the (suitably normalized) vector state $\Gamma(T)^*\Omega$.

For $\frac{1}{2} < \alpha < 1$, however, the situation is different. The diagonalizing transformation T_α cannot in this case be implemented in the Fock representation by an isometric operator, and the natural state (on the algebra $\mathscr{W}$) that is invariant under the interacting dynamics is not a vector state in the Fock representation. In particular, any search for the "interacting ground state" in the Fock representation would be fruitless. We have seen that the reason for the inequivalence of the representations π_I and π_T for $\frac{1}{2} < \alpha < 1$ lies in the strength of the low-energy coupling of the oscillator to the massless field, and is thus a type of "infrared problem."

We have seen, though, that for this model the inequivalence of the free and interacting ground states is no impediment to the concurrent unitary implementation of the two time-development automorphism groups β° and β. In fact, we may implement both β° and β in each of the two natural representations π_I and π_T. Suppose, for example, that β_t° and β_t are implemented in the Fock representation by the continuous unitary groups $\Gamma(\beta_t^\circ)$ and $\Gamma(\beta_t)$, respectively, that is, $\Gamma(\beta_t^\circ)W(f)\Gamma(\beta_t^\circ)^* = \beta_t^\circ(W(f))$ for all $f \in \mathscr{H}$, with a similar formula for $\Gamma(\beta_t)$. As in [I], the (second-quantized) Møller wave operators $W_\pm$ would then be given by the limits $W_\pm \psi = \lim_{t \to \pm\infty} \Gamma(\beta_t)\Gamma(\beta^\circ_{-t})\psi$ for ψ in a suitable subspace of the Fock space $\mathscr{F}(\mathscr{H})$.

These limits, however, cannot possibly exist. We saw in [I] that $W_\pm$, if they were to exist, would be implementations of the partial symplectic transformations Ω_+ on $\mathscr{H}$. We have seen here, however, that $\Omega_\pm$ are not implementable in π_I. Neither are they implementable in π_T. Thus attempts to formulate time-dependent scattering theory in either of these representations would result in nonconvergent expressions for the wave operators.

The cure for these apparent difficulties is, of course, to formulate the scattering theory in terms of wave morphisms on the CCR algebra $\mathscr{W}$. As we have seen, the wave morphisms induced by the partial symplectic transformations $\Omega_\pm$ yield a scattering morphism induced by the transformation $S = \Omega_+^+ \Omega_-$ on $\mathscr{H}$. Because S is unitary on $T\mathscr{H}$, it has a partial isometric implementation $\Gamma(S)$ on Fock space. That is, $\Gamma(S)$ is unitary on the Fock asymptotic scattering state vectors $\mathscr{F}(T\mathscr{H})$ (which, speaking intuitively, consist of all field excitations with the oscillator ground state), and $\Gamma(S)$ is the S matrix of the theory.

Therefore, despite the fact that the Møller wave operators for this model fail to exist in either natural representation π_I or π_T, it is possible to formulate a well-defined scattering theory by working in a representation-independent framework to construct a scattering morphism. We have thus demonstrated that the failure to converge of second-quantized limit expressions for wave operators does not preclude the existence of an S matrix (nor does it preclude the existence of wave morphisms). The nonexistence of wave operators in some representation of the observable algebra can, as we have seen, be due to the fact that the wave morphisms happen not to be implementable in that particular representation, despite the concurrent unitary implementation of the two constituent time-development automorphism groups. These facts show that an algebraic treatment is essential, even for the linear models here.

In this connection we make three remarks. First, the scattering morphism induced by the partial isometry S is not unitarily implementable in the representation π_T. Thus the S matrix is not a unitary operator in the representation induced by the natural invariant state for the interacting system. Second, the Fock vacuum state is the asymptotic scattering-state vacuum, is invariant under the S matrix, and is invariant under the uncoupled time development. It is easy to see, however, that the Fock vacuum is not invariant under the interacting time development, because the symplectic transformation $T^+ V_t T$ is not for all times t a real isometry. Third, the convergence as $|t| \to \infty$ of the morphisms τ_t induced by the partial symplectic transformations $\Omega_t \equiv T^+ V_t T V^\circ_{-t} P^\circ_{\rm ac}$ is rather weak. In particular, the family $\{\tau_t | t \in \mathbb{R}\}$ is not strongly continuous because the map $\mathscr{H} \ni f \to W(f) \in \mathscr{W}$ is not (C^*) norm continuous. We have only that if E is a quasifree state on $\mathscr{W}$, then the strong convergence s-$\lim_{t \to \pm\infty} \Omega_t = \Omega_\pm$ on $\mathscr{H}$ induces the convergence $\lim_{t \to \pm\infty} \| \{\pi_E(\tau_t(A)) - \pi_E(\tau_\pm(A))\}\psi \| = 0$ for

any $A\in\mathscr{W}$ and any $\psi\in\mathscr{H}_E$. Here $\tau_\pm$ are the morphisms on $\mathscr{W}$ defined by $\tau_\pm(W(f))\equiv W(\Omega_\pm f)$ for $f\in\mathscr{H}$, and π_E is the representation determined by E, with carrier space $\mathscr{H}_E$.

The model presented here is a specific example of a diagonalizable linear system with infinite number of degrees of freedom. The results of [I] are applicable to a variety of systems of this type, and can be directly applied once the particular symplectic transformation T which performs the diagonalization to "normal modes" is found. It is thus clear that even linear model field theories generically exhibit phenomena which necessitate algebraic treatment. Features already present in linear models include inequivalent free and interacting vacua, free and interacting automorphism groups potentially not concurrently implementable, the existence of Møller wave morphisms not implementable in the representations determined by the vacua, and S matrices implementable only in certain representations. These phenomena can occur even in a setting free of complications involved in the specification of more realistic dynamical laws.

APPENDIX A: PROPERTIES OF INTEGRAL KERNELS

In the first half of this appendix, we verify the assertions made in Sec. III A regarding the operator $\Delta_\gamma(\epsilon)$. In the second half, we construct the functions $F_L(\epsilon)(\mathbf{p},\mathbf{q})$ arising in Sec. III C.

In Sec. III A, we defined the function $\Delta_\gamma(\epsilon)(\mathbf{p},\mathbf{q})$ for $0<\gamma<1$. We consider first the case $\epsilon=0$.

Lemma: For fixed γ with $0<\gamma<1$, let

$$\Delta_\gamma(0)(\mathbf{p},\mathbf{q})\equiv(\omega_p\omega_q)^{1/2}\omega_p^{-\gamma}(\omega_p^\gamma-\omega_q^\gamma)/(\omega_p^2-\omega_q^2).$$

Then for all $f,g\in L_2(\mathbb{R}^3)$, the integral

$$I_\gamma(f,g)\equiv\int d^3p\,d^3q\,\Delta_\gamma(0)(\mathbf{p},\mathbf{q})\,\overline{f(p)}g(\mathbf{q})$$

converges absolutely, and $|I_\gamma(f,g)|\leqslant(\text{const})\|f\|\cdot\|g\|$.

Proof: To simplify notation, we define two auxiliary bounded operators on $L_2(\mathbb{R}^3)$, the spherical average Ψ and the dilatation δ_a.

Let $f,g\in L_2(\mathbb{R}^3)$ and define Ψ: $L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$ by $(\Psi f)(\mathbf{p})\equiv(4\pi)^{-1}\int d\Omega f(|\mathbf{p}|\Omega)$. Clearly $\Psi^2=\Psi=\Psi^*$ and $\|\Psi\|=1$. Since $(\Psi f)(\mathbf{p})$ depends only on $|\mathbf{p}|$, we write

$$\langle\Psi f|\Psi g\rangle=4\pi\int_0^\infty dp\,p^2\,\overline{(\Psi f)(p)}(\Psi g)(p).$$

Let $a>0$ and let $\delta_a:L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$ be the dilatation given by $(\delta_a f)(\mathbf{p})\equiv a^{3/2}f(a\mathbf{p})$. Clearly, $[\delta_a,\Psi]=0$, and δ_a is a unitary operator.

We first note that if $0<\gamma<1$, then

$$J_\gamma\equiv\int_0^{\pi/2}d\theta(\cos\theta)^{-\gamma}<\infty.$$

To prove the lemma, consider non-negative functions f and g in $L_2(\mathbb{R}^3)$, and let $0<a<1$ and $0<b<1$. Then $\|f\|\,\|g\|\geqslant\langle\Psi\delta_a f|\Psi\delta_b g\rangle$. Multiply each side by $a^{-\gamma}$, put $a\equiv\cos\theta$ and $b\equiv\sin\theta$ for $0<\theta<\pi/2$, and integrate to get

$$J_\gamma\|f\|\,\|g\|>\int_0^{\pi/2}d\theta(\cos\theta)^{-\gamma}\langle\Psi\delta_{\cos\theta}f|\Psi\delta_{\sin\theta}g\rangle.$$

Because $(\sin\theta+\cos\theta)\geqslant1$ in the integration range, we have

$$J_\gamma\|f\|\,\|g\|\geqslant\int_0^{\pi/2}d\theta\frac{(\sin\theta\cos\theta)^{3/2}}{(\cos\theta)^\gamma(\sin\theta+\cos\theta)^{2-\gamma}}\times4\pi\int_0^\infty r^2\,dr\,(\Psi f)(r\cos\theta)\,(\Psi g)(r\sin\theta).$$

Now, for positive a and b, and for $0<\gamma<1$, we have $(a^\gamma-b^\gamma)/(a-b)<(a+b)^{\gamma-1}$. Substituting this ratio for $(\sin\theta+\cos\theta)^{\gamma-1}$ in the above, and making the change of variables $x\equiv r\cos\theta$ and $y\equiv r\sin\theta$ in this absolutely convergent integral, we get

$$\begin{aligned}(4\pi)^{-1}J_\gamma\|f\|\,\|g\|&>\int_0^\infty dx\int_0^\infty dy\frac{(xy)^{3/2}}{x^\gamma(x+y)}\frac{x^\gamma-y^\gamma}{x-y}(\Psi f)(x)\,(\Psi g)(y)\\&=(4\pi)^{-2}\int d^3p\,d^3q\,\Delta_\gamma(0)(\mathbf{p},\mathbf{q})f(\mathbf{p})g(\mathbf{q}).\end{aligned}$$

Because the kernel $\Delta_\gamma(0)(\mathbf{p},\mathbf{q})$ is positive, the consideration of non-negative f and g suffices to show that for arbitrary $f,g\in L_2(\mathbb{R}^3)$, the integral $I_\gamma(f,g)$ is absolutely convergent and satisfies $|I_\gamma(f,g)|<4\pi J_\gamma\|f\|\,\|g\|$ for all $f,g\in L_2(\mathbb{R}^3)$. ///

Because $I_\gamma:L_2(\mathbb{R}^3)\times L_2(\mathbb{R}^3)\to\mathbb{C}$ is a bounded quadratic form, for each γ between 0 and 1 there exists a bounded operator $\Delta_\gamma:L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$ such that $\langle f|\Delta_\gamma g\rangle=I_\gamma(f,g)$ for all $f,g\in L_2(\mathbb{R}^3)$. Furthermore, because the double integral $I_\gamma(f,g)$ is absolutely convergent for arbitary f and g in $L_2(\mathbb{R}^3)$, by Fubini's theorem the single integral $\int d^3q\,\Delta_\gamma(0)(\mathbf{p},\mathbf{q})g(\mathbf{q})$ exists for almost all $\mathbf{p}$, and $(\Delta_\gamma g)(\mathbf{p})=\int d^3q\,\Delta_\gamma(0)(\mathbf{p},\mathbf{q})g(\mathbf{q})$. Thus the function $\Delta_\gamma(0)(\mathbf{p},\mathbf{q})$ is the integral kernel for the bounded operator Δ_γ.

We now consider the case $\epsilon\neq0$. Because $|\Delta_\gamma(\epsilon)(\mathbf{p},\mathbf{q})|<\Delta_\gamma(0)(\mathbf{p},\mathbf{q})$, it is clear from the analysis for the operator Δ_γ that the integral kernel $\Delta_\gamma(\epsilon)(\mathbf{p},\mathbf{q})$ induces a bounded operator $\Delta_\gamma(\epsilon):L_2(\mathbb{R}^3)\to L_2(\mathbb{R}^3)$ given by

$$(\Delta_\gamma(\epsilon)g)(\mathbf{p})\equiv\int d^3q\Delta_\gamma(\epsilon)(\mathbf{p},\mathbf{q})g(\mathbf{q}),$$

where the integral is absolutely convergent for almost all $\mathbf{p}$. Clearly $\Delta_\gamma(0)=\Delta_\gamma$, and $\|\Delta_\gamma(\epsilon)\|<\|\Delta_\gamma\|$ for all $\epsilon>0$. Furthermore, it follows easily that s-$\lim_{\epsilon\to+0}\Delta_\gamma(\epsilon)=\Delta_\gamma$ and s-$\lim_{\epsilon\to+0}\Delta_\gamma(\epsilon)^*=\Delta_\gamma^*$.

We turn next to the construction of the functions $F_L(\epsilon)(\mathbf{p},\mathbf{q})$. Consider first the operator $(M(\epsilon)-I)(M(\epsilon)^*-I)$. It has the kernel

$$(M(\epsilon)-I)(M(\epsilon)^*-I)(\mathbf{p},\mathbf{q})=\frac{\lambda\omega_p^{1/2}\omega_q^{1/2}(\omega_0^2-\omega_p^2)(\omega_0^2-\omega_q^2)\rho(\mathbf{p})\rho(\mathbf{q})}{D_+(\omega_p^2)D_-(\omega_q^2)}J(\omega_p^2,\omega_q^2),$$

where

$$J(\omega_p^2,\omega_q^2)\equiv\int d^3k\frac{\lambda\rho(\mathbf{k})^2}{\omega_k(\omega_p^2-\omega_k^2+i\epsilon)(\omega_q^2-\omega_k^2-i\epsilon)}.$$

It is convenient to rewrite this integral as follows. Using the identity for ρ^2, we find that $J(\omega_p^2,\omega_q^2)=J_0(\omega_p^2,\omega_q^2)$, where

$$J_\delta(s,t)\equiv(2\pi i)^{-1}\int_0^\infty dy\times\frac{D_-(y)-D_+(y)}{y^{1/2}(y-s-i\epsilon)(y-t+i\epsilon)(y-\omega_0^2-i\delta)}.$$

Note that because there is no singularity in the integrand even when $\delta = 0$, we have $\lim_{\delta \to 0} J_\delta(s,t) = J_0(s,t) = J(s,t)$ for $s > 0$ and $t > 0$.

We next rewrite $J_\delta(s,t)$ as a contour integral. Let $0 < \delta < \epsilon$, and choose the square root function $z \to z^{1/2}$ to have branch cut along the positive real axis, with $0 \leqslant \arg(z^{1/2}) < \pi$. Consider the following contours in the complex plane, for $R > 1/\delta$:

$$\gamma_1 \equiv \{x + i/R \mid x \in [0,R]\},$$
$$\gamma_2 \equiv \{z + i/R \mid \mathrm{Im}\, z \geqslant 0 \text{ and } |z| = R\},$$
$$\gamma_3 \equiv \{x + i/R \mid x \in [-R,0]\},$$
$$\gamma_4 \equiv \{x - i/R \mid x \in [0,R]\},$$
$$\gamma_5 \equiv \{z - i/R \mid \mathrm{Im}\, z \leqslant 0 \text{ and } |z| = R\},$$
$$\gamma_6 \equiv \{x - i/R \mid x \in [-R,0]\}.$$

We take the line segments γ_1, γ_3, γ_4, and γ_6 to be oriented in the positive Re z direction, and we take the semicircles γ_2 and γ_5 to have counterclockwise and clockwise orientations, respectively. Thus $\gamma_1 + \gamma_2 + \gamma_3$ encloses both points $s + i\epsilon$ and $\omega_0^2 + i\delta$ in the positive sense, whereas $\gamma_4 + \gamma_5 + \gamma_6$ encloses the point $t - i\epsilon$ in the negative sense. In terms of these contours,

$$J_\delta(s,t) = \lim_{R \to \infty} (2\pi i)^{-1} \int_{\gamma_1 + \gamma_4} dz \times \frac{-D(z)}{z^{1/2}(z - s - i\epsilon)(z - t + i\epsilon)(z - \omega_0^2 - i\delta)}.$$

Because the corresponding integrals over γ_2 and γ_5 vanish as $R \to \infty$, we find

$$\begin{aligned} J(s,t) = {} & \frac{-D_+(\omega_0^2)}{\omega_0(s - \omega_0^2 + i\epsilon)(t - \omega_0^2 - i\epsilon)} \\ & + \frac{-D(s + i\epsilon)}{(s + i\epsilon)^{1/2}(s - t + 2i\epsilon)(s - \omega_0^2 + i\epsilon)} \\ & + \frac{D(t - i\epsilon)}{(t - i\epsilon)^{1/2}(t - s - 2i\epsilon)(t - \omega_0^2 - i\epsilon)} \\ & + \lim_{R \to \infty} (2\pi i)^{-1} \int_{\gamma_3 + \gamma_6} dz \times \frac{D(z)}{z^{1/2}(z - s - i\epsilon)(z - t + i\epsilon)(z - \omega_0^2)}, \end{aligned}$$

where the first three terms are residues. Here we have taken the limit $\delta \to 0$ after the contour rearrangement. The fourth (integral) term may be written as $Y_M(s + i\epsilon, t - i\epsilon)/\pi$, where

$$Y_M(z,w) \equiv \int_0^\infty dy \frac{D(-y)}{y^{1/2}(y + \omega_0^2)(y + z)(y + w)}.$$

Thus

$$\begin{aligned} & (M(\epsilon) - I)(M(\epsilon)^* - I)(\mathbf{p},\mathbf{q}) \\ & \quad = -\omega_0^{-1}\omega_p^{1/2}\omega_q^{1/2} Q(\mathbf{p}) Q(\mathbf{q}) \\ & \qquad \times \left\{ \frac{(\omega_p^2 - \omega_0^2)(\omega_q^2 - \omega_0^2)}{(\omega_p^2 - \omega_0^2 + i\epsilon)(\omega_q^2 - \omega_0^2 - i\epsilon)} \right\} \\ & \qquad - \overline{\mu(\epsilon,\mathbf{q})}(M(2\epsilon) - I)(\mathbf{p},\mathbf{q}) \\ & \qquad - \mu(\epsilon,\mathbf{p})(M(2\epsilon)^* - I)(\mathbf{p},\mathbf{q}) \\ & \qquad + \frac{\lambda}{\pi} \frac{\rho(\mathbf{p})(\omega_0^2 - \omega_p^2)}{D_+(\omega_p^2)} \frac{\rho(\mathbf{q})(\omega_0^2 - \omega_q^2)}{D_-(\omega_q^2)} \\ & \qquad \times (\omega_p \omega_q)^{1/2} Y_M(\omega_p^2 + i\epsilon, \omega_q^2 - i\epsilon), \end{aligned}$$

where

$$\mu(\epsilon,\mathbf{p}) \equiv \frac{\omega_p(\omega_0^2 - \omega_p^2) D(\omega_p^2 + i\epsilon)}{(\omega_p^2 + i\epsilon)^{1/2}(\omega_0^2 - \omega_p^2 - i\epsilon) D_+(\omega_p^2)}.$$

Because the expression in curly brackets and the function $\mu(\epsilon,\mathbf{p})$ are bounded functions with limits equal to 1 almost everywhere as $\epsilon \to +0$, the strong limit of the first term is the dyadic $-|\omega_0^{-1/2}\omega^{1/2}Q\rangle\langle\omega_0^{-1/2}\omega^{1/2}Q|$, and the middle two terms are kernels for operators which have strong limits equal to $(I - M)$ and $(I - M^*)$, respectively.

Now consider the last term, which we denote by $F_M(\epsilon)(\mathbf{p},\mathbf{q})$. We have $F_M(\epsilon)(\mathbf{p},\mathbf{q}) = K_M(\epsilon)(\omega_p^2, p_q^2)$, with the functions $K_M(\epsilon)$ defined by

$$K_M(\epsilon)(s,t) \equiv \frac{\lambda}{\pi} \frac{(\omega_0^2 - s)}{D_+(s)} \frac{(\omega_0^2 - t)}{D_-(t)} \times \rho(s^{1/2})\rho(t^{1/2})(st)^{1/4} Y_M(s + i\epsilon, t - i\epsilon).$$

It follows from the form of $Y_M(s + i\epsilon, t - i\epsilon)$ that the function $F_M(\epsilon)(\mathbf{p},\mathbf{q})$ is a jointly continuous function of the variables $\mathbf{p},\mathbf{q}$, and ϵ in the region $\mathbf{p} \neq 0$, $\mathbf{q} \neq 0$, $\epsilon \geqslant 0$, and that, furthermore, on any compact subset of $\mathbb{R}^3 \times \mathbb{R}^3$ which excludes the points with $\mathbf{p} = 0$ or $\mathbf{q} = 0$, $F_M(\epsilon)(\mathbf{p},\mathbf{q})$ tends uniformly to $F_M(0)(\mathbf{p},\mathbf{q})$ as ϵ tends to zero. Let D be the dense subspace of $L_2(\mathbb{R}^3)$ consisting of functions with compact support not including the origin. Then for any $\epsilon \geqslant 0$ the function $F_M(\epsilon)(\mathbf{p},\mathbf{q})$ defines a quadratic form $\langle |F_M(\epsilon)| \rangle$ with form domain $D \times D$, and for any f and g in D, we have

$$\lim_{\epsilon \to +0} \langle f | F_M(\epsilon) | g \rangle = \langle f | F_M(0) | g \rangle.$$

Now, because the strong limits as $\epsilon \to 0$ of the uniformly bounded families $M_\alpha(\epsilon)$ and $M_\alpha(\epsilon)^*$ are equal to M_α and M_α^*, respectively, it follows that s-$\lim_{\epsilon \to +0} M_\alpha(\epsilon) M_\alpha(\epsilon)^* = M_\alpha M_\alpha^*$. Therefore, because of the strong-limit properties of the other terms in the formula for $(M(\epsilon) - I)(M(\epsilon)^* - I)$ above, we have

$$\langle f | F_M(0) | g \rangle = \langle f | F_M\, g \rangle, \text{ for } f \text{ and } g \text{ in } D,$$

where F_M is the bounded operator

$$F_M \equiv MM^* - I + |\omega_0^{-1/2}\omega^{1/2}Q\rangle\langle\omega_0^{-1/2}\omega^{1/2}Q|$$

defined in Sec. III C. It now follows from the continuity properties of the function $F_M(0)$ that $F_M \in B_2(L_2(\mathbb{R}^3))$ if and only if the function $F_M(0)(\mathbf{p},\mathbf{q})$ is an element of $L_2(\mathbb{R}^6)$.

In exactly the same way, we show that the operator F_L defined above is in $B_2(L_2(\mathbb{R}^3))$ if and only if $F_L(0)(\mathbf{p},\mathbf{q})$ is in $L_2(\mathbb{R}^6)$, where $F_L(\epsilon)(\mathbf{p},\mathbf{q}) \equiv K_L(\epsilon)(\omega_p^2, \omega_q^2)$ for $\epsilon \geqslant 0$, with

$$K_L(\epsilon)(s,t) \equiv \frac{-\lambda}{\pi} \frac{(\omega_0^2 - s)}{D_+(s)} \frac{(\omega_0^2 - t)}{D_-(t)} \frac{\rho(s^{1/2})\rho(t^{1/2})}{(st)^{1/4}} \times Y_L(s + i\epsilon, t - i\epsilon),$$

and

$$Y_L(z,w) \equiv \int_0^\infty dy \frac{y^{1/2} D(-y)}{(y + \omega_0^2)(y + z)(y + w)}.$$

We thus conclude that

$$(LL^* - I) \in B_2(L_2(\mathbb{R}^3)) \text{ iff } F_L(0) \in L_2(\mathbb{R}^6),$$
$$(MM^* - I) \in B_2(L_2(\mathbb{R}^3)) \text{ iff } F_M(0) \in L_2(\mathbb{R}^6).$$

APPENDIX B: ESTIMATES FOR INTEGRAL KERNELS

In this appendix we derive some bounds for the integral kernels F which appear in the text. First we establish a lemma which is of use in this appendix and elsewhere in the text.

Let z and w be complex numbers which are neither negative real numbers nor zero, with arguments taken to lie in the interval $(-\pi,\pi)$. For $-1<\beta<1$, define

$$E_\beta(z,w) \equiv \int_0^\infty \frac{y^\beta\, dy}{(y+z)(y+w)}.$$

It is not difficult to show that

$$E_\beta(z,w) = \pi(\sin\pi\beta)^{-1}(z^\beta - w^\beta)/(z-w),$$

where the arguments of z^β and w^β lie in the interval $(-\pi/2,\pi/2)$. For $\beta = 0$ we have $E_0(z,w) = (\ln z - \ln w)/(z-w)$, and for $z = w$ we have $E_\beta(z,z) = \pi\beta(\sin\pi\beta)^{-1}z^{-(1-\beta)}$.

We now specialize to the situation in which z and w are positive real numbers and $0<\beta<1$.

Lemma. Let $s>0$, $t>0$ and $0<\beta<1$. Then,

(1) $2^{1-\beta}A_\beta(s+t)^{-(1-\beta)}$
$$\leqslant E_\beta(s,t) \leqslant \beta^{-1}A_\beta(s+t)^{-(1-\beta)},$$

where $A_\beta \equiv \pi\beta(\sin\pi\beta)^{-1}$, and

(2) $2^{1+\beta}A_\beta(s+t)^{-(1+\beta)}(st)^\beta$
$$\leqslant E_\beta(s,t) \leqslant \frac{B_\beta(\theta)}{s^{\theta(1-\beta)}t^{(1-\theta)(1-\beta)}},$$

where $0<\theta<1$ and where

$$B_\beta(\theta) \equiv \left[\frac{\pi(1-2\theta(1-\beta))}{\sin\pi(1-2\theta(1-\beta))} \times \frac{\pi(1-2(1-\theta)(1-\beta))}{\sin\pi(1-2(1-\theta)(1-\beta))}\right]^{1/2}.$$

Proof: The left inequality in (1) is due to the fact that $(y+s)(y+t) \leqslant (y+(s+t)/2)^2$, and thus holds for $-1<\beta\leqslant 0$ as well. The right inequality in (1) follows from the fact that for $s>0$, $t>0$, and $0<\beta<1$, $(s^\beta - t^\beta)/(s-t) < (s+t)^{\beta-1}$. The left inequality in (2) follows from the left inequality in (1) and the identity $E_\beta(s,t) = (st)^{-1}E_{-\beta}(s^{-1},t^{-1})$. The right inequality in (2) follows from the application of Schwartz' inequality

$$E_\beta(s,t) = \int_0^\infty dy \frac{y^{1/2-\theta(1-\beta)}}{y+s}\frac{y^{1/2-(1-\theta)(1-\beta)}}{y+t}$$
$$\leqslant \left[\int_0^\infty dy \frac{y^{1-2\theta(1-\beta)}}{(y+s)^2}\right]^{1/2} \times \left[\int_0^\infty dy \frac{y^{1-2(1-\theta)(1-\beta)}}{(y+t)^2}\right]^{1/2}$$

and from the fact that $E_\beta(s,s) = \pi\beta(\sin\pi\beta)^{-1}s^{-(1-\beta)}$. ///

Note that estimates for β negative can be obtained using the identity $E_\beta(s,t) = (st)^{-1}E_{-\beta}(s^{-1},t^{-1})$. In particular, for β negative, $E_\beta(s,t) \leqslant |\beta|^{-1}A_{|\beta|}(st)^{-|\beta|}(s+t)^{-(1-|\beta|)}$.

We now derive estimates for the functions $F_L(\epsilon)(\mathbf{p},\mathbf{q})$ and $F_M(\epsilon)(\mathbf{p},\mathbf{q})$ which are defined for $\epsilon\geqslant 0$ in Appendix A. Because the behavior of the function $D(\alpha;-y)$ changes at the parameter values $\alpha = \frac{1}{2}$, it is convenient to treat the cases $0<\alpha<\frac{1}{2}$ and $\frac{1}{2}<\alpha<1$ separately in deriving bounds for the functions Y and K.

Suppose first that $0<\alpha<\frac{1}{2}$. From the explicit form of $D(-y)$ it is easy to see that in this case the function $|(y+\omega_0^2)^{-1}D(-y)|$ is bounded by a constant a_1 for $0\leqslant y<\infty$, because $(y^{1/2-\alpha}-1)/(y-1) < (y+1)^{-(\alpha+1/2)}$. Thus for $s>0$, $t>0$, and $\epsilon\geqslant 0$,

$$|Y_{\underset{M}{L}}(s+i\epsilon,t-i\epsilon)|$$
$$\leqslant a_1\int_0^\infty dy \frac{y^{\pm 1/2}}{|(y+s+i\epsilon)(y+t-i\epsilon)|}$$
$$\leqslant a_1\int_0^\infty dy \frac{y^{\pm 1/2}}{(y+s)(y+t)} = a_1E_{\pm 1/2}(s,t).$$

Now, $E_{1/2}(s,t) \leqslant \pi(s+t)^{-1/2}$ and

$$E_{-1/2}(s,t) = (st)^{-1}E_{1/2}(s^{-1},t^{-1}) < \pi(st)^{-1/2}(s+t)^{-1/2}.$$

Thus for $0<\alpha<\frac{1}{2}$, $s>0$, $t>0$ and $\epsilon\geqslant 0$,

$$|Y_L(s+i\epsilon,t-i\epsilon)| \leqslant \pi a_1(s+t)^{-1/2},$$
$$|Y_M(s+i\epsilon,t-i\epsilon)| \leqslant \pi a_1(st)^{-1/2}(s+t)^{-1/2}.$$

To estimate $K_{\underset{M}{L}}$, recall that $|D_+(t)| > b_1 > 0$ for $0<t<\infty$. Because $D_+(t)$ is continuous and $\lim_{t\to\infty} D_+(t)/t = -1$, it follows that the quantity $|(\omega_0^2 - t)/D_+(t)|$ is bounded by a fixed constant c_1 for $0<t<\infty$. Taking into account the fact that $\rho(s^{1/2}) = s^{-\alpha/2}(1+s)^{-1/2}$, we find, for $0<\alpha<\frac{1}{2}$, $s>0$, $t>0$, and $\epsilon\geqslant 0$,

$$|K_{\underset{M}{L}}(\epsilon)(s,t)|$$
$$\leqslant d_1(st)^{-1/4}(1+s)^{-1/2}(1+t)^{-1/2}(st)^{-\alpha/2}(s+t)^{-1/2},$$

where $d_1 \equiv \lambda a_1 c_1^2$ is a positive constant. Note that this estimate is the same for K_L and K_M, and is independent of ϵ. For future convenience we set

$$W(s,t) \equiv (st)^{-1/4}(1+s)^{-1/2}(1+t)^{-1/2}.$$

Then the above estimate becomes

$$|K_{\underset{M}{L}}(\epsilon)(s,t)| \leqslant d_1W(s,t)(st)^{-\alpha/2}(s+t)^{-1/2}.$$

We now consider the situation when $\frac{1}{2}<\alpha<1$. In this case it is helpful to decompose each of the functions Y and K into two terms, a tame term and a more singular term which reflects the essential behavior of the functions near the origin.

Rewrite the explicit form for $D(-y)$ as

$$\frac{D(-y)}{\omega_0^2+y} = \zeta_\alpha(y) + \frac{2\pi^2\lambda}{\sin\pi(\alpha-\frac{1}{2})}\frac{1}{y^{\alpha-1/2}},$$

where

$$\zeta_\alpha(y) \equiv 1 + \frac{\lambda}{\omega_0^2+y} - \frac{2\pi^2\lambda}{\sin\pi(\alpha-\frac{1}{2})}\frac{y^{(3/2-\alpha)}-1}{y-1}.$$

Note that, because $\frac{1}{2}<\alpha<1$, the function $\zeta_\alpha(y)$ is bounded in magnitude for all $y\geqslant 0$ by some positive constant, say a_2.

Corresponding to this decomposition of $D(-y)(\omega_0^2+y)^{-1}$, we may write

$$Y_{\underset{M}{L}}(z,w) = Y^{(1)}_{\underset{M}{L}}(z,w) + Y^{(2)}_{\underset{M}{L}}(z,w),$$

where

$$Y^{(1)}_{\substack{L\\M}}(z,w) \equiv \int_0^\infty dy\, y^{\pm 1/2}\zeta_\alpha(y)(y+z)^{-1}(y+w)^{-1}$$

and

$$Y^{(2)}_{\substack{L\\M}}(z,w) \equiv 2\pi^2\lambda\,(\sin\pi(\alpha-\tfrac{1}{2}))^{-1} \times\int_0^\infty dy\,\frac{y^{\pm 1/2}}{y^{\alpha-1/2}}(y+z)^{-1}(y+w)^{-1}.$$

Then $K_{\substack{L\\M}}(\epsilon)(x,t) = K^{(1)}_{\substack{L\\M}}(\epsilon)(s,t) + K^{(2)}_{\substack{L\\M}}(\epsilon)(s,t)$, with, of course,

$$K^{(\beta)}_{\substack{L\\M}}(\epsilon)(s,t) \equiv \frac{\mp\lambda}{\pi}\frac{(\omega_0^2-s)}{D_+(s)}\frac{(\omega_0^2-t)}{D_-(t)}\frac{\rho(s^{1/2})\rho(t^{1/2})}{(st)^{\pm 1/4}} \times Y^{(\beta)}_{\substack{L\\M}}(s+i\epsilon,t-i\epsilon),$$

and $F^{(\beta)}_{\substack{L\\M}}(\epsilon)(\mathbf{p},\mathbf{q}) \equiv K^{(\beta)}_{\substack{L\\M}}(\epsilon)(\omega_p^2,\omega_q^2)$.

First we analyze $Y^{(1)}$ and $K^{(1)}$. Because $|\zeta_\alpha(y)| < a_2$ for $y \geqslant 0$, we note that as above $|Y^{(1)}_{\substack{L\\M}}(s+i\epsilon,t-i\epsilon)| \leqslant a_2 E_{\pm 1/2}(s,t)$ for $s,t>0$ and $\epsilon\geqslant 0$. From the explicit form of $D_+(t)$, we see that for $\frac{1}{2}<\alpha<1$, the quantity $|\omega_0^2 - t|\,|t^{\alpha-1/2}D_+(t)|^{-1}$ is bounded by some positive constant c_2 for all $t>0$. Thus we find, similar to the above estimate, for $\frac{1}{2}<\alpha<1$, $s>0$, $t>0$, and $\epsilon\geqslant 0$,

$$|K^{(1)}_{\substack{L\\M}}(\epsilon)(s,t)| < d_2 W(s,t)(st)^{-(1-\alpha)/2}(s+t)^{-1/2},$$

where $d_2 \equiv \lambda a_2 c_2^2$ is a positive constant.

We now analyze $Y^{(2)}$ and $K^{(2)}$. We have

$$Y^{(2)}_L(z,w) = 2\pi^2\lambda\,(\sin\pi(\alpha-\tfrac{1}{2}))^{-1}E_{1-\alpha}(z,w) = b_2(\alpha)(z^{1-\alpha}-w^{1-\alpha})/(z-w),$$

where $b_2(\alpha) \equiv 2\pi^3\lambda\,(\sin\pi(\alpha-\frac{1}{2})\sin\pi(1-\alpha))^{-1}$. Similarly,

$$Y^{(2)}_M(z,w) = 2\pi^2\lambda\,(\sin\pi(\alpha-\tfrac{1}{2}))^{-1}E_{-\alpha}(z,w) = b_2(\alpha)(z^{-\alpha}-w^{-\alpha})/(w-z).$$

We note that for $s,t>0$ and $\epsilon\geqslant 0$, we have the upper bounds

$$|Y^{(2)}_L(s+i\epsilon,t-i\epsilon)| \leqslant b_2(\alpha)(s+t)^{-\alpha},$$
$$|Y^{(2)}_M(s+i\epsilon,t-i\epsilon)| \leqslant b_2(\alpha)(st)^{-\alpha}(s+t)^{-(1-\alpha)}.$$

These imply, for $s>0$, $t>0$, and $\epsilon\geqslant 0$,

$$|K^{(2)}_L(\epsilon)(s,t)| \leqslant k_2(\alpha)W(s,t)(st)^{-(1-\alpha)/2}(s+t)^{-\alpha},$$
$$|K^{(2)}_M(\epsilon)(s,t)| \leqslant k_2(\alpha)W(s,t)(st)^{-\alpha/2}(s+t)^{-(1-\alpha)},$$

where $k_2(\alpha) \equiv \lambda c_2^2 b_2(\alpha)/\pi$ is a positive constant.

We require one further estimate, a lower bound for $K^{(2)}_{\substack{L\\M}}(0)(s,t)$. We note that according to the lemma above,

$$Y^{(2)}_L(s,t) = b_2(\alpha)(s^{1-\alpha}-t^{1-\alpha})/(s-t) \geqslant b_2(\alpha)(1-\alpha)2^\alpha(s+t)^{-\alpha},$$
$$Y^{(2)}_M(s,t) = b_2(\alpha)(t^{-\alpha}-s^{-\alpha})/(s-t) \geqslant \alpha b_2(\alpha)(st)^{-\alpha}((s+t)/2)^{-(1-\alpha)}.$$

From the explicit form of $D_+(s)$ it is easy to see that $|s^{\alpha-1/2}D_+(s)|$ is bounded on any finite interval. Thus there exists a constant $e_2>0$ such that $|\omega_0^2 - s|\,|s^{\alpha-1/2}D_+(s)|^{-1} > e_2$ for all s between zero and $\nu \equiv \omega_0^2/2$, say.

This implies that for $0\leqslant s<\nu$ and $0\leqslant t<\nu$,

$$|K^{(2)}_L(0)(s,t)| > (1-\alpha)2^\alpha h_2(\alpha)W(s,t)(st)^{-(1-\alpha)/2}(s+t)^{-\alpha},$$
$$|K^{(2)}_M(0)(s,t)| > \alpha 2^{1-\alpha}h_2(\alpha)W(s,t)(st)^{-\alpha/2}(s+t)^{-(1-\alpha)}$$

where $h_2(\alpha) \equiv (\pi/\lambda)e_2^2 b_2(\alpha)$ is a positive constant.

In the second half of this appendix, we derive estimates for the functions $\tilde{F}_L(\epsilon)(\mathbf{p},\mathbf{q})$ and $\tilde{F}_M(\epsilon)(\mathbf{p},\mathbf{q})$ which are defined for $\epsilon\geqslant 0$ in the text by

$$\tilde{F}_{\substack{L\\M}}(\epsilon)(\mathbf{p},\mathbf{q}) \equiv \tilde{K}_{\substack{L\\M}}(\epsilon)(\omega_p^2,\omega_q^2),$$

where

$$\tilde{K}_{\substack{L\\M}}(\epsilon)(s,t) \equiv \pm(-\lambda/\pi)(st)^{\pm 1/4}\rho(s^{1/2})\rho(t^{1/2}) \times\tilde{Y}_{\substack{L\\M}}(s+i\epsilon,t-i\epsilon),$$

with

$$\tilde{Y}_{\substack{L\\M}}(z,w) \equiv \int_0^\infty dy\,\frac{(y+\omega_0^2)}{y^{\pm 1/2}D(-y)(y+z)(y+w)}.$$

These estimates are substantially easier than those in the first half.

To obtain upper bounds, note that from the explicit form for $D(\alpha;z)$ we have

$$D(\alpha;-y) > y+\omega_0^2, \quad \text{for all } \alpha\in(0,1).$$

Thus $|\tilde{Y}_{\substack{L\\M}}(s+i\epsilon,t-i\epsilon)| \leqslant E_{\pm 1/2}(s,t)$, whence as before

$$|\tilde{Y}_L(s+i\epsilon,t-i\epsilon)| \leqslant \pi(st)^{-1/2}(s+t)^{-1/2},$$
$$|\tilde{Y}_M(s+i\epsilon,t-i\epsilon)| \leqslant \pi(s+t)^{-1/2}.$$

Therefore we find that for $0<\alpha<1$, $s>0$, $t>0$, and $\epsilon\geqslant 0$,

$$|\tilde{K}_{\substack{L\\M}}(\epsilon)(s,t)| \leqslant \lambda W(x,t)(st)^{-\alpha/2}(s+t)^{-1/2}.$$

To obtain lower bounds on $\tilde{Y}_{\substack{L\\M}}(s,t)$ for $\frac{1}{2}<\alpha<1$, we recall that for these values of α,

$$\frac{D(-y)}{\omega_0^2+y} \leqslant a_2 + \frac{a_2(l_2-1)}{y^{\alpha-1/2}},$$

where

$$l_2(\alpha) \equiv 1 + 2\pi^2\lambda/a_2|\sin\pi(\alpha-\tfrac{1}{2})|.$$

Then, using the fact that $y^\beta < y+1$ for $0<\beta<1$ and $y\geqslant 0$, we conclude that

$$\frac{\omega_0^2+y}{D(-y)} \geqslant \frac{1}{a_2}\frac{y^{\alpha-1/2}}{y+l_2}.$$

Therefore,

$$\tilde{Y}_L(s,t) \geqslant a_2^{-1}\int_0^\infty \frac{dy}{y^{1-\alpha}(y+s)(y+t)(y+l_2)}$$

and

$$\tilde{Y}_M(s,t) \geqslant a_2^{-1}\int_0^\infty \frac{y^\alpha\,dy}{(y+s)(y+t)(y+l_2)}.$$

We next use the inequality $(y+s)(y+t) < (y+s+t)^2$ for positive s, t, and y, and upon differentiation of the explicit

formula for $E_\beta(z,w)$ with respect to z, we find

$$\tilde{Y}_L(s,t) \geqslant \tilde{h}(-(1-\alpha))(s+t)^{-(2-\alpha)} \times F_{-(1-\alpha)}((s+t)/l_2(\alpha)),$$

$$\tilde{Y}_M(s,t) \geqslant \tilde{h}(\alpha)(s+t)^{-(1-\alpha)} F_\alpha((s+t)/l_2(\alpha)),$$

where the positive constant $\tilde{h}(\beta)$ is given by

$$\tilde{h}(\beta) \equiv \pi\beta/a_2\, l_2(\beta)\sin\pi\beta,$$

and where

$$F_\beta(x) \equiv \beta^{-1}(1-x)^{-2}\{(1-\beta)x - x^{1-\beta} + \beta\}.$$

This function $F_\beta(x)$ is a continuous strictly positive monotonically decreasing function of x on $[0,\infty)$ for every value of β in $(-1,1)$, and $F_\beta(0) = 1$. The behavior at the origin of the (s,t)-plane of $\tilde{Y}_L$ is thus given by the factors $(s+t)^{-(2-\alpha)}$ and $(s+t)^{-(1-\alpha)}$ in the expressions above.

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Gauge theory of the post-Galilean groups

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By means of an extension of the field of real numbers we construct post-Galilean groups, which in a sense lay between the Galilean group and the Lorentz group. By gauging these groups we obtain a frame theory of gravitation, which comprises Newton–Cartan theory, general relativity, and an infinite number of intermediate theories. This leads to a better understanding of how the structural differences of the two main theories of gravitation arise.

I. INTRODUCTION

The purpose of this paper is the structural comparison of the Newtonian theory of gravitation and the general theory of relativity. Notwithstanding the quantitative differences of the two theories, interest rested, almost from the first days of general relativity, also on their qualitative structural differences.[1,2] The four-dimensional covariant formulation of the Newtonian theory of gravitation leads us to apply the mathematical tools and the conceptual content of general relativity to the Newtonian theory of gravitation. After the recognition that general relativity is a kind of gauge theory of the Lorentz group an improvement of this approach is possible: first formulate the Newtonian theory as a gauge theory of the Galilean group and then compare the two theories using the concepts of gauge theories, now common to both. This course is not straightforward, however, since, first, general relativity is not quite a canonical gauge theory[3] and, second, the gauge theory of the Galilean group, called here the Newton–Cartan theory of gravitation, is not exactly the Newtonian theory of gravitation.[4,5] Both complications are not insurmountable, since, first, the additional structural element of general relativity, the metric tensor, in comparison to other gauge theories, appears also in the Newton–Cartan theory. Second, this theory is just a little bigger than Newtonian theory—it contains, in addition to the Newtonian potential, a kind of "magnetic" gravitational potential.

The principle motivation for the comparison of the two theories is the question raised in Ref. 4: if and in what sense the Newtonian theory of gravitation is a limit of the general theory of relativity. To answer this question one notices that the Galilean group is the limit of the Lorentz group as the parameter $\epsilon(=c^{-2})$ tends to zero. If this limiting process of the group can be carried over to the corresponding gauge theories, then the limit of general relativity as $\epsilon \to 0$ must be the Newton–Cartan theory. That, strictly speaking, this is not the case can be seen from an independent formulation of the Newton–Cartan theory. Differences appear both in the mathematical structure and in the physical interpretation of the two theories. The main differences are (i) the metric tensor of the Newton–Cartan theory does not uniquely determine a Newtonian torsion-free connection, (ii) there is no variational principle as Hilbert's for the field equations of Newton–Cartan theory, (iii) the equations of motion of the matter fields do not follow from the field equations of Newton–Cartan theory, and (iv) the metric field of the Newton–Cartan theory does not correspond to the gravitational potential, as is the case in general relativity.

To see how these and other differences arise we formulate, as in Ref. 4, a frame theory, comprising Newton–Cartan theory, general relativity, and an infinity of intermediate theories. To obtain this we must carefully study the role played by the parameter ϵ in the limit "Lorentz group$\to$Galilean group" and in the less precisely defined limit of the corresponding gauge theories. The fundamental objects laying behind the two groups and their gauge theories, and which characterize their structural differences are without doubt the Minkowski metric $g^M = g(\epsilon = c^{-2})$, $h^M = h(\epsilon = c^{-2})$ and the Galilean metric $g^G = g(\epsilon = 0)$, $h^G = h(\epsilon = 0)$[4].

Relating the differences of the groups to differences of the metrics, we find that these are expressed by integers, particularly by their ranks and signatures. These numbers change discretely, when ϵ becomes zero. In this process there is nothing like a continuous limit, but only a transition from $\epsilon > 0$ to $\epsilon = 0$. On the other hand, between these two cases we find the various post-Newtonian approximations of general relativity. These approximations have nothing to do with the numerical value of the parameter ϵ, as long as ϵ remains small and positive. But ϵ plays a decisive role in this process. Its powers ϵ^N, $N > n$ are neglected, i.e., set equal to zero, in the nth post-Newtonian approximation. We conclude that it is not the analytic, but the algebraic properties of ϵ, which are of importance here. The relevant algebraic properties of ϵ are (i) $\epsilon^N \neq 0$, $N = 0,\ldots, n$, $(\epsilon^0 := 1)$, (ii) $\epsilon^{n+1} = 0$, and (iii) $1\epsilon = \epsilon$.

From (i) and (ii) it follows immediately that, for finite $n \neq 0$, ϵ cannot be a real number. Thus, in the following we introduce the symbol $\varnothing$ in place of ϵ.

We extend the field of real numbers $\mathbf{R}$ by adding to it the new "number" $\varnothing$ and denote the new set by $\mathbf{R}^{[n]}$. Here, $\mathbf{R}^{[n]}$ is a commutative ring with unit element. To obtain groups, which in some sense lay between the Lorentz group and the Galilean group, we introduce, for $n = 0,1,\ldots$, the n-post Galilean metrics by means of the definition $g^{[n]} := g(\epsilon = \varnothing)$, $h^{[n]} := h(\epsilon = \varnothing)$. Since the components of the n-post-Galilean metric are $\mathbf{R}^{[n]}$ numbers, the space on which they are defined must be a $\mathbf{R}^{[n]}$ module. We obtain such a module from a real linear space by a method similar to the complexification of real linear space. The isometry group of the n-post-Galilean metric is the n-post-Galilean group. The next step is the definition of an n-post-Galilean manifold. We take

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as basis a real differentiable manifold M, and, as in the construction of the $\mathbf{R}^{[n]}$ module, we "complexify" its tangential bundle. We can now define an n-post-Galilean metric field on M and with its help construct n-post-Galilean connections and gauge theories, for $n = 0,1,\ldots$. For the field equations we postulate a variational principle similar to Hilbert's for general relativity. The field equations, obtained, are brought in a form appropriate for solution and physical interpretation.

In this way we obtain, for every n, an exact gravitational theory, laying "between" the Newton–Cartan theory and general relativity and showing some of the characteristic features of both theories. Clearly, for $n = 0$ we expect the Newton–Cartan theory and for $n = \infty$ in some sense, general relativity. That the latter is true can be seen from the properties of ϵ listed above. For $n = \infty$, ϵ may be any nonzero real number and thus can be set equal to c^{-2}. In this way we find how the structural peculiarities of the Newton–Cartan theory are shifted from step to step to finally coincide with those of general relativity as n tends to ∞. Therefore, we actually reversed the direction of the question stated above and are now asking if and in what sense the post-Galilean gauge theories tend to general relativity.

II. THE RING OF n-POST-REAL NUMBERS

Let $\{\varnothing^N : N = 0,1,\ldots,n\}$ denote the standard basis of $\mathbf{R}^{n+1}$. We define a multiplication on $\mathbf{R}^{n+1}$ as the bilinear map

$$\mathbf{R}^{n+1}\times\mathbf{R}^{n+1}\to\mathbf{R}^{n+1};\ (p,q)\to pq,$$

with the following properties.

(i) $\varnothing^0 := 1$ is the unit element of the multiplication.

(ii) $\varnothing^N\varnothing^M = \varnothing^{N+M}$, $N,M = 0,1,\ldots$.

(iii) $\varnothing^{n+1} = 0$.

The linear space $\mathbf{R}^{n+1}$ with the above defined multiplication becomes a commutative ring with unit element. We call it the ring of n-post real numbers and denote it by $\mathbf{R}^{[n]}$.

One can easily prove that $\mathbf{R}^{[n]}$ is isomorphic[6] to $\mathbf{R}[x]/I^{n+1}$, where $\mathbf{R}[x]$ is the ring of real polynomials of one variable and I^{n+1} is the ideal of $\mathbf{R}[x]$ defined by

$$I^{n+1} := \left\{ \sum_{N=0}^{\infty} \alpha_N x^N : \alpha_0 = \cdots = \alpha_n = 0 \right\}.$$

From the definition above we see that $\varnothing$ is fixed in $\mathbf{R}^{[n]}$ but not in $\mathbf{R}[x]/I^{n+1}$. So for every element α of $\mathbf{R}^{[n]}$ we have a unique decomposition

$$\alpha = \sum_{N=0}^{n} \varnothing^N \alpha^{(N)}, \quad \alpha^{(N)}\in\mathbf{R}. \tag{2.1}$$

Here, $\alpha^{(N)}$ is called the N-part of α. For later use we introduce also the notation

$$\alpha^{[m]} := \sum_{M=0}^{m} \varnothing^M \alpha^{(M)}, \quad m\leqslant n. \tag{2.2}$$

We call $\alpha^{[m]}$ the $[m]$-part of α. Clearly $\alpha^{[n]} = \alpha$. If ϵ is a fixed real number we define the real linear map

$$\mathscr{P}_\epsilon : \mathbf{R}^{[n]}\to\mathbf{R};\quad \mathscr{P}_\epsilon(\varnothing^N) = \epsilon^N,\quad N = 0,1,\ldots,n. \tag{2.3}$$

Here, $\mathscr{P}_\epsilon$ is not a homomorphism of rings. If we let ϵ be a real parameter, then we have the following useful identities:

$$\alpha^{(N)} = \frac{1}{n!}\frac{d^N}{d\epsilon^N}(\mathscr{P}_\epsilon(\alpha))\Big|_{\epsilon=0},\quad N = 0,\ldots,n. \tag{2.4}$$

For convenience we also write α_ϵ in place of $\mathscr{P}_\epsilon(\alpha)$. Using (2.4) we can easily prove that for $\alpha,\beta\in\mathbf{R}^{[n]}$

$$(\alpha\beta)^{(N)} = \frac{1}{N!}\frac{d^N}{d\epsilon^N}(\alpha_\epsilon\beta_\epsilon)\Big|_{\epsilon=0},\quad N = 0,\ldots,n \tag{2.5}$$

and, if $\alpha^{(0)}\neq 0$, then

$$(\alpha^{-1})^{(N)} = \frac{1}{N!}\frac{d^N}{d\epsilon^N}(\alpha_\epsilon)^{-1}\Big|_{\epsilon=0},\quad N = 0,\ldots,n. \tag{2.6}$$

Otherwise, α^{-1} is not defined.

In order to generalize the above formulas let f be a $\mathbf{R}^{[n]}$-valued C^∞ function on $\mathbf{R}$

$$f:\mathbf{R}\to\mathbf{R}^{[n]}.$$

Setting $f_\epsilon := \mathscr{P}_\epsilon \circ f$ we extend f on $\mathbf{R}^{[n]}$ by means of the definition

$$f^{[n]}:\mathbf{R}^{[n]}\to\mathbf{R}^{[n]};\quad \alpha\to f^{[n]}(\alpha), \tag{2.7}$$

$$f^{[n]}(\alpha) := \sum_{N=0}^{n} \varnothing^N [f(\alpha)]^{(N)}, \tag{2.7'}$$

with

$$[f(\alpha)]^{(N)} := \frac{1}{N!}\frac{d^N}{d\epsilon^N}[f_\epsilon(\alpha_\epsilon)]\Big|_{\epsilon=0},\quad N = 0,\ldots,n, \tag{2.8}$$

where we assume that (2.8) is well defined.

Letting g be a real-valued function on $\mathbf{R}$ we can easily prove the consistency of this definition with the composition of functions, that is,

$$[f\circ g]^{[n]} = f^{[n]}\circ g^{[n]}. \tag{2.9}$$

Finally, we find a real $(n+1)$-square matrix representation of $\mathbf{R}^{[n]}$ in terms of the correspondence, for $N = 0,1,\ldots,n$,

$$\varnothing^N\to(\varnothing^N)^r{}_s := \delta^r{}_{s+N},\quad r,s = 0,1,\ldots,n, \tag{2.10}$$

where $\delta^r{}_s$ is the Kronecker symbol.

III. THE n-POST-LINEAR ALGEBRA

Let V be a finite-dimensional real linear space. We set

$$V^{[n]} := \mathbf{R}^{[n]}\otimes_{\mathbf{R}} V, \tag{3.1}$$

the tensor product of $\mathbf{R}^{[n]}$ and V over the reals. On $V^{[n]}$ we define an operation for the elements of $\mathbf{R}^{[n]}$ by means of

$$\mathbf{R}^{[n]}\times V^{[n]}\to V^{[n]},\quad p(q\otimes v) := (pq)\otimes v, \tag{3.2}$$

where $p,q,\in\mathbf{R}^{[n]}$ and $v\in V$. With this operation $V^{[n]}$ becomes a $\mathbf{R}^{[n]}$ module, an n-postlinear space. Because of (2.1) we have a unique decomposition of $V^{[n]}$ in N-parts and so we may identify V with the 0-part of $V^{[n]}$. Here, $V^{[n]}$ is a free module since every linear basis of V becomes an n-postlinear basis of $V^{[n]}$ by means of the above identification. One can also prove that the 0-parts of the elements of an n-postlinear basis of $V^{[n]}$ make a linear basis of V. So $V^{[n]}$ over $\mathbf{R}^{[n]}$ has the same dimension[7] as V over $\mathbf{R}$.

For the space $L^{[n]}(V^{[n]},V^{[n]})$ of n-postlinear transformations of $V^{[n]}$,

$$L^{[n]}(V^{[n]},V^{[n]}) = \mathbf{R}^{[n]}\otimes L(V,V) \tag{3.3}$$

holds, where $L(V,V)$ is the space of real linear transformations of V. Thus, for an element $A \in L^{[n]}(V^{[n]},V^{[n]})$ we have a unique decomposition

$$A = \sum_{N=0}^{n} \varnothing^N A^{(N)}, \quad A^{(N)} \in L(V,V). \tag{3.4}$$

As for the n-post-real numbers the map A is invertible if and only if $A^{(0)}$ is invertible. The set of invertible elements of $L^{[n]}(V^{[n]},V^{[n]})$ forms a group $\mathrm{GL}^{[n]}(V)$, the general n-post-linear group. One can also show that under n-post similarity transformations of A the rank of only $A^{(0)}$ remains invariant.

The space $L^{[n]}(V^{[n]},\mathbf{R}^{[n]}) =: V^{[n]*}$ will be called the dual of $V^{[n]}$. If $\{a_\mu : \mu = 1,\ldots\}$ is any n-postlinear basis of $V^{[n]}$, then by means of the relations

$$\eta^\mu(a_\nu) = \delta^\mu{}_\nu; \eta^\mu \in V^{[n]*}, \quad \mu,\nu = 1,\ldots,\dim V, \tag{3.5}$$

an n-postlinear basis of $V^{[n]*}$ is uniquely defined as the dual basis of $\{a_\mu\}$.

IV. THE n-POST-GALILEAN METRIC

Let V be a four-dimensional real linear space. The pair of symmetric n-postlinear maps

$$g := (g_{\mu\nu}): V^{[n]} \to V^{[n]*},$$
$$h := (h^{\mu\nu}): V^{[n]*} \to V^{[n]}, \tag{4.1}$$

with decompositions

$$g_{\mu\nu} = \sum_{N=0}^{n} \varnothing^N g^{(N)}{}_{\mu\nu}, \quad h^{\mu\nu} = \sum_{N=0}^{n} \varnothing^N h^{(N)\mu\nu},$$

is called an n-post-Galilean metric, if the following conditions hold:

$g^{(0)}$ and $-h^{(0)}$ are positive semidefinite of rank 1 and 3, respectively, (4.2a)

and

$$h^{\mu\rho} g_{\rho\nu} = \varnothing \delta^\mu{}_\nu. \tag{4.2b}$$

Condition (4.2a) is motivated from the definition of a Galilean metric.[4,8,9] Since $g^{(0)}$ is positive semidefinite of rank 1, we can find a one-form $\psi^{(0)}$, such that

$$g^{(0)}{}_{\mu\nu} = \psi^{(0)}{}_\mu \psi^{(0)}{}_\nu. \tag{4.3a}$$

We also write

$$h^{(0)\mu\nu} = -\gamma^{(0)\mu\nu}. \tag{4.3b}$$

Theorem: There exists a not-uniquely determined invertible 4×4 matrix

$$\theta^i{}_\mu = \sum_{N=0}^{n} \varnothing^N \theta^{(N)i}{}_\mu, \tag{4.4a}$$

with the inverse

$$e^\mu{}_j = \sum_{N=0}^{n} \varnothing^N e^{(N)\mu}{}_i, \tag{4.4b}$$

i.e.,

$$e^\mu{}_j \theta^i{}_\mu = \delta^i_j, \tag{4.4c}$$

such that

$$g_{ij} := g_{\mu\nu} e^\mu{}_i e^\nu{}_j = \psi_i \psi_j - \varnothing \gamma_{ij}$$
$$[= \mathrm{diag}(1, -\varnothing, -\varnothing, -\varnothing)], \tag{4.5a}$$

$$h^{ij} := h^{\mu\nu} \theta^i{}_\mu \theta^j{}_\nu = -\gamma^{ij} + \varnothing v^i v^j$$
$$[= \mathrm{diag}(\varnothing, -1, -1, -1)]. \tag{4.5b}$$

For later convenience we have introduced the symbols

$$\psi_i = \delta^0{}_i, \quad v^i = \delta^i{}_0, \quad \gamma^{ij} = \delta^i{}_A \delta^j{}_B \delta^{AB}, \quad \gamma_{ij} = \delta^A{}_i \delta^B{}_j \delta_{AB}, \tag{4.6}$$

with $i,j = 0,1,2,3$ and $A,B = 1,2,3$.

For the proof see Appendix A.

Now let $\{a_\mu : \mu = 0,1,2,3\}$ be the linear basis of $V \subset V^{[n]}$ and $\{\eta^\mu : \mu = 0,1,2,3\}$ its dual to which the components of the metric $(g_{\mu\nu}, h^{\mu\nu})$ refer. From the above theorem we obtain an orthonormal basis[10] $\{e_i := e^\mu{}_i a_\mu : i = 0,1,2,3\}$ and its dual $\{\theta^i := \theta^i{}_\mu \eta^\mu : i = 0,1,2,3\}$.

For some pair of matrices (θ,e) satisfying the conditions of the above theorem, we set

$$\psi_\mu := \psi_i \theta^i{}_\mu, \quad \gamma^{\mu\nu} := \gamma^{ij} e^\mu{}_i e^\nu{}_j,$$
$$v^\mu := v^i e^\mu{}_i, \quad \gamma_{\mu\nu} := \gamma_{ij} \theta^i{}_\mu \theta^j{}_\nu. \tag{4.7}$$

From these definitions we find from (4.5) and (4.6) the decomposition

$$g_{\mu\nu} = \psi_\mu \psi_\nu - \varnothing \gamma_{\mu\nu}, \tag{4.8a}$$
$$h^{\mu\nu} = -\gamma^{\mu\nu} + \varnothing v^\mu v^\nu \tag{4.8b}$$

of the n-post-Galilean metric. We note that $\psi_\mu, \gamma^{\mu\nu}, \gamma_{\mu\nu}$, and v^μ are n-post-real numbers. We also stress that the decomposition (4.8) of the metric depends on the pair (θ,e), which is not uniquely determined.

The tensors defined in (4.7) satisfy the relations

$$\gamma^{\mu\nu}\psi_\nu = 0, \tag{4.9a}$$
$$v^\mu \psi_\mu = 1, \tag{4.9b}$$
$$\gamma_{\mu\nu} v^\nu = 0, \tag{4.9c}$$
$$\gamma^{\mu\rho}\gamma_{\rho\nu} = \delta^\mu{}_\nu - v^\mu \psi_\nu. \tag{4.9d}$$

From (4.9a) follows that the pair $(\gamma^{\mu\nu},\psi_\mu)$ formally is a Galilean metric. From the rest of (4.9) follows also that $\gamma_{\mu\nu}$ formally is the v-associated covariant space metric of $(\gamma^{\mu\nu},\psi_\mu)$.[8]

V. THE n-POST-GALILEAN GROUP

An n-postlinear map $\Lambda: V^{[n]} \to V^{[n]}$ is called an n-post-Galilean transformation if it is an isometry of the n-post-Galilean metric, that is,

$$h^{kl} \Lambda^i{}_k \Lambda^j{}_l = h^{ij}, \quad g_{kl} \Lambda^k{}_i \Lambda^l{}_j = g_{ij}. \tag{5.1}$$

With the aid of (4.5) we determine the general form of an n-post-Galilean transformation to be

$$\Lambda^i{}_j = (\delta^i{}_k - \varnothing[v^i B_k/(1 - \varnothing v^l B_l)]) R^k{}_j$$
$$+ (1 - \varnothing v^l B_l) v^i \psi_j + \gamma^{ik} B_k \psi_j, \tag{5.2}$$

where the parameters R^i and B_k are restricted by the conditions

$$v^i B_i + \tfrac{1}{2}(\gamma^{ij} - \varnothing v^i v^j) B_i B_j = 0, \tag{5.3}$$
$$\gamma^{kl} R^i{}_k R^j{}_l = \gamma^{ij} + \varnothing \gamma^{ik}\gamma^{jl} B_k B_l, \tag{5.4}$$

and

$$R^i{}_j \psi_i = 0, \quad R^i{}_j v^j = 0. \tag{5.5}$$

One also has the following useful relations:

$$R^i{}_j = (\delta^i{}_k - v^i\psi_k)\Lambda^k{}_l(\delta^l{}_j - v^l\psi_j), \tag{5.6a}$$

and

$$B_i = \gamma_{ik}\Lambda^k{}_l v^l - \frac{\gamma_{kl}\Lambda^k{}_r\Lambda^l{}_s v^r v^s}{1 + v^k\Lambda^l{}_k\psi_l}\psi_i. \tag{5.6b}$$

From (5.2)–(5.4) we recognize that $R^i{}_j$ is the spatial rotational part and B_i the boost part of $\Lambda^i{}_j$. Here, $\Lambda^{[n]}$ is obtained from a Lorentz transformation $\Lambda(c^{-2})$ through the substitution $c^{-2}\to\varnothing$.

The symbols defined in (4.6) are not invariant under n-post-Galilean transformations. They transform as follows:

$$\psi'_i = \psi_i - \varnothing B_i, \tag{5.7a}$$

$$v'^i = (1 - \varnothing v^j B_j)v^i + \gamma^{ij}B_j, \tag{5.7b}$$

$$\gamma'^{ij} = \gamma^{ij} + \varnothing\gamma^{ik}\gamma^{jl}B_kB_l + \varnothing(1 - \varnothing v^kB_k)v^{(i}\gamma^{j)l}B_l + \varnothing^3(\gamma^{kl}B_kB_l)v^iv^j, \tag{5.7c}$$

and

$$\gamma'_{ij} = \gamma_{ij} - \psi_{(i}B_{j)} + \varnothing B_iB_j. \tag{5.7d}$$

Here and in the following the (anti-)symmetrization symbols are used without numerical coefficients.

As we see from these formulas these symbols are transformed only by the boost part of the n-post-Galilean transformations. The special case of (5.7), in which $\varnothing B_i = 0$ holds, is of particular interest. We have

$$\psi'_i = \psi_i, \quad \gamma'^{ij} = \gamma^{ij}, \tag{5.8a}$$

$$v'^i = v^i + \gamma^{ij}B_j, \quad \gamma'_{ij} = \gamma_{ij} - \psi_{(i}B_{j)}, \tag{5.8b}$$

and from (5.3)

$$v^iB_i + \tfrac{1}{2}\gamma^{ij}B_iB_j = 0, \tag{5.8c}$$

where the second term of (5.8c) is present only for $n = 0$.

The set of all n-post-Galilean transformations forms a group, the n-post-Galilean group $SO^{[n]}(1,3)$. (We restrict our discussion to the special n-post-Galilean group.) The $SO^{[n]}(1,3)$ is a subgroup of $GL^{[n]}(4,\mathbb{R})$. In general $SO^{[m]}(1,3)$ is not a subgroup of $SO^{[n]}(1,3)$ for $m < n$. From (5.2) we obtain the Galilean group for $n = 0$ and the Lorentz group for $n = \infty, \varnothing = c^{-2}$.

An element $\omega^i{}_j$ of the Lie algebra $\mathfrak{so}^{[n]}(1,3)$ of the n-post-Galilean group must satisfy the relations

$$h^{k(i}\omega^{j)}{}_k = 0, \quad g_{k(i}\omega^k{}_{j)} = 0. \tag{5.9}$$

From these relations, or from (5.2), we find

$$\omega^i{}_j = r^i{}_j + \gamma^{ik}b_k\psi_j + \varnothing v^ib_j, \tag{5.10}$$

where

$$r^i{}_jv^j = 0, \quad \psi_jr^j{}_i = \gamma^{k(i}r^{j)}{}_k = 0, \tag{5.11a}$$

and

$$v^ib_i = 0. \tag{5.11b}$$

A $\mathbb{R}^{[n]}$-linear basis of $\mathfrak{so}^{[n]}(1,3)$ is given by the six matrices L^{ab}, $a,b = 0,1,2,3$, with

$$(L^{ab})^i{}_j := -h^{i[a}\delta^{b]}{}_j. \tag{5.12}$$

The commutation relations of these generators are as for the orthogonal groups

$$[L^{ab},L^{cd}] = -h^{ad}L^{bc} + h^{ac}L^{bd} - h^{bc}L^{ad} + h^{bd}L^{ac}. \tag{5.13}$$

The structure constants are n-post-real numbers. Here, $\mathfrak{so}^{[n]}(1,3)$ is a $\mathbb{Z}$-graded Lie algebra over the reals. We set for $N\in\mathbb{Z}$

$$\mathcal{L}^{(2N)} := \{\varnothing^N L^{AB} : A,B = 1,2,3\},$$
$$\mathcal{L}^{(2N+1)} := \{\varnothing^N L^{A0} : A = 1,2,3\}, \quad \mathcal{L}^{(N)} := \{0\}, \ N<0. \tag{5.14}$$

From these definitions we easily find

$$\mathfrak{so}^{[n]}(1,3) = \bigoplus_{N\in\mathbb{Z}} \mathcal{L}^{(N)}; \quad [\mathcal{L}^{(N)},\mathcal{L}^{(M)}] \subset \mathcal{L}^{(N+M)}. \tag{5.15}$$

In the limit $n\to\infty, \varnothing = c^{-2}$, we have a $\mathbb{Z}_2$ gradation with

$$\mathfrak{so}(1,3) = m^{(0)} \oplus m^{(1)}, \quad [m^{(a)},m^{(b)}] \subset m^{(a+b)}, \tag{5.16}$$

where $m^{(0)}$ denotes the set of spacelike rotations, $m^{(1)}$ the boosts, and a,b, $a+b\in\mathbb{Z}_2$.

VI. THE n-POST-GALILEAN MANIFOLDS

On a real four-dimensional C^∞ manifold M we define the n-post-tangential bundle as

$$TM^{[n]} := \bigcup_{p\in M} (\mathbb{R}^{[n]} \otimes T_pM), \tag{6.1}$$

where T_pM is the tangential space on $p\in M$. In an obvious way we also define the n-post-tensor bundles on M. A real four-dimensional C^∞ manifold with an n-post Galilean metric field $(g^{[n]},h^{[n]})$ will be called an n-post-Galilean manifold. As in (2.3) we introduce the map $\mathcal{P}_\epsilon : TM^{[n]}\to TM, \epsilon\in\mathbb{R}$,

$$\pi\circ\mathcal{P}_\epsilon = \pi^{[n]}, \tag{6.2}$$

where $\pi : TM\to M$, $\pi^{[n]} : TM^{[n]}\to M$ are the obvious bundle projections. As in Sec. III we identify TM with the zero-part of $TM^{[n]}$.

Since M is a real manifold the coordinate transformations are real maps and the holonomic bases of T_pM have vanishing N-parts, $N>0$. We introduce now the concept of an n-post diffeomorphism. Let f be a $(\mathbb{R}^4)^{[n]}$-valued C^∞ map on $\mathbb{R}^4$ with the decomposition

$$f = \sum_{N=0}^{n} \varnothing^N f^{(N)}. \tag{6.3}$$

Then f is called an n-post-diffeomorphism of $\mathbb{R}^4$ if $f_\epsilon := \mathcal{P}_\epsilon\circ f$ is a diffeomorphism of $\mathbb{R}^4$ for all ϵ in an open neighborhood of $\epsilon = 0\in\mathbb{R}$. Suppose $f_{\alpha\alpha'}$ is an n-post-diffeomorphism of $\mathbb{R}^4$ and (V_α,ϕ_α), $(V_{\alpha'},\phi_{\alpha'})$ are charts of M, such that $\phi_\alpha^{-1}\circ(\mathcal{P}_\epsilon\circ f_{\alpha\alpha'})\circ\phi_{\alpha'}$ is defined for all ϵ in some open neighborhood of $\epsilon = 0$. Also let $f_{\beta\beta'}$, (V_β,ϕ_β), and $(V_{\beta'},\varphi_{\beta'})$ be another triple, which satisfies the above condition. We call the two triples *equivalent* $f_{\alpha\alpha'}\sim f_{\beta\beta'}$, if the following relation

$$f_{\beta\beta'} = \varphi^{[n]}_{\beta\alpha}\circ f_{\alpha\alpha'}\circ\phi_{\alpha'\beta'} \tag{6.4}$$

holds, whenever the coordinate transformations $\phi_{\alpha'\beta'} := \phi_{\alpha'}\circ\phi_{\beta'}^{-1}$, $\phi_{\beta\alpha} := \phi_\beta\circ\phi_\alpha^{-1}$ are defined. Here, $\phi^{[n]}_{\alpha\beta}$ is defined as in (2.7). With the aid of (2.9) it is easy to prove that $\sim$ is an equivalence relation. The equivalence classes of $\sim$ define objects on M, which will be called n-post-diffeomorphisms of M.

Setting

$$f^{\alpha\alpha'}_\epsilon := \phi_\alpha^{-1}\circ(\mathcal{P}_\epsilon\circ f_{\alpha\alpha'})\circ\phi_{\alpha'}, \tag{6.5}$$

one can easily prove, using (2.8), that if $f_{\alpha\alpha'} \sim f_{\beta\beta'}$, then $f^{\alpha\alpha'}_{\epsilon}$ and $f^{\beta\beta'}_{\epsilon}$ meet at $\epsilon = 0$ to the nth order. That is, for any pair of charts (V_γ,ϕ_γ), $(V_{\gamma'},\phi_{\gamma'})$ the relations

$$\frac{1}{N!}\frac{d^N}{d\epsilon^N}(f^{\alpha\alpha'}_{\epsilon})_{\gamma\gamma'}\Big|_{\epsilon=0} = \frac{1}{N!}\frac{d^N}{d\epsilon^N}(f^{\beta\beta'}_{\epsilon})_{\gamma\gamma'}\Big|_{\epsilon=0}, \quad N=0,1,\ldots,n \tag{6.6}$$

hold, whenever the maps $(f^{\alpha\alpha'}_{\epsilon})_{\gamma\gamma'} = \phi_\gamma \circ f^{\alpha\alpha'}_{\epsilon} \circ \phi^{-1}_{\gamma'}$ and $(f^{\beta\beta'}_{\epsilon})_{\gamma\gamma'}$ are defined. In this case

$$f^{(N)}_{\gamma\gamma'} = \frac{1}{N!}\frac{d^N}{d\epsilon^N}(f^{\alpha\alpha'}_{\epsilon})_{\gamma\gamma'}\Big|_{\epsilon=0}, \tag{6.7}$$

where $f_{\gamma\gamma'}$ is defined with the aid of (6.4). This allows us to simply write f_ϵ instead of $f^{\alpha\alpha'}_{\epsilon}$.

We now give the transformational behavior of scalar functions, vector fields, and one-forms under an n-post diffeomorphism f. We derive them in analogy to the real case. Let S be a $\mathbb{R}^{[n]}$-valued C^∞ function on M. We then have the decomposition

$$S = \sum_{N=0}^{n} \varnothing^N S^{(N)}. \tag{6.8}$$

Then f transforms S into

$$f_* S = \sum_{N=0}^{n} \varnothing^N (f_* S)^{(N)}, \tag{6.9a}$$

with

$$(f_* S)^{(N)} := \left\{ \frac{1}{N!}\frac{d^N}{d\epsilon^N}(S_\epsilon \circ f_\epsilon^{-1} \circ \phi_\alpha^{-1})\Big|_{\epsilon=0} \right\} \circ \phi_\alpha, \tag{6.9b}$$

where $S_\epsilon := \mathscr{P}_\epsilon \circ S$ and ϕ_α is an appropriate chart of M. Since $d/d\epsilon$ commutes with the exterior derivative, we obtain from (6.9) the transformation of a one-form. Let χ_μ be an n-post-one-form. Then

$$(f_* \chi)_\mu = \sum_{N=0}^{n} \varnothing^N (f_* \chi)^{(N)}_\mu, \tag{6.10a}$$

with

$$(f_* \chi)^{(N)}_\mu := 1/N! \frac{d^N}{d\epsilon^N}\{[(J_{f_\epsilon}^{-1})^\nu{}_\mu (\chi_\epsilon)_\nu] \circ f_\epsilon^{-1}\}\Big|_{\epsilon=0}, \tag{6.10b}$$

where J_{f_ϵ} is the Jacobian of f_ϵ. Similarly, for an n-post vector field X^μ we obtain

$$(f_* X)^\mu = \sum_{N=0}^{n} \varnothing^N (f_* X)^{(N)}\mu, \tag{6.11a}$$

with

$$(f_* X)^{(N)}\mu := \frac{1}{N!}\frac{d^N}{d\epsilon^N}\{[(J_{f_\epsilon})^\mu{}_\nu (X_\epsilon)^\nu] \circ f_\epsilon^{-1}\}\Big|_{\epsilon=0}. \tag{6.11b}$$

From these formulas we obtain the transformational behavior of any tensor.

By an extension of the arguments used on $\mathbb{R}$ we can show that any closed $\mathbb{R}^{[n]}$-valued one-form, whose zero-part never vanishes, can be locally transformed to δ^0_μ.

The definitions given here can be naturally formulated by use of jet-bundle formalism.

VII. TORSION-FREE n-POST-GALILEAN CONNECTIONS

Let $\Gamma^\rho_{\mu\nu}$ denote the components of an n-postlinear connection with respect to some coordinate system. If the connection is to be torsion-free, then we must have

$$\Gamma^\rho_{[\mu\nu]} = 0 \Rightarrow \Gamma^{(N)\rho}_{[\mu\nu]} = 0, \quad N = 0,\ldots,n. \tag{7.1}$$

Such a connection will be called an n-post-Galilean connection if the n-post-Galilean metric is covariantly constant with respect to it, that is,

$$\nabla_\rho g_{\mu\nu} = 0, \quad \nabla_\rho h^{\mu\nu} = 0, \tag{7.2}$$

where ∇ denotes the covariant derivative, with respect to Γ.

In the following we solve these equations for the connection coefficients. Substituting the decomposition (4.8) of the metric in (7.2) we obtain

$$(\nabla_\rho \psi_{(\mu})\psi_{\nu)} = \varnothing \nabla_\rho \gamma_{\mu\nu}, \tag{7.3a}$$

$$\nabla_\rho \gamma^{\mu\nu} = \varnothing v^{(\mu} \nabla_\rho v^{\nu)}. \tag{7.3b}$$

Using (4.9) we find

$$\nabla_\rho \psi_\mu = -\varnothing \gamma_{\mu\nu} \nabla_\rho v^\nu, \tag{7.4a}$$

$$\varnothing \nabla_\rho v^\mu = -\gamma^{\mu\nu} \nabla_\rho \psi_\nu, \tag{7.4b}$$

and, since the connection is torsion-free,

$$\psi_{[\mu,\nu]} = -\varnothing \gamma_{\rho[\mu} \nabla_{\nu]} v^\rho. \tag{7.5a}$$

From this equation the condition

$$\psi^{(0)}_{[\mu,\nu]} = 0 \tag{7.5b}$$

follows immediately. We now introduce the two-form

$$\chi_{\mu\nu} := \gamma_{\rho[\mu} \nabla_{\nu]} v^\rho. \tag{7.6a}$$

Then we have

$$\psi_{[\mu,\nu]} = -\varnothing \chi_{\mu\nu}. \tag{7.6b}$$

Using (7.1), (7.2), and (4.2b) we easily find

$$\varnothing \Gamma^\rho{}_{\mu\nu} = \tfrac{1}{2} h^{\rho\sigma}(g_{\sigma(\mu,\nu)} - g_{\mu\nu,\sigma}). \tag{7.7}$$

We see that, for finite n, the n-part of the connection is not determined from (7.7). Substituting (4.8) in (7.7) we find

$$\varnothing \Gamma^\rho{}_{\mu\nu} = \varnothing\{\overset{v}{\Gamma}{}^\rho{}_{\mu\nu} + \varnothing v^\rho \gamma_{\sigma\mu} \overset{v}{\nabla}{}_\nu v^\sigma - \tfrac{1}{2} h^{\rho\sigma} \chi_{\sigma(\mu}\psi_{\nu)}\}, \tag{7.8}$$

where

$$\overset{v}{\Gamma}{}^\rho{}_{\mu\nu} = \tfrac{1}{2}\gamma^{\rho\sigma}(\gamma_{\sigma(\mu,\nu)} - \gamma_{\mu\nu,\sigma}) \tfrac{1}{2} v^\rho \psi_{(\mu,\nu)} \tag{7.9}$$

is formally the v-special "Galilean" connection of $(\psi_\mu,\gamma^{\mu\nu})$ (see Ref. 11), and $\overset{v}{\nabla}$ is the covariant derivative with respect to $\overset{v}{\Gamma}$. For this connection we have the following identities:

$$\gamma_{\sigma[\mu} \overset{v}{\nabla}{}_{\nu]} v^\sigma = 0 \tag{7.10}$$

and

$$\overset{v}{\nabla}{}_\mu \psi_\nu = -\tfrac{1}{2}\psi_{[\mu,\nu]} = \varnothing \tfrac{1}{2}\chi_{\mu\nu}, \tag{7.11a}$$

$$\overset{v}{\nabla}{}_\rho \gamma^{\mu\nu} = \varnothing \tfrac{1}{2} v^{(\mu} \chi^{\nu)\sigma} \chi_{\rho\sigma}, \tag{7.11b}$$

$$\overset{v}{\nabla}_\rho \gamma_{\mu\nu} = -\psi_{(\mu}\gamma_{\nu)\sigma}\overset{v}{\nabla}_\rho v^\sigma. \tag{7.11c}$$

We also have

$$\nabla_\rho \gamma_{\mu\nu} = -\psi_{(\mu}\gamma_{\nu)\sigma}\nabla_\rho v^\sigma. \tag{7.12}$$

Using these identities, after lengthy calculations, we obtain

$$\Gamma^\rho{}_{\mu\nu} = \overset{v}{\Gamma}{}^\rho{}_{\mu\nu} + \varnothing v^\rho \gamma_{\sigma\mu}\overset{v}{\nabla}_\nu v^\sigma - \tfrac{1}{2}h^{\rho\sigma}\chi_{\sigma(\mu}\psi_{\nu)}. \tag{7.13}$$

This does not mean that the n-post-Galilean, torsion-free connection is completely determined, since because of (7.6a) Γ appears also on the right-hand side of (7.13).

Freeing ourselves from (7.6a) and letting (7.6b) be the definition of $\chi_{\mu\nu}$, we see that its n-part $\chi^{(n)}{}_{\mu\nu}$ is undetermined. Thus, there remains an indeterminacy in Γ expressed by the free choice of the real two-form $\chi^{(n)}{}_{\mu\nu}$. This is a characteristic of the Galilean theory, which is retained here. With the aid of (7.7) and (5.8) it can be shown that (7.13) is independent of the particular decomposition of the metric used in (4.8).

We can now simplify (7.13) by choosing the decomposition (4.8) such that

$$\psi_{[\mu,\nu]} = 0 \tag{7.14}$$

holds. It is shown in Appendix B that this choice is locally possible. It restricts the $[n-1]$-part of the boost B_i in (5.7).

Using (7.14) we find

$$\Gamma^\rho{}_{\mu\nu} = \overset{v}{\Gamma}{}^\rho{}_{\mu\nu} + \varnothing v^\rho \gamma_{\sigma\mu}\overset{v}{\nabla}_\nu v^\sigma + \tfrac{1}{2}\gamma^{\rho\sigma}\chi_{\sigma(\mu}\psi_{\nu)}, \tag{7.15}$$

with

$$\chi_{\mu\nu} = \varnothing^n \chi^{(n)}{}_{\mu\nu}, \tag{7.16}$$

where $\chi^{(n)}{}_{\mu\nu}$ is an arbitrary real two-form. In the following we always use a decomposition of the metric for which (7.14) holds.

From the transformational behavior of the connection Γ under an n-post diffeomorphism f we find, as in the real case, that

$$f_* \overset{\Gamma}{\nabla} = \overset{f_*\Gamma}{\nabla} f_* \tag{7.17}$$

holds.

VIII. THE CURVATURE TENSOR AND THE NEWTONIAN CONDITION

Setting

$$\Sigma_{\mu\nu} := \gamma_{\sigma\mu}\overset{v}{\nabla}_\nu v^\sigma, \tag{8.1}$$

we find for the curvature tensor

$$\begin{aligned} R^\rho{}_{\sigma\mu\nu} = {} & \overset{v}{R}{}^\rho{}_{\sigma\mu\nu} + \varnothing \overset{v}{\nabla}_{[\mu}(v^\rho \Sigma_{\nu]\sigma}) \\ & + \frac{1}{2}\left(\overset{v}{\nabla}_{[\mu}\chi^\rho_{\cdot\nu]}\right)\psi_\sigma - \frac{1}{2}\psi_{[\mu}\overset{v}{\nabla}_{\nu]}\chi^\rho_{\cdot\sigma} \\ & + \tfrac{1}{4}\chi^{\rho\lambda}_{\cdot\cdot}\chi_{\lambda[\mu}\psi_{\nu]}\psi_\sigma, \end{aligned} \tag{8.2}$$

where

$$\overset{v}{R}{}^\rho{}_{\sigma\mu\nu} := -\overset{v}{\Gamma}{}^\rho{}_{\sigma[\mu,\nu]} - \overset{v}{\Gamma}{}^\lambda{}_{\sigma[\mu}\overset{v}{\Gamma}{}^\rho{}_{\nu]\lambda} \tag{8.3}$$

is the curvature tensor of $\overset{v}{\Gamma}$ and

$$\chi^\rho_{\cdot\sigma} := \gamma^{\rho\lambda}\chi_{\lambda\sigma}. \tag{8.4}$$

The last term of (8.2) (quadratic in χ) is present only for $n = 0$ because of (7.16). Since the connection is torsion-free we have the identity

$$R^\mu{}_{[\nu\rho\sigma]} = 0. \tag{8.5}$$

From the metric compatibility of the connection we also obtain

$$h^{\lambda(\mu}R^{\nu)}{}_{\lambda\rho\sigma} = 0, \quad g_{\lambda(\mu}R^\lambda{}_{\nu)\rho\sigma} = 0. \tag{8.6}$$

Using these identities we find the condition

$$\varnothing(h^{\rho\lambda}R^\mu{}_{\nu\lambda\sigma} - h^{\mu\lambda}R^\rho{}_{\sigma\lambda\nu}) = 0. \tag{8.7}$$

If we set

$$P^\mu{}_{\nu\rho\sigma} = \overset{v}{R}{}^\mu{}_{\nu\rho\sigma} + \varnothing \overset{v}{\nabla}_{[\rho}(v^\mu \Sigma_{\sigma]\nu}), \tag{8.8}$$

then, because of (7.16) and (8.2)

$$\varnothing(h^{\rho\lambda}P^\mu{}_{\nu\lambda\sigma} - h^{\mu\lambda}P^\rho{}_{\sigma\lambda\nu}) = 0. \tag{8.9}$$

Adding to the n-post-Galilean metric $(n+1)$-parts, such as to obtain an $(n+1)$-post-Galilean metric for which $\psi^{[n+1]}{}_{[\mu,\nu]} = 0$ holds, we find that the $[n]$-part of $P^{[n+1]\mu}{}_{\nu\rho\sigma}$ equals $P^{[n]\mu}{}_{\nu\rho\sigma}$. Since we proved (8.9) for every n, it also holds for $n+1$, hence it follows that in place of (8.9) the stricter result

$$h^{\rho\lambda}P^\mu{}_{\nu\lambda\sigma} - h^{\mu\lambda}P^\rho{}_{\sigma\lambda\nu} = 0 \tag{8.10}$$

holds, where $P = P^{[n]}$. From (8.2) and (8.10) we find that

$$h^{\rho\lambda}R^\mu{}_{\nu\lambda\sigma} - h^{\mu\lambda}R^\rho{}_{\sigma\lambda\nu} = 0 \tag{8.11}$$

is equivalent to the condition that the two-form $\chi_{\mu\nu}$ is closed, or

$$\chi_{[\mu\nu,\rho]} = 0. \tag{8.12}$$

In this case we can choose the n-part of the boost freedom remaining after the assumption (7.14) such as to make $\chi_{\mu\nu}$ locally disappear (see Appendix C).

Definition: An n-post-Galilean connection is called an n-post-Newtonian connection if its curvature tensor is the $[n]$-part of the curvature tensor, an $(n+1)$-post-Galilean connection. We summarize the above results in the following theorem.

Theorem: An n-post-Galilean connection is Newtonian if and only if

$$h^{\rho\lambda}R^\mu{}_{\nu\lambda\sigma} = h^{\mu\lambda}R^\rho{}_{\sigma\lambda\nu}.$$

In this case there is a decomposition (4.8) of the metric, such that

$$\Gamma^\rho{}_{\mu\nu} = \overset{v}{\Gamma}{}^\rho{}_{\mu\nu} + \varnothing v^\rho \gamma_{\mu\sigma}\overset{v}{\nabla}_\nu v^\sigma \tag{8.13}$$

and

$$R^\rho{}_{\sigma\mu\nu} = \overset{v}{R}{}^\rho{}_{\sigma\mu\nu} + \varnothing \overset{v}{\nabla}_{[\mu}(v^\rho \Sigma_{\nu]\sigma}) \tag{8.14}$$

(for $n = 0$ see Ref. 8).

In the following we restrict ourselves to Newtonian connections and use the decomposition of the metric for which (8.13) and (8.14) hold. In this case, the Ricci tensor is

$$R_{\mu\nu} := R^{\rho}{}_{\mu\nu\rho} = \overset{v}{R}{}_{\mu\nu} - \varnothing \overset{v}{\nabla}{}_{\rho}(v^{\rho}\Sigma_{\mu\nu}) \tag{8.15}$$

and the curvature scalar

$$R := h^{\mu\nu}R_{\mu\nu} = \overset{v}{R} + \varnothing \overset{v}{\nabla}{}_{\rho}v^{\rho}, \tag{8.16}$$

where $\overset{v}{R} := h^{\mu\nu}\overset{v}{R}{}_{\mu\nu}$.

IX. VARIATIONAL PRINCIPLE AND FIELD EQUATIONS

In order to postulate a variational principle similar to Hilbert's principle for general relativity, we need some scalar density as is the determinant of the metric tensor. Since here the components of the metric tensor are $\mathbb{R}^{[n]}$-valued functions, it is not obvious how to construct from them such a scalar density. Note that the formal determinant of $g_{\mu\nu}$ vanishes for $n<3$. To avoid this problem, we use tetrad fields and the calculus of differential forms adapted to our problem.[12]

Let $\{e_i : i = 0,1,2,3\}$ be a local n-post-Galilean orthonormal tetrad field with its dual $\{\theta^i : i = 0,1,2,3\}$. We write η_{ijkl} for the totally antisymmetric tensor, with $\eta_{0123} = 1$. (Latin indices refer to $\{e_i\}$, $\{\theta^i\}$). Here, η_{ijkl} is numerically invariant under n-post-Galilean transformations. We now introduce the differential forms

$$\eta = (1/4!)\eta_{ijkl}\theta^i \wedge \theta^i \wedge \theta^k \wedge \theta^l, \tag{9.1a}$$

$$\eta_i = (1/3!)\eta_{ijkl}\theta^j \wedge \theta^k \wedge \theta^l, \tag{9.1b}$$

$$\eta_{ij} = (1/2!)\eta_{ijkl}\theta^k \wedge \theta_l, \tag{9.1c}$$

$$\eta_{ijk} = \eta_{ijkl}\theta^l. \tag{9.1d}$$

Here, η is the volume four-form. With the aid of these definitions, we can prove the following identities:

$$(\theta^{i_1} \wedge \cdots \wedge \theta^{i_r}) \wedge \eta_{j_1\cdots j_s} = \frac{1}{r!}\frac{1}{(s-r)!}\eta_{[j_1\cdots j_{s-r}}\delta^{i_1\cdots i_r}_{j_{r-s+1}\cdots j_s]}, \tag{9.2}$$

with $r,s = 1,\ldots,4$ and

$$\delta^{i_1\cdots i_r}_{j_1\cdots j_r} := \delta^{i_1}_{[j_1}\cdots\delta^{i_r}_{j_r]}. \tag{9.3}$$

These identities are independent of the metric. If $R^{i}{}_{jkl}$ are the components of the curvature tensor referred to $\{\theta^i\}$ and $\{e_i\}$, we set

$$\Omega^{i}{}_{j} := \tfrac{1}{2}R^{i}{}_{jkl}\theta^k \wedge \theta^l \tag{9.4}$$

for the curvature two-from. As in general relativity we set for the Lagrangian density

$$\mathcal{L} = h^{jk}\Omega^{i}{}_{j} \wedge \eta_{ik} + 2\varnothing\Lambda\eta + 2\varnothing\kappa\mathcal{L}_M, \tag{9.5}$$

where Λ is the cosmological constant, $\mathcal{L}_M$ the Lagrangian density of the gravitating matter fields, and $2\varnothing\kappa$ the coupling constant chosen in analogy to general relativity. With the aid of (9.2) one can easily prove that the first term of (9.5) equals $R\eta$.

Using the fact that h^{ij} and η_{ijkl} are numerical constants, and the identities

$$\delta\eta_{i_1\cdots i_r} = \delta\theta^{r+1} \wedge \eta_{i_1\cdots i_{r+1}}, \tag{9.6}$$

we find after varying (9.5) (see Refs. 12 and 13)

$$h^{jk}\Omega^{l}{}_{j} \wedge \eta_{lki} + 2\varnothing\Lambda\eta_i + 2\varnothing\kappa t_i = 0, \tag{9.7}$$

where t_i is the energy-momentum three-form defined by

$$\delta\mathcal{L}_M = \delta\theta^i \wedge t_i. \tag{9.8}$$

Using (9.4) and the identities (9.2) we find for the first summand of (9.7)

$$h^{jk}\Omega^{l}{}_{j} \wedge \eta_{lki} = 2(h^{jk}R_{ki} - \tfrac{1}{2}h^{kl}R_{kl}\delta^{j}_{i})\eta_j. \tag{9.9}$$

Also setting

$$t_i = g_{ik}T^{kj}\eta_j, \tag{9.10}$$

where T^{ij} is the energy-momentum tensor, we find from (9.7) the field equations

$$h^{jk}R_{ki} - \tfrac{1}{2}\delta^{j}_{i}R + \varnothing\delta^{j}_{i}\Lambda = -\varnothing\kappa g_{ik}T^{kj}. \tag{9.11}$$

Referring these equations to a coordinate system, we have

$$h^{\mu\rho}R_{\rho\nu} - \tfrac{1}{2}\delta^{\mu}{}_{\nu}R + \varnothing\delta^{\mu}{}_{\nu}\Lambda = -\varnothing\kappa g_{\nu\rho}T^{\mu\rho}. \tag{9.12}$$

A more useful form is

$$h^{\mu\rho}R_{\rho\nu} = \varnothing\delta^{\mu}{}_{\nu}\Lambda - \varnothing\kappa(g_{\nu\rho}\delta^{\mu}{}_{\sigma} - \tfrac{1}{2}g_{\rho\sigma}\delta^{\mu}{}_{\nu})T^{\sigma\rho}. \tag{9.13}$$

Using the Bianchi identities we also derive the equations of motion for the matter fields

$$\varnothing g_{\mu\rho}\nabla_{\nu}T^{\mu\nu} = 0. \tag{9.14}$$

Using the decomposition (4.8) of the metric and the Newtonian condition (8.11) we deduce from (9.13) the two equations

$$R_{\mu\nu} - \psi_{\mu}\psi_{\nu}(v^{\rho}v^{\sigma}R_{\rho\sigma}) = -\varnothing\gamma_{\mu\nu}\Lambda + \varnothing\kappa(\psi_{\rho}\psi_{(\mu}\gamma_{\nu)\sigma} - \varnothing\gamma_{\mu\rho}\gamma_{\mu\sigma} - \tfrac{1}{2}g_{\rho\sigma}\gamma_{\mu\nu})T^{\rho\sigma} \tag{9.15a}$$

and

$$\varnothing v^{\rho}v^{\sigma}R_{\rho\sigma} = \varnothing\Lambda - \varnothing(\kappa/2)(\psi_{\rho}\psi_{\sigma} + \gamma_{\rho\sigma})T^{\rho\sigma}. \tag{9.15b}$$

From (9.15) we see that the n-part of $v^{\rho}v^{\sigma}R_{\rho\sigma}$ remains undetermined by the field equations. This becomes critical for $n = 0$, since it is Eq. (9.15b) which corresponds to the Poisson equation. From (9.14) we obtain the two equations

$$\varnothing\psi_{\rho}\nabla_{\nu}T^{\rho\nu} = 0 \tag{9.16a}$$

and

$$\varnothing^2\nabla_{\nu}T^{\mu\nu} = 0. \tag{9.16b}$$

Therefore the full equations of motion follow from the field equations only for $n \geqslant 2$.

X. DECOMPOSITION OF THE FIELD EQUATIONS IN VACUUM

Since ψ_{μ} is a closed one-form with never-vanishing zero-part we can transform it by means of an n-post-diffeomorphism to $\psi_{\mu} = \psi^{(0)}{}_{\mu}$, where all N-parts with $N = 1, \ldots, n$ vanish. This does not induce a restriction of the coordinate system, since coordinate transformations do not mix parts of different order. In what follows ψ_{μ} will be of this particular form.

Let u^{μ} be an arbitrary real vector field for which

$$u^{\mu}\psi_{\mu} = 1 \tag{10.1}$$

holds. Setting

$$p_\mu := -\gamma_{\mu\nu}u^\nu + \tfrac{1}{2}(\gamma_{\alpha\beta}u^\alpha u^\beta)\psi_\mu, \tag{10.2}$$

we find

$$v^\mu = u^\mu + \gamma^{\mu\nu}p_\nu. \tag{10.3}$$

We also define the tensor field

$$\overset{u}{\gamma}_{\mu\nu} := \gamma_{\mu\nu} + \psi_{(\mu}p_{\nu)}. \tag{10.4}$$

The four tensors $\psi_\mu, \gamma^{\mu\nu}, u^\mu$, and $\overset{u}{\gamma}_{\mu\nu}$ satisfy the relations (4.9), but they do not form a decomposition (4.8) of the metric. Conversely, if we postulate (10.3) and (10.4), then the tensors $\psi_\mu, \gamma^{\mu\nu}, u^\mu, \overset{u}{\gamma}_{\mu\nu}$ satisfy (4.9), if and only if

$$u^\mu p_\mu + \tfrac{1}{2}\gamma^{\mu\nu}p_\mu p_\nu = 0. \tag{10.5}$$

With the aid of (10.3) and (10.4) we find[14]

$$\overset{v}{\Gamma}{}^{\rho}{}_{\mu\nu} = \overset{u}{\Gamma}{}^{\rho}{}_{\mu\nu} + \tfrac{1}{2}\gamma^{\rho\sigma}\kappa_{\sigma(\mu}\psi_{\nu)}, \tag{10.6}$$

where

$$\overset{u}{\Gamma}{}^{\rho}{}_{\mu\nu} = \frac{1}{2}\gamma^{\rho\sigma}\left(\overset{u}{\gamma}_{\sigma(\mu,\nu)} - \overset{u}{\gamma}_{\mu\nu,\sigma}\right) + \frac{1}{2}\tfrac{1}{2}u^\rho\psi_{(\mu,\nu)} \tag{10.7}$$

and

$$\kappa_{\nu\mu} := -p_{[\mu,\nu]}. \tag{10.8}$$

Using this decomposition of $\overset{v}{\Gamma}$ we easily find

$$\overset{v}{R}{}_{\mu\nu} = \overset{u}{R}{}_{\mu\nu} - \frac{1}{2}\left(\overset{u}{\nabla}{}_\rho\kappa^\rho_{\cdot(\mu}\right)\psi_{\nu)} - \frac{1}{4}(\kappa^{\rho\sigma}_{\cdot\cdot}\kappa_{\rho\sigma})\psi_\mu\psi_\nu, \tag{10.9}$$

where $\overset{u}{R}{}_{\mu\nu}$ is the Ricci tensor of $\overset{u}{\Gamma}$, and $\overset{u}{\nabla}$ the covariant derivative with respect to it. In the derivation of (10.9) we used the fact that $\overset{u}{\Gamma}$ is formally the u-special "Galilean" connection of $\psi_\mu, \gamma^{\mu\nu}$.

With the aid of $\psi_\mu, \gamma^{\mu\nu}, u^\mu$, and $\overset{u}{\gamma}_{\mu\nu}$ we can decompose the Ricci tensor as follows:

$$R_{\mu\nu} = r\psi_\mu\psi_\nu + r^\alpha\overset{u}{\gamma}_{\alpha(\mu}\psi_{\nu)} + r^{\alpha\beta}\overset{u}{\gamma}_{\alpha\mu}\overset{u}{\gamma}_{\beta\nu}, \tag{10.10a}$$

where

$$r := R_{\mu\nu}u^\mu u^\nu, \quad r^\alpha := R_{\mu\nu}u^\mu\gamma^{\nu\alpha}, \quad r^{\alpha\beta} := R_{\mu\nu}\gamma^{\mu\alpha}\gamma^{\nu\beta}. \tag{10.10b}$$

Substituting (10.9) in (10.10b) we obtain

$$\overset{v}{r} = \overset{u}{r} - \left(\overset{u}{\nabla}{}_\rho\kappa^\rho_{\cdot\mu}\right)u^\mu - \frac{1}{4}(\kappa^{\rho\sigma}_{\cdot\cdot}\kappa_{\rho\sigma}), \tag{10.11a}$$

$$\overset{v}{r}{}^\alpha = \overset{u}{r}{}^\alpha - \frac{1}{2}\left(\overset{u}{\nabla}_\rho\kappa^{\rho\alpha}_{\cdot\cdot}\right), \tag{10.11b}$$

$$\overset{v}{r}{}^{\alpha\beta} = \overset{u}{r}{}^{\alpha\beta}, \tag{10.11c}$$

where $\overset{v}{r}, \overset{v}{r}{}^\alpha, \overset{v}{r}{}^{\alpha\beta}$ and $\overset{u}{r}, \overset{u}{r}{}^\alpha, \overset{u}{r}{}^{\alpha\beta}$ are defined as in (10.10b) from $\overset{v}{R}{}_{\mu\nu}$ and $\overset{u}{R}{}_{\mu\nu}$, both with u^μ. Setting

$$\sigma^{\alpha\beta} := \gamma^{\alpha\mu}\gamma^{\beta\nu}\Sigma_{\mu\nu}, \tag{10.12a}$$

we find from (8.1)

$$\sigma^{\alpha\beta} = \tfrac{1}{2}\gamma^{\rho(\alpha}\overset{u}{\nabla}_\rho v^{\beta)}, \tag{10.13}$$

and if $\Sigma_{\mu\nu}$ is decomposed in the same manner as $R_{\mu\nu}$ in (10.10b), then

$$\sigma^\alpha = -p_\beta\sigma^{\alpha\beta}, \quad \sigma = p_\alpha p_\beta\sigma^{\alpha\beta}. \tag{10.12b}$$

We also have

$$\overset{v}{\nabla}_\rho(v^\rho\sigma^{\alpha\beta}) = \overset{u}{\nabla}_\rho(v^\rho\sigma^{\alpha\beta}) + \tfrac{1}{2}\sigma^{\rho(\alpha}\kappa^{\beta)}_{\cdot\rho}. \tag{10.14}$$

Using these relations, we find for the decomposition of $R_{\mu\nu}$

$$r^{\alpha\beta} = \overset{u}{r}{}^{\alpha\beta} - \varnothing\left[\overset{u}{\nabla}_\rho(v^\rho\sigma^{\alpha\beta}) + \frac{1}{2}\sigma^{\rho(\alpha}\kappa^{\beta)}_{\cdot\rho}\right], \tag{10.15a}$$

$$r^\alpha = \overset{u}{r}{}^\alpha - \frac{1}{2}\left(\overset{u}{\nabla}_\rho\kappa^{\rho\alpha}_{\cdot\cdot}\right) + p_\beta\left(\overset{u}{r}{}^{\alpha\beta} - r^{\alpha\beta}\right), \tag{10.15b}$$

$$r = \overset{u}{r} - \left(\overset{u}{\nabla}_\rho\kappa^\rho_{\cdot\mu}\right)u^\mu - \frac{1}{4}\kappa^{\rho\sigma}_{\cdot\cdot}\kappa_{\rho\sigma} + p_\alpha p_\beta\left(r^{\alpha\beta} - \overset{u}{r}{}^{\alpha\beta}\right). \tag{10.15c}$$

With the aid of these equations we find from the field equations (9.15) with $\Lambda = 0 = T^{\mu\nu}$

$$\varnothing\left[\overset{u}{\nabla}_\rho(v^\rho\sigma^{\alpha\beta}) + \frac{1}{2}\sigma^{\rho(\alpha}\kappa^{\beta)}_{\cdot\rho}\right] = \overset{u}{r}{}^{\alpha\beta}, \tag{10.16a}$$

$$\tfrac{1}{2}\overset{u}{\nabla}_\rho\kappa^{\rho\alpha}_{\cdot\cdot} = \overset{u}{r}{}^\alpha + \overset{u}{r}{}^{\alpha\beta}p_\beta, \tag{10.16b}$$

and

$$\varnothing\left[\left(\overset{u}{\nabla}_\rho\kappa^\rho_{\cdot\mu}\right)u^\mu + \frac{1}{4}\kappa^{\rho\sigma}_{\cdot\cdot}\kappa_{\rho\sigma}\right] = \varnothing\left(\overset{u}{r} - \overset{u}{r}{}^{\alpha\beta}p_\alpha p_\beta\right). \tag{10.16c}$$

These equations must be complemented by (10.5). Of particular importance is the case in which

$$p_\mu = U\psi_\mu + S_{,\mu} \tag{10.17}$$

holds, where U, S are $\mathbb{R}^{[n]}$-valued functions on M. Substituting (10.17) in (10.8) and (10.16) we find

$$\varnothing\overset{u}{\nabla}_\rho(v^\rho\sigma^{\alpha\beta}) = \overset{u}{r}{}^{\alpha\beta}, \tag{10.18a}$$

$$\overset{u}{r}{}^\alpha = -\overset{u}{r}{}^{\alpha\beta}S_{,\beta}, \tag{10.18b}$$

$$\varnothing\Delta U = \varnothing\left(\overset{u}{r} - \overset{u}{r}{}^{\alpha\beta}S_{,\alpha}S_{,\beta}\right), \tag{10.18c}$$

where

$$\Delta U := \gamma^{\rho\sigma}\overset{u}{\nabla}_\rho U_{,\sigma} \tag{10.19}$$

is the Laplace operator formed with $\overset{u}{\Gamma}$. From (10.5) we also have the Hamilton–Jacobi equation

$$u^\rho S_{,\rho} + \tfrac{1}{2}\gamma^{\rho\sigma}S_{,\rho}S_{,\sigma} + U = 0. \tag{10.20}$$

As we see from (10.18c), U corresponds to the Newtonian potential. The n-post-Galilean metric we obtain from these equations has the form

$$h^{\mu\nu} = -\gamma^{\mu\nu} + \varnothing(u^\mu + S^{,u}_{,\cdot})(u^\nu + S^{,\nu}_{,\cdot}) \tag{10.21a}$$

and

$$g_{\mu\nu} = (1 + 2\varnothing U)\psi_\mu\psi_\nu + \varnothing\psi_{(\mu}S_{,\nu)} - \varnothing\overset{u}{\gamma}_{\mu\nu}. \tag{10.21b}$$

XI. CONCLUSIONS

In Sec. VII we found that as in the Newton–Cartan theory, the n-post-Galilean metric does not uniquely determine an n-post-Galilean connection nor even a Newtonian connection. However, the indeterminacy, which is expressed by a real two-form, is present only in the last (n-) part of the connection. At every step $n \to n+1$ it is shifted from the n-part to the $(n+1)$-part of the connection and disappears when n tends to infinity.

In Sec. IX we postulated a variational principle which for $n = \infty$ goes over into Hilbert's variational principle of general relativity. For finite n the field equations, obtained from it, do not determine all field variables up to the n-part. Although the metric is completely determined by these equations, since it does not contain $v^{(n)\mu}$ and $\gamma^{(n)}{}_{\mu\nu}$, the connection, which contains such terms, remains undetermined. For $n = 0$, the field equations (9.15) are not those of the Newton–Cartan theory $R_{\mu\nu} = -(\kappa/2)\psi_\mu\psi_\nu(\psi_\rho\psi_\sigma T^{\rho\sigma})$ (see Ref. 8); moreover, the variational principle does not even give the Poisson equation.

The full equations of motion follow from the field equations only for $n \geqslant 2$. For $n = 1$ we obtain only a part of them (9.16a), which can be identified with the continuity equation.

As can be seen from (10.17) the gravitational potential is not contained in ψ_μ or $\gamma^{\mu\nu}$, but in v^μ. This vector field enters the metric only for $n \geqslant 1$. For $n = 0$, we can interpret v^μ as part of the orthonormal Galilean tetrad field, but not as part of the metric.

Finally, we remark that the n-post-Galilean theories of gravitation can be seen as exact gauge theoretic formulations of the n-post-Newtonian approximations of general relativity. The missing $n\frac{1}{2}$-post-Newtonian approximations can be obtained if we allow the holonomic (but not the anholonomic) components of the metric and consequently also the components of the tetrad field to depend on the square root of $\varnothing$. This is also necessary for the formulation of the n-post-Galilean Dirac equation.

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APPENDIX A: CANONICAL FORM FOR THE n-POST-GALILEAN METRIC

Proof of the theorem in Sec. IV.

Since in the proof we use induction on n we write $(g^{[n]}, h^{[n]})$ for the n-post-Galilean metric. We also write $e^{[n]\mu}{}_i$ and $\theta^{[n]i}{}_\mu$ for the pair of matrices to be constructed in the nth step.

From (4.2b) and (4.3) follows immediately

$$\gamma^{(0)\mu\nu}\psi^{(0)}{}_\nu = 0.$$

Therefore the pair $(\gamma^{(0)}, \psi^{(0)})$, which is equivalent to $(g^{[0]}, h^{[0]})$, is a Galilean metric, for which the pair $(e^{[0]}, \theta^{[0]})$ can be constructed up to Galilean transformations.

Now let $e^{[m]}, \theta^{[m]}$ be constructed, such that $g^{[m]}, h^{[m]}$ take the form (4.5). Clearly $e^{[m]}$ is the $[m]$-part of $e^{[m+1]}$, that is,

$$e^{[m+1]\mu}{}_i = e^{[m]\mu}{}_i + \varnothing^{m+1} e^{(m+1)\mu}{}_i.$$

Hence, we only need to construct $e^{(m+1)}$. Since $e^{[m]}$ is invertible, we may write

$$e^{[m+1]\mu}{}_i = e^{[m]\mu}{}_j(\delta^j{}_i + \varnothing^{m+1} e^{(m+1)j}_{[m]}{}_i),$$

where

$$e^{(m+1)j}_{[m]}{}_i := (e^{[m+1]\mu}{}_i \theta^{[m]j}{}_\mu)^{(m+1)}.$$

From a similar definition of $\theta^{(m+1)i}_{[m]}{}_j$ we find that (4.4c) is equivalent to

$$e^{(m+1)i}_{[m]}{}_j + \theta^{(m+1)i}_{[m]}{}_j = 0. \tag{A1}$$

If we now set

$$g^{(m+1)}_{[m]}{}_{ij} := [g^{[m+1]}{}_{\mu\nu} e^{[m]\nu}{}_i e^{[m]\mu}{}_j]^{(m+1)},$$

and similarly for h, we find

$$g^{[m+1]}{}_{ij} = g^{[m]}{}_{ij} + \varnothing^{m+1}(g^{(m+1)}_{[m]}{}_{ij} + \psi_k e^{(m+1)k}_{[m]}{}_{(i}\psi_{j)}) \tag{A2}$$

and

$$h^{[m+1]ij} = h^{[m]ij} + \varnothing^{m+1}(h^{(m+1)ij}_{[m]} - \theta^{(m+1)(i}_{[m]}{}_k \gamma^{j)k}). \tag{A3}$$

From (4.2b) we now find

$$h^{[m]ik} g^{[m]}{}_{kj} + \varnothing^{m+1}(-\gamma^{ik} g^{(m+1)}_{[m]}{}_{kj} + \psi_j\psi_k h^{(m+1)ki}_{[m]}) = \varnothing\delta^i{}_j. \tag{A4}$$

We must distinguish now between the two cases $m = 0$ and $m > 0$. In both cases Eqs. (A1) to (A4) reduce to consistency conditions for $e^{(m+1)}$ and $\theta^{(m+1)}$, which can be used to produce $e^{[m+1]}$ and $\theta^{[m+1]}$.

APPENDIX B: CLOSENESS OF ψ_μ

We prove here that it is possible to choose the decomposition (4.8) of the n-post-Galilean metric such that $\psi_{[\mu,\nu]} = 0$ holds.

Equations (5.7a) and (5.3) in the coordinate system used are

$$\psi'_\mu = \psi_\mu - \varnothing B_\mu \tag{B1}$$

and

$$v^\mu B_\mu + \tfrac{1}{2}(\gamma^{\mu\nu} - \varnothing v^\mu v^\nu) B_\mu B_\nu = 0. \tag{B2}$$

Since $\psi^{(0)}{}_\mu$ is a closed one-form, we demand

$$\psi'_\mu = \psi^{(0)}{}_\mu - \varnothing K_{,\mu}, \tag{B3}$$

where K is a $\mathbf{R}^{[n]}$-valued function on M. Also setting

$$\psi_\mu = \psi^{(0)}{}_\mu + \varnothing\tilde{\psi}_\mu, \tag{B4}$$

we find from (B1)

$$\varnothing B_\mu = \varnothing(\tilde{\psi}_\mu + K_{,\mu}). \tag{B5}$$

Multiplying (B2) by $\varnothing$ and substituting from (B5) we obtain

$$\varnothing[v^\mu(K_{,\mu} + \tilde{\psi}_\mu) + \tfrac{1}{2}(\gamma^{\mu\nu} - \varnothing v^\mu v^\mu) \times (K_{,\mu} + \tilde{\psi}_\nu)(K_{,\nu} + \tilde{\psi}_\nu)] = 0.$$

This is a partial differential equation of the form of the Hamilton–Jacobi equation, which can be locally solved to give $\varnothing K$. From (B5) we obtain B_μ up to its n-part, which is free. With this B we have $\psi'_{[\mu,\nu]} = 0$.

APPENDIX C: ELIMINATION OF $\chi_{\mu\nu}$

Equations (5.8) in the coordinate system we use are

$$\psi'_{\mu} = \psi_{\mu}, \quad \gamma'^{\mu\nu} = \gamma^{\mu\nu}, \tag{C1}$$

$$v'^{\mu} = v^{\mu} + \gamma^{\mu\nu}B_{\nu}, \quad \gamma'_{\mu\nu} = \gamma_{\mu\nu} - \psi_{(\mu}B_{\nu)}, \tag{C2}$$

and

$$v^{\mu}B_{\mu} + \tfrac{1}{2}\gamma^{\mu\nu}B_{\mu}B_{\nu} = 0, \tag{C3}$$

where we assumed that

$$\varnothing B_{\mu} = 0 \tag{C4}$$

holds also. For the v-special "Galilean" connection (7.9) related to $(v'^{\mu},\gamma'_{\mu\nu})$ we find

$$\overset{v'}{\Gamma}{}^{\rho}{}_{\mu\nu} = \overset{v}{\Gamma}{}^{\rho}{}_{\mu\nu} + \tfrac{1}{2}\gamma^{\rho\sigma}K_{\sigma(\mu}\psi_{\nu)}, \tag{C5}$$

where

$$K_{\mu\nu} := -B_{[\mu,\nu]}. \tag{C6}$$

Since $\chi_{\mu\nu}$ is closed and $\varnothing\chi_{\mu\nu} = 0$ [cf. (7.16)] we can choose B_{μ} such that

$$K_{\mu\nu} + \chi_{\mu\nu} = 0. \tag{C7}$$

Now substituting (C5) in (7.15) we find with (C4)

$$\Gamma^{\rho}{}_{\mu\nu} = \overset{v'}{\Gamma}{}^{\rho}{}_{\mu\nu} + \varnothing v'^{\rho}\gamma'_{\sigma\mu}\overset{v'}{\nabla}{}_{\nu}v'^{\sigma}.$$

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Kantowski–Sachs cosmological models as big-bang models

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In the presence of a nonzero cosmological constant Λ, we classify the anisotropic cosmological models of the Kantowski–Sachs type by means of the quantities ϵ_0^2, q_0, Σ_0 corresponding, respectively, to the relative root-mean-square deviation from isotropy, the deceleration parameter, and the density parameter of the perfect fluid at a given time $t = t_0$. We obtain for $\Lambda > 0$ a set of big-bang models of zero measure as well as a set of cosmological models of nonzero measure evolving toward the de Sitter solution.

I. INTRODUCTION

In a recent article,[1] we have analyzed the anisotropic cosmological models of the Kantowski–Sachs (KS) type[2] in the presence of a nonzero cosmological constant Λ and containing a perfect fluid. These models are an exceptional case in the class of spatially homogeneous cosmologies, in that they contain an isometry group G_3 whose orbits are two dimensional and of constant positive curvature, contrary to the Bianchi classification, whose isometry groups G_3 have a simply transitive action on the three-dimensional spacelike hypersurfaces.

The evolution of the KS models was analyzed by means of a three-dimensional autonomous system. The method transforms the Einstein field equations together with the conservation equation into an autonomous system of differential equations and it is well known in the two-dimensional case, both in theory[3] and in its applications to cosmology.[4,6] It is not so familiar, however, in the three-dimensional case. The study is mainly qualitative, except around the singularity points, where we obtain a quantitative asymptotic behavior for quantities like the average distance $l(t)$, where t is the cosmic time, or the density $\mu(t)$ of the perfect fluid. The main results are, besides two new singularity points, two sets of solutions (one of measure zero, one of positive measure), which become isotropic in an infinite cosmic time.

In this paper we reexpress those results in the formalism of the Stabell–Refsdal[7] classification generalized[8] to three dimensions. We obtain that the two sets of KS solutions tend asymptotically to the de Sitter model (dS) when $\Lambda > 0$. This is an interesting complementary result to the one of Wald[9] (even if it was derived earlier[10]), but obtained by a different method. Let us indicate that our matter stress-energy tensor satisfies Wald's assumptions of dominant and strong energy conditions. The classification is based on physical quantities close to observation, like the deceleration parameter q and the density parameter Σ. The third parameter, ϵ^2, describes the relative root-mean-square deviation from isotropy.

II. THE $(\epsilon_0^2, q_0, \Sigma_0)$ CLASSIFICATION

We take the Kantowski–Sachs metric[2] in the form

$$ds^2 = dt^2 - X^2(t)dr^2 - Y^2(t)(d\theta^2 + \sin^2\theta\, d\varphi^2) \quad (2.1)$$

in coordinates (t,r,θ,ϕ), where r is a radial coordinate and θ, ϕ the usual spherical coordinates. Here $X(t)$ and $Y(t)$ are two unknown functions of t. The Einstein field equations[1] become functions of X, Y and their first and second derivatives with respect to t, which are related to the density of matter μ and the pressure p.

Using the geometric quantities[11] $\theta = \dot{X}X^{-1} + 2\dot{Y}Y^{-1}$, the volume expansion, and $\sigma = 3^{-1/2}(\dot{X}X^{-1} - \dot{Y}Y^{-1})$, the shear, we can express the field equations as follows:

$$\dot{\theta} + \tfrac{1}{3}\theta^2 + 2\sigma^2 + \tfrac{1}{2}(\mu + 3p) - \Lambda = 0, \quad (2.2)$$

$$\dot{\sigma} + \sigma\theta - 1/\sqrt{3}Y^2 = 0, \quad (2.3)$$

$$\theta^2/3 - \sigma^2 + 1/Y^2 - \Lambda = \mu. \quad (2.4)$$

Equation (2.2) is the well-known Raychaudhuri equation for the case of a perfect fluid and a nonzero cosmological constant. Together with Eq. (2.4), it transforms to

$$\dot{\theta} + \tfrac{1}{3}\theta^2 + 2\sigma^2 + ((3\gamma - 2)/2)\mu - \Lambda = 0 \quad (2.5)$$

and

$${}^3R = 2(\mu + \Lambda + \sigma^2 - \theta^2/3), \quad (2.6)$$

where we use the barotropic equation of state $p = (\gamma - 1)\mu$ and the Ricci scalar ${}^3R = 2Y^{-2}$. The values of the constant γ lie in the range $1 \leqslant \gamma \leqslant 2$.

In terms of the average distance $l = l(t)$ $(= XY^2$ in the case of the KS models), the Hubble parameter H may be generalized to anisotropic cosmological models:

$$H = \theta/3 = \dot{l}/l.$$

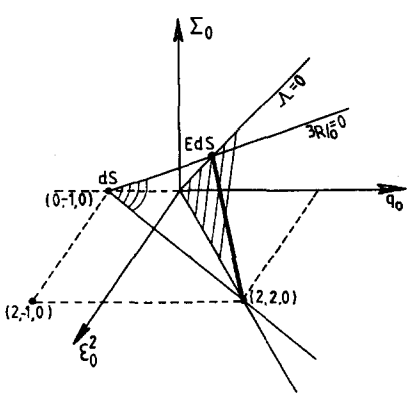

FIG. 1. The planes $\Lambda = 0$ and ${}^3R|_0 = 0$, and their intersection for $\gamma = 1$ in the $(\epsilon_0^2, q_0, \Sigma_0)$ coordinates; dS and EdS denote, respectively, the de Sitter and Einstein–de Sitter models.

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TABLE I. We have indicated the different singularity points at finite distance as well as the asymptotic behavior of the average length scale l, the fluid density μ, and the fluid expansion θ. These variables are expressed as functions of the cosmic time t.

$p=(\gamma-1)\mu$ Λ	(x,β',z)	l	μ	θ
$1<\gamma<2$ $\Lambda>0$ $\Lambda<0$	(0,2,0) (0, − 2,0) (1,0,0)	$(\pm t)^{1/3}$ $(\pm t)^{1/3}$ $(+t)^{2/3\gamma}$	$(\pm t)^{-\gamma}$ $(\pm t)^{-\gamma}$ $(\pm t)^{-2}$	t^{-1} t^{-1} t^{-1}
$\gamma=2$ $\Lambda>0$ $\Lambda<0$	$(x=1-\beta'^2/4,$ $-2<\beta'<2,$ $z=0)$	$(\pm t)^{1/3}$	$(\pm t)^{-2}$	t^{-1}
$1<\gamma<2$ $\Lambda>0$	(0,0,3/Λ) (0, − 2,9/Λ)	$e^{\pm(\Lambda/3)^{1/2}t}$ $e^{\pm(\Lambda/3)^{1/2}t}$	$e^{\pm(3\Lambda)^{1/2}\gamma t}$ $e^{\pm(\Lambda)^{1/2}\gamma t}$	$\mp\sqrt{3\Lambda}$ $\mp\sqrt{\Lambda}$

The deceleration parameter q becomes

$$q=-\ddot{l}l/\dot{l}^2=-(\dot{\theta}+\tfrac{1}{3}\theta^2)/3H^2.$$

We define the density parameter Σ by

$$\Sigma=\mu/6H^2.$$

The shear σ will be replaced by the relative root-mean-square deviation from isotropy,[8] defined as

$$\epsilon^2=\tfrac{1}{3}\sum_{\nu=1}^{3}\epsilon_\nu^2$$

and related to σ by $\epsilon^2=\tfrac{2}{3}\sigma^2/H^2$.

In terms of these parameters, Eqs. (2.5) and (2.6) become

$$\Lambda=3H^2[(3\gamma-2)\Sigma+\epsilon^2-q]$$
$$=3H_0^2[(3\gamma-2)\Sigma_0+\epsilon_0^2-q_0] \tag{2.7}$$

and

$${}^3R\,|_0=6H_0^2\left[3\gamma\Sigma_0+\tfrac{3}{2}\epsilon_0^2-q_0-1\right], \tag{2.8}$$

where the index 0 indicates the value of the parameter at a time $t=t_0$, which can be our present time.

Equations (2.7) and (2.8) generalize the (Σ_0,q_0) equations of Stabell–Refsdal to the case of anisotropic but spatially homogeneous cosmological models.

When we put $\Lambda=0$ in (2.7) and ${}^3R\,|_0=0$ in (2.8) we obtain in the two cases a plane instead of a straight line. When $\gamma=1$ the equations of the two planes (see Fig. 1) read

$$\Sigma_0+\epsilon_0^2-q_0=0,\quad \text{for } \Lambda=0$$

and

$$3\Sigma_0+\tfrac{3}{2}\epsilon_0^2-q_0-1=0,\quad \text{for } {}^3R\,|_0=0.$$

Analyzing the evolution of the KS models by means of a three-dimensional autonomous system, we obtained[1] the following singularity points at finite distance in the coordinates (x,β',z), where x is the dynamical importance of the fluid, i.e., $x=3\mu/\theta^2$, β' the dynamical importance of the shear, i.e., $\beta'=-2\sqrt{3}\sigma/\theta$, and z is defined as $z=3x/\mu$. For $1<\gamma<2$, $\Lambda>0$, we have the set $\{(1,0,0),(0,2,0),(0,-2,0),(0,0,3/\Lambda),(0,-2,9/\Lambda)\}$; for $1<\gamma<2$, $\Lambda<0$, we have only $\{(1,0,0),(0,2,0),(0,-2,0)\}$; for $\gamma=2$ we have, both for $\Lambda>0$ and $\Lambda<0$, a continuous line of singularity points ($z=0$, $4-4x-\beta'^2=0$) as well as the points $\{(0,0,3/\Lambda),(0,-2,9/\Lambda)\}$ when $\Lambda>0$.

Using the parameters ϵ_0^2, q_0, Σ_0 and the quantitative asymptotic behavior around the singularity points (see Table I), we get the following points in the $(\epsilon_0^2,q_0,\Sigma_0)$ classification (see Table II): $\{(2,2,0),(0,(3\gamma-2)/2,\tfrac{1}{2}),(0,-1,0),(2,-1,0)\}$ when $1<\gamma<2$ and $\{(0,2,\tfrac{1}{2}),(0,-1,0),(2,-1,0)\}$ when $\gamma=2$.

The global picture of the integral curves of the three-dimensional system[1] contains a double infinity of cosmological models for $\Lambda<0$ starting at $(\epsilon_0^2=2,q_0=2,\Sigma_0=0)$ and coming back to that point. There is a simple infinity of models starting at the point $(\epsilon_0^2=0,q_0=(3\gamma-2)/2,\Sigma_0=\tfrac{1}{2})$, which corresponds to the Einstein–de Sitter (EdS) model, and tending to $(\epsilon_0^2=2,q_0=2,\Sigma_0=0)$ in a finite cosmological time. When $\Lambda>0$ there is a simple infinity of models

TABLE II. The singularity points, presented in the (x,β',z) coordinates of the three-dimensional autonomous system and in the $(\epsilon_0^2,q_0,\Sigma_0)$ coordinates of the generalized Stabell–Refsdal classification.

	(x,β',z)	$(\epsilon_0^2,q_0,\Sigma_0)$
$1<\gamma<2$	(0,2,0) (0, − 2,0)	(2,2,0)
	(1,0,0)	$(0,(3\gamma-2)/2,\tfrac{1}{2})$
	(0,0,3/Λ)	(0, − 1,0)
	(0, − 2,9/Λ)	(2, − 1,0)
$\gamma=2$	$(1-\beta'^2/4,-2<\beta'<2,0)$	$(0,2,\tfrac{1}{2})$
	(0,0,3/Λ)	(0, − 1,0)
	(0, − 2,9/Λ)	(2, − 1,0)

starting at EdS and tending to $(\epsilon_0^2 = 0, q_0 = -1, \Sigma_0 = 0)$, which represents the de Sitter (dS) model, in an infinite cosmological time. These are nonempty big-bang models. Notice that these models become anisotropic during the evolution and isotropize finally in an infinite cosmic time. Finally, there is a double infinity of KS models starting at $(\epsilon_0^2 = 2, q_0 = 2, \Sigma_0 = 0)$ and tending to the point dS. These models have an important anisotropy at the beginning of their evolution where the matter is negligible; in the end both the anisotropy and the density parameter are zero although matter is not negligible between these two points.

For $\gamma = 2$ and $\Lambda \leqslant 0$, all the KS models start at EdS and come back to it; when $\Lambda > 0$ there are, in addition, cosmological KS models evolving from EdS to dS.

For empty KS models $(\Sigma_0 = 0)$ we may restrict the discussion to the plane (ϵ_0^2, q_0). There are KS models starting at $(\epsilon_0^2 = 2, q_0 = 2, \Sigma_0 = 0)$ and coming back to it for $\Lambda < 0$ and $\Lambda > 0$. Some start at (2,2,0) and tend to dS. There is only one model starting at $(\epsilon_0^2 = 2, q_0 = -1, \Sigma_0 = 0)$ and tending to dS, and only one from $(\epsilon_0^2 = 2, q_0 = 2, \Sigma_0 = 0)$ to $(\epsilon_0^2 = 2, q_0 = -1, \Sigma_0 = 0)$.

III. CONCLUSION

We have classified Kantowski–Sachs models with a cosmological constant and containing a perfect fluid, in terms of the parameters ϵ_0^2, q_0, Σ_0. From the interpretation of the cosmological models found by the method of three-dimensional autonomous system in these parameters, we have obtained, in particular, a class of big-bang models for the KS line element, which evolve toward the de Sitter model in an infinite cosmological time. Clearly anisotropic cosmological models, i.e., the Bianchi models, can be analyzed by the same method. This will be reported on elsewhere.[12]

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Weak rigidity in almost-thermodynamic material schemes

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To avoid the restrictions that the Born rigidity supposes for the motions in relativity, the definition of a weakly rigid almost-thermodynamic material scheme is proposed. From it the relativistic incompressibility condition given by Ferrando and Olivert is obtained. Moreover, it is proved that, for the weakly rigid irrotational and geodesic almost-thermodynamic material schemes, the scalar curvature of the Landau manifolds is constant along the streamlines.

I. INTRODUCTION

In a previous paper,[1] we proposed a definition of rigidity for the almost-thermodynamic material schemes that fulfilled the incompressibility condition given by Ferrando and Olivert.[2] There, we joined to the Born condition the vanishing of the spatial change of the relativistic stress tensor of the scheme and we obtained, for the hypoelastic Carter–Quintana almost-thermodynamic material schemes and for the hypoelastic Maugin ones, the inexistence of principal shock waves associated with Hadamard's discontinuities of the four-velocity of the scheme.

Since the Born-rigidity condition supposes a strong restriction to the motions described in general relativity, as Pirani shows in Ref. 3, we propose in this work a less restricted definition of rigid almost-thermodynamic material schemes. This definition also fulfills the relativistic incompressibility condition. Moreover, some specifications on the congruence of scheme world lines will lead to the primitive definition.

In Sec. II we propose (Definition 2.1) the definition of a weakly rigid almost-thermodynamic material scheme. In Proposition 2.2 we prove that such schemes verify the incompressibility condition of Ferrando and Olivert. We close this section with an equivalence theorem (Theorem 2.3) that expresses, in the absence of the expansion velocity scalar, the weak rigidity condition by means of the vanishing of the Ricci tensor Fermi derivative with respect to the four-velocity of the scheme.

This equivalence is used in Sec. III in a very particular kind of weakly rigid congruences. We work there in geodesic irrotational almost-thermodynamic material schemes (Definition 3.1). The use of Gaussian normal coordinates associated to the Landau manifolds and to the streamlines of one of these schemes allows us to prove (Theorem 3.2) that in such a scheme, weak rigidity leads to the constant character of the Landau manifolds scalar curvature along the streamlines. We relate this fact to the Gauss egregium theorem.

Let us explain now some questions of general type.

We will consider the space-time as a set of three components (M,g,∇), where M stands for a connected four-dimensional pseudo-Riemannian manifold of Hausdorff type,[4] g will be a hyperbolic metric tensor field [of signature (3,1)], and ∇ is the unique linear connection that M possesses, compatible with g and without torsion.

Everywhere throughout this paper we will work in an almost-thermodynamic metal scheme D in the space-time manifold M; D is a domain of the space-time in which a second-order energy momentum tensor T is defined which is normal with four-velocity u and associated eigenvalue $-\rho$ ($\rho > 0$). We will also admit the Taub decomposition,[5]

$$\rho = r(1+\epsilon), \tag{1.1}$$

ρ being the proper mass-energy density of the scheme, r its matter density, and ϵ its specific internal energy.

The spatial projector tensor is given by

$$\gamma = g + u \otimes u; \tag{1.2}$$

thus, the energy-momentum tensor has the form

$$T = \rho(u \otimes u) + t, \tag{1.3}$$

where t is the relativistic stress tensor, spatial projection of T by means of the projector γ.

In every case, Latin labels symbolize values of indices from 1 to 4 and Greek labels are used for indices from 1 to 3.

We will introduce now the strain rate tensor d and the rotation tensor Ω of the scheme. They are defined, respectively, by means of the tensor symmetrization and skew symmetrization of

$$e_{ij} = \gamma^k{}_i \gamma^l{}_j \nabla_k u_l. \tag{1.4}$$

(Note that the strain rate tensor is given by

$$d = \tfrac{1}{2} L_u \gamma, \tag{1.5}$$

where L_u symbolizes the Lie derivative with respect to the four-velocity u of the tensor that follows it.)

The tangent space of $p \in M$ will be represented by $T_p M$. By the spatial tensor field in D we will mean the one which, in every point, is orthogonal to the four-velocity u of D. To conclude this section let us say that measure units have been chosen in such way that the light speed in the vacuum has the constant value 1.

II. WEAK RIGIDITY

As we indicate above, we have been interested in the study of the rigid motions in almost-thermodynamic material schemes with the purpose of obtaining a definition from which we could derive the relativistic incompressibility condition[2] and the absence of perturbations. The Born rigidity, given in general relativity by the vanishing of the strain rate tensor d of the scheme, was enough for these purposes in elastic Synge almost-thermodynamic material schemes[1] but not for the elastic Carter–Quintana ones[6] nor for the elastic Maugin ones.[7] To pass over these insufficiencies, in Ref. 1 we

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added to the Born condition the vanishing of the spatial change of the relativistic stress tensor.

However, we know the critiques that in the relativistic literature[8] are outlined about the restrictions that suppose, for the motions of a scheme, the Born condition. Thus, in Ref. 3, is obtained, from this condition and after some dynamical considerations, the constant character of the angular velocity along the streamlines; this scalar being defined by

$$w^2 = \tfrac{1}{2}\Omega_{ij}\Omega^{ij}. \tag{2.1}$$

Let us remember that, according to Ref. 1, a rigid almost-thermodynamic material scheme D in the space-time manifold M verifies the following conditions:

$$\text{(i)}\quad d = 0, \tag{2.2}$$

$$\text{(ii)}\quad F_u t = 0. \tag{2.3}$$

In the expression of Eq. (2.3) the formalism of the Fermi derivative with respect to the four-velocity of the scheme,[4,9] besides the spatial character of the relativistic stress tensor t, have been used.

We now suggest the following definition as a less strong rigidity condition than the one proposed in Ref. 1.

Definition 2.1: An almost-thermodynamic material scheme D in the space-time manifold M will be called weakly rigid if the next conditions fulfill in it

$$\text{(i)}\quad F_u t = 0, \tag{2.4}$$

$$\text{(ii)}\quad \nabla_u r = 0, \tag{2.5}$$

$$\text{(iii)}\quad \nabla_u \epsilon = 0. \tag{2.6}$$

As a first consequence of Definition 3.1 we derive a result already obtained in Ref. 1.

Proposition 2.2: Every weakly rigid almost-thermodynamic material scheme is incompressible.

Proof: Let us consider the dynamic volume tensor[2] defined by

$$K = f/r, \tag{2.7}$$

f being the tensor index of the scheme, given by

$$f = (1+\epsilon)\gamma + t/r. \tag{2.8}$$

Remember that the incompressibility condition of Ferrando and Olivert, written in the Fermi derivative formalism, gives

$$F_u K = 0. \tag{2.9}$$

Thus, our purpose is to verify Eq. (2.9). Taking into account that

$$\begin{aligned} F_u K &= F_u(f/r) = F_u(1/r)f + (1/r)F_u f \\ &= F_u(1/r)f + 1/r[(F_u\epsilon)\gamma + (1+\epsilon)F_u\gamma \\ &\quad + F_u(1/r)t + (1/r)F_u t\,], \end{aligned}$$

which follows from the Fermi derivative properties, the result claimed is obtained after simple application of Definition 3.1.

This section concludes with a result which will be used below and that may be considered as an equivalent definition of weakly rigid; it follows from the consideration in our material scheme, weakly rigid, of the Einstein equations.

Theorem 2.3: A necessary and sufficient condition for an almost-thermodynamic material scheme D to be weakly rigid is the fulfillment of the following relations:

$$\text{(i)}\quad F_u\ \mathrm{Ric} = 0, \tag{2.10}$$

$$\text{(ii)}\quad \nabla\cdot u = 0. \tag{2.11}$$

Proof: Here, Ric symbolizes the Ricci tensor of the space-time defined in the scheme D. Equation (2.11) expresses the vanishing of the expansion velocity scalar of the scheme,[3,6] given by

$$\theta = d_i{}^i = \nabla_i u^i. \tag{2.12}$$

We first consider the weak rigidity hypothesis. After using the Taub decomposition it is possible to assert, from Eqs. (2.5) and (2.6),

$$F_u\rho = 0 \tag{2.13}$$

and, by virtue of the form of the scheme energy-momentum tensor [Eq. (1.3)], we obtain

$$F_u T = 0 \tag{2.14}$$

from the Fermi derivative properties and weak rigidity hypothesis.

Now we use Einstein's equations

$$\mathrm{Ric} - \tfrac{1}{2}Rg = ET, \tag{2.15}$$

where E is the Einstein constant and R stands for the scalar Riemannian curvature

$$R = (\mathrm{Ric})_i{}^i. \tag{2.16}$$

Taking into account the Fermi derivative properties and Eq. (2.15), we derive

$$F_u R = 0, \tag{2.17}$$

after applying Fermi derivatives with respect to u in Eq. (2.16) and contracting with the metric tensor field g.

From Eqs. (2.17) and (2.15), we deduce

$$F_u\ \mathrm{Ric} = 0. \tag{2.18}$$

Besides, from the continuity equation

$$\nabla\cdot(ru) = 0, \tag{2.19}$$

we obtain the vanishing of the expansion after considering Eq. (2.5).

To prove the converse we start from Eqs. (2.10) and (2.11); the continuity equation (2.19) leads us to Eq. (2.5).

Moreover, by contracting Eq. (2.10) with g, we derive Eq. (2.17); consequently, from Einstein's equations we obtain Eq. (2.14).

Since the scheme is normal with four-velocity u and associated eigenvalue $-\rho$,

$$T(u) = -\rho u, \tag{2.20}$$

thus,

$$F_u T(u) + T(F_u u) = -(F_u\rho)u - \rho(F_u u) \tag{2.21}$$

and so

$$\nabla_u\rho = F_u\rho = 0, \tag{2.22}$$

which implies, by virtue of Taub's decomposition, the fulfillment of Eq. (2.6).

If we now develop Eq. (2.14), making use of the decomposition (1.3), we arrive, after consideration of the Fermi derivative properties, at Eq. (3.4) which completes the con-

cept of a weakly rigid almost-thermodynamic material scheme.

After this result, the weak rigidity can be expressed by means of purely geometric quantities: the Ricci tensor associated to a congruence of world lines in the absence of expansion. In the next section, this version will be used.

III. GEODESIC IRROTATIONAL WEAKLY RIGID ALMOST-THERMODYNAMIC MATERIAL SCHEMES

In the present section we will consider a very special kind of almost-thermodynamic material schemes that, under the weak rigidity hypothesis proposed in Sec. II, will verify a geometrical condition on the scalar curvature of the hypersurfaces orthogonal to their four-velocity. At the end of this section we intend to give a signification to this condition.

Everywhere throughout this section we will work in almost-thermodynamic material schemes which fulfill the following definition.

Definition 3.1: An almost-thermodynamic material scheme D will be called irrotational and geodesic if the following conditions are verified.

(i) The scheme D has irrotational motion,[10] i.e., for every $x \in D$,

$$\Omega_x = 0. \tag{3.1}$$

(ii) The congruence of streamlines of the scheme is geodesic, so

$$\nabla_u u = 0, \text{ in } D. \tag{3.2}$$

Let us remember that under the irrotationality hypothesis on an almost-thermodynamic material scheme D, every Landau manifold L_p associated to an arbitrary point $p \in D$ (see Ref. 11) is orthogonal to the four-velocity u of the scheme at every point.

Previous to proving the result we claimed, let us consider a point $q \in D$ and a system of Gaussian normal coordinates[10,12] in a neighborhood of q, associated to the Landau manifolds of the scheme and to the geodesic congruence of the steamlines of it.

In this particular coordinate system, we get

$$u^\alpha = 0, \quad u^4 = 1. \tag{3.3}$$

Moreover, by virtue of the orthogonality of the Landau manifolds to the four-velocity u,

$$g_{4\alpha} = 0, \quad g_{44} = -1. \tag{3.4}$$

So, noting by

$$\bar{g}_p = i_p^* g \tag{3.5}$$

the induced metric of L_p, $p \in D$, by the natural immersion[11]

$$i_p : L_p \to D,$$

we can also assure[12] the relations

$$g_{\alpha\beta}/L_p = \bar{g}_{p^{\alpha\beta}}. \tag{3.6}$$

Besides, the Christoffel symbols of the second kind associated to the Riemann connection ∇ calculated in the chosen coordinate system, have the values

$$\Gamma_{44}^4 = \Gamma_{4\alpha}^4 = \Gamma_{44}^\alpha = 0, \tag{3.7}$$

$$\Gamma_{4\beta}^\alpha = g^{\alpha\gamma}\Gamma_{\gamma\beta}^4. \tag{3.8}$$

Here,

$$\Gamma_{\alpha\beta}^4/L_p = -H_{p^{\alpha\beta}} \tag{3.9}$$

are the components of the extrinsic curvature or the hypersurface L_p (see Refs. 12 and 13). Also take into account that, in the chosen coordinate system,

$$H_{p^{\alpha\beta}} = -\bar{d}_{p^{\alpha\beta}} = \bar{d}_{\alpha\beta}/L_p, \tag{3.10}$$

$d_{\alpha\beta}$ being the spatial components (components nonzero in our coordinate system) of the strain rate tensor of D, according to its definition given in the Introduction.[12]

Now we state the following theorem.

Theorem 3.2: In every geodesic irrotational weakly rigid almost-thermodynamic material scheme D, the scalar Riemannian curvature $\bar{R}_p$ of the L_p hypersurfaces (Landau manifolds), $p \in D$, is constant along the steamlines of D.

Proof: We work in a Gaussian normal coordinate system as it is shown above and, to simplify the notation, we will omit the p subindices everywhere; it must be clear that, in each point of the considered neighborhood, the barred expressions will be the ones induced from those corresponding to D on the (unique) Landau manifold that contains it. According to Definition 2.1, and by virtue of the equivalence theorem (Theorem 2.3), every weakly rigid almost-thermodynamic material scheme verifies the relations

$$F_u \text{ Ric} = 0, \tag{3.11}$$

$$\nabla \cdot u = 0. \tag{3.12}$$

Note that, in the general case,

$$F_u R_{ij} = \nabla_u R_{ij} - R_{kj}(u_i \nabla_u u^k - u^k \nabla_u u_i) - R_{ik}(u_j \nabla_u u^k - u^k \nabla_u u_j),$$

taking into account the congruence geodesic character

$$F_u R_{ij} = \nabla_u R_{ij}. \tag{3.13}$$

In particular, after using Eq. (3.7), we get

$$F_u R_{44} = \nabla_u R_{44} = \partial_4 R_{44} - 2\Gamma_{44}^\alpha R_{\alpha 4} = \partial_4 R_{44}. \tag{3.14}$$

Besides, we can use the following coordinate expression[10,12]:

$$R_{44} = -\partial_4 \Gamma_{\alpha 4}^\alpha - \Gamma_{4\beta}^\alpha \Gamma_{\alpha 4}^\beta. \tag{3.15}$$

From Eqs. (3.9)–(3.11), (3.14), and (3.15), we obtain

$$\partial_4[\partial_4(d_\alpha{}^\alpha) + d_{\alpha\beta} d^{\alpha\beta}] = 0. \tag{3.16}$$

As from Eq. (3.12) we deduce

$$d_\alpha{}^\alpha = 0, \tag{3.17}$$

Eq. (3.16) gives

$$\partial_4(d_{\alpha\beta} d^{\alpha\beta}) = 0. \tag{3.18}$$

Take into account the Gauss relation[12,13]

$$2G_4^4 = -\bar{R} - d_{\alpha\beta} d^{\alpha\beta} + (d_\alpha{}^\alpha)^2, \tag{3.19}$$

where G_{ij} is the Einstein tensor

$$G_{ij} = R_{ij} - \tfrac{1}{2} R g_{ij} = E T_{ij}. \tag{3.20}$$

By virtue of Eq. (2.14) and working in our Gaussian normal coordinate system, we obtain, as in the Ricci case,

$$F_u G_4^4 = \partial_4 G_4^4 = 0, \tag{3.21}$$

which applied to Eq. (3.19) gives us the result expected if previous use of Eqs. (3.17) and (3.18) has been made.

The theorem just proved suggests to us the result of the egregium theorem of Gauss in the sense that the Gauss curvature of a surface is invariant with respect to the flexions[14]; these are understood as some kind of deformations in the surface which maintain the distance of points in it. Thus, the Gauss theorem considers, in a certain way, a classical rigidity for surfaces.

In the theorem just presented, the scalar curvature of the L_p seems to replace the Gauss curvature and some weakly rigid motions (not all of them) would take the role of the flexions.

It should be noted that the absence of expansions or contractions is already implicit in Eq. (3.12) but we need to add irrotationality conditions and assume the congruence of steamlines to be geodesic, so restricting the weakly rigid motions considered, in order to prove Theorem 3.2 after also taking into account Eq. (3.11).

These restrictions make of Theorem 3.2 a generalization of the well-known result for rigid congruences in the Minkowski space, i.e., for congruences of straight parallel world lines. Here, the Landau manifolds would be replaced by hyperplanes orthogonal to the straight lines of the conguence and, obviously, have zero scalar curvature in every point; thus, Eq. (3.11) is evidently verified.

IV. DISCUSSION

We have proposed in this paper a definition of weakly rigid almost-thermodynamic material schemes (Sec. II) which leads us in a straightforward manner to the relativistic incompressibility condition of Ferrando and Olivert. This definition does not present the restrictions on the strain rate tensor that the one given in Ref. 1 does. Besides, for the geodesic irrotational weakly rigid almost-thermodynamic material schemes (Sec. III), the scalar Riemannian curvature of the Landau manifolds is constant along the steamlines. With respect to this point, note that the equivalence theorem 2.3 and the vanishing of the Fermi derivative of the metric tensor field g allows us to obtain this result for the scalar curvature R of the scheme without additional hypothesis. So, the irrotationality of D and the geodesic character of the congruence modify the outcome in the explained way.

We now indicate some particular cases in which the imposition of additional restrictions to a weakly rigid almost-thermodynamic material scheme D leads us to a rigid scheme in the way proposed in Ref. 1.

Assume first that the four-velocity u of D moves parallel to the Landau manifolds, i.e., for every $v \in T_pL_p$, $p \in D$,

$$\nabla_v u = 0, \tag{4.1}$$

and suppose that the motion is irrotational. The assertion made above follows from a result of Ref. 1. A trivial example of such a situation would be a congruence of parallel straight lines in the Minkowski space as the one quoted in Sec. III.

The physical meaning of Eq. (4.1) could be the vanishing of the relative velocities of the points of L_p with respect to p if we use a similar definition to the one established in Ref. 15.

A case in which a weaky rigid almost-thermodynamic material scheme D becomes rigid in the sense given in Ref. 1 would be found if D were irrotational and its four-velocity a Killing vector field.[1]

A deeper analysis of Definition 2.1 of weak rigidity may be the subject of later work. In it, the method of Hadamard's discontinuities for the study of the velocities of the shock waves associated to the infinitesimal discontinuities of the four-velocity u would be used. Furthermore, the application of techniques of parametrized post-Newtonian approximation in general relativity is being considered.

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Static gravitational field in generalized scalar tensor theory

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A useful relation between the metric component g_{00} and the scalar field ϕ is obtained for a static gravitational field in Nordtvedt's general scalar tensor theory where the parameter ω is a variable. A simple method for generating the solutions of Nordtvedt's field equations from the corresponding Einstein's vacuum solutions is obtained. Static axially symmetric field equations are solved in prolate and oblate spheroidal coordinates. Simple cylindrically symmetric solutions are also given.

I. INTRODUCTION

Nordtvedt[1] proposed a modification of the Brans–Dicke[2] theory to the effect that in the former the parameter ω is no longer a constant quantity. It is rather a variable being a function of the scalar field. A fairly large number of static and nonstatic solutions are obtained in the modified theory (Banerjee and Duttachoudhury,[3] Banerjee and Santos,[4,5] Barkar,[6] Rao *et al.*,[7] and Van den Bergh[8,9]). Banerjee *et al.*[10] have recently discussed a static spherically symmetric field in this general scalar tensor theory for charged and uncharged sources, where all possible exact solutions for coupled Einstein–Maxwell–Nordtvedt fields are obtained and their properties analyzed. The present paper refers to a static axially symmetric metric in Nordtvedt's theory. Field equations are written in Dicke's conformally transformed units.[11] Though less appealing compared to the original Brans–Dicke[2] version, the revised units are advantageous in many respects. The field equations now look simpler and for axial symmetry one can use Weyl's canonical coordinates in view of the fact that $R^3_3 + R^0_0 = 0$ in new units, while in the original Brans–Dicke version it is not possible.

In Sec. II a relation between g_{00} and the scalar field is deduced under certain physical conditions. This relation is useful for providing a technique to generate exact solutions in Nordtvedt's scalar tensor theory provided the corresponding Einstein's vacuum solutions are known. The procedure is described in Sec. III. In Sec. IV explicit monopole and dipole solutions are given using prolate and oblate spheroidal coordinates as was done by Misra,[12] Zipoy,[13] and others for Einstein's field. The only assumption made in order to obtain such solutions is that the scalar field ϕ is a function of only one of several variables such as u in spheroidal coordinates. It implies that ϕ remains constant over any ellipsoidal surface. These particular solutions can be verified to be asymptotically flat and their behavior is like that of Schwarzchild's solution of a large distance. Last, in Sec. V simple cylindrically symmetric solutions are given as special cases.

The solutions are dependent on the functional form of $\omega(\phi)$ only when they are expressed in the original atomic units.

II. STATIC FIELD EQUATIONS AND g_{00}–ϕ RELATION IN NORDTVEDT'S THEORY

The field equations in the metric formulation of Nordtvedt's general scalar tensor theory can be written as

$$\bar{G}_{\mu\nu} \equiv \bar{R}_{\mu\nu} - \tfrac{1}{2}\bar{R}\bar{g}_{\mu\nu} = -\frac{8\pi}{\phi}\bar{T}_{\mu\nu} - \frac{\omega}{\phi^2}\left(\phi_\mu\phi_\nu - \frac{1}{2}\bar{g}_{\mu\nu}\phi_\alpha\phi^\alpha\right) - (1/\phi)(\phi_{\mu;\nu} - \bar{g}_{\mu\nu}\Box\phi), \tag{2.1}$$

$$\Box\phi \equiv \phi^{\ \mu}_{;\mu} = -\frac{\phi_\alpha\phi^\alpha}{(2\omega+3)}\frac{d\omega}{d\phi}, \tag{2.2}$$

where $\bar{T}_{\mu\nu}$'s are the components of the energy-momentum tensor. The subscript in ϕ_μ, etc. corresponds to the ordinary derivative and a semicolon corresponds to the covariant derivative. The bars indicate that the variables are in the units where G varies and particle masses remain fixed (Brans and Dicke[2]). The line element for a static space-time is given by

$$ds^2 = \bar{g}_{00}\,dt^2 + \bar{g}_{ik}\,dx^i\,dx^k, \tag{2.3}$$

where i, j, run from 1 to 3 and g_{00}, g_{ik} are functions of the space coordinates.

From the field equations one can obtain a relation like

$$\phi\bar{R}^0_0 = -(\omega/\phi)\phi^{\ 0}\phi_0 - \phi^{\ 0}_{;0} - \tfrac{1}{2}\Box\phi. \tag{2.4}$$

Again for a static metric (2.3) we have

$$\bar{R}^0_0 = (1/2\sqrt{-\bar{g}})(\bar{g}^{00}\bar{g}^{ij}\sqrt{-\bar{g}}\bar{g}_{00,j})_{,i}. \tag{2.5}$$

Here the time derivative of ϕ, that is, ϕ_0, is zero and $\phi^{\ 0}_{;0} = \frac{1}{2}\bar{g}^{00}\bar{g}_{00,i}\phi^{\ i}$. Using these and Eqs. (2.2) and (2.5) in (2.4), one obtains

$$(\bar{g}^{ij}\sqrt{-\bar{g}})_{,i}\bar{g}^{00}\bar{g}_{00,j}\phi + \bar{g}^{ij}\sqrt{-\bar{g}}(\bar{g}^{00}\bar{g}_{00,j}\phi)_{,i} = \frac{1}{2}\bar{g}^{ij}\sqrt{-\bar{g}}\,\frac{(d/d\phi)(2\omega+3)}{(2\omega+3)}\phi_i\phi_j. \tag{2.6}$$

Now,

$$\Box\phi \equiv \phi^{\ \mu}_{;\mu} = (1/\sqrt{-\bar{g}})(\sqrt{-\bar{g}}\bar{g}^{ij}\phi_j)_{,i} = (1/\sqrt{-\bar{g}})[(\sqrt{-\bar{g}}\bar{g}^{ij})_{,i}\phi_j + \sqrt{-\bar{g}}\bar{g}^{ij}\phi_{ij}]. \tag{2.7a}$$

So, from (2.2)

$$(\bar{g}^{ij}\sqrt{-g})_{,i}\phi_j = \bar{g}^{ij}\sqrt{-\bar{g}}\phi_{ij} - \frac{\frac{1}{2}(d/d\phi)(2\omega+3)}{(2\omega+3)} \times\sqrt{-\bar{g}}\bar{g}^{ij}\phi_i\phi_j. \tag{2.7b}$$

With (2.7) and the fact that $[d(2\omega+3)/d\phi]\phi_i$ can be written as $(2\omega+3)_{,i}$, Eq. (2.6) results in

$$\bar{g}^{ij}(X-Y)_{,i}\phi_j = 0, \tag{2.8}$$

where

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$$X = \ln[(\bar{g}^{00}\bar{g}_{00,j}\phi)/\phi_j + 1], \tag{2.9a}$$

$$Y = \ln[(2\omega + 3)^{1/2}]. \tag{2.9b}$$

For a nonvanishing scalar field $\phi_j \neq 0$, Eq. (2.8) implies that either $(X - Y)_{,i}$ is zero or the two vectors $(X - Y)_{,i}$ and ϕ_j are mutually orthogonal. However, for a bounded distribution of matter as a source, the gradients of both $(X - Y)$ and ϕ would tend to be orthogonal to $r = \text{const}$ hypersurface in the asymptotic region and thus would be parallel to each other in that region (Raychaudhuri and Bandyopadhyay[14]). So, in order that relation (2.8) is valid everywhere in space we must have $(X - Y)_{,i} = 0$. Or, in other words, $X = Y + \ln A$, where A is a constant of integration. With X and Y given by (2.9), we have

$$\bar{g}^{00}\bar{g}_{00,j}\phi + \phi_j = A(2\omega + 3)^{1/2}\phi_j. \tag{2.10}$$

The same relation can also be derived for any arbitrary source when $\bar{g}_{00}$ and ϕ are functionally related (see Banerjee and Duttachoudhury[3]) and $\bar{g}^{ij}\phi_j \neq 0$.

In Dicke's conformally transformed units, where $g_{ij} = \phi\bar{g}_{ij}$ (variables without a bar indicate that they are in the transformed version), particle masses vary and G remains constant (Dicke[11]). In this version, the field equations assume the much simpler form (Raychaudhuri[15])

$$R_{ij} = [(2\omega + 3)/2]\psi_i\psi_j, \tag{2.11}$$

where ψ is equal to $\ln\phi$ and plays the role of the scalar field in the revised version. On the other hand, expressing the scalar field and the metric in the transformed units, one can write Eq. (2.10) as

$$e^{\psi}g^{00}(e^{-\psi}g_{00,j} - e^{-\psi}g_{00}\psi_j) + \psi_j = A(2\omega + 3)^{1/2}\psi_j. \tag{2.12}$$

Now, since $g_{00}g^{00} = 1$, Eq. (2.12) immediately leads us to

$$(g_{00})^{-2}g_{00,i}g_{00,j} = A^2(2\omega + 3)\psi_i\psi_j. \tag{2.13}$$

Combining (2.11) and (2.13), one arrives at the relation

$$R_{ij} = -(1/2A^2)(1/g_{00})^2 g_{00,i}g_{00,j}. \tag{2.14}$$

III. GENERATION OF SOLUTIONS IN NORDTVEDT'S THEORY FROM EINSTEIN'S VACUUM SOLUTIONS

A very simple technique for generating solutions in the presence of a scalar field in Nordtvedt's theory from the corresponding Einstein's vacuum solutions in axial symmetry is described in what follows.

The general axially symmetric static metric is given by (Synge[16])

$$ds^2 = e^{2\alpha}dt^2 - e^{2\beta}(d\rho^2 + dz^2) - \rho^2 e^{2\nu}d\Phi^2, \tag{3.1}$$

where the metric components are functions of ρ and z. In Dicke's revised units ($g_{\mu\nu} = \phi\bar{g}_{\mu\nu}$ and $\psi = \ln\phi$), the field equations are given by Eq. (2.11) and the wave equation becomes

$$\Box\psi = -\frac{1}{(2\omega + 3)}\psi_\lambda\psi^\lambda\frac{d\omega}{d\psi}. \tag{3.2}$$

In the case of axial symmetry, ψ is a function of ρ and z, and using (2.11) one can write

$$R^3_3 + R^0_0 = 0,$$

allowing us to write the metric in Weyl's canonical form

$$ds^2 = e^{2\lambda}dt^2 - e^{(2\nu - 2\lambda)}(d\rho^2 + dz^2) - \rho^2 e^{-2\lambda}d\Phi^2, \tag{3.3}$$

where λ and ν are functions of ρ and z. Ricci tensor components, calculated from the metric (3.3), are

$$R_{33} = -\rho^2 e^{-2\nu}(\lambda_{11} + \lambda_{22} + \lambda_1/\rho), \tag{3.4}$$

$$R_{11} - R_{22} = 2(\lambda_1^2 - \lambda_2^2) - 2\nu_1/\rho, \tag{3.5}$$

$$R_{12} = 2\lambda_1\lambda_2 - \nu_2/\rho. \tag{3.6}$$

Subscripts 1 and 2 on λ, ν represent differentiation with respect to ρ and z, respectively. In view of (3.4) to (3.6), the field equations (2.14) in scalar tensor theory can now be written explicitly as

$$\lambda_{11} + \lambda_{22} + \lambda_1/\rho = 0, \tag{3.7a}$$

$$\nu_1 = \rho(\lambda_1^2 - \lambda_2^2)(1 + 1/A^2), \tag{3.7b}$$

$$\nu_2 = 2\rho\lambda_1\lambda_2(1 + 1/A^2). \tag{3.7c}$$

On the other hand, Einstein's field equations in the absence of the scalar field are $R_{ij} = 0$, which explicitly yield

$$\lambda_{11} + \lambda_{22} + \lambda_1/\rho = 0, \tag{3.8a}$$

$$\nu_1 = \rho(\lambda_1^2 - \lambda_2^2), \tag{3.8b}$$

$$\nu_2 = 2\rho\lambda_1\lambda_2. \tag{3.8c}$$

It is now possible to conclude that if λ_E and ν_E are solutions of the set of equations (3.8) for empty space, the corresponding scalar field solutions are given in view of (3.7a)–(3.7c) as

$$\lambda_N = \lambda_E, \quad \text{and } \nu_N = \nu_E(1 + 1/A^2),$$

where the subscripts N and E correspond to Nordtvedt's and Einstein's solutions, respectively.

Later, in Sec. IV, a method for generating such simple solutions in spheroidal coordinates is given.

IV. STATIC SOLUTIONS IN PROLATE AND OBLATE SPHEROIDAL COORDINATES

In this section, static solutions of the field equations will be obtained directly in prolate and oblate spheroidal coordinates. In Dicke's revised version, the field equations are given by (2.11). For static axially symmetric case $\psi_3 = \psi_0 = 0$, and the metric can be written in the form (3.3). Suitable combinations of the field equations would look like

$$\lambda_{11} + \lambda_{22} + \lambda_1/\rho = 0, \tag{4.1a}$$

$$\nu_1 = \rho(\lambda_1^2 - \lambda_2^2) + \tfrac{1}{4}\rho(2\omega + 3)(\psi_1^2 - \psi_2^2), \tag{4.1b}$$

$$\nu_2 = 2\rho\lambda_1\lambda_2 + \tfrac{1}{2}\rho(2\omega + 3)\psi_1\psi_2, \tag{4.1c}$$

$$\nu_{11} + \nu_{22} + \lambda_1^2 + \lambda_2^2 = -[(2\omega + 3)/4](\psi_1^2 + \psi_2^2). \tag{4.1d}$$

The wave equation is

$$\psi_{11} + \psi_{22} + \frac{\psi_1}{\rho} = -\frac{1}{(2\omega + 3)}\frac{d\omega}{d\psi}(\psi_1^2 + \psi_2^2). \tag{4.2}$$

Equation (4.1d) is a consequence of the other three field equations in empty space-time in the absence of the scalar field, but in the presence of the scalar field, it is an independent equation with the wave equation being a consequence of the field equations.

A. Solutions in prolate spheroidal coordinates

If we transform the equations in prolate spheroidal coordinates [(x,y) or (u,θ)] defined by

$$\rho = a(x^2-1)^{1/2}(1-y^2)^{1/2} = a \sinh u \sin\theta, \tag{4.3a}$$

$$z = axy = a \cosh u \cos\theta, \tag{4.3b}$$

the field equations will take up the form

$$\frac{\partial}{\partial x}[(x^2-1)\lambda_x] + \frac{\partial}{\partial y}[(1-y^2)\lambda_y] = 0, \tag{4.4a}$$

$$\frac{\partial \nu}{\partial x} = \frac{(1-y^2)}{(x^2-y^2)}[x(x^2-1)\lambda_x^2 - x(1-y^2)\lambda_y^2 - 2y(x^2-1)\lambda_x\lambda_y + [(2\omega+3)/4]\{x(x^2-1)\psi_x^2 - x(1-y^2)\psi_y^2 - 2y(x^2-1)\psi_x\psi_y\}], \tag{4.4b}$$

$$\frac{\partial \nu}{\partial y} = \frac{(x^2-1)}{(x^2-y^2)}[y(x^2-1)\lambda_x^2 - y(1-y^2)\lambda_y^2 + 2x(1-y^2)\lambda_x\lambda_y + [(2\omega+3)/4]\{y(x^2-1)\psi_x^2 - y \times (1-y^2)\psi_y^2 + 2x(1-y^2)\psi_x\psi_y\}], \tag{4.4c}$$

$$(x^2-1)\nu_{xx} + (1-y^2)\nu_{yy} + x\nu_x - y\nu_y + (x^2-1)\lambda_x^2 + (1-y^2)\lambda_y^2 = -[(2\omega+3)/4][(x^2-1)\psi_x^2 + (1-y^2)\psi_y^2], \tag{4.4d}$$

and the wave equation becomes

$$(x^2-1)\psi_{xx} + (1-y^2)\psi_{yy} + 2x\psi_x - 2y\psi_y = -\frac{1}{(2\omega+3)}[(x^2-1)\psi_x^2 + (1-y^2)\psi_y^2]\frac{d\omega}{d\psi}, \tag{4.5}$$

where subscripts x and y indicate differentiation with respect to x and y, respectively.

For the sake of simplicity, we would assume that ψ depends on x alone. Physically it implies that the scalar field ψ is uniform on the ellipsoidal surfaces $u = \text{const}$. Now the integration of Eq. (4.5) directly gives (with $\psi_y = 0$)

$$(2\omega+3)^{1/2}\psi_x = c_1/(x^2-1), \tag{4.6}$$

where c_1 is a constant of integration.

Equation (4.4a) is the Laplace equation in prolate spheroidal coordinates and has the solution

$$\lambda = \sum_{l=0}^{\infty} a_l Q_l(x) P_l(y),$$

where a_l's are constants and $Q_l(x)$ and $P_l(y)$ are Legendre functions of the second and first kind of different orders. If $l = 0$, one obtains the so-called monopole solution for λ

$$\lambda = -(m_1/2)\ln((x+1)/(x-1)), \tag{4.7}$$

m_1 being a constant of integration.

Using (4.7) and (4.6), one can obtain by integration of the Eq. (4.4b),

$$\nu = [(4m_1^2 + c_1^2)/8]\ln((x^2-1)/(x^2-y^2)) + f(y), \tag{4.8}$$

where $f(y)$ is an arbitrary function of y. Differentiating (4.8) with respect to y and comparing it with (4.4c), one finds that $f(y)$ is a constant. This constant may be put equal to zero from the consideration of asymptotic flatness. Therefore, we obtain

$$\nu = [(4m_1^2 + c_1^2)/8]\ln((x^2-1)/(x^2-y^2)). \tag{4.9}$$

Then $l = 1$ gives the dipole solutions of the Laplace equation (4.4a),

$$\lambda = m_2 y[1 - (x/2)\ln((x+1)/(x-1))], \tag{4.10}$$

m_2 being an arbitrary constant. With (4.6) and (4.10), the corresponding solution for ν can be obtained from (4.4b) and (4.4c),

$$\nu = -\frac{m_2^2}{8}(x^2-1)(1-y^2)\left\{\ln\left(\frac{x+1}{x-1}\right)\right\}^2 + \frac{m_2^2 y^2}{2} + \frac{m_2^2}{2}\ln\left(\frac{x^2-1}{x^2-y^2}\right) + \frac{m_2^2}{2}x(1-y^2)\ln\left(\frac{x+1}{x-1}\right) + \frac{c_1^2}{8}\ln\left(\frac{x^2-1}{x^2-y^2}\right) + A, \tag{4.11}$$

where A is an arbitrary integration constant.

B. Solutions for the scalar field ϕ

Assuming the exact functional dependence of ω on ϕ one can integrate Eq. (4.6) to get the solutions for ψ and hence ϕ ($\phi = \exp\psi$) in the prolate spheroidal coordinates as follows.

(1) For Brans–Dicke[2] theory, $\omega = \omega_0$ (const),

$$\phi = e^{\psi} = a_1((x-1)/(x+1))^{c_1/\sqrt{2\omega_0+3}}. \tag{4.12a}$$

(2) For Barkar[6] theory, $2\bar{\omega} + 3 = 1/(\phi-1)$,

$$\phi = e^{\psi} = 1 + \tan^2\{(c_1/4)\ln a_2((x-1/x+1))\}. \tag{4.12b}$$

(3) For Schwinger theory, $2\omega + 3 = 1/\alpha\phi$,

$$\phi = e^{\psi} = [(c_1\sqrt{\alpha}/4)\ln a_3((x+1)/(x-1))]^{-2}. \tag{4.12c}$$

(4) For curvature coupling, $2\omega + 3 = 3/(1-\phi)$,

$$\phi = e^{\psi} = \frac{4a_4((x-1)/(x+1))^{c_1/\sqrt{3}}}{[1 - a_4((x-1)/(x+1))^{c_1/\sqrt{3}}]^2}. \tag{4.12d}$$

Here a_1, a_2, a_3, a_4 are arbitrary constants. For Schwinger theory and curvature coupling, see Van den Bergh[8] and references therein.

C. Solutions in oblate spheroidal coordinates

Solutions can be obtained in the oblate spheroidal coordinates also, where

$$\rho = a(x^2+1)^{1/2}(1-y^2)^{1/2} = a \cosh u \cos\theta, \tag{4.13}$$

$$z = axy = a \sinh u \sin\theta, \tag{4.14}$$

x and y being $\sinh u$ and $\sin\theta$, respectively. Here we would present the solutions directly without giving details of the procedure. The wave equation becomes, with the transformation of coordinates,

$$(x^2+1)\psi_{xx} + (1-y^2)\psi_{yy} + 2x\psi_x - 2y\psi_y = -\frac{1}{(2\omega+3)}[(x^2+1)\psi_x^2 + (1-y^2)\psi_y^2]\frac{d\omega}{d\psi}. \tag{4.15}$$

With the assumption that ψ depends on x alone, Eq. (4.15) readily integrates into

$$(2\omega+3)^{1/2}\psi_x = c_2/(x^2+1), \tag{4.16}$$

c_2 being a constant of integration.

Proceeding in the same way as had been done in the case of prolate spheroidal coordinates, one obtains the corresponding solutions in the oblate spheroidal coordinates.

For monopole solutions

$$\lambda = -n_1 \tan^{-1}\left(\frac{1}{x}\right), \tag{4.17a}$$

$$\nu = [(4n_1^2 + c_2^2)/8]\ln((x^2+y^2)/(x^2+1)). \tag{4.17b}$$

For dipole solutions

$$\lambda = n_2 y\left[1 - x\tan^{-1}\left(\frac{1}{x}\right)\right], \tag{4.17c}$$

$$\begin{aligned}\nu = &-(n_2^2/2)(x^2+1)(1-y^2)\left\{\tan^{-1}\left(\frac{1}{x}\right)\right\}^2 + \tfrac{1}{2}n_2^2 y^2 \\ &+ \tfrac{1}{2}n_2^2 \ln((x^2+1)/(x^2+y^2)) + n_2^2 x(1-y^2)\tan^{-1}\left(\frac{1}{x}\right) \\ &+ \tfrac{1}{8}c_2^2 \ln((x^2+y^2)/(x^2+1)) + B,\end{aligned} \tag{4.17d}$$

where n_1, n_2, B are arbitrary integration constants.

D. Solutions for the scalar field ϕ

Equation (4.6) will lead to the solutions for the scalar field ϕ in oblate spheroidal coordinates if the functional dependence of ω on ϕ is given as follows.

(1) For Brans–Dicke theory,

$$\phi = e^{\psi} = \exp[c_2 \tan^{-1}x/\sqrt{2\omega_0 + 3} + a_5]. \tag{4.18a}$$

(2) For Barkar theory,

$$\phi = e^{\psi} = [1 + \tan^2\{1 + \tfrac{1}{2}(c_2 \tan^{-1}x + a_6)\}]. \tag{4.18b}$$

(3) For Schwinger theory,

$$\phi = e^{\psi} = [(\sqrt{\alpha}/2)(c_2 \tan^{-1}x + a_7)]^{-2}. \tag{4.18c}$$

(4) For curvature coupling,

$$\phi = e^{\psi} = \left[\frac{4a_8 \exp(c_2 \tan^{-1}x/\sqrt{3})}{1 - a_8 \exp(c_2 \tan^{-1}x/\sqrt{3})}\right]. \tag{4.18d}$$

Here a_5, a_6, a_7, a_8 are constants of integration.

Therefore, $g_{\mu\nu}$ can be obtained from Eqs. (4.7), (4.9), (4.10), (4.11), (4.17), and (4.18) in spheroidal coordinates. With the solutions for ϕ at hand, the corresponding $\bar{g}_{\mu\nu}$ in the unrevised version can be obtained from the relation $g_{\mu\nu} = \phi\bar{g}_{\mu\nu}$. By suitable choice of the integration constant it is possible to show that λ and ν vanish as $x \to \infty$, which implies that the metric is asymptotically flat. Chatterjee[17] had previously considered dipole solutions for a special case of Nordtvedt's theory, that is for Barkar's choice of $\omega(\phi)$. The solutions given by him for ν and the scalar field ψ are, however, incorrect. The modification in the relation between the parameter ω and the scalar field, introduced due to the choice of Dicke's revised units, was apparently ignored. The solution for the scalar field was therefore wrong, leading to an incorrect set of metric components in the original atomic units of Brans and Dicke.

The constants c_1 and c_2 appearing in the solutions take care of the contributions from the scalar field. When these constants are put equal to zero one gets back corresponding Einstein's solutions for spheroidal symmetry (see Misra[12] and Zipoy[13]).

In the following we give examples of obtaining very simple spheroidal solutions in Nordtvedt's theory by using the technique presented in the previous section for generating them from corresponding Einstein's solutions.

In prolate spheroidal coordinates, the solutions of (3.7a) and (3.7b) corresponding to the monopole solution of λ_E are given by (Zipoy[13])

$$\lambda_E = -\frac{k_1}{2}\ln\left(\frac{x+1}{x-1}\right), \quad \nu_E = \frac{k_1^2}{2}\ln\left(\frac{x^2-1}{x^2-y^2}\right), \tag{4.19}$$

k_1 being a constant of integration which determines λ_E. From (3.9b), the corresponding solution in Nordtvedt theory would be

$$\lambda_N = \lambda_E, \quad \nu_N = \frac{k_1^2}{2}(1+A^2)\ln\left(\frac{x^2-1}{x^2-y^2}\right), \tag{4.20}$$

which is consistent with the solution (4.9).

In oblate spheroidal coordinates monopole solutions of λ_E and ν_E are given by (Misra[12] and Zipoy[13])

$$\begin{aligned}\lambda_E &= -k_2 \tan^{-1}\left(\frac{1}{x}\right), \\ \nu_E &= (k_2^2/2)\ln((x^2+y^2)/(x^2+1)),\end{aligned} \tag{4.21}$$

where k_2 is a constant of integration which determines λ_E. The corresponding Nordtvedt solution of Eqs. (3.8b) and (3.8c) will be

$$\lambda_N = \lambda_E, \quad \nu_N = \frac{k_2^2}{2}\left(1 + \frac{1}{A^2}\right)\ln\left(\frac{x^2+y^2}{x^2+1}\right), \tag{4.22}$$

which is consistent with the solution (4.16b).

V. STATIC CYLINDRICALLY SYMMETRIC SOLUTIONS IN NORDTVEDT'S THEORY

If the static line element exhibits cylindrical symmetry (the variables are functions of ρ alone), the field equations (4.1a)–(4.1d) become

$$\lambda_{11} + \lambda_1/\rho = 0, \tag{5.1a}$$

$$\nu_1 = \rho\lambda_1^2 + \tfrac{1}{4}\rho(2\omega+3)\psi_1^2, \tag{5.1b}$$

$$\nu_{11} + \lambda_1^2 = \tfrac{1}{4}(2\omega+3)\psi_1^2. \tag{5.1c}$$

Equation (4.1c) will be trivially satisfied. The wave equation becomes

$$\psi_{11} + \psi_1/\rho = -\omega_1\psi_1/(2\omega+3). \tag{5.2}$$

With (5.1a) and (5.1b), (5.1c) gives

$$\nu_{11} + \nu_1/\rho = 0. \tag{5.3}$$

Integration of (5.1a) and (5.3) directly gives us

$$\lambda = b_1 \ln\rho + c_1, \tag{5.4}$$

$$\nu = b_2 \ln\rho + c_2, \tag{5.5}$$

where b_1, b_2, c_1, c_2 are constants of integration. These solutions can also be obtained following the method described in Sec. III.

A. Solutions for the scalar field ϕ

In view of (5.4) and (5.5) one easily obtains from (5.1b) or (5.1c) the following relation:

$$(2\omega + 3)\psi_1^2 = p^2/\rho^2, \tag{5.6}$$

where $p^2 = 4(b_2 - b_1^2)$.

We solve (5.6) for ψ in the following cases, an exact functional form of $\omega = \omega(\psi)$ being already known in each case.

(1) For Brans–Dicke theory,

$$\phi = e^{\psi} = A_1 \rho^{p\sqrt{2\omega_0 + 3}}. \tag{5.7a}$$

(2) For Barkar theory,

$$\phi = e^{\psi} = \sec^2[\ln(A_2 \rho^{p/2})]. \tag{5.7b}$$

(3) For Schwinger theory,

$$\phi = e^{\psi} = \ln[A_3 \rho^{(1/2)p\sqrt{\alpha}}]^{-2}. \tag{5.7c}$$

(4) For curvature coupling,

$$\phi = e^{\psi} = 4A_4 \rho^p/(1 + A_4 \rho^p)^2. \tag{5.7d}$$

Here A_1, A_2, A_3, and A_4 are constants of integration.

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Spherically symmetric vacuum field in the general scalar–tensor theory

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The field equations in the general scalar–tensor theory of gravitation proposed by Nordtvedt are studied for a static and spherically symmetric vacuum field. Closed-form exact solutions of the field equations are presented for the scalar–tensor theories in the form given by Barker and Schwinger.

I. INTRODUCTION

Brans and Dicke[1] have proposed a modification of Einstein's theory of gravitation through the introduction of a scalar field ϕ in the field equations to make things more consistent with Mach's principle and less reliant on the absolute properties of space. But in view of the recent experimental evidence it is argued that if the Brans–Dicke theory of gravitation is to be a correct theory, the value of the parameter ω in this theory has to be as large as, or even greater than, 30 (see Ref. 2). With such a large value for ω it is difficult to distinguish between the Brans–Dicke theory of gravitation and the general theory of relativity, at least from their consequences. On the other hand, since there is no *a priori* reason to exclude the introduction of any long-range scalar field in the evolution of the universe, which might be quite important at some epoch, one may explore the possibility of a general scalar–tensor theory with ω as a time-dependent function. Nordtvedt[3] modified the Brans–Dicke theory where ω now becomes a function of scalar field ϕ instead of being a constant. Within the framework of Nordtvedt's general scalar–tensor theory Barker[4] proposed a particular ω-ϕ relation, which has a consequence that the local gravitational constant in the Newtonian approximation does not change with time. Also, Schwinger[5] and Kimball and Yee[6] have formulated a scalar–tensor theory as a mass-varying theory, but it can be put in the form of a standard scalar–tensor theory with a suitable choice of the function $\omega(\phi)$ and after a transformation to "particle units" has been carried out.[6]

Spherically symmetric static conformally flat solutions in the general scalar–tensor theory have been discussed by Rao and Reddy[7] and Singh and Singh.[8] Recently Van den Bergh[9] has given a conformal technique to generate exact solutions for the spherically symmetric vacuum field in the general scalar–tensor theory with vanishing cosmological constant in the frame in which particle masses vary but the gravitational "constant" G does not. By this method, one can generate exact vacuum solutions for general scalar–tensor theory from the corresponding solutions in Brans–Dicke theory. At the same time, he expressed doubt that even in the extremely simple case of a spherically symmetric vacuum field, equations do not lend themselves directly for analytic manipulations.

In this paper with a quite different approach, we have obtained exact solutions of Nordtvedt's general scalar–tensor theory in the conformal frame in which G varies but the particle masses are constant. We take $\omega(\phi)$ in the forms given by Barker and Schwinger. These solutions are simple and different from the solution given by Van den Bergh.[9]

II. FIELD EQUATIONS

The vacuum field equations in the general scalar–tensor theory of Nordtvedt[3] can be expressed as

$$R_{ij} - \tfrac{1}{2}g_{ij}R = -(\omega/\phi^2)(\phi_{,i}\phi_{,j} - \tfrac{1}{2}g_{ij}\phi_{,h}\phi^{,h}) - (1/\phi)(\phi_{,i;j} - g_{ij}\Box\phi) \tag{1}$$

and

$$\Box\phi = -\frac{\phi_{,h}\phi^{,h}}{(2\omega+3)}\frac{d\omega}{d\phi}. \tag{2}$$

Here a comma and semicolon denote partial and covariant derivatives, respectively.

In the following section, we solve the field equations (1) and (2) for a static spherically symmetric metric in isotropic coordinates,

$$ds^2 = e^{\alpha}dt^2 - e^{\beta}(d\rho^2 + \rho^2 d\theta^2 + \rho^2\sin^2\theta\, d\phi^2), \tag{3}$$

where α and β are functions of ρ only.

Taking ϕ as a function of ρ only and using (3) the field equations (1) and (2) can be written as

$$\beta'' + \tfrac{1}{4}\beta'^2 + (2/\rho)\beta' = -\frac{\omega}{2}\left(\frac{\phi'}{\phi}\right)^2 + \frac{\phi'\alpha'}{2\phi} + \frac{\phi'^2}{(2\omega+3)\phi}\frac{d\omega}{d\phi}, \tag{4}$$

$$\tfrac{1}{4}\beta'^2 + \tfrac{1}{2}\alpha'\beta' + (1/\rho)(\alpha'+\beta') = \frac{\omega}{2}\left(\frac{\phi'}{\phi}\right)^2 + \frac{\phi''}{\phi} - \frac{\phi'\beta'}{2\phi} + \frac{\phi'^2}{(2\omega+3)\phi}\frac{d\omega}{d\phi}, \tag{5}$$

$$\tfrac{1}{2}\beta'' + \tfrac{1}{4}\alpha'' + \tfrac{1}{4}\alpha'^2 + (1/2\rho)(\alpha'+\beta') = -\frac{\omega}{2}\left(\frac{\phi'}{\phi}\right)^2 + \frac{\phi'\beta'}{2\phi} + \frac{\phi'}{\rho\phi} + \frac{\phi'^2}{(2\omega+3)\phi}\frac{d\omega}{d\phi}, \tag{6}$$

and

$$\frac{d}{d\rho}\left[\exp\left(\frac{\alpha+\beta}{2}\right)\rho^2\phi'\right] = -\frac{\exp[(\alpha+\beta)/2]\rho^2\phi'}{2\omega+3}\frac{d\omega}{d\phi}. \tag{7}$$

Here a superscript prime indicates differentiation with respect to ρ.

Equation (7) can be integrated at once to give

$$\phi' = Ke^{-(\alpha+\beta)/2}/\rho^2(2\omega+3)^{1/2}, \tag{8}$$

where K is an integration constant.

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Adding Eqs. (5) and (6) and using (7) we have the solution

$$\phi e^{(\alpha+\beta)/2} = C[1-(B^2/\rho^2)], \tag{9}$$

where C and B are integration constants. Substituting Eq. (9) into (8) we obtain

$$(2\omega+3)^{1/2}\phi'/\phi = K/C(\rho^2-B^2). \tag{10}$$

Differentiating Eq. (9) once with respect to ρ and using Eq. (8), we have

$$\beta' = -\alpha' - \frac{2\phi'}{\phi}\left\{1-\frac{2CB^2(2\omega+3)^{1/2}}{\rho K}\right\}. \tag{11}$$

Also, Eq. (9) can be written in the form

$$e^{-\beta}/\phi\rho^4 = \phi e^{\alpha}/C^2(\rho^2-B^2). \tag{12}$$

III. SOLUTIONS OF THE FIELD EQUATIONS IN BARKER'S THEORY

We now discuss the solutions of the field equations (4)–(7) in the special case proposed by Barker[4] with $\omega(\phi)$ in the form

$$\omega = (4-3\phi)/2(\phi-1). \tag{13}$$

Using (13) in (10) and (11) we have, respectively,

$$\phi'/\phi(\phi-1)^{1/2} = K/C(\rho^2-B^2), \tag{14}$$

$$\beta' = -\alpha' - \frac{2\phi'}{\phi}\left\{1-\frac{2CB^2}{\rho K(\phi-1)^{1/2}}\right\}. \tag{15}$$

Integrating (14) we have

$$\phi = \sec^2[\tfrac{1}{2}\log\{\phi_0[(\rho-B)/(\rho+B)]^{A/\lambda}\}], \tag{16}$$

where

$$A/\lambda = K/2BC, \tag{17}$$

and ϕ_0 is another integration constant. Then A and λ are also constants.

Making the substitution

$$Y = e^{-\alpha/2} \tag{18}$$

and using Eqs. (13), (14), (15), and (17), Eq. (5) can be rewritten in the form

$$(Y'')^2 + 2F(\rho)YY' + H(\rho)Y^2 = 0, \tag{19}$$

where

$$2F(\rho) = -\frac{2AB(\phi-1)^{1/2}}{\lambda(\rho^2-B^2)}, \tag{20}$$

$$H(\rho) = -\frac{4B^2}{(\rho^2-B^2)^2}\left[1-\frac{\phi}{4}\left(\frac{A}{\lambda}\right)^2\right]. \tag{21}$$

The differential equation (19) can be expressed in a simple form if the variables are changed to $\eta(\xi)$ and ξ by the transformations

$$Y(\rho) = \eta(\xi)\exp(-\int F\,d\rho), \tag{22}$$

$$\xi = \int (H-F^2)^{1/2}\,d\rho. \tag{23}$$

Then Eq. (19) becomes

$$\left(\frac{d\eta}{d\xi}\right)^2 + \eta^2 = 0, \tag{24}$$

which in turn gives us the solution

$$e^{\alpha}\phi = \frac{1}{D^2}\exp\left\{\frac{p(A^2-4\lambda^2)^{1/2}}{2\lambda}\log\left(\frac{\rho-B}{\rho+B}\right)\right\}, \tag{25}$$

$$e^{\beta}\phi = C^2D^2\left(1-\frac{B^2}{\rho^2}\right)^2 \times\exp\left\{\frac{-p(A^2-4\lambda^2)^{1/2}}{2\lambda}\log\left(\frac{\rho-B}{\rho+B}\right)\right\}, \tag{26}$$

where D is a constant of integration and p is another constant.

The question of overdeterminacy in solving the field equations is settled by satisfaction of all the field equations by actual substitution of the values of α, β, and ϕ.

It can be seen that as $\rho\to\infty$ the solution given by (16), (25), and (26) leads to e^{α}, e^{β}, and ϕ, all of them tending to constants, which can be transformed to the standard form flat space-time of Einstein's theory with $\phi = \text{const}$.

IV. SOLUTIONS OF THE FIELD EQUATIONS IN SCHWINGER'S THEORY

We now discuss the solutions of the field equations (4)–(7) in Schwinger's theory[5,6] with $\omega(\phi)$ in the form

$$2\omega + 3 = 1/\gamma\phi, \tag{27}$$

where γ is a constant.

Using Eq. (27) in (10) and (11) we have

$$\phi'/\phi(\gamma\phi)^{1/2} = K/C(\rho^2-B^2), \tag{28}$$

$$\beta' = -\alpha' - \frac{2\phi'}{\phi}\left\{1-\frac{2CB^2}{\rho K(\gamma\phi)^{1/2}}\right\}. \tag{29}$$

Integrating Eq. (28) one has

$$\phi = 4/\gamma\left\{\log\left[\phi_0\left(\frac{\rho-B}{\rho+B}\right)^{A/\lambda}\right]\right\}^2, \tag{30}$$

where A/λ is given by (17) and ϕ_0 is an integration constant. From Eqs. (18), (27), (28), and (29), Eq. (5) can be written in the form

$$(Y'')^2 + 2F(\rho)YY' + H(\rho)Y^2 = 0, \tag{31}$$

where

$$2F(\rho) = -2AB(\gamma\phi)^{1/2}/\lambda(\rho^2-B^2), \tag{32}$$

$$H(\rho) = -\frac{4B^2}{(\rho^2-B^2)^2}\left[1-\frac{(1+\gamma\phi)}{4}\left(\frac{A}{\lambda}\right)^2\right]. \tag{33}$$

Following the method adopted in Sec. III, the solution of Eq. (31) can be obtained in the form

$$e^{\alpha}\phi = \frac{4}{\gamma D_1^2}\exp\left\{\frac{p(A^2-4\lambda^2)^{1/2}}{2\lambda}\log\left(\frac{\rho-B}{\rho+B}\right)\right\} \tag{34}$$

$$e^{\beta}\phi = C^2D_1^2\left(1-\frac{B^2}{\rho^2}\right)^2 \times\exp\left\{\frac{-p(A^2-4\lambda^2)^{1/2}}{2\lambda}\log\left(\frac{\rho-B}{\rho+B}\right)\right\}, \tag{35}$$

where D_1 is a constant of integration.

On actual verification it is found that the values α, β, and ϕ satisfy all the field equations. It can be seen that as $\rho\to\infty$, the solution given by (30), (34), and (35) leads to e^{α}, e^{β}, and ϕ, all the three tending to constants which can be brought to the standard form of flat space-time of Einstein's theory with $\phi = \text{const}$.

V. CONCLUSIONS

The complete solutions are, therefore, obtained for a spherically symmetric matter-free space-time in the general scalar–tensor theory of Nordtvedt, which in a special case includes the Brans–Dicke theory. The solutions have the property of asymptotic flatness and reduce to the corresponding Brans–Dicke solutions in spherically symmetric matter-free space-time when we put $\omega = \text{const}$. It may be noted that one can obtain a vacuum solution to the general scalar–tensor theory from a corresponding solution in Brans–Dicke theory by a conformal technique given by Van den Bergh.[9] In this paper a vacuum solution has been obtained by directly solving the field equations.

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The vacuum Einstein equations and deformations of the Bianchi identity

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The Einstein equations in vacuum are written as a closed differential ideal of matrix-valued differential forms with constant coefficients. Several properties of the resulting equations, such as the existence of an associated integrability system and of conserved matrix currents, as well as the treatment of specific Petrov types, are briefly considered. We also show that the field equations can be expressed as a deformation (depending on a complex parameter λ) of the Bianchi identity for an adequate Poincaré or de Sitter connection.

I. INTRODUCTION

It is the purpose of the present work to formulate the Einstein equations in vacuum in such a way that the study and use of their geometric and invariance properties becomes quite simple. In particular, we are thinking of the possible generalization of the solution-generating techniques already in use in general relativity to generic cases (no isometries and no special algebraic type of the gravitational field). The formulation in terms of Lie-algebra-valued differential forms seems to be quite appropriate to this end. In Sec. II, we discuss the vacuum field equations written in terms of matrix-valued differential forms, as well as an integrability system associated with them.[1] Some points that are discussed briefly are the group-theoretical aspects, as well as the conserved currents that appear naturally in this formulation, and the mechanism for dealing with specific Petrov types.

The two Cartan structural equations on which the formulation presented in Sec. II is based may be united into a single entity. In other words, torsion and curvature play a role in the theory which is, up to a certain point, symmetrical. The similarity between torsion and curvature has been emphasized by many authors; let us mention Ne'eman[2] and Regge,[3] where this point of view is adopted. In order to give a concrete meaning to this idea, the next section deals with central extensions and graded Lie algebras, which involve both the Lie and the Grassmann algebra structures.

Such structures are used in Sec. IV, where the Einstein equations are formulated in terms of a Poincaré connection. The field equations turn out to be a generalization of the usual Bianchi equation for the curvature Ω, involving now a deformation $\Omega(\lambda)$ of the curvature depending on the complex deformation parameter λ. As we are interested in the conventional Einstein theory, which is invariant only under the Lorentz subgroup of the Poincaré group, it is appropriate that the resulting equations break the Poincaré gauge transformation properties of the connection ω down to gauge invariance under the SL(2,C) subgroup only.

Finally, in Sec. V we introduce a slightly different approach, using again the structures described in Sec. III. A de Sitter connection depending on a contraction parameter μ is considered, and the field equations are written in terms of a single Bianchi-type equation for $\Omega_0(\lambda)$, the latter being a contraction and deformation of the curvature Ω with values in the de Sitter algebra.

II. EINSTEIN EQUATIONS IN VACUUM

The Einstein equations may be formulated as Cartan's structural equations by means of differential forms. Different versions of the equations put in this language may be seen in Refs. 4–6. We shall take Ref. 6 as our starting point. The basic ingredients are the vierbein of one-forms $\{k,m,t,\bar{t}\}$ (where k and m are real, and $\bar{t}$ is the complex conjugate of t) (see Ref. 7), and the complex-valued connection one-forms $\{u,v,w\}$. The structural equations take the form

$$dk = \tfrac{1}{2}(u+\bar{u})\wedge k + \bar{v}\wedge t + v\wedge\bar{t}, \tag{2.1a}$$

$$dm = -\tfrac{1}{2}(u+\bar{u})\wedge m + w\wedge t + \bar{w}\wedge\bar{t}, \tag{2.1b}$$

$$dt = -\bar{w}\wedge k - v\wedge m + \tfrac{1}{2}(u-\bar{u})\wedge t, \tag{2.1c}$$

$$\begin{aligned} dv - u\wedge v = {} & C_2 m\wedge\bar{t} + C_1(k\wedge m + t\wedge\bar{t}) \\ & + C_0 k\wedge t - \tfrac{1}{12}Rk\wedge t + \tfrac{1}{2}S_{kk}m\wedge t \\ & + \tfrac{1}{2}S_{kt}(k\wedge m - t\wedge\bar{t}) + \tfrac{1}{2}S_{tt}k\wedge\bar{t}, \end{aligned} \tag{2.2a}$$

$$\begin{aligned} du - 2w\wedge v = {} & -2C_1 m\wedge\bar{t} - 2C_0(k\wedge m + t\wedge\bar{t}) \\ & - 2C_{-1}k\wedge t - \tfrac{1}{12}R(k\wedge m + t\wedge\bar{t}) \\ & + \tfrac{1}{2}S_{k\bar{t}}m\wedge t \\ & + \tfrac{1}{2}S_{\bar{t}\bar{t}}(k\wedge m - t\wedge\bar{t}) - \tfrac{1}{2}S_{mt}k\wedge\bar{t}, \end{aligned} \tag{2.2b}$$

$$\begin{aligned} dw - w\wedge u = {} & C_0 m\wedge\bar{t} + C_{-1}(k\wedge m + t\wedge\bar{t}) + C_{-2}k\wedge t \\ & - \tfrac{1}{12}Rm\wedge\bar{t} + \tfrac{1}{2}S_{\bar{t}\bar{t}}m\wedge t \\ & - \tfrac{1}{2}S_{m\bar{t}}(k\wedge m - t\wedge\bar{t}) + \tfrac{1}{2}S_{mm}k\wedge\bar{t}, \end{aligned} \tag{2.2c}$$

where the coefficients C_i, S_{ij}, and R correspond to the decomposition of the Riemann tensor into its Weyl, traceless Ricci, and scalar-curvature parts. The vacuum equations are obtained from (2.1a)–(2.1c), (2.2a)–(2.2c) by setting $S_{ij} = 0$, $R = 0$. Equations (2.2a)–(2.2c) take the form

$$dv - u\wedge v = C_2 m\wedge\bar{t} + C_1(k\wedge m + t\wedge\bar{t}) + C_0 k\wedge t, \tag{2.3a}$$

$$\begin{aligned} du - 2w\wedge v = {} & -2C_1 m\wedge\bar{t} - 2C_0(k\wedge m + t\wedge\bar{t}) \\ & - 2C_{-1}k\wedge t, \end{aligned} \tag{2.3b}$$

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$$dw - w\wedge u = C_0 m\wedge\bar{t} + C_{-1}(k\wedge m + t\wedge\bar{t}) + C_{-2}k\wedge t. \tag{2.3c}$$

The field equations (2.1a)–(2.1c), (2.3a)–(2.3c) may be put in a very compact form by introducing the matrix-valued one-forms

$$\eta = \begin{bmatrix} -k & t \\ \bar{t} & m \end{bmatrix}, \quad \gamma = \begin{bmatrix} \frac{1}{2}u & -v \\ w & -\frac{1}{2}u \end{bmatrix}.$$

The forms η and γ may be characterized in a coordinate and tetrad-free way by imposing their defining conditions

$$\eta^\dagger = \eta, \quad \tilde{\gamma} = \gamma, \tag{2.4}$$

where the dagger denotes Hermitian conjugation, and the tilde of any two-by-two matrix p form M is defined by

$$\tilde{M} = \epsilon M^t \epsilon,$$

where t denotes transpose and ϵ is given by

$$\epsilon = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

The connection form γ is thus a sl(2,C)-valued one-form ($\operatorname{tr}\gamma = 0$).

The field equations (2.1a)–(2.1c) and (2.3a)–(2.3c) are now expressed as

$$d\eta = \gamma\wedge\eta - \eta\wedge\gamma^\dagger, \tag{2.5a}$$

$$d\gamma - \gamma\wedge\gamma = W\wedge\eta, \tag{2.5b}$$

where

$$W = \begin{bmatrix} -C_0(k+m) - C_{-1}t + C_1\bar{t} & -C_1(k+m) - C_0 t + C_2\bar{t} \\ C_{-1}(k+m) + C_{-2}t - C_0\bar{t} & C_0(k+m) + C_{-1}t - C_1\bar{t} \end{bmatrix}. \tag{2.6}$$

In (2.5a), (2.5b), and in the sequel, the wedge product of matrix-valued forms is understood as matrix multiplication, with the ordinary product substituted by the exterior product.

The fact that the spinor components of the Weyl tensor appear explicitly in Eq. (2.5b) through W has the following consequence: If one wants to consider a closed differential system, the integrability conditions for (2.5b) should be added to (2.5a) and (2.5b). [The integrability conditions for (2.5a) are satisfied by virtue of $W\wedge\eta\wedge\eta = 0$, with W given by Eq. (2.6).] Such integrability conditions (Bianchi conditions) are in the present case

$$dW\wedge\eta = W\wedge\gamma\wedge\eta + \gamma\wedge W\wedge\eta - W\wedge\eta\wedge\gamma - W\wedge\eta\wedge\gamma^\dagger. \tag{2.7}$$

In order to avoid the extra equation (2.7), whose explicit consideration is unnecessary for the purposes of the present work, it is convenient to write Eq. (2.5b) in an implicit form. The vacuum field equation as expressed by (2.5b) is somewhat unpleasant in that W does not transform in a simple way under the SL(2,C) gauge transformations (see below); on the other hand, it is rather remarkable that W is traceless and such that only three basic independent one-forms appear (the combination $k - m$ is missing).

It turns out that Eq. (2.5b), with W having the algebraic structure given by (2.6), is precisely equivalent to the condition

$$(d\gamma - \gamma\wedge\gamma)\wedge\eta = 0. \tag{2.8}$$

A trivial computation indeed shows that the general expression for $d\gamma - \gamma\wedge\gamma$ satisfying Eq. (2.8) is of the type (2.5b) and (2.6).

The field equations (2.5a) and (2.5b) are now substituted for by the equivalent formulation[1]

$$d\eta = \gamma\wedge\eta - \eta\wedge\gamma^\dagger, \tag{2.9a}$$

$$(d\gamma - \gamma\wedge\gamma)\wedge\eta = 0. \tag{2.9b}$$

The system (2.9a) and (2.9b) is now closed under exterior differentiation. Furthermore, the SL(2,C) invariance of the equations under the gauge transformations

$$\eta \to \eta' = S\eta S^\dagger, \tag{2.10a}$$

$$\gamma \to \gamma' = S\gamma S^{-1} + dS\,S^{-1} \tag{2.10b}$$

[where S is a matrix function with values in SL(2,C)] is now manifest.[8]

The space-time metric g is given by the expression

$$g = \operatorname{tr}(\eta\otimes\tilde{\eta}),$$

where the tensor product symbol refers to the product to be used among entries belonging to the matrix one-forms η and $\tilde{\eta}$. In order to obtain a physically meaningful metric, Eqs. (2.9a) and (2.9b) should be supplemented by the requirement

$$\eta\wedge\tilde{\eta}\wedge\eta\wedge\tilde{\eta} \neq 0,$$

which expresses the fact that the one-forms entering into η should be independent, or, alternatively, that the space-time volume element should be nondegenerate.

Equations (2.9a) and (2.9b) may be formulated in the algebraically equivalent form[1]

$$d\eta = \gamma\wedge\eta - \eta\wedge\gamma^\dagger, \tag{2.11a}$$

$$d(\gamma\wedge\eta) = \gamma\wedge\eta\wedge\gamma^\dagger. \tag{2.11b}$$

Let us define the torsion and curvature forms by

$$\mathcal{T} = d\eta - \gamma\wedge\eta + \eta\wedge\gamma^\dagger, \quad \mathcal{R} = d\gamma - \gamma\wedge\gamma.$$

Equations (2.9a) and (2.9b) may be expressed as a system of homogeneous degree by writing

$$\tilde{\eta}\wedge\mathcal{T} = 0, \tag{2.12a}$$

$$\tilde{\eta}\wedge\mathcal{R} = 0. \tag{2.12b}$$

This is due to the fact that $\tilde{\eta}\wedge\mathcal{T} = 0 \Leftrightarrow \mathcal{T} = 0$ for Hermitian $\mathcal{T}$. [Here $\tilde{\eta}$ has been used instead of η in Eq. (2.12a) in order to have the correct gauge transformation properties, as $\tilde{\eta} \to \tilde{\eta}' = (S^\dagger)^{-1}\tilde{\eta}S^{-1}$; Eq. (2.12b) is the tilde transform of Eq. (2.9b).] An alternative system of homogeneous degree, equivalent to (2.12a) and (2.12b), is the following:

$$d(\tilde{\eta}\wedge\eta)=\tilde{\eta}\wedge\eta\wedge\gamma^{\dagger}-\gamma^{\dagger}\wedge\tilde{\eta}\wedge\eta,$$

$$d(\gamma\wedge\eta)=\gamma\wedge\eta\wedge\gamma^{\dagger}.$$

Again, this is due to the fact that $\mathscr{T}\wedge\eta-\tilde{\eta}\wedge\mathscr{T}=0\Leftrightarrow\mathscr{T}=0$ for nonsingular η. The field equations written in this form imply the existence of the conserved matrix currents $*\mathscr{P}$ and $*\mathscr{J}$, where $*$ is the Hodge duality operator and

$$\mathscr{P}=\gamma\wedge\eta\wedge\gamma^{\dagger},$$

$$\mathscr{J}=\tilde{\eta}\wedge\eta\wedge\gamma^{\dagger}-\gamma^{\dagger}\wedge\tilde{\eta}\wedge\eta.$$

The form $\mathscr{P}$ satisfies $\mathscr{P}^{\dagger}=-\mathscr{P}$, and as a consequence it contains four real scalar forms, while $\tilde{\mathscr{J}}=\mathscr{J}$, so that it contains six scalar forms.

Let us mention here that the transformation $\eta\mapsto\tilde{\eta}$ corresponds to time inversion in the flat space case, and has a related meaning in the general case, as it corresponds to the interchange $k\leftrightarrow m$ in the explicit form of η given above. This in turn corresponds to an inversion of the exact one-form induced by the time coordinate when Gaussian normal coordinates are used, such coordinates satisfying $d(\mathrm{tr}\,\eta)=0$. Equations (2.9a) and (2.9b) are invariant under the discrete transformation $\eta\mapsto\tilde{\eta}$, $\gamma\mapsto-\gamma^{\dagger}$.

Equation (2.9b) has the following group-theoretic interpretation: The curvature $\mathscr{R}$ transforms under gauge transformation as

$$\mathscr{R}\mapsto\mathscr{R}'=S\mathscr{R}S^{-1},$$

thus belonging to a representation space of SL(2,C). Equation (2.9b) selects an invariant subspace, which in fact corresponds to an irreducible spin-2 representation of SL(2,C). The spin-2 representation becomes manifest when the spinor components of the Weyl tensor are explicitly introduced. Equation (2.9b) is a coordinate-free expression of this fact.

Equations (2.9a) and (2.9b) were introduced in Ref. 1 in order to facilitate the development of solution-generating techniques for the general vacuum case, such techniques possibly being the generalization of certain methods already known for the special case when two commuting isometries exist: Bäcklund transformations[9–11] and the inverse scattering method.[12] Integrability systems associated to nonlinear partial differential equations are at the root of the inverse scattering and Bäcklund transformation methods currently in use for equations in two independent variables. In searching for an integrability system of this type, related to the general case of the Einstein equations in vacuum, one is guided by the following observation: The trivial solution to the equations (Minkowski space) is characterized by the special case of Eqs. (2.9a) and (2.9b), given by

$$d\eta=\gamma\wedge\eta-\eta\wedge\gamma^{\dagger}, \tag{2.13a}$$

$$d\gamma-\gamma\wedge\gamma=0. \tag{2.13b}$$

It is then easily checked that (2.13a) and (2.13b) are the integrability conditions for the system

$$\phi\eta\phi^{\dagger}=d\xi, \tag{2.14a}$$

$$d\phi=-\phi\gamma, \tag{2.14b}$$

where ϕ and ξ are matrix zero-forms with $\phi\in\mathrm{SL}(2,\mathbb{C})$ and $\xi^{\dagger}=\xi$. The general solution of Eqs. (2.13a) and (2.13b) is obtained from (2.14a) and (2.14b):

$$\eta=\phi^{-1}\,d\xi\,(\phi^{\dagger})^{-1}, \tag{2.15a}$$

$$\gamma=-\phi^{-1}\,d\phi. \tag{2.15b}$$

Now η and γ given by (2.15a) and (2.15b) may be reduced to the standard form by using the gauge transformations (2.10a) and (2.10b) with $S=\phi$:

$$\eta_0=d\xi,\quad \gamma_0=0.$$

Given the relation that exists between Eqs. (2.13a) and (2.13b) and (2.9a) and (2.9b), one could be tempted to think that the integrability system associated with Eqs. (2.9a) and (2.9b) would be

$$\phi\eta\phi^{\dagger}=d\xi,$$

$$(d\phi+\phi\gamma)\wedge\eta=0.$$

However, this naive procedure fails due to the fact that $A\wedge\eta=0\Rightarrow A=0$ for any matrix one-form A, so one would be led back to the trivial case (2.14a) and (2.14b). Fortunately, this can be avoided by using a one-form Φ instead of the zero-form ϕ. The relevant equations are[1]

$$\Phi\wedge\eta\wedge\Phi^{\dagger}=d\xi, \tag{2.16a}$$

$$d\Phi\wedge\eta=\Phi\wedge\gamma\wedge\eta, \tag{2.16b}$$

where ξ is now a two-form satisfying $\xi^{\dagger}=-\xi$. It can be easily checked that the field equations (2.9a) and (2.9b) are a sufficient condition for the integrability of Eqs. (2.16a) and (2.16b). They will also be a necessary condition if enough solutions of (2.16a) and (2.16b) exist. The existence of nontrivial solutions is guaranteed by the fact that $\Phi=\gamma$ is always a solution by virtue of (2.9a) and (2.9b). Other integrability systems, with varying degrees of strength, have been considered in the literature (see Refs. 13–17). Notice that *both* (16a) and (16b) have to be considered in order to obtain Eqs. (2.9a) and (2.9b). In particular, Eq. (2.16a) is crucial for the metric condition (2.9a).

The Hilbert–Einstein action for the gravitational field in vacuum takes on the simple expression

$$SI=-i\int\tilde{\eta}\wedge(d\gamma-\gamma\wedge\gamma)\wedge\eta,$$

where I is the identity matrix.

One of the attractive features of the Newman–Penrose formalism is the ability to control the Petrov type under investigation by explicitly involving in the equations the spinor components of the Weyl tensor. Equations (2.5a), (2.5b), (2.6), and (2.7) are the exterior form analog of such equations. It is of interest to point out that, in spite of the fact that the Weyl components no longer appear explicitly in Eqs. (2.9a) and (2.9b), the possibility still exists of controlling the Petrov type of the solution. This may be achieved by incorporating additional conditions to the equations. For instance, for Petrov type N the additional equation is

$$P(d\gamma-\gamma\wedge\gamma)=0, \tag{2.17}$$

where

$$P=\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}.$$

The complete set of equations, forming a closed differential ideal, is in this case

$$d\eta=\gamma\wedge\eta-\eta\wedge\gamma^{\dagger},\quad (d\gamma-\gamma\wedge\gamma)\wedge\eta=0,$$
$$P(d\gamma-\gamma\wedge\gamma)=0,\quad P\gamma\wedge(d\gamma-\gamma\wedge\gamma)=0.$$

Alternatively, one may specify the residual gauge subgroup of SL(2,ℂ) that survives when a certain additional fixing condition such as (2.17) is given.

III. CENTRAL EXTENSIONS, THE POINCARÉ GROUP, AND LIE SUPERALGEBRAS

The results stated in the preceding section take an invariant form when one introduces some concepts related to the theory of group extensions and the theory of Lie superalgebras. A comprehensive exposition of the topics involved here can be found in Refs. 18–21.

Let us consider the exact sequence of multiplicative groups

$$1\to G_0\to G\to G_1\to 1.$$

The elements of the group G can be written as pairs (g_1,g_0) of elements g_1 and g_0 in the groups G_1 and G_0, respectively. Let a map $\psi: G_1\to \mathrm{Aut}\ G_0$ be given, so that we can define the multiplication law in G as

$$(g_1,g_0)(g_1',g_0')=(g_1g_1',[\psi(g_1')^{-1}g_0]g_0').$$

This is known as a central extension of G_1 by G_0. In the present context G_0 will be a normal Abelian subgroup of G and $G_1=G/G_0$, the subgroup of equivalence classes determined by G_0 in G. Thus, G_1 acts in G_0 by conjugation, and this permits us to define the map ψ as an element of $\mathrm{Hom}(G_1,\mathrm{Aut}\ G_0)$ given by

$$\psi(h_1)g_0=h_1g_0h_1^{-1},\quad h_1\in G_1,\quad g_0\in G_0.$$

We apply the construction above to the Poincaré group. By identifying G_1 with SL(2,ℂ) and G_0 with the translation group T_4, the elements of the Poincaré group are given by products g_Ag_M, $A\in \mathrm{SL}(2,\mathbb{C})$; $M\in \mathrm{Mat}_2^{\#}(\mathbb{C})$ $(M=M^{\dagger})$ [i.e., to the vector $(M^i)_0^3$, $M^i\in\mathbb{R}$ of T_4 we assign the self-adjoint matrix $M=\Sigma_0^3 M^i\sigma_i$, $\sigma_0=I$, σ^i, $i=1,2,3$ the Pauli matrices]. Thus, the product rule is defined by

$$g_Ag_Mg_Bg_N=g_Ag_Bg_B^{-1}g_Mg_Bg_N=g_{AB}[\psi(g_B)^{-1}g_M]g_N,$$
$$A,B\in \mathrm{SL}(2,\mathbb{C}),\quad M,N\in \mathrm{Mat}_2^{\#}(\mathbb{C}).$$

The homomorphism ψ is constructed with the help of the following outer automorphism θ of SL(2,ℂ):

$$\theta(A)=(A^{\dagger})^{-1}.$$

We take for ψ the natural action of SL(2,ℂ) in $\mathrm{Mat}_2^{\#}(\mathbb{C})$, $M\to BMB^{\dagger}$,

$$\psi(g_B)g_M=g_{BMB^{\dagger}},$$

and we get the desired extension by realizing the group elements g_A,g_M through the matrices

$$g_A=\begin{bmatrix}A & 0\\ 0 & \theta(A)\end{bmatrix},\quad g_M=\begin{bmatrix}I & M\\ 0 & I\end{bmatrix},\tag{3.1}$$

for which

$$\psi(g_B)g_M=g_Bg_Mg_B^{-1}=g_{BMB^{\dagger}}=\begin{bmatrix}I & BMB^{\dagger}\\ 0 & I\end{bmatrix}.\tag{3.2}$$

In this way we have reduced the product rule for the elements (g_A,g_M) of the extension of SL(2,ℂ) by the translation group to the multiplication of ordinary matrices in GL(4,ℂ) determined by the formula

$$g_Ag_Mg_Bg_N=\begin{bmatrix}A & AM\\ 0 & \theta(A)\end{bmatrix}\begin{bmatrix}B & BN\\ 0 & \theta(B)\end{bmatrix}$$
$$=\begin{bmatrix}AB & AB(N+B^{-1}M(B^{\dagger})^{-1})\\ 0 & \theta(AB)\end{bmatrix}.\tag{3.3}$$

Next, we describe the Lie algebra structure induced by the extension above. It is given by the exact sequence

$$0\to\mathfrak{g}_0\to\mathfrak{g}\to\mathfrak{g}_1\to 0.$$

We denote by $a\in \mathrm{sl}(2,\mathbb{C})$ and $m\in \mathrm{Mat}_2^{\#}(\mathbb{C})$ the elements on the Lie algebras parametrizing the Lie algebra of the Poincaré group $\mathfrak{g}$. Let $X, X'\in\mathfrak{g}$ be given by

$$X=(X_a,X_m),\quad X'=(X_b,X_n),$$
$$a,b,\in \mathrm{sl}(2,\mathbb{C}),\quad m,n\in \mathrm{Mat}_2^{\#}(\mathbb{C}).$$

The corresponding formulas to (3.1)–(3.3) in the Lie algebra are now

$$X_a=\begin{bmatrix}a & 0\\ 0 & \sigma(a)\end{bmatrix},\quad X_m=\begin{bmatrix}0 & m\\ 0 & 0\end{bmatrix},\tag{3.4}$$

σ being the Lie algebra automorphism of sl(2,ℂ): $\sigma(a)=-a^{\dagger}$ determined by θ in the group. We have also

$$\phi(X_b)\cdot X_m=\mathrm{ad}\,X_b\cdot X_m=\begin{bmatrix}0 & bm+mb^{\dagger}\\ 0 & 0\end{bmatrix},\tag{3.5}$$

where the Lie algebra homomorphism $\phi:\mathrm{sl}(2,\mathbb{C})\to \mathrm{Der}\ \mathrm{Mat}_2^{\#}(\mathbb{C})$ from sl(2,ℂ) into the Lie algebra of derivations of $\mathrm{Mat}_2^{\#}(\mathbb{C})$ is the derivative at the identity of the group homomorphism ψ. Hence, the commutation rule for the Lie algebra extension of sl(2,ℂ) by $\mathrm{Mat}_2^{\#}(\mathbb{C})$ takes the following form:

$$[X,X']=([X_a,X_b],\ \phi(X_a)\cdot X_n-\phi(X_b)X_m).$$

In terms of matrices in gl(4,ℂ) we have

$$[X,X']=\begin{bmatrix}[a,b] & an+na^{\dagger}-(bm+mb^{\dagger})\\ 0 & \sigma([a,b])\end{bmatrix},$$
$$\sigma(a)=-a^{\dagger}.\tag{3.6}$$

These formulas are all we need in order to get a consistent Lie-algebraic description for the Einstein equations.

In Sec. II, use has been made of Lie-algebra-valued exterior differential forms. We shall now discuss in a somewhat more elaborate way some of the properties of vector-valued differential forms.

Let $\mathfrak{g}$ be a Lie algebra with linear basis $\{e_i\}$. Let M be a smooth differentiable manifold and $\Lambda(M)=\oplus_{k>0}\Lambda_k(M)$ the Grassmann algebra of differential forms defined on it. We shall denote by $\bar{\mathfrak{g}}=\Lambda(M)\otimes\mathfrak{g}$ the $\mathbb{Z}$-graded algebra of differential forms on M with values in $\mathfrak{g}$. Thus, we have a $\mathbb{Z}$ grading on $\mathfrak{g}$ induced by that of $\Lambda(M)$: $\mathfrak{g}=\oplus_{k>0}\bar{\mathfrak{g}}_k$, $\deg\mathfrak{g}=0$, $\deg\bar{\mathfrak{g}}_k=k$.

For each $\omega_k\in\bar{\mathfrak{g}}_k$ we have an expression of the form $\omega_k=\Sigma_i\omega_k^i\otimes e_i$, which we shall write simply as

$\omega_k = \Sigma_i \omega_k^i e_i$, the ω_k^i's being elements of $\Lambda_k(M)$. Moreover, in $\bar{\mathfrak{g}}$ is defined a natural product

$$[\omega_k,\omega_l] = \sum_{i,j} \omega_k^i \wedge \omega_l^j [e_i,e_j] \tag{3.7}$$

determining a mapping $\bar{\mathfrak{g}}_k \times \bar{\mathfrak{g}}_l \to \bar{\mathfrak{g}}_{k+l}$. It is easily seen that $[\omega_k,\omega_l]$ is the $(k+l)$-form with values in $\mathfrak{g}$ given by

$$[\omega_k,\omega_l]:(X_1,\ldots,X_{k+l}) \to \frac{1}{(k+l)!} \sum_{\sigma\in\mathfrak{S}} \epsilon(\sigma)[\omega_k(X_{\sigma(1)},\ldots,X_{\sigma(k)}), \omega_l(X_{\sigma(k+1)},\ldots,X_{\sigma(k+l)})],$$

with the usual notation conventions, the $X_1,\ldots,X_{k+l}$ being tangent vectors to the manifold M.

The following proposition is trivial.

Proposition: (i) The algebra $\bar{\mathfrak{g}}$ is a Lie superalgebra[21]

$$\bar{\mathfrak{g}} = \bar{\mathfrak{g}}_{\bar{0}} \oplus \bar{\mathfrak{g}}_{\bar{1}},$$

with

$$\bar{\mathfrak{g}}_{\bar{0}} = \bigoplus_{k>0} \bar{\mathfrak{g}}_{2k}, \quad \bar{\mathfrak{g}}_{\bar{1}} = \bigoplus_{k>0} \bar{\mathfrak{g}}_{2k+1}.$$

(ii) The algebra $\bar{\mathfrak{g}} = \bar{\mathfrak{g}}_{\bar{0}} \oplus \bar{\mathfrak{g}}_{\bar{1}}$ is a $\mathbb{Z}$-graded Lie superalgebra with the $\mathbb{Z}$ gradation $(\bar{\mathfrak{g}}_k)_{k>0}$ consistent with the $\mathbb{Z}_2$ gradation of $\bar{\mathfrak{g}}$.

In fact, the commutation rule for $\bar{\mathfrak{g}}$ is determined by (3.7), and as it is easily verified, the following relations hold: (a) graded skew symmetry,

$$[\omega_k,\omega_l] = (-1)^{kl+1}[\omega_l,\omega_k];$$

and (b) graded Jacobi identity,

$$(-1)^{km}[\omega_k,[\omega_l,\omega_m]] + (-1)^{lk}[\omega_l,[\omega_m,\omega_k]] + (-1)^{ml}[\omega_m,[\omega_k,\omega_l]] = 0.$$

It easily follows from these relations that $\bar{\mathfrak{g}}_{\bar{0}}$ is a Lie algebra for the commutation given by the formula (3.7).

IV. LIE ALGEBRA FORM OF THE EINSTEIN EQUATIONS

In this section we consider the Lie superalgebra $\bar{\mathfrak{g}} = \Lambda(M) \otimes \mathfrak{g}$, where $M = \mathbb{R}^4$ and $\mathfrak{g}$ is the Lie algebra of the Poincaré group. A connection in $\bar{\mathfrak{g}}$ will be given by a one-form on M with values in $\mathfrak{g}$. According to the description of $\mathfrak{g}$ made in Sec. III as the central extension of sl(2,C) by the Abelian Lie algebra $\mathbb{R}^4$, a connection ω is specified by a pair $\omega = (\gamma,\eta)$, where γ takes values in sl(2,C) and η in $\mathbb{R}^4$ [equivalently, in $\mathrm{Mat}_2^*(\mathbb{C})$], the notation being the same we used in Sec. III. In order to get a more convenient expression for ω we shall write it in the form

$$\omega = \omega_\gamma + \omega_\eta, \tag{4.1}$$

following Eq. (3.4), and setting

$$\omega_\gamma = \begin{bmatrix} \gamma & 0 \\ 0 & -\gamma^\dagger \end{bmatrix}, \quad \omega_\eta = \begin{bmatrix} 0 & \eta \\ 0 & 0 \end{bmatrix}, \tag{4.2}$$

η being the same self-adjoint matrix differential one-form we were using previously.

We define the curvature two-form by the expression

$$\Omega = d\omega - \tfrac{1}{2}[\omega,\omega], \tag{4.3}$$

with "components" $\mathscr{R}$ and $\mathscr{T}$ corresponding to the curvature and torsion in Sec. II, $\Omega = (\mathscr{R},\mathscr{T})$. The explicit expression in terms of the matrices γ and η is given by the formulas

$$\mathscr{R} = d\gamma - \tfrac{1}{2}[\gamma,\gamma] = d\gamma - \gamma\wedge\gamma,$$
$$\mathscr{T} = d\eta - \phi(\gamma)\cdot\eta = d\eta - \gamma\wedge\eta + \eta\wedge\gamma^\dagger.$$

Furthermore, we can write

$$\Omega = \Omega_{\mathscr{R}} + \Omega_{\mathscr{T}}, \tag{4.4}$$

with

$$\omega_{\mathscr{R}} = \begin{bmatrix} \mathscr{R} & 0 \\ 0 & -\mathscr{R}^\dagger \end{bmatrix}, \quad \Omega_{\mathscr{T}} = \begin{bmatrix} 0 & \mathscr{T} \\ 0 & 0 \end{bmatrix},$$

and the Bianchi identity for the curvature two-form Ω reads

$$d\Omega = [\omega,\Omega].$$

We are now in a position to get the result we are looking for. Let λ be a complex variable and define the λ-dependent two-form $\Omega(\lambda) = (\lambda\mathscr{R},\mathscr{T})$ starting from the curvature Ω. This can be put as

$$\Omega(\lambda) = \Omega_{\lambda\mathscr{R}} + \Omega_{\mathscr{T}}. \tag{4.5}$$

Notice that $\Omega(\lambda)$ may be obtained by means of the linear map

$$\Omega \to \Omega(\lambda) = \begin{bmatrix} I & 0 \\ 0 & \bar{\lambda} I \end{bmatrix} \Omega \begin{bmatrix} \lambda I & 0 \\ 0 & I \end{bmatrix},$$

where I is the 2×2 identity matrix. One can think of $\Omega(\lambda)$ as a deformation of the curvature Ω depending on the deformation parameter λ.

The main result of this section may be formulated as the following theorem.

Theorem: Let ω be the connection form given by Eqs. (4.1) and (4.2), and let $\Omega(\lambda)$ be the deformation of the curvature defined above. Then, the Einstein equations in vacuum are given by

$$d\Omega(\lambda) = [\omega,\Omega(\lambda)], \tag{4.6a}$$
$$\Omega(0) = 0. \tag{4.6b}$$

Proof: From (4.6b) and (4.5) we get $\mathscr{T} = 0$, which gives Eq. (2.9a). Thus, $\Omega(\lambda) = \Omega_{\lambda\mathscr{R}}$ for the solutions of system (4.6a) and (4.6b). By taking into account this special form of $\Omega(\lambda)$, Eq. (4.6a) reduces to

$$d\Omega_{\lambda\mathscr{R}} = [\omega,\Omega_{\lambda\mathscr{R}}]$$

or

$$d\Omega_{\lambda\mathscr{R}} = [\omega_\gamma,\Omega_{\lambda\mathscr{R}}] + [\omega_\eta,\Omega_{\lambda\mathscr{R}}],$$

after introducing the decomposition $\omega = \omega_\gamma + \omega_\eta$ given by Eq. (4.1). From this last equation we obtain the relations

$$d\Omega_{\lambda\mathscr{R}} = [\omega_\gamma,\Omega_{\lambda\mathscr{R}}], \quad [\omega_\eta,\Omega_{\lambda\mathscr{R}}] = 0,$$

by separating sl(2,C) and $\mathrm{Mat}_2^*(\mathbb{C})$ "components." The first of the last two equations is identically satisfied by virtue of the Bianchi identity for the sl(2,C) curvature $\mathscr{R}$ and the second one results in $\phi(\lambda\mathscr{R})\cdot\eta = 0$, or in terms of the matrices $\mathscr{R}$ and η reads

$$\lambda\mathscr{R}\wedge\eta + \bar{\lambda}\eta\wedge\mathscr{R}^\dagger = 0,$$

which is nothing else but Eq. (2.9b) in view of the arbitrariness of λ. This finally proves our assertion.

In the preceding formulation, the tetrad η and connection γ are combined into a single connection form ω taking values in the Lie algebra of the Poincaré group. Equation (4.6a) expresses the fact that the deformation of the curvature, $\Omega(\lambda)$, is covariantly constant for any value of λ. This generalizes the Bianchi identity for $\Omega \equiv \Omega(1)$, which is kinematical and holds irrespective of the field equations, being a consequence of its definition (4.3). The second equation (4.6b) may be considered as an initial condition. It is worth pointing out that under a gauge transformation the connection ω undergoes the usual change

$$\omega \to \omega' = g\omega g^{-1} + dg \cdot g^{-1},$$

where g is an element of the Poincaré group, of the form given by Eq. (3.1),

$$g = \begin{bmatrix} A & AM \\ 0 & (A^\dagger)^{-1} \end{bmatrix}.$$

This gauge transformation induces the following transformation properties of η and γ:

$$\eta \to \eta' = A(\eta - \gamma M - M\gamma^\dagger + dM)A^\dagger,$$

$$\gamma \to \gamma' = A\gamma A^{-1} + dA\,A^{-1}.$$

The field equation (4.6a) is *not* invariant under a gauge transformation with arbitrary g; only those elements g with $M = 0$ leave it invariant. This has the effect of breaking down the Poincaré symmetry to the SL(2,C) symmetry of Einstein's gravity.

V. DE SITTER CONNECTIONS AND CONTRACTIONS

The Einstein equations (4.6a) and (4.6b) admit an alternative formulation which makes use of a contraction from the de Sitter to the Poincaré Lie algebra. The use of a deformation of the curvature introduced in the last section is now supplemented by the introduction of a de Sitter connection depending on a contraction parameter μ. This has the effect of combining (4.6a) and the vanishing torsion equation (4.6b) into a single equation.

Let us consider the 4×4 complex matrix

$$H = \begin{bmatrix} \alpha I & B \\ \tilde{B} & -\alpha I \end{bmatrix}, \tag{5.1}$$

where $\alpha \in \mathbb{R}$, $B = B^\dagger$ is a self-adjoint 2×2 matrix, and I is the identity in two dimensions. The (double covering of the connected component of the identity of the) de Sitter group SO(4,1) may be defined as the set of those matrices $\Sigma \in GL(4,C)$ acting as a group of transformations as

$$H' = \Sigma H \Sigma^{-1} \tag{5.2}$$

and leaving the algebraic form of H invariant. The algebraic restrictions on H [which are equivalent to the generic form given by Eq. (5.1)] are the following:

$$H^t = -\sigma H \sigma, \quad \overline{H} = \rho H \rho, \quad \operatorname{tr} H = 0, \tag{5.3}$$

where

$$\sigma = \begin{bmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{bmatrix}, \quad \rho = \begin{bmatrix} 0 & \epsilon \\ \epsilon & 0 \end{bmatrix},$$

ϵ being the 2×2 matrix defined in Sec. II. The transformation (5.2) leaves invariant the traces of the successive powers of H. From (5.1) or (5.3) we have $\operatorname{tr} H = \operatorname{tr} H^3 = 0$; $\operatorname{tr} H^2 = 2(\alpha^2 - \det B)$; $\operatorname{tr} H^4 = \frac{1}{2}(\operatorname{tr} H^2)^2$. Thus, there is only one nonvanishing independent invariant of H under the transformation (5.2); such an invariant is in fact a nondegenerate quadratic form in $\mathbb{R}^5$ with signature $(+\,+\,+\,+\,-)$. Conditions (5.3) impose the following restrictions on Σ, which may be taken as the definition of the group:

$$\Sigma^t \sigma \Sigma = \sigma, \quad \Sigma^{-1} \rho \overline{\Sigma} = \rho. \tag{5.4}$$

The explicit form of the group elements Σ may be easily calculated from Eq. (5.4). The corresponding elements ξ in its Lie algebra, so(4,1), will satisfy the conditions

$$\xi^t \sigma + \sigma \xi = 0, \quad \xi \rho - \rho \overline{\xi} = 0. \tag{5.5}$$

The Lie algebra consists then of matrices ξ of the form

$$\xi = \begin{bmatrix} a & b \\ -\tilde{b} & -a^\dagger \end{bmatrix}, \tag{5.6}$$

with a,b complex 2×2 matrices with $\tilde{a} = a(\operatorname{tr} a = 0)$ and $b^\dagger = b$. It is easy to see that the Lie algebra, whose generic element is of the form (5.6), has the isomorphic realization

$$\xi = \begin{bmatrix} a & b \\ -\mu\tilde{b} & -a^\dagger \end{bmatrix}, \tag{5.7}$$

with $\mu > 0$ and a,b as before. A contraction of the so(4,1) to the Poincaré algebra takes place when $\mu \to 0$. Let us now consider a so(4,1) connection of the form

$$\omega_\mu = \begin{bmatrix} \gamma & \eta \\ -\mu\tilde{\eta} & -\gamma^\dagger \end{bmatrix}. \tag{5.8}$$

We have the following theorem.

Theorem: Let

$$\Omega_\mu(\lambda) = \begin{bmatrix} I & 0 \\ 0 & \lambda I \end{bmatrix} (d\omega_\mu - \omega_\mu \wedge \omega_\mu) \begin{bmatrix} \lambda I & 0 \\ 0 & I \end{bmatrix},$$

ω_μ a de Sitter connection given by Eq. (5.8), and denote by $\Omega_0(\lambda)$ the contraction $\lim_{\mu\to0} \Omega_\mu(\lambda)$. The Einstein equations in vacuum are equivalent to the equation

$$d\Omega_0(\lambda) = [\omega_\mu, \Omega_0(\lambda)] \quad (\forall \mu > 0, \quad \forall \lambda \in \mathbb{C}). \tag{5.9}$$

Proof: Equation (5.9) is equivalent to the following set of equations:

$$\tilde{\eta} \wedge \mathcal{T} = 0, \quad \tilde{\eta} \wedge \mathcal{R} = 0,$$

$$d\mathcal{T} = \gamma \wedge \mathcal{T} + \mathcal{T} \wedge \gamma^\dagger, \quad d\mathcal{R} = \gamma \wedge \mathcal{R} - \mathcal{R} \wedge \gamma.$$

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A class of solutions of the Einstein–Maxwell equations

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We present all the exact solutions of the Einstein–Maxwell equations for a special case of the Robinson–Trautman metric form. Gaussian curvature of the angularlike part of the chosen metric form is equal to zero. The solutions are of the Petrov types D or II. Eight of them are probably new.

I. INTRODUCTION

In this paper we present all the exact solutions of the Einstein–Maxwell equations (without currents)

$$G_{\mu\nu} = -\lambda g_{\mu\nu} + 2(F_{\rho\mu}F_{\nu}{}^{\rho} + \tfrac{1}{4}g_{\mu\nu}F_{\rho\tau}F^{\rho\tau}),$$

$$F_{[\mu\nu,\rho]} = 0, \quad F^{\mu\nu}{}_{;\nu} = 0, \tag{1.1}$$

assuming only the limitation

$$ds^2 = 4p^2\,dY\,d\overline{Y} + 2\,dp\,dq + p^{-2}(2mp + f)dq^2. \tag{1.2}$$

The meanings of symbols are as follows: $G_{\mu\nu}$, $g_{\mu\nu}$, and $F_{\mu\nu}$ are the Einstein, metric, and electromagnetic field tensors, respectively, λ is the cosmological constant, Y is a complex coordinate, p and q are real coordinates, m is an arbitrary real constant, and $f = f(Y,\overline{Y},p,q)$ is a disposable real function that belongs to class C^2. Here and below every symbol with an overbar means a complex conjugate quantity of the given symbol.

The signature is $+\ +\ +\ -$.

The metric form (1.2) is a special case of the Robinson–Trautman one.[1] The Gaussian curvature of every two-dimensional surface $p,q = \text{const}$ $(p \neq 0)$ is equal to zero for space-times (1.2).[2] Such a geometrical property of space-time has a special physical interpretation in the case of the Robinson–Trautman type space-times. Namely, the interpretation has been given that the sources of fields, that produce the Riemannian curvature of these space-times, move with the speed of light.[1,2] Thus the solutions presented below make it possible to find explicitly the detailed properties of all such space-times admitted by the Einstein–Maxwell theory within the limitation (1.2).

In Sec. II some general properties of the solutions are briefly reviewed. In Sec. III a list of the explicit solutions and Petrov's classification are given.

II. SOME GENERAL PROPERTIES

When solving Eqs. (1.1) under condition (1.2) we used the known results[3] that include expressions ready for integration.[4] After easy integration of a part of those expressions one finds that

$$f = -\tfrac{1}{3}\lambda p^4 + pA - B\overline{B} \tag{2.1}$$

and

$$A = \overline{A}, \quad A_{,Y} = A_{,\overline{Y}} = A_{,p} = 0,$$
$$C_{,Y} = C_{,\overline{Y}} = C_{,p} = 0, \quad A_{,q} = 2C\overline{C} \tag{2.2}$$

for $B = 0$, where C is an arbitrary complex function of q only, and

$$A = \overline{A}, \quad A_{,p} = 0, \quad B_{,\overline{Y}} = B_{,p} = 0, \tag{2.3a}$$
$$A_{,Y\overline{Y}}\overline{B} - A_{,Y}\overline{B}_{,\overline{Y}} + 4\overline{B}^2 B_{,q} = 0, \tag{2.3b}$$
$$A_{,Y}A_{,\overline{Y}} - 8A_{,q}B\overline{B} = 0 \tag{2.3c}$$

for $B \neq 0$.

The electromagnetic field is given by the following equations:

$$F_{Y\overline{Y}} = F_{Yp} = F_{pq} = 0, \quad F_{Yq} = C \tag{2.4}$$

for $B = 0$, and

$$F_{Yp} = 0, \quad F_{Y\overline{Y}} = B - \overline{B}, \quad F_{pq} = -\tfrac{1}{2}p^{-2}(B + \overline{B}),$$
$$F_{Yq} = \tfrac{1}{2}p^{-1}B_{,Y} - \tfrac{1}{4}A_{,Y}\overline{B}^{-1} \tag{2.5}$$

for $B \neq 0$.

It is well known that λ is introduced into the Robinson–Trautman metrics in a very simple way.[5] This causes the absence of λ in Eqs. (2.2) and (2.3). Thus Eqs. (2.2)–(2.5) are special cases of the more general equations that have been given by Robinson *et al.*[6]

It is easy to see from Eqs. (1.2) and (2.1) that real function A is determined with an accuracy up to an arbitrary additive real constant since m is arbitrary. Thus condition $A = \text{const}$ is equivalent to condition $A = 0$.

The following transformations:

$$Y = Y' + \alpha, \quad Y = Y'e^{ia}, \quad q = q' + b \tag{2.6}$$

do not change Eqs. (1.2) and (2.1)–(2.5) for arbitrary constants α, a, and b, where α is complex and a and b are real.

In each of our space-times the vector field $k^{\mu} := \delta^{\mu}_{p}$ determines a congruence of the principal null curves of the electromagnetic field since it is a conclusion from Eqs. (1.2), (2.4), and (2.5) that $k_{[\mu}F_{\nu]\rho}k^{\rho} = 0$ and $k_{\mu}k^{\mu} = 0$. The last equation means that metric form (1.2) is also the Kerr–Schild

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metric form since $dq = k_\mu dx^\mu$. It is easy to prove (see, e.g., Refs. 3 and 4) that vector k^μ is geodetic, shear-free, rotation-free, its expansion does not vanish, and that it is a double Debever–Penrose vector.

III. LIST OF SOLUTIONS AND PETROV'S CLASSIFICATION

The explicit solutions of Eqs. (2.2) and (2.3) are as follows:

$$A = 2\int C\bar{C}\,dq, \quad B = 0, \tag{3.1}$$

$$A = 0, \quad B = \phi(Y), \tag{3.2}$$

where ϕ is an arbitrary analytic function of Y only,

$$A = 4ab(Y+\bar{Y}) + 2a^2q, \quad B = be^{ic}, \tag{3.3}$$

$$A = 4abY\bar{Y} + 2a^2q, \quad B = bY, \tag{3.4}$$

$$A = -8a^2q^{-1}e^{Y+\bar{Y}}, \quad B = ae^{Y}, \tag{3.5}$$

$$A = -\tfrac{2}{3}a^2(Y+\bar{Y})^2q^{-1/3} + 4abi(Y-\bar{Y}) + 6b^2q^{1/3},$$
$$B = ae^{ic}q^{1/3}, \tag{3.6}$$

$$A = 2a^2[-2xY\bar{Y} + b(Y^2+\bar{Y}^2)](x^2-b^2)^{-1}$$
$$+ [2ac(Y+\bar{Y}) - c^2](x+b)^{-1}$$
$$+ [2agi(Y-\bar{Y}) - g^2](x-b)^{-1},$$
$$B = ae^{ih}(x^2-b^2), \tag{3.7a}$$

where the auxiliary real variable x is determined by the equation

$$q = \tfrac{2}{5}x^5 - \tfrac{4}{3}b^2x^3 + 2b^4x, \tag{3.7b}$$

$$A = 4a^2bi(\ln\bar{Y} - \ln Y) + 2a^2b^2q, \quad B = ae^{ibq}Y^{-1}, \tag{3.8}$$

$$A = -2a^2(1+bi)\ln Y - 2a^2(1-bi)\ln\bar{Y}$$
$$+ \tfrac{1}{2}a^2(1+b^2)\ln q,$$
$$B = aq^{(1+bi)/2}Y^{-1}, \tag{3.9}$$

$$A = -4ab^2e^{a(\alpha+\bar{\alpha})q}Y^\alpha\bar{Y}^{\bar{\alpha}},$$
$$B = be^{a\alpha q}Y^{\alpha-1}, \quad \alpha\bar{\alpha} + 2(\alpha+\bar{\alpha}) = 0, \tag{3.10}$$

$$A = -8a^2kq^{-\alpha\bar{\alpha}k}Y^\alpha\bar{Y}^{\bar{\alpha}}, \quad B = aq^{2\alpha k}Y^{\alpha-1},$$
$$k^{-1} = \alpha\bar{\alpha} + 2(\alpha+\bar{\alpha}) \neq 0, \tag{3.11}$$

$$A = 2ab(Y^{-2}+\bar{Y}^{-2}) + 2a^2q(Y\bar{Y})^{-2},$$
$$B = e^{ic}(aqY^{-3} + bY^{-1}), \tag{3.12}$$

$$A = -\tfrac{2}{3}q^{-1/3}(aY\bar{Y}+b)^2, \quad B = aq^{1/3}Y, \tag{3.13}$$

where α is a complex constant arbitrary up to the appropriate limitations given in relations (3.10) and (3.11), and a, b, c, g, and h are arbitrary real constants. When integrating Eqs. (2.3) one obtains more complicated expressions for A and B than ours at right-hand sides of Eqs. (3.3)–(3.13). Those expressions include more arbitrary constants but they can be reduced to Eqs. (3.3)–(3.13) by means of transformations (2.6). When obtaining solution (3.5) the transformation $Y = cY'$, $p = c^{-1}p'$, $q = cq'$ has also been used. The same transformation has also been used to get a special case of solution (3.11), i.e., when $\mathrm{Re}\,\alpha = 1$ and $\mathrm{Im}\,\alpha \neq 0$. If $\alpha = 1$, then solution (3.11) is a special case of solution (3.7).

The above list includes *all* the exact solutions of Eqs. (1.1) with limitation (1.2). A proof of this theorem is given in Appendices A, B, and C.

Solution (3.1) has been given by Robinson and Trautman,[1] solution (3.2) by many authors,[3,6,7] and solutions (3.4), (3.5), and (3.13) have been given by Leroy.[8] The remaining solutions seem to be new [special cases of solutions (3.9), (3.10), and (3.11) have also been given in Ref. 8].

Each of our metrics is conformally flat if and only if $2m + A = B = 0$ (or equivalently $m = A = B = 0$).

When determining the Petrov types of our solutions we used Lemma 1 from Ref. 3 (cf. Ref. 4) since the premise of that lemma holds in the case of our metrics. It appears that only solution (3.1) is of type [2,2] (Penrose's notation). The remaining solutions are of type [2,1,1] with possibilities of further degenerating to type [2,2]. More precisely, for each one of our solutions we have the following: if it is not conformally flat, then it is of type [2,2] if and only if all equations

$$2(2m+A)A_{,YY} - 3(A_{,Y})^2 = 0, \tag{3.14a}$$

$$(2m+A)B_{,YY} + 2A_{,YY}B - 4A_{,Y}B_{,Y} = 0, \tag{3.14b}$$

$$3BB_{,YY} - 4(B_{,Y})^2 = 0 \tag{3.14c}$$

hold together.

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APPENDIX A: INTRODUCTORY REMARKS AND THE FIRST STEP OF THE PROOF

Our proof of the theorem, saying that Eqs. (2.1) and (3.1)–(3.13) are all solutions of Eqs. (1.1) with limitation (1.2), is too long to allow its presentation here in totality. Therefore, we give here only its scheme, putting emphasis on the more important items so as to permit anybody interested to easily carry out the proof himself in detail.

Notation: $D, E, F, \ldots$ are complex functions of two variables, Y and q, analytic in Y (or of $\bar{Y}$ and q analytic in $\bar{Y}$ for the symbol with an overbar). $K, L, M, \ldots$ are disposable complex functions of one real variable q; α is an arbitrary complex constant; a and b are arbitrary real constants. An integer subscript at any symbol does not change the above meaning of the symbol.

Assuming $B = 0$ one immediately obtains (3.1) from (2.2). Thus, henceforth, we put

$$B \neq 0. \tag{A1}$$

Integrating (2.3b) we get

$$A_{,Y} = -4\bar{B}(D + \bar{Y}B_{,q}), \tag{A2}$$

where D is a disposable function.

Assuming $B_{,q} = B_{,Y} = 0$ we easily obtain from (A2) and (2.3c) that $D = \alpha$ and then solution (3.3).

Let us assume $B_{,q} = 0$ and $B_{,Y} \neq 0$. If $D = 0$, then by (A2), (2.3c), and (A1) we immediately obtain solution (3.2). If $D \neq 0$, then by the fact that $A_{,Y\bar{Y}} = \bar{A}_{,\bar{Y}Y}$ and by (A2) we get $B_{,\bar{Y}}{}^{-1}D = K_1 = \bar{K}_1 \neq 0$, and then from (2.3c) we obtain $B_{,YY}\bar{B}_{,\bar{Y}}K_1^2 + 2B_{,Y}\bar{B}K_{1,q} = 0$. Assuming $B_{,YY} = 0$ we easi-

ly get solution (3.4). Assuming $B_{,YY} \neq 0$ we obtain solution (3.5) after a short calculation.

Thus all possibilities are exhausted for $B_{,q} = 0$ and henceforth, we put

$$B_{,q} \neq 0. \tag{A3}$$

Assuming $B_{,Y} = 0$ we obtain by the fact that $A_{,Y\bar{Y}} = \bar{A}_{,\bar{Y}Y}$ and by (A2) that $B = L_1 e^{i\alpha}$ and $L_1 = \bar{L}_1$, and then taking (2.3c)$_{,Y\bar{Y}}$ and (A2) we find that $D = YM_1 + N_1$. Now from (2.3c) we obtain among others that $M_1 = \alpha L_1^{-2}$ and $L_{1,q} L_1^2 = (bL_1 + \alpha\bar{\alpha})^{1/2}$. Then after simple calculations we find solution (3.6) for $b = 0$ and solution (3.7) for $b \neq 0$.

Thus all possibilities are exhausted for $B_{,Y} = 0$ and henceforth, we put

$$B_{,Y} \neq 0. \tag{A4}$$

Assumption:

$$1 + (B_{,Y}^{-1} B)_{,Y} = 0. \tag{A5}$$

From (A5) we have $B = (Y + K_2)^{-1} L_2$ and then by the fact that $A_{,Y\bar{Y}} = \bar{A}_{,\bar{Y}Y}$ and by (A2) we obtain $D = (Y + K_2)^{-2}(\bar{L}_2^{-1} M_2 - K_{2,q}\bar{K}_2 L_2) + (Y + K_2)^{-1} L_{2,q}\bar{K}_2$, where M_2 is real. Then from (2.3c) we get $M_2 = K_{2,q} = 0$ and $L_{2,q}\bar{L}_2 = \alpha \neq 0$. Putting $L_2 = N_2 \exp iP_2$, where N_2 and P_2 are real, we obtain among others $(N_2^2)_{,q} = a$ and then after short calculations we get solution (3.8) for $a = 0$ and solution (3.9) for $a \neq 0$.

Now we begin the more complicated part of the proof.

Assumption:

$$1 + (B_{,Y}^{-1} B)_{,Y} \neq 0. \tag{A6}$$

Since $A_{,Y\bar{Y}} = \bar{A}_{,\bar{Y}Y}$ we obtain from (A2) and (A6) that

$$D = (BE)_{,Y}, \tag{A7a}$$

$$B_{,q} = (BF)_{,Y}, \tag{A7b}$$

where

$$E := Y\bar{L} + K, \quad K = \bar{K}, \tag{A8a}$$

$$F := YM + L \neq 0, \quad M = \bar{M}. \tag{A8b}$$

Inequality $F \neq 0$ results from (A3) and (A7b).[9] Then the integration of (A2) gives us

$$A = -4[B\bar{B}(K + L\bar{Y} + \bar{L}Y + MY\bar{Y}) + N], \quad N = \bar{N}, \tag{A9}$$

and by (A2) and (A7)–(A9) we get from (2.3c) that

$$B_{,Y}[\bar{G}(Y + \bar{J})^2 + 3\bar{B}P(Y + \bar{J})] + B[\bar{H}(Y + \bar{J}) + \bar{B}(P + 2\bar{F}J_{,q})] + 2N_{,q} = 0, \tag{A10}$$

where

$$G := B_{,Y} F^2 + 3BFM, \tag{A11}$$

$$H := 3G + B(2F_{,q} - 4FM), \tag{A12}$$

$$J := EF^{-1} = (Y\bar{L} + K)(YM + L)^{-1}, \tag{A13}$$

$$P := L\bar{L} - KM = \bar{P}. \tag{A14}$$

Assuming $G = 0$ we obtain $M \neq 0$ and $B = QF^{-3}$ from (A11) and then from (A10) we get $N_{,q} = H = P = J_{,q} = 0$, which leads via a short calculation to a special case of solution (3.12) (i.e., if $b = c = 0$ there).

Henceforth, we put

$$G \neq 0. \tag{A15}$$

APPENDIX B: CONTINUATION OF ASSUMPTION (A6) FOR $P = 0$

Relations (A1)–(A4) and (A6)–(A15) hold here. Assumption $P = 0$ gives us

$$M \neq 0, \quad J = \bar{L}M^{-1}, \quad A = -4(B\bar{B}F\bar{F}M^{-1} + N). \tag{B1}$$

Integrating (A10) we find B and then differentiating the result once with respect to $\bar{Y}$ and several times with respect to Y we get rid of B and the integrals. In consequence we obtain a product equal to zero of an expression different from zero and of a polynomial of Y. Thus the coefficients of the polynomial, which depend on $\bar{Y}$ and q, are equal to zero. This procedure should be conducted twice, separately for $N_{,q} = 0$ and $N_{,q} \neq 0$.

This gives us among others

$$H = Q_1 G, \quad BFJ_{,q} = Q_2 G \tag{B2}$$

for $N_{,q} = 0$, and

$$J_{,q} = 0, \quad H(H_{,Y} - G_{,Y}) = 0 \tag{B3}$$

for $N_{,q} \neq 0$.

Assumption:

$$N_{,q} = 0. \tag{B4}$$

Assuming $J_{,q} \neq 0$ ($\Leftrightarrow Q_2 \neq 0$) and taking into account (A11) we find B from the second equation of (B2) and then substituting such a B into (A10) we obtain a contradictory result $J_{,q} = 0$. Thus $J_{,q} = 0$, which after the first transformation from (2.6) gives us

$$F = MY. \tag{B5}$$

Assuming $Q_1 = 3$ we get from (B2), (A12), and (B5) that $M = -(2q)^{-1}$ and then from (A10), (B1), and (2.3c) we obtain a special case of solution (3.12) (i.e., if $b = c = 0$ there).

Assuming $Q_1 \neq 3$ we get from (B2) that $\ln B = \ln Q_3 - [M^2(5 - 3Q_1) + 2M_{,q}]M^{-2}(3 - Q_1)^{-1} \ln Y$ and then by (B1) we obtain $Q_{1,q} = 0$ and an explicit expression of $Q_3(q)$ from (A2), (A7a), and (2.3c). Putting $Q_1 = 1 - \alpha$ we get $2M_{,q} + M^2[\alpha\bar{\alpha} + 2(\alpha + \bar{\alpha})] = 0$ from (A10) and then we obtain solution (3.10) for $M_{,q} = 0$ and solution (3.11) for $M_{,q} \neq 0$.

Assumption:

$$N_{,q} \neq 0. \tag{B6}$$

Since $J_{,q} = 0$ [see (B3)] thus (B5) holds also here.

If we assume $H = 0$, then it is easy to see that B which fulfills both (A10) and (A12) contradicts (A6). Thus, $H \neq 0$ and we obtain $H_{,Y} = G_{,Y}$ from (B3). Assuming $G_{,Y} \neq 0$ and differentiating (A10) with respect to $\bar{Y}$ we get a contradiction with (A6). Thus we have $G_{,Y} = H_{,Y} = 0$.

Inequality $H \neq 3G$ contradicts (A6) by (A12) and (B5). Thus, $H = 3G$ and we obtain $M = -(2q)^{-1}$ from (A12) and (B5). Then integrating (A10) we get from (B1) and (2.3c), after a simple calculation, solution (3.12).

APPENDIX C: CONTINUATION OF ASSUMPTION (A6) FOR $P \neq 0$

Relations (A1)–(A4) and (A6)–(A15) hold here. Applying for $P \neq 0$, the procedure that is described in the second

paragraph of Appendix B, we obtain

$$(HG^{-1})_{,Y}=0, \tag{C1a}$$

$$P+2FJ_{,q}=0 \tag{C1b}$$

for $N_{,q}=0$, and among others

$$(HG^{-1})_{,Y}(G_{,Y}-H_{,Y})=0 \tag{C2}$$

for $N_{,q}\neq 0$.

Let us assume $N_{,q}=0$. Relations (A4), (A10), (A15), and (C1b) give us then $H\neq 0$. Thus, from (C1a) we obtain $H=\bar{R}G$ and $R\neq 0$. Then (A10) and (C1b) give us $B=R_1(Y+\bar{R}_2)^{-R}$, where $R_2=J+3BPG^{-1}$. Substituting such a B into the latter [taking into account (A11)] we get a polynomial of Y equal to zero. Its coefficients (equal to zero) give us a system of algebraic equations involving L, $\bar{L}$, M, R, R_2, and $\bar{R}_2$. The system appears to be self-contradictory by the fact that $F, P, R\neq 0$. Thus we have

$$N_{,q}\neq 0. \tag{C3}$$

Let us assume $H=0$ and split our considerations into two separate cases $M=0$ and $M\neq 0$. The procedures are the same in both cases. We integrate (A12) getting B's and then after substitution of those B's into (A10) we obtain contradictions with (A4) for $M=0$ by (C3), and with (A6) for $M\neq 0$ by (C3), (A4), and (A15).

Thus we have $H\neq 0$ and assuming $H_{,Y}=0$ we get $G_{,Y}=0$ from (C2). If $H\neq 3G$, then from (A12) we obtain contradictions with (A4) for $M_{,q}=2M^2$ and with (A6) for $M_{,q}\neq 2M^2$. Thus we have $H=3G$. Integrating (A11) we get B that after substitution into (A10) gives us a polynomial of Y equal to zero. Its coefficients give us a self-contradictory system of equations depending on $\bar{Y}$ and q. The contradictions are caused by (A15) and equation $H=3G$ for $M=0$ and by (A6) and assumption $P\neq 0$ for $M\neq 0$. Thus we have

$$H_{,Y}\neq 0. \tag{C4}$$

The most general solution of (C2) is

$$H=GS+T,\quad (S-1)T=0, \tag{C5}$$

which by (C4) gives us

$$G_{,Y}S\neq 0. \tag{C6}$$

Differentiating (A10) with respect to $\bar{Y}$, then dividing it by $B_{,Y}\bar{G}_{,\bar{Y}}$ and differentiating once again with respect to Y and $\bar{Y}$ we obtain

$$\bar{E}_1+\bar{E}_2(B_{,\bar{Y}}^{-1}B)_{,Y}=0. \tag{C7}$$

Assumption:

$$E_2=0. \tag{C8}$$

This gives us by (C7)

$$E_1=0. \tag{C9}$$

Integrating (C8) and (C9) we get

$$2GJ+3BP=GU_1+U_2, \tag{C10}$$

$$HJ+B(P+2FJ_{,q})=GV_1+V_2. \tag{C11}$$

Using (C10) and (C11) in (A10) and differentiating (A10) with respect to $\bar{Y}$, and then dividing (A10) by $\bar{G}_{,\bar{Y}}$ and differentiating once again with respect to $\bar{Y}$ we obtain by (A4) an equation that after integration gives us

$$J(GU_1+U_2-GJ)=GW_1+W_2. \tag{C12}$$

Now let us use J as a new variable instead of Y. This is possible since $J_{,Y}=F^{-2}P\neq 0$. In the new variable language there is $F=P(\bar{L}-JM)^{-1}$.

Integrating (C10) and (C12) with respect to J [see (A11)] we obtain two expressions for B. Equating those expressions and differentiating the obtained equation with respect to J to get rid of integrals we obtain a polynomial of J equal to zero. Its coefficients give us a system of algebraic equations involving $\bar{L}$, M, U_1, U_2, W_1, and W_2. If $M=0$, then the system gives us $U_2=W_2=0$, which contradicts (A15) by (C12). If $M\neq 0$, then the system gives us $U_2\neq 0$ by (A15) and (C12) and then it gives us $U_1^2=4W_1$ and $U_1U_2=2W_2$ (if $L=0$, then $U_1=W_1=W_2=0$). This leads to a contradiction with (A4) by (C10) and (C12). Thus, the case $E_2=0$ is empty.

Assumption:

$$E_2\neq 0. \tag{C13}$$

Relations (C7) and (C13) give us $(B_{,\bar{Y}}^{-1}B)_{,YY}=0$. This equation has only two solutions with respect to Y. The first one is $B=U_3e^{UY}$ but it contradicts (A10) by (A4) and (C3). The second solution is

$$B=V_3(Y+V_4)^V. \tag{C14}$$

Substituting such a B into (A10) and taking into account (A6), which implies $V\neq -1$, we analyze (A10). Simple analysis gives us

$$T=0,\quad S=-1,\quad V=1 \tag{C15}$$

by (C5) and (C6). Then substituting B from (C14) into (A12) and using (A11), (C5), and (C15) we obtain a polynomial of Y equal to zero. Its coefficients give us a system of differential (with respect to q) equations involving L, M, and V_4. Solving the system with the use of (A8b) we get $M=(6q)^{-1}$, $L=\alpha q^{-1}$, and $V_4=6\alpha$. Then we obtain after a short calculation solution (3.13) by (A7b), (A9), and (2.3c).

This terminates the proof since all possibilities have been exhausted.

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Chiral and gravitational anomalies in any dimension

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Gravitational contributions to the chiral anomaly in $4N$ space-time dimensions as well as the purely gravitational anomaly in $4N-2$ dimensions are expressed in terms of the Riemann–Christoffel tensor. Using this formula, we give a simple proof that if $N \geqslant 4$ there is no way to cancel the gravitational anomalies using fields of spin-$\frac{1}{2}$, -$\frac{3}{2}$, and -1.

I. INTRODUCTION

It seems that physicists and mathematicians have independently developed the same theory of the chiral anomaly.[1,2] Motivated by the unification of gravity with other gauge fields in higher dimensions, many physicists have recently calculated the chiral anomalies due to gauge fields[3] as well as the gravitational field[4] in higher dimensions. They have searched for a consistent theory in which anomalies are canceled among fields of different representations of a gauge group and/or different spin. To arrive at their results they have resorted to Feynman diagram or path integral methods, neither procedure being too difficult to apply for external spin-1 fields. In the case of a gravitational field, however, it seems that the higher the dimension the more complicated the calculation becomes.[4,5] On the other hand, mathematicians[2] have studied the subject in arbitrary dimensions from the beginning but have expressed their results in their own fashion, in a terminology slightly unfamiliar to physicists. The mathematicians' results have often preceded the physicists' derivation.

Recognizing this fact, we shall express the mathematicians' expressions for the chiral anomaly (for "spin"-$\frac{1}{2}$ and -$\frac{3}{2}$ fields) in terms of the Riemann–Christoffel tensor more familiar to physicists. The newly discovered pure gravitational anomaly[6] receives contributions from spinor fields and antisymmetric tensor fields among others and it can also be written out in terms of the curvature tensor in a similar way to the chiral case. Finally, using the explicit formulas derived by us, we can discuss a cancellation of the gravitational anomaly among fields of different spin in arbitrary dimensions.

II. THE GENERATING FUNCTION AND THE COEFFICIENTS

Let us start by describing the mathematical terminology for the chiral anomaly in a gravitational background. The index theorem[2] tells us that the contributions of one left-handed spin-$\frac{1}{2}$ and one left-handed spin-$\frac{3}{2}$ field to the chiral anomaly in $D = 4N$ space-time dimensions are given, respectively, by

$$A_D^{1/2} = C_D \prod_{i=1}^{D/2} \frac{x_i/2}{\sinh(x_i/2)} \tag{1}$$

and

$$A_D^{3/2} = C_D \prod_{i=1}^{D/2} \frac{x_i/2}{\sinh(x_i/2)} \left[2 \sum_{j=1}^{D/2} \cosh x_j - 1 \right], \tag{2}$$

where

$$C_D = (4\pi)^{-D/2} \tag{3}$$

and the x_i's are defined as follows. The curvature tensor can be regarded as an antisymmetric two-form matrix R,

$$(R)^{ab} = R^{ab}{}_{\mu\nu} dx^\mu \wedge dx^\nu . \tag{4}$$

This antisymmetric $D \times D$ matrix can be expressed in terms of "eigenvalues" x_i's:

$$R = \begin{pmatrix} 0 & x_1 & & & & & \\ -x_1 & 0 & & & & & \\ & & 0 & x_2 & & & \\ & & -x_2 & 0 & & & \\ & & & & \ddots & & \\ & & & & & 0 & x_{D/2} \\ & & & & & -x_{D/2} & 0 \end{pmatrix}. \tag{5}$$

Given (1)–(5), the anomaly is written as

$$\int d^D x \, \partial_\mu (\sqrt{-g} J_5^\mu) = \int (A_D^{1/2} + A_D^{3/2}) \tag{6}$$

in the presence of one left-handed spin-$\frac{1}{2}$ and one left-handed spin-$\frac{3}{2}$ field in extended Minkowski space [i.e., one-time and $(D-1)$-space dimensions]. Here J_5^μ is a contravariant axial current composed of the spin-$\frac{1}{2}$, spin-$\frac{3}{2}$, and associated Fadeev–Popov–Nielsen ghosts.

The problem is to express (1) and (2) in terms of R in (5). Instead of treating each case separately, let us develop the problem in a more general way. We define

$$A_D = C_D \prod_{i=1}^{D/2} f(x_i), \tag{7}$$

where the function $f(x)$ is even in x and may take one of the forms (1) or (2) say. A simple computation, using (5), provides the relation between x and R:

$$\sum_{i=1}^{D/2} x_i^{2m} = \frac{1}{2} \mathrm{Tr}(iR)^{2m} . \tag{8}$$

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In terms of the lhs of (8), (7) is expanded and expressed in terms of R:

$$A_D = C_D \exp[\tfrac{1}{2}\,\mathrm{Tr}\ln f(iR)]\,. \tag{9}$$

Suppose the function $f(x)$ possesses the series expansion

$$f(x) = 1 + \sum_{n=1}^{\infty} b_n x^{2n}\,. \tag{10}$$

Then, with the help of the logarithmic function series, we may write (9) as

$$A_D = C_D \sum_{l=0}^{\infty} \frac{1}{l!}\left[\mathrm{Tr}\sum_{m=1}^{\infty} -\frac{1}{2m}\left\{-\sum_{n=1}^{\infty} b_n (iR)^{2n}\right\}^m\right]^l . \tag{11}$$

Hence the quantity A_D assumes the form

$$A_D = C_D \sum_{l=0}^{\infty} \frac{1}{l!}\left[\mathrm{Tr}\sum_{m=1}^{\infty} a_m R^{2m}\right]^l , \tag{12}$$

whereupon the desired final expression which includes only D-form terms reads

$$A_D = C_D \sum_{\{n_i\}}^{n_1+2n_2+\cdots+Nn_N=N} \frac{1}{n_1!n_2!\cdots n_N!} \times (a_1\,\mathrm{Tr}\,R^{\,2})^{n_1}(a_2\,\mathrm{Tr}\,R^{\,4})^{n_2}\cdots(a_N\,\mathrm{Tr}\,R^{\,2N})^{n_N}\,. \tag{13}$$

Here the summation over n_i runs from zero to a certain integer such that the constraint

$$n_1 + 2n_2 + 3n_3 + \cdots + Nn_N = N$$

is obeyed.

The problem is thus reduced to discovering how to express the $\{a_m\}$ in terms of the $\{b_n\}$. This can be done by picking up only $R^{\,2m}$ terms within the square brackets of (11). The answer is

$$a_m = \frac{(-1)^{m+1}}{2} \sum_{\{n_i\}}^{\Sigma jn_j = m} \frac{(n_1+n_2+\cdots+n_N-1)!}{n_1!n_2!\cdots n_N!} \times(-b_1)^{n_1}(-b_2)^{n_2}\cdots(-b_N)^{n_N}\,, \tag{14}$$

where one should notice that the summation is actually over a set of $\{n_i : 1\leqslant i\leqslant m\}$. The last step to our goal consists in replacing the constraint over the $\{n_i\}$, essentially a Kronecker delta, by

$$\delta_{m,n_1+2n_2+\cdots+Nn_N} = \frac{1}{2\pi}\int_0^{2\pi} d\theta\, e^{2i\theta(n_1+2n_2+\cdots+Nn_N-m)}\,. \tag{15}$$

[The factor of 2 in the exponent on the rhs of (15) is chosen for later convenience.] Then (14) can be written as

$$\begin{aligned} a_m &= \frac{(-1)^{m+1}}{4\pi}\int_0^{2\pi} d\theta\, e^{-2im\theta} \times\sum_{n=1}^{\infty}\frac{(-1)^n}{n}(b_1e^{2i\theta}+b_2e^{4i\theta}+\cdots+b_Ne^{2iN\theta})^n \\ &= \frac{i(-1)^{m+1}}{4\pi}\oint dz\, z^{-2m-1} \times\sum_{n=1}^{\infty}\frac{(-1)^n}{n}(b_1z^2+b_2z^4+\cdots+b_Nz^{2N})^n\,. \end{aligned} \tag{16}$$

Since $m\leqslant N$, we may add terms like $z^{2N+l}(l\geqslant 1)$ within the brackets of (16) without affecting the residue. In other words the interior of the bracket can be replaced by $f(z)-1$. This finally yields the elegant result

$$\begin{aligned} a_m &= \frac{i(-1)^{m+1}}{4\pi}\oint dz\, z^{-2m-1}\ln f(z) \\ &= \frac{i(-1)^{m+1}}{8\pi m}\oint dz\, z^{-2m}\frac{d}{dz}\ln f(z)\,, \end{aligned} \tag{17}$$

where the second line is obtained by partially integrating the first line and observing that $\ln f(z)/z^{2m}\to 0$ as $z\to\infty$. Summarizing, the answer is given by (13) with coefficients a_m's calculated by (17).

Now we are in a position to compute each case quickly.

(i) Spin-$\frac{1}{2}$ field: Here (1) provides the function

$$f(x) = (x/2)/\sinh(x/2) \tag{18}$$

and (17) reduces to

$$a_m^{1/2} = \frac{i(-1)^m}{8\pi m}\oint \frac{dz}{z^{2m}(e^z-1)}\,. \tag{19}$$

Since

$$\frac{z}{e^z-1} = \sum_{n=0}^{\infty} B_n\frac{z^n}{n!}\,,$$

where B_n is the Bernoulli number, we obtain

$$a_m^{1/2} = \frac{(-1)^{m+1}}{4m(2m)!}B_{2m}\,. \tag{20}$$

This result agrees with the one in Ref. 5 which was derived by a complicated Feynman graph calculation.

(ii) Spin-$\frac{3}{2}$ field: This case resembles the spin-$\frac{1}{2}$ field. The difference lies in the extra factor on the right of (2), which can be manipulated with the help of (8); viz.

$$\begin{aligned} 2\sum_j \cosh x_j &= \sum_{n=0}^{\infty}\frac{1}{(2n)!}\mathrm{Tr}(iR)^{2n} \\ &= \mathrm{Tr}(e^{iR}) \end{aligned} \tag{21}$$

where the last line is obtained because $\mathrm{Tr}(R^{\,2n+1})=0$. Recalling how we derived (13), and combining (12) with (21), we arrive at

$$A_D^{3/2} = C_D \sum_{\{n_i\}}^{n_0+n_1+2n_2+\cdots+Nn_N=N} \frac{1}{(2n_0)!n_1!n_2!\cdots n_N!} \times\left[\mathrm{Tr}(-R^{\,2})^{n_0} - \delta_{n_0,0}\right] \times(a_1^{1/2}\,\mathrm{Tr}\,R^{\,2})^{n_1}(a_2^{1/2}\,\mathrm{Tr}\,R^{\,4})^{n_2}\cdots(a_N^{1/2}\,\mathrm{Tr}\,R^{\,2N})^{n_N}\,. \tag{22}$$

The answer involves the spin-$\frac{1}{2}$ coefficients of (20). The first term in the square bracket in (22) represents the pure spin-$\frac{3}{2}$ part while the second term corresponds to the contribution of the fictitious particles.

Next we consider the purely gravitational anomaly[6] which arises in $(4N-2)$ dimensions in the context

$$\begin{aligned} &-\frac{1}{2}\int d^{\,4N-2}x\sqrt{-g}\;T^{\mu\nu}(D_\mu\epsilon_\nu + D_\nu\epsilon_\mu) \\ &\quad = 4\pi\int(D_a\epsilon_b - D_b\epsilon_a)\frac{\delta}{\delta R^{\,ab}}(A_{D=4N})\,. \end{aligned} \tag{23}$$

Here the lhs is the variation of the one-loop effective action for matter fields under the infinitesimal general coordinate

transformation $x^\mu \to x^\mu + \epsilon^\mu$, while the rhs comes by differentiating a certain $4N$-form A_{4N} with respect to a matrix element of the two-form matrix R of (4). If the rhs does not vanish it implies that invariance under the infinitesimal coordinate transformation is broken; equivalently when one writes the lhs of (23) as

$$\int d^{4N-2}x \sqrt{-g}\epsilon^\nu D^\mu T_{\mu\nu} ,$$

one infers that the induced energy-momentum tensor is not conserved. Indeed there are at least three kinds of field (spin-$\frac{1}{2}$, spin-$\frac{3}{2}$, and antisymmetric tensor) which can contribute to the rhs of (23). For spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$, A_{4N} is none other than the chiral anomaly (13), explicitly worked out in (20) and (22).

The corresponding quantity for an antisymmetric tensor field in $D = 4N$ dimensions is given by

$$A^{\frac{1}{2}}_D = -\frac{1}{8} C_D \prod_{i=1}^{D/2} \frac{x_i}{\tanh x_i} . \tag{24}$$

We can just as easily apply the former procedure to express (24) in terms of R by setting

$$f(x) = x/\tanh x . \tag{25}$$

This time (17) becomes

$$a^1_n = \frac{i(-1)^m}{2\pi m} \oint dz\, z^{-2m} \frac{e^{2z}}{e^{4z}-1}$$

$$= \frac{(-1)^{m+1}2^{4m}}{4m(2m)!} B_{2m}\left(\frac{1}{2}\right), \tag{26}$$

where we have used the generating function for the Bernoulli polynomial,

$$\frac{ze^{xz}}{e^z - 1} = \sum_{n=0}^{\infty} B_n(x) \frac{z^n}{n!} . \tag{27}$$

Combining (13) with (24), the antisymmetric contribution can be written as

$$A^{\frac{1}{2}}_D = -\frac{C_D}{8} \sum_{\{n_i\}}^{n_1 + 2n_2 + \cdots + Nn_N = N} \frac{1}{n_1! n_2! \cdots n_N!}$$

$$\times (a^1_1 \operatorname{Tr} R^2)^{n_1} (a^1_2 \operatorname{Tr} R^4)^{n_2} \cdots (a^1_N \operatorname{Tr} R^{2N})^{n_N} \tag{28}$$

with the coefficients derived in (26). Incorporating (28) into the rhs of (23) we easily obtain the antisymmetric tensor contribution to the gravitational anomaly.

At last we have all the information needed to look for a cancellation of the gravitational anomaly among fields of different spin. This problem has already been addressed by the authors of Ref. 6 who analyzed the expressions up to 14 dimensions. However, we are armed with general explicit formulas for $A^{1/2}_D$, $A^{3/2}_D$, and $A^{\frac{1}{2}}_D$ in arbitrary dimensions, and can tackle the problem more comprehensively. We give below the simple explicit analysis as an alternative to that of Ref. 6. Since we are seeking a nontrivial solution of the equation

$$c_1 A^{1/2}_D + c_2 A^{3/2}_D + c_3 A^{\frac{1}{2}}_D = 0 , \tag{29}$$

we may set $c_3 = 1$ in general. After obtaining the solution for c_1 and c_2 as rational numbers (if it exists) we can convert the solution to integers by appropriate multiplication.

In order to reveal an inconsistency in a certain dimension we need at least *three* equations for c_1 and c_2. We choose those three equations as the ones that provide the coefficients of $(\operatorname{Tr} R^2)^N$, $(\operatorname{Tr} R^2)^{N-2} \operatorname{Tr} R^4$, and $(\operatorname{Tr} R^2)^{N-3} \operatorname{Tr} R^6$, which are, respectively,

$$c_1 - (20N + 3)c_2 + (-8)^{N-1} = 0 , \tag{30}$$

$$c_1 - (20N - 285)c_2 - \tfrac{7}{2}(-8)^{N-1} = 0 , \tag{31}$$

$$c_1 - (20N + 435)c_2 + \tfrac{31}{4}(-8)^{N-1} = 0 . \tag{32}$$

Amazingly, Eqs. (30)–(32) are linearly dependent and give a unique solution

$$c_1 = (20N - 61)(-8)^{N-3} , \tag{33}$$

$$c_2 = (-8)^{N-3} . \tag{34}$$

This then is perfectly acceptable when $N = 1, 2$, and 3, i.e., in two, six, and ten space-time dimensions. For higher N there are further consistency conditions. It is enough to examine the coefficient of $(\operatorname{Tr} R^2)^{N-4}(\operatorname{Tr} R^4)^2$ which, if it is to vanish, necessitates that

$$c_1 - (20N - 573)c_2 + \tfrac{49}{4}(-8)^{N-1} = 0 . \tag{35}$$

There is now disagreement between (33), (34), and (35). And this proves that there is no way to cancel the gravitational anomalies among spin-$\frac{1}{2}$, spin-$\frac{3}{2}$, and antisymmetric tensor fields if $N \geqslant 4$, or in space-times of dimension $D \geqslant 14$. Of course it is not inconceivable that cancellation can be achieved by including extra fields belonging to even more exotic Lorentz group representations, if we are not deterred by the cause of renormalizability which is anyway lost.

Note added in proof: After submitting this paper, we received a preprint from Osaka by R. Endo and M. Takao who derive the gravitational anomalies for spin-$\frac{1}{2}$ and spin-$\frac{3}{2}$ via Fujikawa's path integral method. They give explicit answers up to 16 dimensions as in Ref. 6, which are particular cases of our general formulas (20), (22), and (28). Their paper is to be published in the Prog. Theor. Phys.

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Realization of latent ensembles of the statistical operator

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The statistical operator is a weighted sum, over eigenvalues of a complete commuting set of observables, of pure states each evolving unitarily from a microstate of the set. For every complete commuting set $\hat{\mathbf{q}}$ there is a latent ensemble, the diagonal projection of the statistical operator in $\hat{\mathbf{q}}$ representation, which determines the probabilities of observables in set $\hat{\mathbf{q}}$. When constraints imposed by a measurement situation makes these observables measurable, the latent $\hat{\mathbf{q}}$ ensemble is realized as the initial state of a new ensemble, which then evolves unitarily. Realization of a latent ensemble is an irreversible process with non-negative entropy increase. Reduced ensembles are realized when the constraints of the measurement situation permit only a subset of $\hat{\mathbf{q}}$ observables to be measurable. Successive realizations in response to changing measurement situations drive the system toward a state of maximum entropy. This mechanism explains the approach to equilibrium, and the change of an equilibrium system to an equilibrium state of increased entropy as constraints are relaxed.

I. INTRODUCTION

When the statistical operator (density matrix) of a system[1,2] evolves by unitary transformation in time, the entropy is constant. The von Neumann formula for the entropy of a system described by statistical operator $\hat{w}_t$ at time t is

$$S[\hat{w}_t] = -\operatorname{tr}[\hat{w}_t \ln(\hat{w}_t)], \tag{1.1}$$

which is invariant to unitary transformations. This appears to be an unsatisfactory result. It is well known, for example, that the entropy of an isolated system increases as the system irreversibly approaches equilibrium. The properties of entropy have been reviewed by Wehrl[3]; many other expressions for entropy have been formulated. However, only the definition given in (1.1) will be used in this paper. We follow von Neumann[4] in proposing a second mechanism, in addition to unitary transformation, for change of the statistical operator; one which increases the entropy of the system. It is the mechanism of realization of latent ensembles.

In Sec. II, a $\hat{\mathbf{v}}$ ensemble is described. It is the most general mixed state which can be formed from the eigenstates of observables in a complete commuting set $\hat{\mathbf{v}}$. It evolves by unitary transformation. Since this ensemble is a compact operator its spectrum must be discrete, which implies that the spectrum of $\hat{\mathbf{v}}$ must also be discrete. The requirement of discrete spectra for observables is discussed in Sec. III; it is a necessary requirement for the von Neumann formula for entropy given in (1.1). In Sec. IV the latent ensemble is defined for a complete commuting set of observables $\hat{\mathbf{q}}$. It is the diagonal projection of the statistical operator in $\hat{\mathbf{q}}$ representation, and it specifies the expectation values of the microstates of $\hat{\mathbf{q}}$ at any time. The latent $\hat{\mathbf{q}}$ ensemble may be realized as a $\hat{\mathbf{q}}$ ensemble, at which time it becomes the initial state of a new statistical operator which then evolves unitarily. As shown in Sec. V the evolution of the state of a system is described as a succession of ensembles each of which is a realization of a latent ensemble in the preceding one. It is proven in Sec. VI that the entropy of the system increases at each realization, unless the system is in equilibrium. In Sec. VII reduced ensembles for observables in a subset $\hat{\mathbf{u}}$ of the complete commuting set $\hat{\mathbf{q}}$ are described; they give the expectation values of the aggregates of microstates belonging to the degenerate eigenvalues $\mathbf{u}$. The microstates in a particular aggregate have equal statistical weights in the ensemble; for equilibrium ensembles this is the basis for the "fundamental postulate of equilibrium statistical mechanics." The entropy for the reduced ensemble for the subset $\hat{\mathbf{u}}$ of $\hat{\mathbf{q}}$ is greater than that for the $\hat{\mathbf{q}}$ ensemble for the complete commuting set $\hat{\mathbf{q}}$ when the statistical weights of the aggregates are specified. Measurement situations and the constraints which they impose are discussed in Sec. VIII; these considerations explain the approach of a system to equilibrium. Equilibrium ensembles are discussed in Sec. IX. The equilibrium state of a system is the state of highest entropy consistent with the constraints of the measurement situation.

II. STATISTICAL OPERATOR FOR A COMPLETE COMMUTING SET OF OBSERVABLES

If $\hat{\mathbf{v}}$ represents a complete commuting set[5] of observables of a quantum system and $|\mathbf{v}\rangle$ is a simultaneous eigenvector belonging to the set of eigenvalues $\mathbf{v}$ of $\hat{\mathbf{v}}$, then the vector at time t,

$$|\mathbf{v},t,t_0\rangle = \hat{U}_{t,t_0}|\mathbf{v}\rangle, \quad t \geqslant t_0 \tag{2.1}$$

evolves from its initial value $|\mathbf{v}\rangle$ at time t_0 as determined by the unitary time-evolution operator $\hat{U}_{t,t_0}$. For a system with time-dependent Hamiltonian $\hat{H}_t$,

$$\hat{U}_{t,t_0} = T\exp\left[\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t}\hat{H}_{t'}\,dt'\right], \tag{2.2}$$

where T is the Dyson time-ordering operator. A statistical operator (density matrix), which we term the $\hat{\mathbf{v}}$ ensemble, can be constructed from the vectors of (2.1) as

$$\begin{aligned} w_{t,t_0}(\hat{\mathbf{v}}) &= \int_{\mathbf{v}}|\mathbf{v},t,t_0\rangle w(\mathbf{v})\langle\mathbf{v},t,t_0| \\ &= \hat{U}_{t,t_0}w(\hat{\mathbf{v}})\,\hat{U}_{t,t_0}^{-1}, \quad t \geqslant t_0. \end{aligned} \tag{2.3}$$

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The notation $\int_{\mathbf{v}} \cdots$ indicates a spectral sum over the eigenvalues $\mathbf{v}$ of $\hat{\mathbf{v}}$. Since these eigenvalues are nondegenerate, the $\hat{\mathbf{v}}$ ensemble is the most general mixed state which can be formed from the eigenstates of observables in the commuting set $\hat{\mathbf{v}}$. The $\hat{\mathbf{v}}$ ensemble evolves unitarily from its initial value $w(\hat{\mathbf{v}})$ at $t = t_0$,

$$w(\hat{\mathbf{v}}) = \int_{\mathbf{v}} |\mathbf{v}\rangle w(\mathbf{v}) \langle \mathbf{v}|, \quad \hat{\mathbf{v}} = \int_{\mathbf{v}} |\mathbf{v}\rangle \mathbf{v} \langle \mathbf{v}|. \tag{2.4}$$

In (2.3) the time-independent eigenvalues $w(\mathbf{v})$ of $w_{t,t_0}(\hat{\mathbf{v}})$ are the statistical weights of the eigenstates $|\mathbf{v},t,t_0\rangle$ in the $\hat{\mathbf{v}}$ ensemble. They satisfy

$$w(\mathbf{v}) \geqslant 0, \quad \int_{\mathbf{v}} w(\mathbf{v}) = \mathrm{tr}[w_{t,t_0}(\hat{\mathbf{v}})] = 1. \tag{2.5}$$

Accordingly, $w_{t,t_0}(\hat{\mathbf{v}})$ is a positive Hermitian operator. It is also a compact (Hilbert–Schmidt) operator[6] so that its spectrum must be discrete; $w(\mathbf{v})$ can assume at most a denumerable infinity of real values. In (2.4) $|\mathbf{v}\rangle$ is an eigenvector of $w(\hat{\mathbf{v}})$ belonging to the discrete eigenvalue $w(\mathbf{v})$, and $|\mathbf{v}\rangle$ is also an eigenvector of $\hat{\mathbf{v}}$ belonging to the eigenvalue $\mathbf{v}$. It follows that the spectrum of the set of observables $\hat{\mathbf{v}}$, as well as that of $w(\hat{\mathbf{v}})$, must be discrete. The eigenvectors $|\mathbf{v}\rangle$ of $\hat{\mathbf{v}}$ and $w(\hat{\mathbf{v}})$, as well as the eigenvectors $|\mathbf{v},t,t_0\rangle$ of $w_{t,t_0}(\hat{\mathbf{v}})$, are normalized to unity, not to the Dirac delta or other distribution.

III. DISCRETE SPECTRUM OF OBSERVABLES

Many of the observables of quantum systems have spectra which are continuous, or continuous in part, with Dirac-delta normalization of their eigenvectors. However it has been shown[7] that over a continuous interval of its spectrum an observable is a "generalized coordinate" for which a conjugate "generalized momentum" can be found. A continuous interval in the spectrum of an observable can be replaced, to an arbitrary degree of accuracy, by a discrete spectrum and a parameter. The parameter is the length of the interval over which the spectrum of the conjugate observable extends. The eigenvalues of the discrete spectrum depend on the parameter, which controls the spacing between them, the spectrum becoming continuous only in the physically unattainable limit when the parameter becomes infinite. All parameters are finite, and therefore the spectra of all observables are discrete. Accordingly, the complete commuting set of observables $\hat{\mathbf{v}}$ with discrete spectra, which specifies the $\hat{\mathbf{v}}$ ensemble $w_{t,t_0}(\hat{\mathbf{v}})$, may comprise any commuting observables of the system. We shall ignore the dependence of the statistical operator on the parameters, treating them as constants. It should be noted that if the Hamiltonian depends on such parameters, then the changes in energy of the system which would occur if these parameters were varied would constitute work in the thermodynamic sense.

Since the spectrum of observables $\hat{\mathbf{v}}$ is discrete, the operator

$$\hat{P}(\mathbf{v}) = |\mathbf{v}\rangle \langle \mathbf{v}|, \quad \mathrm{trace}\, \hat{P}(\mathbf{v}) = 1, \tag{3.1}$$

is a projector. It specifies a microstate, a spectral state of a complete commuting set of observables. The $\hat{\mathbf{v}}$ ensemble of (2.3) becomes

$$w_{t,t_0}(\hat{\mathbf{v}}) = \int_{\mathbf{v}} w(\mathbf{v}) \hat{P}_{t,t_0}(\mathbf{v}), \tag{3.2}$$

where the pure state

$$\hat{P}_{t,t_0}(\mathbf{v}) = \hat{U}_{t,t_0} \hat{P}(\mathbf{v}) \hat{U}^{-1}_{t,t_0} \tag{3.3}$$

evolves unitarily from the microstate $\hat{P}(\mathbf{v})$ according to the von Neumann equation,

$$i\hbar\, \partial_t \hat{P}_{t,t_0}(\mathbf{v}) = \hat{\mathscr{L}}_t \hat{P}_{t,t_0}(\mathbf{v}), \quad \hat{P}_{t_0,t_0}(\mathbf{v}) = \hat{P}(\mathbf{v}), \tag{3.4}$$

in which $\hat{\mathscr{L}}_t$ is the commutation operator, $\hat{\mathscr{L}}_t = [\hat{H}_t, \ldots]$.

Since the spectrum of $\hat{\mathbf{v}}$ is discrete, the entropy of the $\hat{\mathbf{v}}$ ensemble can be defined by the von Neumann formula, (1.1),

$$\begin{aligned} S[w_{t,t_0}(\hat{\mathbf{v}})] &= -\mathrm{tr}\{w_{t,t_0}(\hat{\mathbf{v}}) \ln[w_{t,t_0}(\hat{\mathbf{v}})]\} \\ &= -\int_{\mathbf{v}} w(\mathbf{v}) \ln[w(\mathbf{v})], \end{aligned} \tag{3.5}$$

independently of time. Note that the entropy is constant when the statistical operator evolves by unitary transformation even though the Hamiltonian $\hat{H}_t$ may be time dependent.

IV. LATENT ENSEMBLES

Let $\hat{\mathbf{q}}$ represent a complete commuting set of observables of the system (other than, or the same as, $\hat{\mathbf{v}}$). In spectral representation,

$$\hat{\mathbf{q}} = \int_{\mathbf{q}} \mathbf{q} \hat{P}(\mathbf{q}), \quad \hat{1} = \int_{\mathbf{q}} \hat{P}(\mathbf{q}), \tag{4.1}$$

where $\hat{P}(\mathbf{q})$ is the projector

$$\hat{P}(\mathbf{q}) = |\mathbf{q}\rangle \langle \mathbf{q}|, \quad \mathrm{tr}\, \hat{P}(\mathbf{q}) = 1, \tag{4.2}$$

which specifies a $\mathbf{q}$ microstate belonging to the eigenvalue $\mathbf{q}$ in the discrete, nondegenerate spectrum of $\hat{\mathbf{q}}$.

The expectation of the $\mathbf{q}$ microstate when the statistical operator is the $\hat{\mathbf{v}}$ ensemble is

$$\begin{aligned} w_{t,t_0}(\hat{\mathbf{v}};\mathbf{q},\mathbf{q}) &= \mathrm{tr}\,[\hat{P}(\mathbf{q}) w_{t,t_0}(\hat{\mathbf{v}})] \\ &= \int_{\mathbf{v}} w(\mathbf{v}) |\langle \mathbf{q}| \hat{U}_{t,t_0} |\mathbf{v}\rangle|^2, \end{aligned} \tag{4.3}$$

which is a diagonal matrix element of $w_{t,t_0}(\hat{\mathbf{v}})$ in $\hat{\mathbf{q}}$ representation. Only these diagonal elements enter into the calculation of expectation values of functions of $\hat{\mathbf{q}}$ in the $\hat{\mathbf{v}}$ ensemble.

We define, within the $\hat{\mathbf{v}}$ ensemble, an ensemble which we term the latent $\hat{\mathbf{q}}$ ensemble. It is the diagonal projection of $w_{t,t_0}(\hat{\mathbf{v}})$ in $\hat{\mathbf{q}}$ representation,

$$\begin{aligned} w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}}) &= \int_{\mathbf{q}} \hat{P}(\mathbf{q}) \mathrm{tr}\,[\hat{P}(\mathbf{q}) w_{t,t_0}(\hat{\mathbf{v}})] \\ &= \int_{\mathbf{q}} |\mathbf{q}\rangle w_{t,t_0}(\hat{\mathbf{v}};\mathbf{q},\mathbf{q}) \langle \mathbf{q}|. \end{aligned} \tag{4.4}$$

From (2.5), (4.3), and (4.4),

$$w_{t,t_0}(\hat{\mathbf{v}};\mathbf{q},\mathbf{q}) \geqslant 0, \tag{4.5}$$

$$\mathrm{tr}\,[w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})] = \int_{\mathbf{q}} w_{t,t_0}(\hat{\mathbf{v}};\mathbf{q},\mathbf{q}) = 1, \tag{4.6}$$

so that the latent $\hat{\mathbf{q}}$ ensemble is a compact, positive, Hermitian operator. The von Neumann entropy of the latent $\hat{\mathbf{q}}$ ensemble is

$$S[w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})] = -\operatorname{tr}\{w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})\ln[w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})]\}$$
$$= -\int_{\mathbf{q}} w_{t,t_0}(\hat{\mathbf{v}};\mathbf{q},\mathbf{q})\ln[w_{t,t_0}(\hat{\mathbf{v}};\mathbf{q},\mathbf{q})]. \quad (4.7)$$

According to (4.3) this entropy depends on time unless both of the following conditions are satisfied: (1) the Hamiltonian is time independent, $\hat{H}_t = \hat{H}$, so that

$$\hat{U}_{t,t_0} = \exp[-i\hat{H}(t-t_0)/\hbar]; \quad (4.8)$$

and (2) $\hat{H}$ commutes with either one of the complete commuting sets $\hat{\mathbf{v}}$ or $\hat{\mathbf{q}}$.

The expectation values of the microstates $\hat{P}(\mathbf{q})$, and of all functions of $\hat{\mathbf{q}}$, are the same in the latent $\hat{\mathbf{q}}$ ensemble, $w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})$, as in the $\hat{\mathbf{v}}$ ensemble itself. Since $\hat{P}(\mathbf{q})$ is a projector in (4.4), its expectation value is

$$\operatorname{tr}[\hat{P}(\mathbf{q})w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})] = \operatorname{tr}[\hat{P}(\mathbf{q})w_{t,t_0}(\hat{\mathbf{v}})]. \quad (4.9)$$

The latent $\hat{\mathbf{q}}$ ensemble predicts the probabilities of the $\mathbf{q}$ microstates at time $t \geqslant t_0$ and, consequently, the results of measurement of any function of $\hat{\mathbf{q}}$, when the system is in a state described by the $\hat{\mathbf{v}}$ ensemble.

V. REALIZATION OF THE LATENT q ENSEMBLE

The latent $\hat{\mathbf{q}}$ ensemble may be realized as a $\hat{\mathbf{q}}$ ensemble, supplanting the $\hat{\mathbf{v}}$ ensemble as the statistical operator of the system at the moment of realization. Let the value of $w_{t,t_0}(\hat{\mathbf{V}};\mathbf{q},\mathbf{q})$ at time t_1 be

$$w_{t_1,t_0}(\hat{\mathbf{v}};\mathbf{q},\mathbf{q}) = w(\mathbf{q}). \quad (5.1)$$

The statistical operator of the system for $t \geqslant t_1$, which is conditional on the set of values of $w(\mathbf{q})$ for all eigenvalues $\mathbf{q}$, is the $\hat{\mathbf{q}}$ ensemble, the state prepared at t_1 from the microstates $\hat{P}(\mathbf{q})$ with statistical weights $w(\mathbf{q})$. The $\hat{\mathbf{q}}$ ensemble for $t \geqslant t_1$ is

$$w_{t,t_1}(\hat{\mathbf{q}}) = \int_{\mathbf{q}} w(\mathbf{q})\hat{P}_{t,t_1}(\mathbf{q}), \quad \hat{P}_{t,t_1}(\mathbf{q}) = \hat{U}_{t,t_1}\hat{P}(\mathbf{q})\,\hat{U}_{t,t_1}^{-1}. \quad (5.2)$$

It is the realization of the latent $\hat{\mathbf{q}}$ ensemble at t_1. According to (5.1) the statistical weights $w(\mathbf{q})$ of the pure states $\hat{P}_{t,t_1}(\mathbf{q})$ in the $\hat{\mathbf{q}}$ ensemble are the expectation values of the $\mathbf{q}$ microstates in the latent $\hat{\mathbf{q}}$ ensemble at t_1. The latent $\hat{\mathbf{q}}$ ensemble is the initial value of the statistical operator $w_{t,t_1}(\hat{\mathbf{q}})$ for $t \geqslant t_1$. The von Neumann entropy of the $\hat{\mathbf{q}}$ ensemble is

$$S[w_{t,t_1}(\mathbf{q})] = -\int_{\mathbf{q}} w(\mathbf{q})\ln[w(\mathbf{q})], \quad (5.3)$$

independent of time for $t \geqslant t_1$, the same as that given in (4.7) for the latent $\hat{\mathbf{q}}$ ensemble at t_1.

In the preceding, the observables $\hat{\mathbf{q}}$ can be any complete commuting set among all the observables of the system. In the statistical operator $w_{t,t_0}(\hat{\mathbf{v}})$ in (2.3), for each such set $\hat{\mathbf{q}}$ there is a latent $\hat{\mathbf{q}}$ ensemble, $w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})$ in (4.4). Any one of these $\hat{\mathbf{q}}$ ensembles has the potentiality for realization at some time $t_1 > t_0$. Realization of a latent ensemble is an actual physical transformation of the system. It is the first step in any measuring process: identification of the set of $\mathbf{q}$ microstates as the set on which measurements will be made. It can be likened to an ideal pass filtration[8] which passes the entire spectrum of $\mathbf{q}$ microstates of the complete commuting set $\hat{\mathbf{q}}$ while preserving their statistical weights.

Comparison of the expression for $w_{t,t_0}(\hat{\mathbf{v}})$ in (3.2) with that for $w_{t,t_1}(\hat{\mathbf{q}})$ in (5.2) shows that $w_{t,t_0}(\hat{\mathbf{v}})$ itself can be considered to have been realized at t_0 from the latent $\hat{\mathbf{v}}$ ensemble of a prior statistical operator. The evolution of the state of a system is described, accordingly, as a succession of ensembles each of which is a realization of a latent ensemble in the preceding one. The initial time for each ensemble is the moment of its realization. Each ensemble is a weighted average of pure states which evolve unitarily from the microstates of some complete commuting set of observables at its initial time. The statistical weight of each pure state in the ensemble is the same as the probability, specified at the initial time, of the microstate from which it evolves, and the entropy of the system, determined by these statistical weights, remains constant.

VI. ENTROPY CHANGE WHEN LATENT ENSEMBLE IS REALIZED

Although the von Neumann entropy of a system which is evolving unitarily is constant, at the moment of realization of a latent ensemble the entropy of the system will increase (unless the system is in equilibrium, in which case the entropy remains constant). The theorem to be demonstrated is

$$S[w_{t,t_1}(\hat{\mathbf{q}})] \geqslant S[w_{t,t_0}(\hat{\mathbf{v}})], \quad (6.1)$$

where the entropy of the $\hat{\mathbf{v}}$ ensemble is given in (3.5) for $t_1 \geqslant t \geqslant t_0$ and that of the $\hat{\mathbf{q}}$ ensemble is given in (5.3) for $t \geqslant t_1$.

Klein's inequality[9] for two real numbers, $x \geqslant 0$, $y \geqslant 0$, is

$$y\ln x - y\ln y \leqslant x - y, \quad (6.2)$$

with the equality holding for $x = y$. (It follows from the inequality, easily demonstrated graphically,

$$\ln x \leqslant x - 1, \quad x \geqslant 0$$

on replacing x by x/y and multiplying the result by y.) Let $y = w(\mathbf{v})$, $x = w(\mathbf{q})$. Then from (6.2),

$$\int_{\mathbf{v}}\int_{\mathbf{q}} |\langle\mathbf{q}|\hat{U}_{t_1,t_0}|\mathbf{v}\rangle|^2\{w(\mathbf{v})\ln[w(\mathbf{q})] - w(\mathbf{v})\ln[w(\mathbf{v})]$$
$$- w(\mathbf{q}) + w(\mathbf{v})\} \leqslant 0. \quad (6.3)$$

But from (5.1) and (4.3),

$$w(\mathbf{q}) = \int_{\mathbf{v}} |\langle\mathbf{q}|\hat{U}_{t_1,t_0}|\mathbf{v}\rangle|^2 w(\mathbf{v}). \quad (6.4)$$

Also,

$$\int_{\mathbf{q}} |\langle\mathbf{q}|\hat{U}_{t_1,t_0}|\mathbf{v}\rangle|^2 = \int_{\mathbf{v}} |\langle\mathbf{q}|\hat{U}_{t_1,t_0}|\mathbf{v}\rangle|^2 = 1. \quad (6.5)$$

Therefore, from (6.3),

$$\int_{\mathbf{q}} w(\mathbf{q})\ln[w(\mathbf{q})] - \int_{\mathbf{v}} w(\mathbf{v})\ln[w(\mathbf{v})] \leqslant 0, \quad (6.6)$$

so that (6.1) follows, and the theorem is proved. The equality holds in (6.1) when $w(\mathbf{q}) = w(\mathbf{v})$ in (6.4). This is the case if the Hamiltonian is time independent so that (4.8) holds, and if both sets $\hat{\mathbf{q}}$ and $\hat{\mathbf{v}}$ are the same and commute with $\hat{H}$. In this case no change occurs in the statistical operator at t_1; the system is in equilibrium.

The physical basis for the inequality (6.1) is the following: when a particular latent $\hat{\mathbf{q}}$ ensemble $w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})$ is realized at t_1 the potentiality for realization of latent ensembles for other complete commuting sets of observables is lost, togeth-

er with the information which they contain regarding the microstates of those observables. This loss of information results on replacement of the statistical operator $w_{t,t_0}(\hat{\mathbf{v}})$ by its diagonal projection in $\hat{\mathbf{q}}$ representation,[10] the statistical operator $w_{t,t_1}(\hat{\mathbf{q}})$ at $t = t_1$. Since $w_{t,t_0}(\hat{\mathbf{v}})$ cannot be reconstructed from its diagonal elements in a single $\hat{\mathbf{q}}$ representation alone, the realization of a latent ensemble is an irreversible process, as indicated by the entropy increase in (6.1).

VII. REDUCED STATISTICAL OPERATORS

The latent $\hat{\mathbf{q}}$ ensemble $w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})$ depends on the expectation values of the microstates $\hat{P}(\mathbf{q})$ for a complete commuting set of observables $\hat{\mathbf{q}}$. We now consider reduced ensembles which depend on probabilities for only a subset $\hat{\mathbf{u}}$ from the set $\hat{\mathbf{q}}$. Let $\hat{\mathbf{u}}_c$ be the complementary set to $\hat{\mathbf{u}}$ in $\hat{\mathbf{q}}$, and let the eigenvalues of $\hat{\mathbf{u}}$ be $\mathbf{u}$, of $\hat{\mathbf{u}}_c$ be $\mathbf{u}_c$. Define the projector

$$\hat{P}(\mathbf{u}) = \int_{\mathbf{u}_c} \hat{P}(\mathbf{q}), \quad g(\mathbf{u}) = \mathrm{tr}[\hat{P}(\mathbf{u})]. \tag{7.1}$$

Here, $\hat{P}(\mathbf{u})$ represents the aggregate of $\mathbf{q}$ microstates belonging to the degenerate eigenvalue $\mathbf{u}$, and $g(\mathbf{u})$ is the multiplicity of $\mathbf{u}$. Accordingly,

$$\int_{\mathbf{u}} \hat{P}(\mathbf{u}) = \int_{\mathbf{q}} \hat{P}(\mathbf{q}) = \hat{1}, \quad \hat{\mathbf{u}} = \int_{\mathbf{u}} \mathbf{u}\hat{P}(\mathbf{u}). \tag{7.2}$$

The expectation values of $\hat{\mathbf{u}}$ and of all functions of $\hat{\mathbf{u}}$ in the $\hat{\mathbf{v}}$ ensemble are determined by the expectations of $\hat{P}(\mathbf{u})$. From (4.3) and (7.1) these are

$$\mathrm{trace}[\hat{P}(\mathbf{u})w_{t,t_0}(\hat{\mathbf{v}})] = \int_{\mathbf{u}_c} w_{t,t_0}(\mathbf{v};\mathbf{q},\mathbf{q}). \tag{7.3}$$

The latent $\hat{\mathbf{u}}$ ensemble is the diagonal projection of $w_{t,t_0}(\hat{\mathbf{v}})$,

$$\begin{aligned} w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{u}}) &= \int_{\mathbf{q}} \mathrm{tr}\left[w_{t,t_0}(\hat{\mathbf{v}})\frac{\hat{P}(\mathbf{u})}{g(\mathbf{u})}\right]\frac{\hat{P}(\mathbf{u})}{g(\mathbf{u})} \\ &= \int_{\mathbf{u}} \hat{P}(\mathbf{u})\mathrm{tr}\left[w_{t,t_0}(\hat{\mathbf{v}})\frac{\hat{P}(\mathbf{u})}{g(\mathbf{u})}\right]. \end{aligned} \tag{7.4}$$

The latent $\hat{\mathbf{u}}$ ensemble is a compact, positive, Hermitian operator with unit trace. Since $\hat{P}(\mathbf{u})$ is a projector, its expectation value (and that of any function of $\hat{\mathbf{u}}$) in the latent $\hat{\mathbf{u}}$ ensemble, $w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{u}})$, is the same as in $w_{t,t_0}(\hat{\mathbf{v}})$.

Realization of the latent $\hat{\mathbf{u}}$ ensemble at a time t_1 gives the $\hat{\mathbf{u}}$ ensemble, the statistical operator for $t \geqslant t_1$,

$$w_{t,t_1}(\hat{\mathbf{u}}) = \int_{\mathbf{u}} \hat{P}_{t,t_1}(\mathbf{u})\frac{w(\mathbf{u})}{g(\mathbf{u})}, \quad \hat{P}_{t,t_1} = \hat{U}_{t,t_1}\hat{P}(\mathbf{u})\,\hat{U}_{t,t_1}^{-1}, \tag{7.5}$$

where

$$w(\mathbf{u}) = \mathrm{tr}[\hat{P}(\mathbf{u})w_{t,t_0}(\hat{\mathbf{v}})]. \tag{7.6}$$

The von Neumann entropy for the $\hat{\mathbf{u}}$ ensemble is

$$S[w_{t,t_1}(\hat{\mathbf{u}})] = -\int_{\mathbf{u}} w(\mathbf{u})\ln\left[\frac{w(\mathbf{u})}{g(\mathbf{u})}\right], \tag{7.7}$$

independent of time for $t \geqslant t_1$.

In (5.3) the entropy of the $\hat{\mathbf{q}}$ ensemble realized at t_1 from the latent ensemble $w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})$ is specified by the statistical weights $w(\mathbf{q})$ of the individual microstates $\hat{P}(\mathbf{q})$. In (7.7) the entropy of the $\hat{\mathbf{u}}$ ensemble is specified by the statistical weights $w(\mathbf{u})$ of the aggregates $\hat{P}(\mathbf{u})$. It can be shown that

$$S[w_{t,t_1}(\hat{\mathbf{u}})] \geqslant S[w_{t,t_1}(\hat{\mathbf{q}})], \tag{7.8}$$

for all $\hat{\mathbf{q}}$ ensembles satisfying the condition that

$$\int_{\mathbf{u}_c} w(\mathbf{q}) = w(\mathbf{u}), \tag{7.9}$$

for specified values of $w(\mathbf{u})$ for the aggregates. We vary $w(\mathbf{q})$ in $S[w_{t,t_1}(\mathbf{q})]$ given by (5.3) to obtain the maximum subject to the constraints (7.9), getting

$$\int_{\mathbf{q}} \{-\ln[w(\mathbf{q})] + \lambda(\mathbf{u})\}\delta w(\mathbf{q}) = 0, \tag{7.10}$$

with Lagrange multipliers $\lambda(\mathbf{u})$. Accordingly, the values of $w(\mathbf{q})$ which maximize $S[w_{t,t_1}(\hat{\mathbf{q}})]$ are

$$w^m(\mathbf{q}) = w(\mathbf{u})/g(\mathbf{u}), \tag{7.11}$$

for the microstates $\hat{P}(\mathbf{q})$ in the aggregate $\hat{P}(\mathbf{u})$. The $\hat{\mathbf{q}}$ ensemble with these statistical weights is

$$w^m_{t,t_1}(\hat{\mathbf{q}}) = \int_{\mathbf{q}} \hat{P}_{t,t_1}(\hat{\mathbf{q}})w^m(\mathbf{q}) = w_{t,t_1}(\hat{\mathbf{u}}). \tag{7.12}$$

Accordingly the theorem of (7.8) and (7.9) is proven. From (7.11) the $g(\mathbf{u})$ microstates $\hat{P}(\mathbf{q})$ which belong to the same degenerate eigenvalue $\mathbf{u}$ of $\hat{\mathbf{u}}$ all have the same expectation value $w^m(\mathbf{q})$ in the initial $\hat{\mathbf{u}}$ ensemble at t_1.

Since the initial values of the $\hat{\mathbf{q}}$ ensemble and the $\hat{\mathbf{u}}$ ensemble are the latent ensembles from which they are realized at t_1, and since t_1 may be any time after t_0, it follows from (7.8) and (7.9) that

$$S[w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{u}})] \geqslant S[w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})], \tag{7.13}$$

for all latent $\hat{\mathbf{q}}$ ensembles $w_{t,t_0}(\hat{\mathbf{v}};\hat{\mathbf{q}})$ satisfying the condition

$$\int_{\mathbf{u}_c} \mathrm{tr}[w_{t,t_0}(\hat{\mathbf{v}})\hat{P}(\mathbf{q})] = \mathrm{tr}[w_{t,t_0}(\hat{\mathbf{v}})\hat{P}(\mathbf{u})], \tag{7.14}$$

for specified values of $\mathrm{tr}[w_{t,t_0}(\hat{\mathbf{v}})\hat{P}(\mathbf{u})]$. In the latent $\hat{\mathbf{u}}$ ensemble, the $g(\mathbf{u})$ microstates $\hat{P}(\mathbf{q})$ belonging to the degenerate eigenvalue $\mathbf{u}$ of $\hat{\mathbf{u}}$ have the same probability, equal to $\mathrm{tr}[w_{t,t_0}(\hat{\mathbf{v}})\hat{P}(\mathbf{u})]/g(\mathbf{u})$.

In Sec. V we likened the realization of the latent ensemble $w(\hat{\mathbf{v}};\hat{\mathbf{q}})$to an ideal pass filtration of the microstates $\hat{P}(\mathbf{q})$; we may liken the realization of a latent $\hat{\mathbf{u}}$ ensemble to a filtration of $\mathbf{q}$ microstates with a coarse filter which passes the aggregates $\hat{P}(\mathbf{u})$ while preserving their statistical weights and allotting an equal fraction $1/g(\mathbf{u})$ of the weight of the aggregate $\hat{P}(\mathbf{u})$ to each of its microstates.

VIII. THE MEASUREMENT SITUATION; APPROACH TO EQUILIBRIUM

A quantum system is described by its observable, a collection of self-adjoint Hermitian operators with a common domain of Hermiticity.[7] If the observables in the complete commuting set $\hat{\mathbf{q}}$ are to be measured, the system must be constrained so that the probabilities of the $\hat{\mathbf{q}}$ microstates can be assessed. Constraints isolate the system, regulating its interactions with its surroundings in order that the observables in $\hat{\mathbf{q}}$ should be measurable. We use the term $\hat{\mathbf{u}}$ measurement situation when the imposed constraints are appropriate to determine the probabilities of the $\hat{P}(\mathbf{u})$ aggregates of the microstates $\hat{P}(\mathbf{q})$. In a $\hat{\mathbf{u}}$ measurement situation the observables in the complementary set $\hat{\mathbf{u}}_c$ in $\hat{\mathbf{q}}$ are not measurable. The

most highly constrained measurement situation is the one in which the subset $\hat{\mathbf{u}}$ is the entire commuting set $\hat{\mathbf{q}}$, and the aggregates $\hat{P}(\mathbf{u})$ each consist of only one microstate $\hat{P}(\mathbf{q})$. The fewer the observables in the subset $\hat{\mathbf{u}}$ to be measurable, the fewer the constraints needed in the measurement situation and the larger the aggregate $\hat{P}(\mathbf{u})$. When the constraints of a $\hat{\mathbf{u}}$ measurement situation are imposed, the response of the system is realization of the latent $\hat{\mathbf{u}}$ ensemble compatible with the imposed constraints. Thereafter the statistical operator evolves by unitary transformation until the next measurement situation occurs. A measurement situation may arise naturally in the development of the interaction between a system and its surroundings, or it may be contrived in the laboratory (the motivation is irrelevant).

These considerations explain the approach of a system to equilibrium. For any statistical operator of the system at a given time, realization of a latent ensemble will increase the entropy of the system according to (6.1) unless the system is in equilibrium. In equilibrium the Hamiltonian $\hat{H}$ is time independent, and the measurement situation permits realization of an ensemble for a set of observables which commute with $\hat{H}$. Until these conditions are met the state of the system will change through successive realization of latent ensembles, which increase the entropy to a maximum value when equilibrium is attained.

IX. EQUILIBRIUM ENSEMBLES

If the constraints imposed by the measurement situation are relaxed so that the Hamiltonian itself is the only measurable observable in the subset $\hat{\mathbf{u}}$ of the commuting set $\hat{\mathbf{q}}$, then the equilibrium ensemble is an $\hat{H}$ ensemble, a state of higher entropy than $w_{\rm eq}(\hat{\mathbf{q}})$ according to (7.8). In this case, from (7.12),

$$w_{\rm eq}(\hat{H}) = \int_E \frac{\hat{P}(E)w(E)}{g(E)} = \int_{\mathbf{q}} \hat{P}(\mathbf{q})w^m(\mathbf{q}) = w^m_{\rm eq}(\hat{\mathbf{q}}), \tag{9.1}$$

where E is an eigenvalue of $\hat{H}$. This ensemble satisfies the so-called fundamental postulate of equilibrium statistical mechanics: all microstates of a given energy have the same probability in a system at equilibrium.[11] According to (7.11) this probability is

$$w^m(\mathbf{q}) = w(E)/g(E). \tag{9.2}$$

The microcanonical ensemble is a special case of the $\hat{H}$ ensemble when the constraints of the measurement situation impose complete isolation of the system from its surroundings. In this case $w(E) = \delta_{E,E_0}$ where E_0 is the energy of the isolated system. The von Neumann entropy for the $\hat{H}$ ensemble is

$$S[w_{\rm eq}(\hat{H})] = \int_E w(E)\ln[g(E)] - \int_E w(E)\ln[w(E)], \tag{9.3}$$

which is greater than the weighted sum of the entropies, $\ln[g(E)]$, for the individual microcanonical ensembles of energy E.

Of the possible equilibrium states of a system, described by statistical operators which commute with the time-independent Hamiltonian, the $\hat{\mathbf{q}}$ ensemble, $w_{\rm eq}(\hat{\mathbf{q}})$, is the state with the lowest entropy. The actual equilibrium state will be the one with the maximum entropy compatible with the constraints of the measurement situation. Any equilibrium state with entropy less than this maximum will contain latent ensembles of higher entropy whose realizations, in accordance with (6.1), will increase the entropy of the system, driving it to the state of maximum entropy consistent with the constraints. Accordingly the statistical operator $w_{\rm eq}(\hat{\mathbf{q}})$ will change to $w_{\rm eq}(\hat{H})$ as the system is driven to the state of higher entropy when the constraints of the $\hat{\mathbf{q}}$ measurement situation are relaxed to those of the $\hat{H}$ measurement situation. The constraints may be relaxed further by requiring, for example, that only the average value of $\hat{H}$ be specified, instead of the probabilities $w(E)$ of each aggregate $\hat{P}(E)$ in $w_{\rm eq}(\hat{H})$. The new equilibrium state with maximum entropy subject to this constraint is, of course, the canonical ensemble whose temperature is determined by the specified average value of $\hat{H}$.

In the $\hat{H}$ ensemble and the canonical ensemble the subset $\hat{\mathbf{u}}$ of the complete commuting set $\hat{\mathbf{q}}$ contains the single observable $\hat{H}$. When the number operator commutes with $\hat{H}$, $\hat{\mathbf{u}}$ may include both $\hat{H}$ and $\hat{N}$. If the constraints permit both to be measurable, then, from (7.12), the equilibrium statistical operator is

$$w_{\rm eq}(\hat{H},\hat{N}) = \int_E \int_N \frac{\hat{P}(E,N)w(E,N)}{g(E,N)}. \tag{9.4}$$

In petit ensembles, the number of particles in the system is a specified number N_0, so that $w(E,N) = w(E,N_0)\delta(N,N_0)$, and $w_{\rm eq}(\hat{H},\hat{N})$ becomes the same as $w_{\rm eq}(\hat{H})$ when reference to N_0 is suppressed. But if the constraints on the system described by (9.4) are relaxed by requiring that only the average values $\langle\hat{H}\rangle$ and $\langle\hat{N}\rangle$ be specified, the new equilibrium state of maximum entropy subject to these constraints is the grand canonical ensemble whose temperature and chemical potential are determined, respectively, by the specified values of $\langle\hat{H}\rangle$ and $\langle\hat{N}\rangle$.

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Tiling, periodicity, and crystals

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A result on nonperiodic tilings is generalized and related to the problem of the origin of crystalline symmetry.

I. INTRODUCTION

It is a very general physical phenomenon that the molecular configurations of matter tend to be crystalline, i.e., periodic, at low temperature (and any pressure, specifically low pressure). There is a major gap in the understanding of this phenomenon[1–4] and it is of a mathematical character of independent interest, as described below.

Using statistical mechanics one can model matter as follows. The possible state of each molecule is viewed as a random variable with the joint distribution of (many molecule) configurations given by a standard Gibbs ensemble, a known probability measure. At low temperature and pressure the measure is concentrated (uniformly) on those configurations with minimal total energy, where the total energy of a configuration is the sum over energy distributions from pairs (and to a minor extent by triplets, etc.) of neighboring molecules. Thus in this low-temperature, low-pressure limit the variables in a sense lose their randomness and one sees that configurations minimizing such a sum are expected to have a strong tendency to be periodic. The feature we wish to emphasize is that solutions of some general class of minimization problems should necessarily exhibit nontrivial symmetries.

It is a major open question in physics to understand the generality in which this scheme (the "crystal problem") is true and the basic mechanisms behind it.[1–4] Aside from its relevance to physics this problem is also of mathematical significance in its relation to the many optimization problems, such as the isoperimetric problem, for which solutions exhibit symmetries which are not easily understood. For the isoperimetric and some related problems a method due to Steiner has elucidated the symmetry of the solutions.[5] Such an approach would be welcome for the crystal problem; perhaps its shadow has appeared.[6]

The first real progress in the crystal problem has emerged in the last decade and consists mostly of rather specific (classical mechanical) models in one and two space dimensions, usually modeling molecular-bonded solids.[6–19] The mathematical framework is the following. One considers a countable family of variables, $\{z_j \mid j \in N\}$, each having values in some space W of the form $W = X \times S$, where X is "physical space," usually either $\mathbb{R}^d$ or a discrete analog such as $\mathbb{Z}^d$, and S is an "internal space," often finite. In this paper we will only consider classical discrete models, with $X = \mathbb{Z}^d$ and $S = \{1, 2, \ldots, N\}$. Since physically two variables may not simultaneously have common X coordinates it is convenient to use $\mathbb{Z}^d$ itself to index the variables. We will only consider two-body, translation-invariant, finite-range potential energy functions, that is, real symmetric ("potential") functions V on $W' \times W'$, $W' \equiv X \times S$, such that for all u, z, w in $\mathbb{Z}^d$ and s, t in S

$$V[(z, s), (w, t)] = V[(z + u, s), (w + u, t)], \tag{1}$$

$$V[(z, s), (w, t)] = 0 \quad \text{unless } 1 \leqslant |z - w|_\infty \leqslant D, \quad D \text{ a fixed constant.} \tag{2}$$

($|V|_p$ denotes the p norm of $V \in \mathbb{Z}^d$; we will be using only $p = 1, \infty$.) Since we are analyzing infinite-molecule configurations the total energy is not directly accessible; we define "ground states" in the DLR sense[20,21] as follows. A "configuration" $f' \in S^{\mathbb{Z}^d} \equiv T$ is a "ground state with respect to (a given potential) V", ($f' \in T_V$), if for every finite subset C of $\mathbb{Z}^d$ and every other configuration f'' such that f'' and f' agree on all sites not in C, it follows that $E_{C,V}(f') \leqslant E_{C,V}(f'')$. Here $E_{C,V}$ is defined for an arbitrary f in T by

$$E_{C,V}(f) = \sum_{\{z,w\}} \sum_{\cap C \neq \varnothing} [V(z, f(z)), (w, f(w))].$$

Note that T_V is nonempty by a simple compactness argument. A configuration f will be called "r-periodic" ($f \in T'$), if there exist (at least) r linearly independent vectors v in $\mathbb{Z}^d$ such that $f(z + v) = f(z)$ for all z in $\mathbb{Z}^d$. Finally, $\tilde{T}_V$ denotes the set, perhaps empty (a situation usually called "frustration"), of $f \in T$ such that for all z, $w \in \mathbb{Z}^d$,

$$V[(z, f(z)), (w, f(w))] = \inf_{f' \in T} V[(z, f'(z)), (w, f'(w))].$$

Note that $\tilde{T}_v \subseteq T_v$ and that the inclusion is often proper even when $\tilde{T}_V$ is nonempty.

In the context of tiling theory Robinson has proven by explicit example[22] that for any $N \geqslant 56$ and $d \geqslant 2$ there exist "nearest neighbor" [see (3) below] potentials V such that $\tilde{T}_V$ is not empty but that no configuration in $\tilde{T}_V$ is $(d-1)$ periodic. The structure of V is as follows. Two subsets K_i of $S \times S$ are determined, and V has the properties (1), (2), and (with $\{e_i\}$ the usual basis of $\mathbb{Z}^d$)

$$V[(z, s), (w, t)] = 0, \quad \text{if } |z - w|_1 > 1, \tag{3}$$

$$V[(z, s), (w, t)] = -1, \quad \text{if } z - w = e_i \text{ and } (s, t) \in K_i, \quad i = 1, 2, \tag{4}$$

$$V[(z, s), (w, t)] > -1, \quad \text{if } z - w = e_i \text{ and } (s, t) \notin K_i \text{ or } i \geqslant 3. \tag{5}$$

[It is almost immediate to translate examples from tiling notation to the above notation. But note that this requires special features in the tiling example to be able to associate it with some simple lattice, such as $\mathbb{Z}^d$, and finite S; this seems to exclude examples such as those of Penrose (see Ref. 23).]

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II. EXTENSION

One purpose of this paper is to generalize the tiling result from $\tilde{T}_V \cap T^{d-1} = \emptyset$ (and $\tilde{T}_V \neq \emptyset$) to $T_V \cap T^{d-1} = \emptyset$.

Proposition: For any $N \geqslant 56$ and $d \geqslant 2$ there are potentials satisfying (1)–(5) for which there are no r-periodic ground states for $r \geqslant d-1$.

Proof: Suppose $\tilde{f} \in T_V \cap T^{d-1}$ for a potential V satisfying (1)–(5). For simplicity we will assume $d=2$ and that $\tilde{f}$ is periodic along an elementary lattice direction, say horizontally; the general case follows easily. This means $\tilde{f}$ consists of a vertical strip, repeated horizontally. Since the strip has finite width the situation is essentially one-dimensional and it then follows immediately from Ref. 6 that there exists $f' \in T_V \cap T^2$. From the above tiling result it then follows that for some z, w, $|z-w|_1 = 1$, $V[(z, f'(z)), (w, f'(w))] > -1$ and, f' being two-periodic, there must be a nonzero *density* of such pairs. But then for any large enough "square" subset C of $\mathbb{Z}^d$, $E_{C,V}(f') > E_{C,V}(f'')$, where f'' coincides with any $f \in \tilde{T}_V$ inside C and with f' outside C. This contradiction with $f' \in T_V$ proves our claim.

Note: Ammann has produced an example, verified in detail by Robinson[24] reducing the (tiling) bound on N from 56 to 16. This immediately carries through for our generalization. The first tiling result of this type (requiring a large N) is due to Berger.[25]

The above examples are somewhat surprising "counter-examples" to the vague thesis of the opening paragraphs. Perhaps they can be attributed to some "unphysical" manner in which the potential V exploits the *shape* of the molecules, shape here being understood either in the literal sense of the tiles or in the general sense of an internal degree of freedom. With this in mind we pose the following reformulation, which emphasizes the invariance group of V.

III. FRACTION SPACE

Let G be a group of l_∞ isometries acting on $\mathbb{Z}^d$, and assume G contains all translations of $\mathbb{Z}^d$. We emphasize two examples: (1) $G_1 = \mathbb{Z}^d$; and (2) G_2 is generated by $\mathbb{Z}^d$ and the reflections through the d planes $z_j = 0$ and the $d(d-1)$ planes $z_j = \pm z_k, j \neq k$. Extend the action of G to $\mathbb{Z}^d \times \mathbb{Z}^d$ by $g(w, z) = (g(w), g(z))$ and let m be the number of orbits of G in $A \equiv \{(w, z) \mid 1 \leqslant |w-z|_\infty \leqslant D\}$. For each f in T^d define $p(f)$ in ("fraction space") $L \equiv \mathbb{R}^{mN^2}$ with coordinate $p(f)_{N^2 j+k}$ being the relative fraction of those points (z, w), in the jth orbit of G in A, such that $(f(z), f(w))$ is the k th point in $S \times S$; here $j = 0, \ldots, m-1$ and $k = 1, \ldots, N^2$. Given a potential V satisfying (2) and invariant under G, i.e.,

$$V[(z, s), (w, t)] = V[(g(z), s), (g(w), t)], \quad \text{for all } g \text{ in } G, \tag{1'}$$

we define $q(V)$ in $L^* = \mathbb{R}^{mN^2}$ with coordinates $q(V)_{N^2 j+k} = V[(z, s), (w, t)]$, where (z, w) lies in the jth orbit of G in A and (s, t) is the k th element in $S \times S$. Let $P = \{p(f) \mid f \in T^d\}$, and let $t(j)$ be the relative fraction in A of points in the jth orbit of G. With this notation the energy per particle is

$$e_V(f) = \sum_{j=0}^{m-1} \sum_{k=1}^{N^2} t(j)\, p(f)_{N^2 j+k}\, q(V)_{N^2 j+k},$$

which we denote by the inner product $\langle p(f), q(V) \rangle$. Now it is a theorem of Sinai[19,21] that f in T^d is a ground state for V if and only if

$$e_V(f) = \inf_{f' \in T^d} e_V(f'),$$

i.e., if and only if $p(f)$ lies in a hyperplane of support for P, of the family (labeled by c) of parallel hyperplanes $\langle p, q(V) \rangle = c$, with the least c. Consider the following problem: For a given invariance group G, and every V satisfying (1'), (2), $D \geqslant 1$, and d, $N \geqslant 2$, does there exist a ground state f for V in T^d? Note that the role of a given potential is precisely to select a given direction in L, so the problem of the existence of such an f in T^d becomes the following.

Problem: For given G (and all $D \geqslant 1$, d, $N \geqslant 2$) does P contain all the exposed points of its closure?

We have seen in the above proposition that this does not hold for $G = G_1$ (at least since we allow $N \geqslant 16$). It is an open problem whether or not this holds for $G = G_2$.

We conclude with the following argument which solves the problem for G_2 under the severe restriction that $D = 1$.

Let $\hat{T}^d$ be the set of all $\hat{f}$ in T^d invariant under reflections through all the hyperplanes of the form $z_j = n$, n in $\mathbb{Z}$. There are exactly N^{2^d} such $\hat{f}$, corresponding to the possible restrictions of an f to the unit cube $K = \{z \in \mathbb{Z}^d \mid z_j = 0 \text{ or } 1\}$. Given f in T^d as h runs through the translation group $\mathbb{Z}^d$ the restriction of the f to the translate $h(K)$ agrees with each of the restrictions of $\hat{f}$ to K with a well-defined frequency, which we denote $H_f(\hat{f})$. It is then easy to check that

$$p(f) = \sum_{\hat{f} \in \hat{T}^d} p(\hat{f}) H_f(\hat{f}),$$

proving our assertion.

IV. CONCLUSION

This last formulation deemphasizes the role of the interaction apart from its spatial invariance group, and this together with construction of "fraction space" unifies important aspects of the crystal problem and tiling theory in a common, simple, algebraic framework. However, this will eventually need generalization. Since molecules with complicated shapes do exist (though presumably not of the type of the tiles referred to above!) it is clear that eventually one must investigate invariance groups acting on $\mathbb{Z}^d \times S$ not just $\mathbb{Z}^d$.

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On Utiyama's invariant theoretical interpretation of interaction

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An invariant theoretical interpretation of the geometry of interacting particle and gauge fields is pursued. To this end a critical investigation on Utiyama's interaction theory, both in coordinate and geometrical formulation, is discussed.

I. INTRODUCTION

The present paper deals with the invariant interpretation of the *geometry* of interacting particle and gauge fields (which have just been the object of geometrical investigations in previous papers[1,2]).

To this end we go back to Utiyama's interaction theory, both in original[3] and current[4] formulation, which studies the invariance properties of the action density—a Lagrangian composed with a jet extension—of a (classical) particle field.

There we find that the invariance of the action density under a Lie group G of gauge transformations leaving the Lagrangian invariant, is ensured by a well-known *strong* condition on the jet extension, namely, to be defined by a connection form on a G-principal fiber bundle (gauge potential).

There we also find, however, that sufficience only—not necessity as is still claimed[5]—has been really proved for the above condition, which would then stress the possible but not yet the essential role of gauge potentials in the theory.

As a consequence, we are led to restate (Sec. II), in a coordinate language close in spirit to Utiyama's, a rigorous setting of the constitutive elements of the theory, i.e., gauge transformations and jet extension of a particle field.

So the gauge invariance of the action density—the gauge invariance principle—can be shown (Sec. III) to be ensured by a sufficient *and* necessary condition, which both forces the gauge transformations to belong to G and forces the jet extension to undergo covariant transformations.

Then the geometrical reading of this theory leads us (Sec. IV) to regard the particle field as living in a phase space (nontrivial vector bundle) which the above twofold invariance condition endows with the known structures[6] of a Higgs metric and a Yang–Mills connection, respectively.

So an additional requirement on them—the minimal coupling principle—can be shown (Sec. V) to be the sufficient and necessary condition for the Yang–Mills connection to be reducible to a gauge potential on a G-principal fiber bundle, namely, the bundle arising from the symmetry breaking of phase space yielded by the Higgs metric.

II. DEFINITIONS

Let M be a (four-dimensional, oriented) space-time manifold,[7] and (U_α) an open covering of M carrying[8] (i) a $\mathrm{GL}(n,R)$-valued cocycle $(g_{\alpha\beta})$ and (ii) a $\mathrm{gl}(n,R)$-valued Cartan one-form (Γ_α).

Transition mappings

$$g_{\alpha\beta}: U_\alpha \cap U_\beta \to \mathrm{GL}(n,R)$$

characterize local vertical vector bundle automorphisms of the local phase space

$$V = M \times R^n$$

of the particle field defined by wave functions[9]

$$\psi_\alpha \in C(V),$$

up to gauge transformations

$$\psi_\alpha = g_{\alpha\beta} \cdot \psi_\beta$$

on nonempty intersections $(U_\alpha \cap U_\beta)$.

Differential forms[10]

$$\Gamma_\alpha: U_\alpha \to L(TM, \mathrm{gl}(n,R))$$

characterize differential operators on wave functions[11]

$$D_\alpha = d + \Gamma_\alpha : C(V) \to C(L(TM,V))$$

or, equivalently, jet extensions of wave functions

$$j_\alpha = \mathrm{id} \oplus D_\alpha : C(V) \to C(\overline{V})$$

into local jet space

$$\overline{V} = V \oplus L(TM,V).$$

A local Lagrangian

$$\mathscr{L}: \overline{V} \to R,$$

composed with jet extension

$$\bar{\psi}_\alpha = j_\alpha \psi_\alpha$$

of a wave function ψ_α, defines the action density

$$J(\psi_\alpha) = \mathscr{L} \circ \bar{\psi}_\alpha$$

of ψ_α (interacting with Γ_α).

III. INVARIANCE THEOREM

Assume $\mathscr{L}$ to be invariant under a local vertical vector bundle automorphism k of $\overline{V}$ iff k is the covariant extension

$$k = \bar{g}$$

of a local vertical vector bundle automorphism of V characterized by a G-valued transition mapping g—G being a Lie group which acts on R^n as a closed subgroup of $\mathrm{GL}(n,R)$.

As a consequence, admissible gauge transformations (i.e., leaving the action density invariant) of wave functions and their jet extensions will be altogether exhibited by the following sufficient and necessary invariance condition.

Theorem: The action density is invariant under the gauge transformations of wave functions, that is,

$$J(\psi_\alpha) = J(\psi_\beta),$$

whenever

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$$\psi_\alpha = g_{\alpha\beta}\cdot\psi_\beta,$$

if (i)′ cocycle $(g_{\alpha\beta})$ is G-valued and (ii)′ Cartan form (Γ_α) is of adjoint pseudotensorial type[12]

$$\Gamma_\beta = \mathrm{ad}\, g_{\alpha\beta}^{-1}\cdot\Gamma_\alpha + g_{\alpha\beta}^{*}\theta.$$

Proof: In fact we have

$$\begin{aligned}\bar\psi_\alpha &= j_\alpha(g_{\alpha\beta}\cdot\psi_\beta)\\ &= g_{\alpha\beta}\cdot\psi_\beta \oplus D_\alpha(g_{\alpha\beta}\cdot\psi_\beta)\\ &= g_{\alpha\beta}\cdot\psi_\beta \oplus (g_{\alpha\beta}\cdot d\psi_\beta + dg_{\alpha\beta}\cdot\psi_\beta + \Gamma_\alpha\cdot g_{\alpha\beta}\cdot\psi_\beta)\\ &= \bar g_{\alpha\beta}\cdot(\psi_\beta \oplus D_\beta\psi_\beta)\\ &\quad + g_{\alpha\beta}\cdot(-\Gamma_\beta + g_{\alpha\beta}^{-1}\cdot dg_{\alpha\beta} + g_{\alpha\beta}^{-1}\cdot\Gamma_\alpha\cdot g_{\alpha\beta})\cdot\psi_\beta,\end{aligned}$$

that is,

$$\bar\psi_\alpha = (\bar g_{\alpha\beta} + h_{\alpha\beta})\cdot\bar\psi_\beta,$$

where

$$h_{\alpha\beta} = g_{\alpha\beta}\cdot(-\Gamma_\beta + g_{\alpha\beta}^{*}\theta + \mathrm{ad}\, g_{\alpha\beta}^{-1}\cdot\Gamma_\alpha)$$

is meant, in a natural way, as a local vertical vector bundle endomorphism of $\bar V$.

Consequently the gauge invariance of the action density can be expressed by

$$\mathcal{L}\circ k_{\alpha\beta} = \mathcal{L},$$

where

$$k_{\alpha\beta} = \bar g_{\alpha\beta} + h_{\alpha\beta}$$

is a local vertical vector bundle automorphism of $\bar V$.

Owing to G invariance of $\mathcal{L}$, the above condition holds true iff $k_{\alpha\beta}$ is the covariant extension of a G-valued transition mapping, that is,

$$k_{\alpha\beta} = \bar g_{\alpha\beta}$$

or, equivalently,

$$h_{\alpha\beta} = 0,$$

$g_{\alpha\beta}$ being G valued.

The latter assertion is just statement (i)′.

The former assertion corresponds to the covariant transformation law of the jet extensions of the wave functions

$$\bar\psi_\alpha = \bar g_{\alpha\beta}\cdot\bar\psi_\beta$$

or, equivalently, to statement (ii)′.

IV. GEOMETRICAL INTERPRETATION

Let E be the quotient of local phase space V under the equivalence relation defined by cocycle $(g_{\alpha\beta})$, together with its natural structure of (nontrivial) vector bundle[13] over M—the only one (up to isomorphisms) carrying $(g_{\alpha\beta})$ as the cocycle of transition mappings of an atlas (Φ_α) of local trivializations

$$\Phi_\alpha : U_\alpha \times R^n \to E.$$

E is the phase space of the particle field, described by its sections.

Then the geometrical reading of the coordinate theory is the following.

Theorem: On phase space E, conditions (i)′ and (ii)′ correspond to[14] (i)″ a Higgs metric

$$\eta : PE \to \mathrm{GL}(n,R)|_G$$

and (ii)″ a Yang–Mills connection

$$\omega : PE \to L(T(PE), \mathrm{gl}(n,R)),$$

respectively.

Proof: In fact, owing to (i)′, there exists[15] a G-principal fiber bundle Q carrying an atlas (s_α) of sections over (U_α) whose cocycle of transition mappings is $(g_{\alpha\beta})$. Let

$$i : Q \to PE$$

be the reduction of structure group $\mathrm{GL}(n,R)$ to G defined by[16]

$$i\circ s_\alpha = \Phi_\alpha.$$

Any other G-principal fiber bundle Q' carrying an atlas (s'_α) of sections over (U_α) with cocycle $(g_{\alpha\beta})$, is related to Q by an isomorphism

$$f : Q \to Q'$$

such that

$$f\circ s_\alpha = s'_\alpha.$$

Consequently, if

$$i' : Q' \to PE$$

denotes the reduction defined by

$$i'\circ s'_\alpha = \Phi_\alpha,$$

it follows that

$$i'\circ f = i,$$

hence

$$i(Q) = i'(Q').$$

Then $(g_{\alpha\beta})$ is the cocycle of transition mappings over (U_α) of a unique G-principal fiber bundle

$$P \subset PE.$$

Now recall that any Higgs metric η on E is characterized by its kernel (which is a G-principal fiber bundle), for its values on $PE - \ker(\eta)$ uniquely follow from the condition on η to be equivariant[17] with respect to the action of $\mathrm{GL}(n,R)$ on PE and $\mathrm{GL}(n,R)|_G$.

Then P is the kernel of a unique Higgs metric η on E,

$$P = \ker(\eta).$$

Statement (i)″ has been so proved.

Statement (ii)″ is then plain,[18] for (Γ_α), owing to (ii)′, is the set of pullbacks

$$\Gamma_\alpha = \Phi_\alpha^{*}\omega$$

of a unique connection form ω on PE. This is just a Yang–Mills connection on E, whose role is that of a coupling field through jet extension[19]

$$j = \mathrm{id} \oplus D^\omega : C(E) \to C(\bar E)$$

of the particle field into jet space

$$\bar E = E \oplus L(TM, E).$$

V. CONCLUDING REMARK

Let $P = \ker(\eta) \subset PE$ be the symmetry breaking from $\mathrm{GL}(n,R)$ to G yielded by Higgs metric η in E.

A gauge tensorial component of Yang–Mills connection ω is the projection of $\omega|_P$ onto any ad(G)-invariant subspace of gl(n,R), complementary of the Lie algebra g of G.

Such a component can be asked to vanish, due to its tensorial character,[20] and then ω will be said to be a minimal coupling field if it is gauge tensorial component-free.

Thus minimality means reducibility of ω to a (g-valued) connection form on P,

$$\omega|_P : P \to L(TP, g),$$

and then it is the additional principle, *beyond* the gauge invariance, which finally entails Utiyama's quoted result.

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[9]$C(\cdot)$ will denote the space of local sections of a fiber bundle.
[10]$L(\cdot,\cdot)$ will denote a space of linear maps (on fibers), T the tangent functor, d the ordinary differentiation, id the identity mapping, and $\oplus$ the Whitney sum.
[11]See Ref. 2, Lemma 1.
[12]ad will denote the adjoint representation of GL(n,R) in gl(n,R) and θ the canonical one-form on G.
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[14]PE will denote the GL(n,R)-principal fiber bundle of vertical linear frames of E.
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Scalar formalism for quantum electrodynamics

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A set of Feynman rules, similar to the rules of scalar electrodynamics, is derived for a full quantum electrodynamics based on the relativistic Klein–Gordon-type wave equation $\{\Pi_\mu\Pi_\mu + m^2 + ie\,\boldsymbol{\sigma}\cdot(\mathscr{E} + i\mathbf{B})\}\phi = 0$, $\Pi_\mu \equiv -i\partial_\mu - eA_\mu$, for spin-$\frac{1}{2}$ particles [J. Math. Phys. **23**, 1179 (1982); J. Math. Phys. **24**, 2366 (1983)]. In this equation, ϕ is a 2×1 Pauli spinor and σ_a, $a = 1,2,3$, are the usual 2×2 Pauli spin matrices. The irreducible self-energy parts are compared to those of conventional quantum electrodynamics.

I. INTRODUCTION

The Klein–Gordon-type wave equation for spin-$\frac{1}{2}$ particles, herein called the "second-order Dirac equation,"

$$\{\Pi_\mu\Pi_\mu + m^2 + ei\boldsymbol{\sigma}\cdot(\mathscr{E} + i\mathbf{B})\}\phi = 0,$$
$$\Pi_\mu \equiv -i\partial_\mu - eA_\mu, \tag{1.1}$$

has been investigated earlier.[1,2] Its connection with the conventional "first-order Dirac equation"[3]

$$(\boldsymbol{\alpha}\cdot\boldsymbol{\Pi} + \beta m + i\Pi_4)\Psi = 0 \tag{1.2}$$

is brought out most simply by assuming a representation

$$\boldsymbol{\alpha} \equiv \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & -\boldsymbol{\sigma} \end{pmatrix}, \quad \beta \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{1.3}$$

of the Dirac matrices. Then the wave function ϕ of the second-order Dirac equation and the dual wave function $\bar{\phi}$ can be defined through the equation

$$\Psi \equiv \begin{pmatrix} \phi \\ \bar{\phi}^\dagger \\ \bar{m} \end{pmatrix}. \tag{1.4}$$

Indeed it can be verified that Eq. (1.1) together with the equation for the dual wave function,

$$\bar{\phi} \equiv -\phi^\dagger(\boldsymbol{\sigma}\cdot\overleftarrow{\boldsymbol{\Pi}} + i\overleftarrow{\Pi}_4), \tag{1.5}$$

are a pair of equations entirely equivalent to the first-order Dirac equation (1.2). We will here extend this equivalence to include arbitrary radiative corrections by constructing a full quantum electrodynamics based on Eq. (1.1).[4] In Sec. II we derive a set of Feynman rules for such a full quantum electrodynamics (QED). These Feynman rules are derived starting from conventional QED, thereby assuring the equivalence of the new and the old formalism. The Feynman rules that emerge from this derivation are summarized in Table II. They turn out to be essentially the rules of scalar electrodynamics, aside from the replacement of the factor $e(p_{f\mu} + p_{i\mu})$ for the one-photon vertex of scalar electrodynamics by the new factor $e[p_f\cdot(1 + i\sigma) + (1 + i\sigma)\cdot p_i]_\mu$ for the one-photon vertex of Eq. (1.1). Here σ signifies a second-rank self-dual spin tensor whose space-time components are the ordinary 2×2 Pauli matrices

$$\sigma_{\mu\nu} \equiv \left(\begin{array}{ccc|c} 0 & \sigma_3 & -\sigma_2 & \sigma_1 \\ -\sigma_3 & 0 & \sigma_1 & \sigma_2 \\ \sigma_2 & -\sigma_1 & 0 & \sigma_3 \\ \hline -\sigma_1 & -\sigma_2 & -\sigma_3 & 0 \end{array}\right). \tag{1.6}$$

Scalar and spinor quantum electrodynamics can thus be treated in a unified fashion.[5]

In addition, the "scalar formalism" for QED appears to have certain computational advantages. Coulomb Green's functions and related structures for Eq. (1.1) have a particularly simple form.[2] For this reason the scalar formalism for QED is expected to provide an efficient means of evaluating radiative corrections in a strong Coulomb potential, where the full Coulomb propagator is needed. A program of calculations of radiative corrections in quantum electrodynamics is planned in which the scalar formalism will be used. The present work lays the theoretical foundation for such a program of calculations.

The application of the scalar formalism is indicated briefly in Sec. III, where the irreducible self-energy parts are compared to those of conventional quantum electrodynamics.

II. SECOND QUANTIZATION: DERIVATION OF FEYNMAN RULES

As indicated in the Introduction, we begin with conventional QED. Since this topic is well known, our presentation can be brief, concentrating on the essential new points. Accordingly, the standard lore of field theory will be employed as needed, sometimes without explicit comment.[6] We use radiation gauge QED. The Hamiltonian of the system is $H = H_e + H_\gamma + H_{\rm INT}$, where

$$H_e = \int d^3r{:}\Psi^\dagger\left(\boldsymbol{\alpha}\cdot\frac{1}{i}\boldsymbol{\nabla} + \beta m\right)\Psi{:} \tag{2.1}$$

and

$$H_\gamma = \int d^3r{:}\left(\frac{1}{2}\dot{\mathbf{A}}\cdot\dot{\mathbf{A}} + \frac{1}{2}(\boldsymbol{\nabla}\times A)^2\right){:} \tag{2.2}$$

are the free Hamiltonians for the matter field and radiation field, respectively, and

$$H_{\rm INT} = -\int d^3r\,\mathbf{A}\cdot(e{:}\Psi^\dagger\boldsymbol{\alpha}\Psi{:} + \mathbf{J}^{\rm EXT}) + \int d^3r\int d^3r' \times \frac{(e{:}\Psi^\dagger\Psi{:} + \rho^{\rm EXT})(e{:}\Psi'^\dagger\Psi'{:} + \rho^{\rm EXT'})}{8\pi|\mathbf{r} - \mathbf{r}'|} - \int d^3r{:}\Psi^\dagger\beta\delta m\Psi \tag{2.3}$$

is the interaction Hamiltonian. The interaction Hamiltonian incorporates a coupling between the electromagnetic field and an external c-number source current.

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Quantum fields ϕ and $\bar{\phi}$ are introduced by defining them in terms of the already-quantized Ψ field. Equation (1.4) provides the prescription for this. It is a standard exercise in field theory to expand the quantized Ψ field as a linear superposition of plane wave spinors. Equation (1.4) then implies corresponding expansions for the fields ϕ and $\bar{\phi}$:

$$\phi = \sum_{\mathbf{p}} \sum_{\rho=1}^{2} \left(\frac{m}{2E}\right)^{1/2} \left(\frac{1}{V}\right)^{1/2} \{C^{\rho}(\mathbf{p},t) u^{\rho}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{r}} + d^{\rho}(\mathbf{p},t)^{\dagger} v^{\rho}(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{r}}\}, \tag{2.4}$$

$$\bar{\phi} = \sum_{\mathbf{p}} \sum_{\rho=1}^{2} \left(\frac{m}{2E}\right)^{1/2} \left(\frac{1}{V}\right)^{1/2} \{C^{\rho}(\mathbf{p},t)^{\dagger} \bar{u}^{\rho}(\mathbf{p}) e^{-i\mathbf{p}\cdot\mathbf{r}} + d^{\rho}(\mathbf{p},t) \bar{v}^{\rho}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{r}}\}. \tag{2.5}$$

The creation and annihilation operators appearing here are by construction those of conventional QED. Accordingly, we know that asymptotically they create or annihilate physical electrons or positrons. The normalization is

$$\{C^{\rho'}(\mathbf{p}',t); C^{\rho}(\mathbf{p},t)^{\dagger}\} = \{d^{\rho'}(\mathbf{p}',t); d^{\rho}(\mathbf{p},t)^{\dagger}\} = \delta_{\mathbf{p}',\mathbf{p}} \delta_{\rho',\rho}. \tag{2.6}$$

The time dependence of the associated in-field operators is simply

$$C_{\mathrm{IN}}(\mathbf{p},t) = C_{\mathrm{IN}}(\mathbf{p},0) e^{-iEt}$$

and

$$d_{\mathrm{IN}}(\mathbf{p},t)^{\dagger} = d_{\mathrm{IN}}(\mathbf{p},0)^{\dagger} e^{iEt}. \tag{2.7}$$

For future reference we also require the explicit expressions for the Pauli spinors[7]

$$u^{\rho}(p) = \frac{E + m + \boldsymbol{\sigma}\cdot\mathbf{p}}{(2m(E+m))^{1/2}} u^{\rho}(0)$$

and

$$v^{\rho}(\mathbf{p}) = \frac{E + m + \boldsymbol{\sigma}\cdot\mathbf{p}}{(2m(E+m))^{1/2}} v^{\rho}(0), \tag{2.8}$$

in which $E \equiv +(\mathbf{p}\cdot\mathbf{p} + m^2)^{1/2}$ and

$$u^1(0) \equiv \begin{pmatrix}1\\0\end{pmatrix}, \quad u^2(0) \equiv \begin{pmatrix}0\\1\end{pmatrix},$$

$$v^1(0) \equiv \begin{pmatrix}0\\1\end{pmatrix}, \quad v^2(0) \equiv \begin{pmatrix}-i\\0\end{pmatrix}.$$

Next we construct an asymptotic state describing an incoming electron with probability amplitude $f^{\rho}(\mathbf{p},0)$ to have linear momentum $\mathbf{p}$ and polarization ρ. This state is

$$|f_{e^-}\,\mathrm{IN}\rangle = \sum f^{\rho}(\mathbf{p},0) C^{\rho}_{\mathrm{IN}}(\mathbf{p},0)^{\dagger} |0,\mathrm{IN}\rangle,$$

or, in view of Eqs.(2.7),

$$|f_{e^-}\,\mathrm{IN}\rangle = \sum f^{\rho}(\mathbf{p},0) \exp(-iEt)\, C^{\rho}_{\mathrm{IN}}(\mathbf{p},t)^{\dagger} |0,\mathrm{IN}\rangle.$$

This may be transformed into

$$|f_{e^-}\,\mathrm{IN}\rangle = -\frac{i}{m^2} \int d^3r\, \bar{\phi}_{\mathrm{IN}} |0,\mathrm{IN}\rangle \overleftrightarrow{\partial}_4 f_{e^-}, \tag{2.9}$$

in which the Schrödinger wave function f_{e^-} is defined as

$$f_{e^-} \equiv \sum_{\mathbf{p},\rho} f^{\rho}(\mathbf{p},0) \left(\frac{m}{2E}\right)^{1/2} \left(\frac{1}{V}\right)^{1/2} u^{\rho}(\mathbf{p}) e^{i\mathbf{p}\cdot x}. \tag{2.10}$$

We can obtain Eq. (2.9) by first solving Eq. (2.5) and the adjoint of Eq. (2.4) for $C^{\rho}(p,t)^{\dagger}$:

$$C^{\rho}(\tilde{p},t)^{\dagger} = \int d^3r \left(\frac{m}{2E}\right)^{1/2} \left(\frac{1}{V}\right)^{1/2} \times \exp(i\mathbf{p}\cdot\mathbf{r}) \left(\phi^{\dagger} u^{\rho}(\mathbf{p}) + \frac{\bar{\phi}\, u^{\rho}(\mathbf{p})^{\dagger}}{m^2}\right).$$

Further simplifications are allowed in the free field case, and we find

$$C^{\rho}_{\mathrm{IN}}(\mathbf{p},t)^{\dagger} = \frac{-i}{m^2} \int d^3r\, \bar{\phi}_{\mathrm{IN}} \overleftrightarrow{\partial}_4 \left(\frac{m}{2E}\right)^{1/2} \left(\frac{1}{V}\right)^{1/2} \times u^{\rho}(\mathbf{p}) \exp(ip\cdot x).$$

Equation (2.9) is a form of this result obtained by multiplication by $f^{\rho}(\mathbf{p},0)$ and summing over $\mathbf{p}$ and ρ. A relation analogous to Eq. (2.9) is

$$\langle g_{e^-}\,\mathrm{OUT}| = -\frac{i}{m^2} \int d^3r\, \bar{g}_{e^-} \overleftrightarrow{\partial}_4 \langle 0,\mathrm{OUT}|\phi_{\mathrm{OUT}}. \tag{2.11}$$

Most of the Feynman rules that we are looking for may be obtained by considering the scattering of an electron by the external potential produced by j^{EXT}_{μ}. The probability amplitude for an electron to make a transition from a state f in the remote past to a state g in the remote future is given by $S_{gf} \equiv \langle g_{e^-}\,\mathrm{OUT}|f_{e^-}\,\mathrm{IN}\rangle$. Using standard reduction techniques this amplitude can be written

$$S_{gf} = \frac{i}{m^2} \int d^4x_2 \frac{i}{m^2} \int d^4x_1 (-im^2) \bar{g}(2) (\tilde{\partial}_2^2 + m^2) \frac{1}{Z_2} \times \tau(2,1) (\tilde{\partial}_1^2 + m^2) f(1), \tag{2.12}$$

in which

$$S = T\left[\exp\left(-i \int_{-\infty}^{\infty} dt\, H_{\mathrm{INT}}\right)\right] \tag{2.13}$$

is the unitary S matrix, and $\sqrt{Z_2}$ is a wave function renormalization constant canceling a corresponding factor in the τ function

$$\tau(2,1) \equiv \frac{\langle 0,\mathrm{IN}|T[\phi_{\mathrm{IN}}(2)\bar{\phi}_{\mathrm{IN}}(1)S]|0,\mathrm{IN}\rangle/(-im^2)}{\langle 0,\mathrm{IN}|S|0,\mathrm{IN}\rangle}. \tag{2.14}$$

Our next step is to evaluate the numerator and denominator in Eq. (2.14). To do this we substitute the expression (2.13) for S, using the interaction Hamiltonian (2.3). The exponential involving

$$-\int d^3r\, \mathbf{A}^{\mathrm{IN}} \cdot (e{:}\, \Psi^{\dagger}_{\mathrm{IN}} \boldsymbol{\alpha} \Psi_{\mathrm{IN}} {:} + \mathbf{J}^{\mathrm{EXT}})$$

is expanded and the vacuum expectation value of products of the vector potential is worked out with the help of the equation

$$\langle 0,\mathrm{IN}|T[A^{\mathrm{IN}}_a(2) A^{\mathrm{IN}}_b(1)]|0,\mathrm{IN}\rangle = \left(\delta_{ab} - \frac{\partial_{2a}\partial_{2b}}{\nabla_2^2}\right)[-iD_F(2,1)], \tag{2.15}$$

in which

$$D_F(2,1) \equiv \int \frac{d^4k}{(2\pi)^4} e^{ik\cdot x} \frac{1}{k^2 - i\epsilon} \tag{2.16}$$

is the scalar photon propagator. The resulting series, in which the photon operators $\mathbf{A}$ have been replaced by expres-

sions involving the c numbers $-iD_F(2,1)$ can then be resummed to give eventually

$$\langle 0,\mathrm{IN}|T[\phi_{\mathrm{IN}}(2)\bar{\phi}_{\mathrm{IN}}(1)S]|0,\mathrm{IN}\rangle/(-im^2)$$
$$=\langle 0,\mathrm{IN}|T\Big[\phi_{\mathrm{IN}}(2)\bar{\phi}_{\mathrm{IN}}(1)\exp\Big[(-i/2)\int d^4x_2\,d^4x_1$$
$$\times i[j_\mu(2)+j_\mu^{\mathrm{EXT}}(2)]D_F(2,1)i[j_\mu(1)+j_\mu^{\mathrm{EXT}}(1)]$$
$$+i\int d^4x{:}\,\bar{\Psi}\delta m\Psi{:}\Big]\Big]|0,\mathrm{IN}\rangle/(-im^2), \tag{2.17}$$

$$j_\mu \equiv ie{:}\Psi_{\mathrm{IN}}\gamma_\mu\Psi_{\mathrm{IN}}{:}. \tag{2.18}$$

The noncovariant terms associated with the Coulomb gauge quantization have been eliminated in Eq. (2.17) by a standard technique involving integration by parts and current conservation. The gamma matrices in Eq. (2.18) are defined by $\gamma_a \equiv -i\beta\alpha_a$, $a=1,2,3$, and $\gamma_4\equiv\beta$. Also, $\bar{\Psi}\equiv\Psi^\dagger\beta$.

To proceed, we first rewrite the expression (2.17) and the corresponding expression for $\langle 0,\mathrm{IN}|S|0,\mathrm{IN}\rangle$ in a form involving only the fields ϕ_{IN} and $\bar{\phi}_{\mathrm{IN}}$. This is made possible by the identity

$$j_\mu=(e/m^2)\bar{\phi}_{\mathrm{IN}}[\vec{p}\cdot(1+i\sigma)+(1+i\sigma)\cdot\vec{p}]_\mu\phi_{\mathrm{IN}}, \tag{2.19}$$

in which σ denotes the spin tensor (1.6), and

$$\bar{\Psi}_{\mathrm{IN}}\delta m\Psi_{\mathrm{IN}}=\frac{1}{m^2}2m\delta m\bar{\phi}_{\mathrm{IN}}\phi_{\mathrm{IN}}-\frac{1}{m^2}\frac{\delta m}{m}\bar{\phi}_{\mathrm{IN}}\cdot$$
$$\times[\overleftarrow{p}\cdot(1+i\sigma)\cdot\vec{p}+m^2]\phi_{\mathrm{IN}}. \tag{2.20}$$

It is the meaning of the time-ordering symbol in Eq. (2.13) that the factors H_{INT} are the objects being time ordered. Similarly, in Eq. (2.17) the factors $j_\mu=ie{:}\bar{\Psi}_{\mathrm{IN}}\gamma_\mu\bar{\Psi}_{\mathrm{IN}}{:}$ and ${:}\bar{\Psi}_{\mathrm{IN}}\delta m\Psi_{\mathrm{IN}}{:}$ as a whole are the objects being time ordered. The substitution of the equivalent objects (2.19) and (2.20) for these factors will leave the time-ordered products in Eq. (2.17) invariant. The time derivatives in Eqs. (2.19) and (2.20) are hereby meant to act before the time ordering in Eq. (2.17). When the substitutions (2.19) and (2.20) are made in Eq. (2.17), we obtain an expression that can be expanded in a Feynman–Dyson perturbation series. The basic contractions needed for this are

$$\langle 0,\mathrm{IN}|T[\phi_{\mathrm{IN}}(2)\bar{\phi}_{\mathrm{IN}}(1)]|0,\mathrm{IN}\rangle$$
$$\equiv -im^2S_F(2,1)$$
$$=-im^2\int\frac{d^4p}{(2\pi)^4}\frac{e^{ip\cdot(x_2-x_1)}}{p^2+m^2-i\epsilon} \tag{2.21}$$

and

$$\langle 0,\mathrm{IN}|T[(1+i\sigma)\cdot\vec{p}_2\phi_{\mathrm{IN}}(2)\bar{\phi}_{\mathrm{IN}}(1)\bar{p}_1\cdot(1+i\sigma)]|0,\mathrm{IN}\rangle$$
$$=(1+i\sigma)\cdot\vec{p}_2\langle 0,\mathrm{IN}|T[\phi_{\mathrm{IN}}(2)\bar{\phi}_{\mathrm{IN}}(1)]$$
$$\times|0,\mathrm{IN}\rangle\bar{p}_1\cdot(1+i\sigma)+im^2\delta^4(21)(1+i\sigma). \tag{2.22}$$

Here, and elsewhere when warranted for simplicity, spinor and Lorentz indices are suppressed. As we know, time ordering and time differentiation do not in general commute. This is manifested in Eq. (2.22) in the additional delta function term. On the other hand, in an expression like $\langle 0,\mathrm{IN}|T((1+i\sigma)\cdot\vec{p}_2\phi(2)\bar{\phi}(1))|0,\mathrm{IN}\rangle$, involving only one time derivative, the derivative can be taken outside the time-ordering symbol without encountering correction terms. The additional delta function term in Eq. (2.22) can cause vertices to coalesce. For example, the merging of two one-photon vertices produces a two-photon vertex, a type of vertex normally associated only with scalar electrodynamics.

It is now a simple exercise to obtain Feynman rules in the scalar formalism. These rules, which are a provisional set of rules only, are summarized in Table I. The rules are expressed in an abstract operator notation. We introduce space-time coordinate eigenkets $|1\rangle\equiv|\mathbf{r}_1,t_1\rangle$ defined through the equations $x_\mu|1\rangle=(x_\mu)_1|1\rangle$ and $\langle 2|1\rangle=\delta(t_2-t_1)\delta^3(\mathbf{r}_2-\mathbf{r}_1)$. The time component of the four-vector x_μ is thus treated as an operator on the same footing as x,y,z (Ref. 8). The propagator $S_F(2,1)$ of Eq. (2.21) is visualized as a coordinate representation of an abstract operator S_F: $S_F(2,1)\equiv\langle 2|S_F|1\rangle$. From the Fourier integral representation (2.21) it follows that the abstract operator in question is just $S_F=1/(p^2+m^2-i\epsilon)$, where $p_\mu=-i\partial_\mu$ is the four-momentum operator canonically conjugate to x_μ. This abstract operator notation is particularly convenient for the external field problems that the present work is geared to. In addition, this operator notation has the advantage of providing a representation-independent way of expressing the Feynman rules.

We have in Table I the result mentioned in the Introduction: that Feynman rules for QED in the new formalism are basically the rules for scalar electrodynamics, aside from a modification of the one-photon vertex to incorporate spin effects. However, we also have in Table I a more complicated set of mass counterterms than one would expect by comparison with scalar QED. There are two basic types of counterterms in this set, giving rise to vertices with factors $2m\,\delta m$ and $(-\delta m/m)(p^2+m^2)$ in Feynman diagrams. For short we shall refer to the latter type of vertex as a "$\delta m/m$" vertex. Other mass counterterms in Table I are formed by merging a $\delta m/m$ vertex with another $\delta m/m$ vertex or with a one-photon vertex. (A $\delta m/m$ vertex cannot merge with a $2m\delta m$ vertex or with a two-photon vertex.)

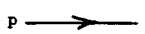
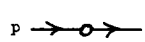
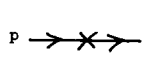
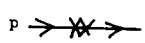
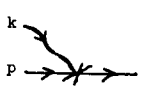
If $2m\delta m$ vertices alone were present, all electron propagators $1/(p^2+m^2)$ would be modified to $1/(p^2+m^2-2m\delta m)$ as a result of the action of the counterterms. Clearly, this is an incomplete renormalization of a scalar propagator, which should become $1/[p^2+m^2-2m\delta m+(\delta m)^2]=1/[p^2+(m-\delta m)^2]$. As can be verified by trying a few special examples, one of the functions of the $\delta m/m$ vertices is to supply the missing $(\delta m)^2$ term in the denominators of the scalar propagators.

Another function of the $\delta m/m$ vertices is to provide an additional overall factor of $[1-(\delta m/m)]$ in the electron propagator, as compared to the propagator expected by analogy with scalar electrodynamics. The appearance of this factor can be demonstrated by means of the following formal argument. The identity

$$\langle 0,\mathrm{IN}|T(\Psi_{\mathrm{IN}}(2)_\alpha\bar{\Psi}_{\mathrm{IN}}(1)_\beta S[\Psi_{\mathrm{IN}},\bar{\Psi}_{\mathrm{IN}},m,\delta m])|0,\mathrm{IN}\rangle$$
$$=\langle 0|T(\Psi_0(2)_\alpha\bar{\Psi}_0(1)_\beta S[\Psi_0,\bar{\Psi}_0,m_0,0])|0\rangle \tag{2.23}$$

expresses the fact that mass renormalization does not formally change the value of the electron propagator at any space-time point, but just reexpresses it in terms of the physical mass m rather than the bare mass m_0. The bracket notation $S[\Psi_{\mathrm{IN}},\bar{\Psi}_{\mathrm{IN}},m,\delta m]$ is functional notation for the S-ma-

TABLE I. Scalar formalism for QED: Feynman rules for the calculation of τ functions, preliminary version.[a,b]

Graph	Name	Factor
	Electron line	$1/(p^2+m^2-i\epsilon)$
	External photon line	$-i\delta_{\mu\nu}/(k^2-i\epsilon)$
	Internal photon line	$\int \frac{d^4k}{(2\pi)^4}\frac{-i\delta_{\mu\nu}}{k^2-i\epsilon}$
	One-photon vertex	$e[p\cdot(1+i\sigma)e^{ik\cdot x}+e^{ik\cdot x}(1+i\sigma)\cdot p]_\mu$
	Two-photon vertex	$-e^2e^{ik_1\cdot x-ik_2\cdot x}2\delta_{\mu\nu}$
	External field interaction	$ij_\mu^{\mathrm{EXT}}(\mathbf{k})$
	$2m\delta m$ vertex	$2m\delta m$
	Simple $\delta m/m$ vertex	$-(\delta m/m)(p^2+m^2)$
	Double $\delta m/m$ vertex	$-(\delta m/m)^2(p^2+m^2)+(\delta m)^2$
	Double one-photon and $\delta m/m$ vertex	$(\delta m/m)e[p\cdot(1+i\sigma)e^{ik\cdot x}+e^{ik\cdot x}(1+i\sigma)\cdot p]_\mu$

[a] See Table II for the final version, in which the mass counterterms are greatly simplified.
[b] In addition there is a rule to take minus the trace over spin and space-time degrees of freedom for each closed electron loop.

trix. In Eq. (2.23) we refer to conventional QED with one type of mass counterterm, a δm vertex. Now restrict α,β in Eq. (2.23) to the range $\alpha,\beta=1,2$. Then in accordance with Eq. (1.4) and the related equation $\bar{\Psi}=(\bar{\phi}/m;\phi^\dagger)$, we have the relations $\Psi_{\mathrm{IN}\alpha}=\phi_{\mathrm{IN}\alpha}$ and $\bar{\Psi}_{\mathrm{IN}\beta}=\bar{\phi}_{\mathrm{IN}\beta}/m$. If we make these substitutions in Eq. (2.23) and further transform the S matrix into an expression referring only to the fields $\bar{\phi}_{\mathrm{IN}},\phi_{\mathrm{IN}}$, as we did above through the use of Eqs. (2.19) and (2.20), we find first

$$\begin{aligned}&\langle 0,\mathrm{IN}|T(\phi_{\mathrm{IN}}(2)[\bar{\phi}_{\mathrm{IN}}(1)/m]\\&\quad\times S[\phi_{\mathrm{IN}},\bar{\phi}_{\mathrm{IN}},m,2m\delta m,\delta m/m])|0,\mathrm{IN}\rangle\\&\quad=\langle 0|T(\phi_0(2)[\bar{\phi}_0(1)/m_0]S[\phi_0,\bar{\phi}_0,m_0,0,0])|0\rangle,\end{aligned}$$

and then (2.24)

$$\begin{aligned}&\langle 0,\mathrm{IN}|T(\phi_{\mathrm{IN}}(2)[\bar{\phi}_{\mathrm{IN}}(1)/(-im^2)]\\&\quad\times S[\phi_{\mathrm{IN}},\bar{\phi}_{\mathrm{IN}},m,2m\delta m,\delta m/m])|0,\mathrm{IN}\rangle\\&\quad=\frac{m_0}{m}\langle 0|T(\phi_0(2)[\bar{\phi}_0(1)/(-im_0^2)]S[\phi_0,\bar{\phi}_0,m_0,0,0])|0\rangle.\end{aligned}$$

We have here the above-mentioned factor of $m_0/m=(m-\delta m)/m=[1-(\delta m/m)]$.

The object

$$\langle 0|T(\phi_0(2)\bar{\phi}_0(1)S[\phi_0,\bar{\phi}_0,m_0,0,0])|0\rangle/(-im_0^2)$$

is precisely the propagator one would expect by comparison with scalar QED: it is the propagator one would obtain using the rules of Table I but ignoring all mass counterterms, and using the bare mass m_0 throughout instead of the physical mass m. Now let us renormalize this propagator the way we would like, writing all factors $1/(p^2+m_0^2)$ in the form

$$1/(p^2+m_0^2)=1/(p^2+m^2-\delta m^2),\quad \delta m^2\equiv m^2-m_0^2,$$

and expanding in ascending powers of δm^2. This gives rise to an expression, which we may call

$$\begin{aligned}&\langle 0,\mathrm{IN}|T(\phi_{\mathrm{IN}}(2)\bar{\phi}_{\mathrm{IN}}(1)\\&\quad\times S[\phi_{\mathrm{IN}},\bar{\phi}_{\mathrm{IN}},m,\delta m^2])|0,\mathrm{IN}\rangle/(-im^2).\end{aligned}$$

By construction, we have the identity [similar to Eq. (2.23)]

$$\begin{aligned}&\langle 0|T(\phi_0(2)[\bar{\phi}_0(1)/(-im_0^2)]\,S[\phi_0,\bar{\phi}_0,m_0,0,0])|0\rangle\\&\quad=\langle 0,\mathrm{IN}|T(\phi_{\mathrm{IN}}(2)[\bar{\phi}_{\mathrm{IN}}(1)/(-im^2)]\\&\qquad\times S[\phi_{\mathrm{IN}},\bar{\phi}_{\mathrm{IN}},m,\delta m^2])|0_{\mathrm{IN}}\rangle.\end{aligned}\tag{2.25}$$

Combining Eqs. (2.24) and (2.25), we get

$$\begin{aligned}&\langle 0,\mathrm{IN}|T(\phi_{\mathrm{IN}}(2)[\bar{\phi}_{\mathrm{IN}}(1)/(-im^2)]\\&\quad\times S[\phi_{\mathrm{IN}},\bar{\phi}_{\mathrm{IN}},m,2m\delta m,\delta m/m])|0,\mathrm{IN}\rangle\\&\quad=(1-\delta m/m)\langle 0_{\mathrm{IN}}|T(\phi_{\mathrm{IN}}(2)[\bar{\phi}_{\mathrm{IN}}(1)/(-im^2)]\\&\quad\times S[\phi_{\mathrm{IN}},\bar{\phi}_{\mathrm{IN}},m,\delta m^2])|0_{\mathrm{IN}}\rangle.\end{aligned}\tag{2.26}$$

On the left-hand side of Eq. (2.26) we have a τ function created according to the original rules of Table I. On the right-hand side we have a τ function created in accordance with a greatly simplified set of rules summarized in Table II. We need no longer deal with the rules of Table I, whose only purpose was to establish contact with conventional QED. The correspondence with scalar electrodynamics can be made complete by absorbing the factor $[1-(\delta m/m)]$ in the electron's wave-function renormalization constant. We define

$$Z_2^{-1}(1-\delta m/m) \equiv Z^{-1}. \tag{2.27}$$

Now when the scattering amplitude (2.12) is computed we can substitute for the τ function in Eq. (2.12) the new τ function

$$\langle 0,\mathrm{IN}|T(\phi_{\mathrm{IN}}(2)\bar{\phi}_{\mathrm{IN}}(1) \times S[\phi_{\mathrm{IN}},\bar{\phi}_{\mathrm{IN}},m,\delta m^2]|0,\mathrm{IN}\rangle/(-im^2),$$

and substitute for the factor $1/Z_2$ in Eq. (2.12) the new factor $1/Z$.

The form of QED embodied in Table II can be expressed in analytical terms by a simple modification of the above equations: In effect we work as though the S matrix were

$$S = T\left[\exp\left(\frac{i}{m^2}\int d^4x\{A\cdot(\mathrm{e}{:}\bar{\phi}\,[\,\tilde{p}\cdot(1+i\sigma) + (1+i\sigma)\cdot\tilde{p}]\phi{:} + m^2 J^{\mathrm{EXT}}) + \delta m^2{:}\bar{\phi}\,\phi{:}\}\right)\right], \tag{2.28}$$

where the field operator A_μ is assumed to have the contractions

$$\langle 0,\mathrm{IN}|T[A_\mu^{\mathrm{IN}}(2)A_\nu^{\mathrm{IN}}(1)]|0,\mathrm{IN}\rangle = -iD_F(2,1)\delta_{\mu\nu}, \tag{2.29}$$

and we use the new electron wave-function renormalization constant Z to convert unrenormalized τ functions into their finite physical counterparts.

III. IRREDUCIBLE SELF-ENERGY PARTS

To illustrate the application of the new Feynman rules we consider briefly the irreducible electron and photon self-energy parts. We now assume $j_\mu^{\mathrm{EXT}} = 0$. The physical free-electron propagator $S_F = 1/(p^2+m^2)$ will be modified by the action of the mass counterterm and by the interaction with the radiation field to $S_F' = 1/(p^2+m^2-\delta m^2+\Sigma)$. Our rules give the expression

$$\Sigma = 4\pi i\alpha\int\frac{d^4k}{(2\pi)^4}\frac{1}{k^2-i\epsilon}\{p\cdot(1+i\sigma)e^{-ik\cdot x} + e^{-ik\cdot x}(1+i\sigma)\cdot p\}_\mu(p^2+m^2-i\epsilon)^{-1} \times\{p\cdot(1+i\sigma)e^{ik\cdot x}+e^{ik\cdot x}(1+i\sigma)\cdot p\}_\mu, \tag{3.1}$$

for the self-energy part Σ to lowest order in α. To evaluate the expression (3.1) we first move plus and minus exponentials together with the help of the identity

$$e^{-ik\cdot x}p_\mu e^{ik\cdot x} = p_\mu + k_\mu. \tag{3.2}$$

The result is

$$\Sigma = 4\pi i\alpha\int\frac{d^4k}{(2\pi)^4}\frac{1}{k^2-i\epsilon} \times\{p\cdot(1+i\sigma)+(1+i\sigma)\cdot(p+k)\}_\mu \times[(p+k)^2+m^2-i\epsilon]^{-1}\{(p+k)\cdot(1+i\sigma) + (1+i\sigma)\cdot p\}_\mu. \tag{3.3}$$

Our next step will deal with the spin algebra. We rearrange the numerator in Eq. (3.3) so that second-rank Lorentz tensors are multiplied in accordance with the laws of matrix algebra

TABLE II. Scalar formalism for QED: Feynman rules for the calculation of τ functions, final version.[a]

Graph	Name	Factor
p →	Electron line	$i/(p^2+m^2-i\epsilon)$
k ~	External photon line	$-i\delta_{\mu\nu}/(k^2-i\epsilon)$
k ~	Internal photon line	$\int\frac{d^4k}{(2\pi)^4}\frac{-i\delta_{\mu\nu}}{k^2-i\epsilon}$
k_1 ~, p →	One-photon vertex	$e[p\cdot(1+i\sigma)e^{ik\cdot x}+e^{ik\cdot x}(1+i\sigma)\cdot p]_\mu$
k_1 ~ k_2 ~, p →	Two-photon vertex	$-e^2e^{ik_1\cdot x-ik_2\cdot x}2\delta_{\mu\nu}$
k ~ ×	External field interaction	$ij_\mu^{\mathrm{EXT}}(k)$
p → × →	Mass counterterm	δm^2

[a] In addition there is a rule to take minus the trace over spin and space-time degrees of freedom for each closed electron loop.

$$\Sigma = 4\pi i\alpha \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 - i\epsilon} \times \{p\cdot(1+i\sigma) + (p+k)\cdot(1-i\sigma)\} \times [(p+k)^2 + m^2 - i\epsilon]^{-1}\{(1-i\sigma)\cdot(p+k) + (1+i\sigma)\cdot p\}. \quad (3.4)$$

The products of tensors appearing here are evaluated with the help of Table III,[9] and we find

$$\Sigma = 16\pi i\alpha \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 - i\epsilon} \frac{k^2 + k\cdot p + p^2}{(p+k)^2 + m^2 - i\epsilon}. \quad (3.5)$$

The integral (3.5) may be evaluated using standard Feynman techniques, with renormalization carried out as in scalar electrodynamics.[10] The result is

$$\Sigma_R = -\frac{\alpha}{2\pi} m^2\rho\left\{2 - \frac{(2-\rho)}{1-\rho}\ln\rho + \ln\left(\frac{\mu^2}{m^2}\right)\right\}, \quad (3.6)$$

$$\rho \equiv (p^2 + m^2)/m^2.$$

Mass and charge renormalization have been carried out, with the subtraction point $p^2 = -m^2$. The result (3.6) is infrared divergent, with $\mu \equiv$ the photon rest mass appearing as an infrared cutoff parameter. Note the complete disappearance of spin structure in Eq. (3.6). This phenomenon is characteristic of the scalar formalism for QED, and holds to all orders in α, as long as there is no external field.

The result (3.6) may be compared to the corresponding result of conventional QED. For this purpose it is convenient to present the latter result in the form[11]

$$\frac{1}{i\not p + m}(-\Sigma_R^{\rm DIRAC})\frac{1}{i\not p + m} = -\frac{\alpha}{2\pi m}\left\{\frac{1}{2(1-\rho)}\left(1 - \frac{2-3\rho}{1-\rho}\ln\rho\right) + \frac{(i\not p - m)}{m} \times\left[\frac{1}{2\rho(1-\rho)}\left(2 - \rho + \frac{-4+4\rho+\rho^2}{1-\rho}\ln\rho\right) - \frac{2}{\rho}\int_0^1 dx\left(\frac{1}{x} - x\right)\right]\right\}, \quad (3.7)$$

representing the change in the conventional Dirac propagator $S_F(2,1) \equiv \langle 0,\mathrm{IN}|T(\Psi_{\rm IN}(2)\bar\Psi_{\rm IN}(1)S)|0,\mathrm{IN}\rangle/i$ due to $\Sigma_R^{\rm DIRAC}$. We have already noted above the relations $\Psi_{1,2}^{\rm IN} = \phi_{1,2}^{\rm IN}, \bar\Psi_{1,2}^{\rm IN} = \bar\phi_{1,2}^{\rm IN}/m$. As a result of these relations the (1,1) sector of the conventional Dirac propagator, viewed as a 2×2 matrix of 2×2 matrices, will be directly proportional to our 2×2 propagator:

$$\left(\frac{1}{i\not p + m - \delta m + \Sigma^{\rm DIRAC}}\right)_{11} = \frac{m}{p^2 + m^2 - \delta m^2 + \Sigma}. \quad (3.8)$$

TABLE III. Some spin algebra: A multiplication table.[a]

	$1+i\sigma$	$1-i\sigma$
$1+i\sigma$	$4(1+i\sigma)$	$-2(1+i\sigma)$
$1-i\sigma$	$-2(1+i\sigma)$	4

[a] Lorentz and spinor indices are suppressed. Written out in more detail with Lorentz indices exhibited explicitly, the relations read $(1+i\sigma)_{\mu\lambda}(1+i\sigma)_{\lambda\nu} = 4(1+i\sigma)_{\mu\nu}$, etc.

Comparing terms proportional to α in an expansion of each side of Eq. (3.8) and carrying out the renormalization gives the requisite connection between the two results (3.6) and (3.7) in the form

$$\left[\frac{1}{i\not p + m}(-\Sigma_R^{\rm DIRAC})\frac{1}{i\not p + m}\right]_{11} = -\frac{\Sigma_R}{m^3\rho^2}. \quad (3.9)$$

Equation (3.9) can be verified by explicit calculation [note that in our representation of the gamma matrices, the (1,1) sector of $i\not p$ in Eq. (3.7) is zero].

The lowest-order photon self-energy part $\Pi_{\mu\nu}$, defined through the equation

$$-iD'_{F_{\mu\nu}} = \frac{-i\delta_{\mu\nu}}{k^2} + \frac{-i\delta_{\mu\alpha}}{k^2} i\Pi_{\alpha\beta}\frac{-i\delta_{\beta\nu}}{k^2},$$

provides an example of an object that should be independent of the representation of the fermion. This will be demonstrated explicitly to lowest order in α. There are two graphs to consider (see Fig. 1). The new rules give

$$i\Pi_{\mu\nu}(k',k) = -4\pi\alpha\,\mathrm{Tr}\int\frac{d^4p}{(2\pi)^4}\langle p|[p\cdot(1+i\sigma)e^{-ik'\cdot x} + e^{-ik'\cdot x}(1+i\sigma)\cdot p]_\mu 1/(p^2+m^2) \times[p\cdot(1+i\sigma)e^{ik\cdot x} + e^{ik\cdot x}(1+i\sigma)\cdot p]_\nu \times(1/(p^2+m^2))|p\rangle + 4\pi\alpha\,\mathrm{Tr}\int\frac{d^4p}{(2\pi)^4}\langle p|2\delta_{\mu\nu} \times e^{ik\cdot x - ik'\cdot x}(1/(p^2+m^2))|p\rangle. \quad (3.10)$$

The exponentials may be eliminated with the help of Eq. (3.2) and the related equation

$$e^{ik\cdot x}|p\rangle = |p+k\rangle. \quad (3.11)$$

Next the orthogonality of the four-momentum eigenstates

$$\langle p_2|p_1\rangle = (2\pi)^4\delta^4(p_2 - p_1) \quad (3.12)$$

is used, leading to an energy-momentum-conserving delta function as an overall factor

$$i\Pi_{\mu\nu}(k',k) = (2\pi)^4\delta^4(k'-k)i\tilde\pi_{\mu\nu}(k). \quad (3.13)$$

The function

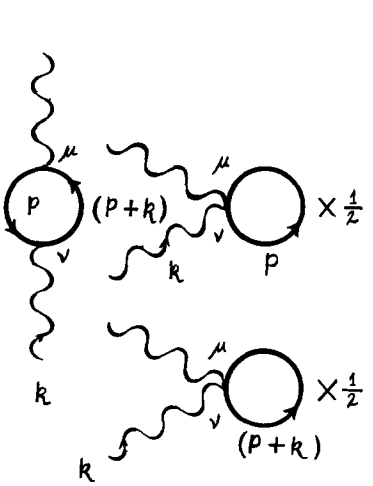


FIG. 1. Graphs contributing to the lowest-order photon self-energy.

$$\tilde{\Pi}_{\mu\nu}(k) = 4\pi i\alpha \,\mathrm{Tr} \int \frac{d^4p}{(2\pi)^4} \frac{[p\cdot(1+i\sigma)+(1+i\sigma)\cdot(p+k)]_\mu [(p+k)\cdot(1+i\sigma)+(1+i\sigma)\cdot p]_\nu}{[(p+k)^2+m^2](p^2+m^2)}$$
$$- 4\pi i\alpha \,\mathrm{Tr} \int \frac{d^4p}{(2\pi)^4} \delta_{\mu\nu}\left(\frac{1}{(p+k)^2+m^2}+\frac{1}{p^2+m^2}\right) \tag{3.14}$$

corresponds to the photon self-energy part familiar from conventional QED. To evaluate the traces we need the equations $\mathrm{Tr}(\sigma_{\mu\nu}) = 0$ and[12]

$$\mathrm{Tr}\,(\sigma_{\mu\nu}\sigma_{\lambda\rho}) = 2(\delta_{\mu\lambda}\delta_{\nu\rho} - \sigma_{\mu\rho}\delta_{\nu\lambda} + \epsilon_{\mu\nu\lambda\rho}). \tag{3.15}$$

The result of taking the trace is

$$\tilde{\pi}_{\mu\nu}(k)$$
$$= 4\pi i\alpha \int \frac{d^4p}{(2\pi)^4} 4 \frac{2p_\mu p_\nu + p_\mu k_\nu + p_\nu k_\mu + \frac{1}{2}\delta_{\mu\nu}k^2}{[(p+k)^2+m^2](p^2+m^2)}$$
$$- 4\pi i\alpha \int \frac{d^4p}{(2\pi)^4} 2\delta_{\mu\nu}\left(\frac{1}{(p+k)^2+m^2}+\frac{1}{p^2+m^2}\right). \tag{3.16}$$

The exponentials in Eq. (3.10) could have been eliminated in a number of different ways, leading to different-looking expressions for $\Pi_{\mu\nu}$. In the second term of Eq. (3.14) we have chosen the average of two such possibilities. This is legitimate, since the two terms become equal after regularization. After taking a common denominator, the expression (3.16) becomes formally identical to the corresponding expression in conventional QED.[13]

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[1]L. Hostler, J. Math. Phys. **23**, 1179 (1982).

[2]L. Hostler, J. Math. Phys. **24**, 2366 (1983).

[3]A third equation $(m^2 + \Pi^2 - 1/2e\,\sigma_{\mu\nu}F_{\mu\nu})\Psi = 0$, where Ψ is a 4×1 Dirac spinor, may be called the "iterated Dirac equation."

[4]The possibility of doing quantum electrodynamics using Eq. (1.1) instead of the first-order Dirac equation has been recognized before. I am grateful to Dr. Peter Mohr for pointing this out to me. Relevant references are R. P. Feynman and M. Gell-Mann, Phys. Rev. **109**, 193 (1958); R. P. Feynman, Rev. Mod. Phys. **20**, 367 (1948); Phys. Rev. **84**, 108 (1951). The last of these references mentions Feynman rules for the iterated Dirac equation, which, aside from the different dimension of the spinors, would be similar to the rules of our Table II.

[5]With the possible exception of the references cited above (Ref. 4), earlier efforts to unify scalar and spinor electrodynamics seem to have moved in the direction of making the spin-zero equations resemble the usual Dirac equation instead of the other way around [N. Kemmer, Proc. R. Soc. London Ser. A **173**, 91 (1939); M. Neuman and W. H. Furry, Phys. Rev. **76**, 1677 (1949); R. G. Moorhouse, Phys. Rev. **76**, 1691 (1949); J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw–Hill, New York, 1964), Sec. 9.7 and other references cited therein].

[6]Our treatment of Coulomb gauge quantization is most like that of J. D. Bjorken and S. D. Drell, *Relativistic Quantum Fields* (McGraw–Hill, New York, 1965). Some other books that may be helpful are S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1961); A. Akhiezer and V. B. Bereztetski, *Quantum Electrodynamics* (Wiley, New York, 1963), 2nd ed.; J. M. Jauch and F. Rohrlich, *The Theory of Photons and Electrons* (Springer, New York, 1976), 2nd ed.

[7]The dual spinors $\bar{u}^\rho(\mathbf{p})$ and $\bar{v}^\rho(\mathbf{p})$ are defined in conformity with Eq. (1.5):

$$\bar{u}^\rho(\mathbf{p}) \equiv -u^\rho(\mathbf{p})^\dagger(-E+\boldsymbol{\sigma}\cdot\mathbf{p}),$$

$$\bar{v}^\rho(\mathbf{p}) \equiv -v^\rho(\mathbf{p})^\dagger(E-\boldsymbol{\sigma}\cdot\mathbf{p}),$$

and turn out to be

$$\bar{u}^\rho(\mathbf{p}) = u^\rho(0)^\dagger m(E+m-\boldsymbol{\sigma}\cdot\mathbf{p})/[2m(E+m)]^{1/2}$$

and

$$\bar{v}^\rho(\mathbf{p}) = -v^\rho(0)^\dagger m(E+m-\boldsymbol{\sigma}\cdot\mathbf{p})/[2m(E+m)]^{1/2}.$$

Also, the spinors $v^\rho(\mathbf{p})$ are defined to be charge conjugates of the spinors $u^\rho(\mathbf{p})$ in the sense that $v^\rho(\mathbf{p})\exp(-i\mathbf{p}\cdot\mathbf{r}+iEt)$ is the charge conjugate of $u^\rho(\mathbf{p})\exp(i\mathbf{p}\cdot\mathbf{r}-iEt)$. Charge conjugation for Eq. (1.1) is defined by $\phi_c \equiv \sigma_y\tilde{\phi}/m$; and $(\tilde{\phi})_c \equiv -m\tilde{\phi}\sigma_y$.

[8]The notation is that of J. Schwinger, Proc. Nat. Acad. Sci. (USA) **37**, 455 (1951).

[9]For completeness we record here another useful relation involving spin algebra. With indices suppressed it reads $(1+i\sigma)0(1+i\sigma) = 2(1+i\sigma)\,\mathrm{tr}\,(0)$. More explicitly, $(1+i\sigma)_{\mu\lambda}0(1+i\sigma)_{\lambda\nu} = 2(1+i\sigma)_{\mu\nu}\,\mathrm{tr}\,(0)$. The object 0 is an arbitrary 2×2 matrix, which may itself carry Lorentz indices, but these are irrelevant to the identity.

[10]F. Rohrlich, Phys. Rev. **80**, 666 (1950); A. Salam, Phys. Rev. **86**, 731 (1952).

[11]J. M. Jauch and F. Rohrlich (see Ref. 6), p. 183, Eqs. (9)–(26). Note that their result is independent of the particular representation of the gamma matrices. By comparing their first-order Dirac equation and ours, it follows that their $i\not{p}$ may be identified with our $i\not{p}$.

[12]This is a consequence of Eq. (2.14) of Ref. 1.

[13]J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics* (McGraw–Hill, New York, 1964), p. 155, Eq. (8.13) before exponentiation of the denominators. Due allowance must be made for the difference between our metric and theirs. Also, their $I_{\mu\nu}(k)$ corresponds to our $i\tilde{\Pi}_{\mu\nu}(k)$.

Relativistic quantum theory of fermions based on the Clifford algebra C_7

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A relativistic quantum theory of spin-½ fermions is presented that includes a charge algebra, as well as an operator that distinguishes between leptons and baryons. This, in effect, extends the Clifford algebra C_4 of Dirac's γ matrices to C_7. Moreover, the particle states Ψ are represented here by elements of C_7 as products of projection operators, instead of column vectors. A number of important results are derived, and the theory serves as a foundation for constructing physical particle states as tensor products of the bare fermion states.

I. INTRODUCTION

The relativistic quantum theory of spin-½ fermions is usually based on Dirac's wave function formalism, in which the γ matrices (belonging a Clifford algebra C_4) act as operators on wave functions represented by column vectors. In the theory presented here the states are represented by elements of the algebra, which are products of projection operators, instead of column vectors. There is no need in this formalism for a matrix representation, and results are obtained in a simpler and more transparent fashion.

Moreover, Dirac's theory is extended to include a charge (isospin) algebra as well as an operator that distinguishes between leptons and baryons. This is accomplished by extending C_4 to C_7.

The four spin-½ fermions described by the theory can be identified with the bare electron, electron neutrino for leptons, and bare proton, and neutron for baryons. It was shown by the authors in a recent publication,[1] referred to from now on as (I), that this theory can be used as a foundation for the synthesis of all other physical particle states, bosons as well as fermions.

A brief review of the intrinsic Clifford algebra C_7 is given in Sec. II. This algebra is then added to the space-time algebra in Sec. III to form the complete algebra A_7.

The spin-½ eigenstates ψ are constructed in Sec. IV from elements of A_7, as products of projection operators instead of column vectors. A massive fermion has four states distinguished by being particle–antiparticle states as well as the helicity eigenvalues $\pm\frac{1}{2}$. For a massless fermion, it is shown that these four states collapse to only two, characterized by the helicity eigenvalues.

Lepton number, baryon number, electric charge, and isospin operators are defined in Sec. V. It is shown there that a massless fermion must have zero electric charge and can only be an isospin singlet.

A reversion operation is defined in Sec. VI; and it is shown that reversion invariance implies that the Dirac subalgebra C_4 is an indecomposable basic subalgebra of A_7.

Conservation laws are formulated in Sec. VII, and an energy-momentum tensor $T^{\mu\nu}$ is defined in Sec. VIII. The states are normalized by equating T^{00} to the energy, and have a unique zero mass limit.

The magnetic moment is discussed in Sec. IX, where it is pointed out that the magnetic moment is not an independent intrinsic property, but a function of the charge and angular momenta, and is determined by the interaction of a particle with an electromagnetic field.

II. THE CLIFFORD ALGEBRA

A Clifford algebra C_n is generated by the identity E and n elements $E_0, E_1,...,E_{n-1}$, satisfying the relations

$$E_A^2 = \alpha_A E, \quad \alpha_A = \pm 1, \quad A = 0,...,n-1; \tag{2.1}$$

$$E_A E_B = -E_B E_A \text{ for } A \neq B. \tag{2.2}$$

In (I) the generators were denoted by $e, e_1,...,e_n$. We changed the symbols so that the elements of C_4 can be denoted by e_μ instead of d_μ used in (I). Moreover, in (I) we took all $\alpha_A = -1$; the additional freedom given in (2.1) is used in several ways that are seen below and in Sec. VI.

The 2^n elements of C_n consist of the generators and all possible products of them. The generators E_A are called one-elements, $E_A E_B (A \neq B)$ are two-elements, etc. An N-element $E_{i_1}\cdots E_{i_N}$ is called an even (odd) element if N is even (odd). The set of even elements and E form a subalgebra C_n^{E} of C_n isomorphic to C_{n-1}, but the set of odd elements do not form a subalgebra.

For any $N = 1,...,n-1$, let

$$F_N \equiv E_0 E_1 \cdots E_N. \tag{2.3}$$

For *odd* n only, the element F_{n-1} of C_n is the only element besides the identity, that commutes with all the other elements, i.e., the center of C_n for odd n consists of E and F_{n-1}. For even n, the center of C_n consists of E only.

If α_A are chosen so that

$$F_N^2 = +E, \tag{2.4}$$

then

$$P_N^{\pm} \equiv \tfrac{1}{2}(E \pm F_N) \tag{2.5}$$

are projection operators (projectors) so that

$$(P_N^{\pm})^2 = P_N^{\pm}, \quad P_N^+ P_N^- = 0, \quad P_N^+ + P_N^- = E. \tag{2.6}$$

The projector F_{n-1} can be used to decompose C_n for odd n, as follows:

$$C_{2n+1} = C_{2n}^+ \oplus C_{2n}^-, \quad C_{2n}^{\pm} \equiv P_{2n}^{\pm} C_{2n+1}^{\mathrm{E}}, \tag{2.7}$$

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where C^{E}_{2n+1} is the even subalgebra of C_{2n+1}. Accordingly,

$$C_7 = C_6^{+} \oplus C_6^{-}, \quad C_6^{\pm} = P_6^{\pm} C_7^{E} \supset C_5^{\pm}$$

$$C_5^{\pm} = (C_6^{\pm})^{E} = P_6^{\pm} C_6^{E};$$

$$C_5^{\pm} = C_4^{\pm\,+} \oplus C_4^{\pm\,-}, \quad C_4^{\pm\,\pm} \equiv P_6^{\pm} P_4'^{\pm} C_5^{E};$$

$$C_4 \equiv C_5^{E} \equiv (C_6^{E})^{E} \equiv ((C_7^{E})^{E})^{E}. \tag{2.8}$$

The subalgebra C_6^{+} is interpreted to be the lepton space, C_6^{-} the bare-baryon space, $C_4^{\pm\,+}$ the spaces of neutral particles, and $C_4^{\pm\,-}$ the spaces of charged particles. The reason for the prime in $P_4'^{\pm}$ is given below (2.11).

The algebra C_7 is generated by $\{E_0,E_1,\ldots,E_6\}$,

$$C_6 \equiv C_7^{E} \text{ by } \{E,E_0E_6,E_1E_6,\ldots,E_5E_6\}, \tag{2.9a}$$

$$C_5 \equiv C_6^{E} \text{ by } \{E,E_0E_6E_5E_6,\ldots,E_4E_6E_5E_6\}$$
$$= \{E,E_0E_5,E_1E_5,\ldots,E_4E_5\}, \tag{2.9b}$$

$$C_4 \equiv C_5^{E} \text{ by } \{E,E_0E_5E_4E_5,\ldots,E_3E_5E_4E_5\}$$
$$\equiv \{E,e_0,e_1,e_2,e_3\}, \tag{2.9c}$$

where

$$e_\mu \equiv E_\mu E_4, \quad \mu = 0,1,2,3; \tag{2.10}$$

$$e_\mu e_\nu = -e_\nu e_\mu, \quad \text{for } \mu \neq \nu. \tag{2.11}$$

Since $(E_0E_5)(E_1E_5)\cdots(E_4E_5) = E_0E_1\cdots E_5 = F_5$, we see that the projector that decomposes C_5 is $P_4'^{\pm} \equiv P_5^{\pm}$.

$$F_6^2 = +E \text{ implies } \alpha_0\alpha_1\cdots\alpha_6 = -1, \tag{2.12a}$$

$$F_5^2 = +E \text{ implies } \alpha_0\alpha_1\cdots\alpha_5 = -1. \tag{2.12b}$$

Moreover, in order for C_4 to serve as a basis for the space-time algebra, we require that it is isomorphic to the Dirac algebra of γ matrices, and assume the metric [see (2.11)]

$$g_{\mu\nu} = \tfrac{1}{2}\{e_\mu,e_\nu\} \equiv \tfrac{1}{2}(e_\mu e_\nu + e_\nu e_\mu), \tag{2.13}$$

$$g_{00} = +1, \quad g_{11} = g_{22} = g_{33} = -1,$$

$$g_{\mu\nu} = 0, \quad \text{for } \mu \neq \nu. \tag{2.14}$$

Making use of (2.1) and (2.2), we deduce from (2.13) that

$$-\alpha_\mu\alpha_4 = g_{\mu\mu}, \quad \alpha_0\alpha_1\alpha_2\alpha_3 = -1.$$

It follows from this and (2.12) that

$$\alpha_\mu = -\alpha_4 g_{\mu\mu}, \quad \alpha_4\alpha_5 = +1, \quad \alpha_6 = +1. \tag{2.15}$$

The parameter α_4 is arbitrary. To fix it, we take

$$E_\mu^2 = g_{\mu\mu}E, \quad \text{or } \alpha_\mu = g_{\mu\mu} \text{ and } \alpha_4 = -1. \tag{2.16}$$

Consequently,

$$\alpha_0 = +1, \quad \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \alpha_5 = -1,$$

$$\alpha_6 = +1, \tag{2.17}$$

i.e., the C_7 matrix is $(+---,---+)$.

From (2.17), (2.1), and (2.2) it follows that

$$F_1^2 = +E, \quad F_2^2 = F_3^2 = -E,$$

$$F_4^2 = F_5^2 = F_6^2 = +E. \tag{2.18}$$

For later purposes we define $g^{\mu\nu}$ and e^μ by

$$g_{\lambda\mu}g^{\mu\nu} \equiv \delta_\lambda^\nu, \tag{2.19}$$

$$e^\mu \equiv g^{\mu\nu}e_\nu^\mu \text{ or } e_\mu = g_{\mu\nu}e^\nu. \tag{2.20}$$

Numerically, the $g^{\mu\nu}$ have the same values as the $g_{\mu\nu}$ in (2.14).

III. THE COMPLETE ALGEBRA

The algebra C_7 is the intrinsic part of the complete algebra A_7, consisting of C_7 and the extrinsic space-time algebra generated by the position and momentum four-vectors x^μ,p^μ. These vectors commute with all elements of C_7, and satisfy the covariant commutation relations

$$[x_\mu,x_\nu] = 0, \quad [p_\mu,p_\nu] = 0, \quad [x_\mu,p_\nu] = -ig_{\mu\nu}; \tag{3.1a}$$

$$[x_\mu,E_A] = 0, \quad [p_\mu,E_A] = 0. \tag{3.1b}$$

Note that $x_0 = ct$ is a q number; whereas the proper time is a Lorentz-invariant c number.

The orbital angular momentum (AM) tensor is defined by

$$L_{\mu\nu} \equiv x_\mu p_\nu - x_\nu p_\mu, \tag{3.2}$$

and the spin AM tensor by

$$S_{\mu\nu} \equiv \tfrac{1}{4}i[e_\mu,e_\nu] = \tfrac{1}{4}i[E_\mu,E_\nu]. \tag{3.3}$$

Note, according to (3.1b), that the $L_{\kappa\lambda}$ commute with the $S_{\mu\nu}$. The total AM is defined by

$$J_{\mu\nu} \equiv L_{\mu\nu} + S_{\mu\nu}. \tag{3.4}$$

The set $\{J_{\mu\nu},p_\lambda\}$ satisfy the commutation relations of the Poincaré algebra.

An invariant momentum is defined in C_4 by

$$\mathfrak{p} \equiv e^\mu p_\mu = e_\mu p^\mu = E_\mu E_4 p^\mu. \tag{3.5}$$

This momentum is Lorentz invariant (scalar) because

$$[S_{\mu\nu},\mathfrak{p}] = -[L_{\mu\nu},\mathfrak{p}] = i(p_\mu e_\nu - p_\nu e_\mu), \tag{3.6a}$$

and hence

$$[J_{\mu\nu},\mathfrak{p}] = 0. \tag{3.6b}$$

According to (2.13) we have

$$\mathfrak{p}^2 = e_\mu e_\nu p^\mu p^\nu = \tfrac{1}{2}\{e_\mu,e_\nu\}p^\mu p^\nu$$
$$= g_{\mu\nu}p^\mu p^\nu E = p_\mu p^\mu E. \tag{3.7}$$

The spin four-vector components are defined, as usual, by

$$w^\kappa \equiv \tfrac{1}{2}\epsilon^{\kappa\lambda\mu\nu}J_{\lambda\mu}p_\nu = \tfrac{1}{2}\epsilon^{k\lambda\mu\nu}S_{\lambda\mu}p_\nu. \tag{3.8}$$

This is a two-element [see (3.3)] of C_4, and the invariant spin

$$\mathfrak{w} \equiv w^\kappa e_\kappa = \tfrac{1}{4}i\epsilon^{\kappa\lambda\mu\nu}e_\kappa e_\lambda e_\mu p_\nu = \tfrac{1}{4}i\epsilon^{\kappa\lambda\mu\nu}E_\kappa E_\lambda E_\mu E_4 p_\nu \tag{3.9}$$

is a three-element of C_4 (but four-element of C_7). Because of this, we have

$$\mathfrak{w}^2 = 3w_\mu w^\mu, \tag{3.10}$$

where according to (3.8), (3.3), and (3.7),

$$w_\mu w^\mu = g_{\mu\nu}w^\mu w^\nu = -\tfrac{1}{2}(\tfrac{1}{2}+1)p_\mu p^\mu E. \tag{3.11}$$

This shows that *all states in A_7 have spin-$\frac{1}{2}$*. An examination of the derivation of this conclusion would show that it is a result of the subalgebra A_4, using the properties of C_4 rather than C_7.

States of spin other than $\frac{1}{2}$ can be constructed from tensor products of A_7 states, as shown in (I).

The spin three-vector components are defined by

$$S^j \equiv \tfrac{1}{2}\epsilon^{jkl}S_{kl}, \tag{3.12}$$

and the helicity by

$$h=\sum_j \frac{S^j p^j}{|\mathbf{p}|}=\frac{-w^0}{|\mathbf{p}|}. \tag{3.13}$$

It can be verified by means of (3.8) that

$$h^2=\tfrac{1}{4}E, \tag{3.14}$$

i.e., the eigenvalues of h are $\pm\frac{1}{2}$, as expected.

The element in C_4 corresponding to Dirac's γ_5 is

$$F_3=E_0E_1E_2E_3=e_0e_1e_2e_3, \quad F_3^2=-E. \tag{3.15}$$

It can be checked by means of (3.9) that

$$F_3\mathfrak{w}=\tfrac{3}{2}\mathfrak{p}, \quad F_3\mathfrak{w}\mathfrak{p}=\tfrac{3}{2}p_\mu p^\mu E. \tag{3.16}$$

A complete set of mutually commuting operators (CSCO) of the complete algebra A_7 is

$$F_6\equiv E_0\cdots E_6, \quad F_5\equiv E_0\cdots E_5, \quad \mathfrak{p}=p^\mu e_\mu=p^\mu E_\mu E_4; \tag{3.17a}$$

$$p_\mu p^\mu, w_\mu w^\mu=-\tfrac{3}{4}p_\mu p^\mu, \mathbf{p}, h. \tag{3.17b}$$

Note that (3.17b) is a CSCO of the Poincaré algebra $\{J_{\mu\nu}, p_\lambda\}$.

IV. EIGENSTATES

If $F\in A_7$ is such that $F^2=+E$, then

$$P_F^{\pm}\equiv\tfrac{1}{2}(E\pm F), \quad F^2=E \tag{4.1}$$

is a projector satisfying (2.6), and

$$FP_F^{\pm}=\tfrac{1}{2}F(E\pm F)=\tfrac{1}{2}(F\pm E)=\pm P_F^{\pm}. \tag{4.2}$$

Thus $P_F^{\pm}$ is an eigenstate of F with the eigenvalues ± 1.

This is clearly the case for F_6 and F_5. Moreover, we see from (3.14) that

$$(2h)^2=+E. \tag{4.3}$$

Thus the helicity projector

$$P_h^{\pm}\equiv\tfrac{1}{2}(E\pm 2h) \tag{4.4}$$

is an eigenstate of the helicity h with eigenvalues $\pm\frac{1}{2}$, i.e.,

$$hP_h^{\pm}=\pm\tfrac{1}{2}P_h^{\pm}. \tag{4.5}$$

The eigenstate ψ of p_μ is obtained by adopting the position representation of p_μ, necessary to satisfy (3.1a), i.e.,

$$p_\mu\psi=i\partial_\mu\psi. \tag{4.6}$$

If $\psi_{p'}$ is an eigenstate of p_μ with eigenvalue p'_μ, then

$$p_\mu\psi_{p'}=p'_\mu\psi_{p'}. \tag{4.7}$$

The last two equations imply

$$\psi_{p'}=u\exp(-ip'_\mu x^\mu)\equiv ue^{-p'\cdot x}. \tag{4.8}$$

From (4.7), (3.7), and (3.11) we see that

$$\mathfrak{p}^2\psi_{p'}=p_\mu p^\mu\psi_{p'}=p'_\mu p'^\mu\psi_{p'}, \tag{4.9}$$

$$w_\mu w^\mu\psi_{p'}=-\tfrac{3}{4}p'_\mu p'^\mu\psi_{p'}. \tag{4.10}$$

Thus $\psi_{p'}$ is a simultaneous eigenstate of p_μ, $\mathfrak{p}^2$, and $w_\mu w^\mu$.

To determine the eigenstates of the remaining operator $\mathfrak{p}$ in (3.17), we define the particle projectors P_a ($a=\nu,e,n,p$), where

$$P_\nu\equiv P_5^+P_6^+, \quad P_e\equiv P_5^-P_6^+,$$
$$P_n\equiv P_5^+P_6^-, \quad P_p\equiv P_5^-P_6^-, \tag{4.11a}$$

$$P_\nu+P_e=P_6^+, \quad P_n+P_p=P_6^-, \quad P_aP_b=P_a\delta_{ab}. \tag{4.11b}$$

The subscripts on the lhs refer, respectively, to the bare electron neutrino, electron, neutron, and proton.

For the particle a, we introduce the rest mass m_a by

$$p'_{a\mu}p'^\mu_a=m_a^2. \tag{4.12}$$

When this is combined with (4.9), it yields

$$\mathfrak{p}^2\psi_{p'_a}=m_a^2\psi_{p'_a}. \tag{4.13}$$

It only remains to distinguish a particle from its antiparticle. In view of (4.9), we can choose a representation of A_7 in which

$$\mathfrak{p}\psi^{\pm}=p_\mu e^\mu\psi^{\pm}=\pm\sum_a m_aP_a\psi^{\pm}, \tag{4.14}$$

where the positive and negative signs refer to the particle and antiparticle states, respectively, and m_a are arbitrary mass parameters. This is the wave equation for the bare fermions.

Equation (4.14) does not imply that $\mathfrak{p}=\pm\Sigma_a m_aP_a$; only that $\mathfrak{p}$ can be represented by $\pm\Sigma_a m_aP_a$ when operating on $\psi^{\pm}$. This equation imposes additional conditions on e_μ.

For composite systems, such as the physical nucleons, ψ is a tensor product of the states of the basic fermions,[1] and (4.14) becomes

$$(\Gamma_\mu p^\mu-K)\psi=0, \tag{4.15}$$

where the Lorentz scalar K and Lorentz vector Γ_μ are operators in the tensor product spaces of C_7.

The state $\psi_a^{\pm}$ of a specific particle a can be projected out of $\psi^{\pm}$ by means of the projectors (4.11), i.e.,

$$\psi_a^{\pm}=P_a\psi^{\pm}. \tag{4.16}$$

Then, according to (4.14), (4.11b), and (4.16),

$$\mathfrak{p}\psi_a^{\pm}=p^\mu e_\mu\psi_a^{\pm}=\pm\sum_b m_bP_bP_a\psi^{\pm}=\pm m_a\psi_a^{\pm}. \tag{4.17}$$

Thus $\psi_a^{\pm}$ is an eigenstate of $\mathfrak{p}$ with the eigenvalues $\pm m_a$. Moreover, it follows from (4.17) that

$$\mathfrak{p}^2\psi_a^{\pm}=\left(\sum_b m_b^2P_b\right)\psi_a^{\pm}=m_a^2\psi_a^{\pm}. \tag{4.18}$$

This confirms the consistency of (4.14) with (4.9).

A simultaneous eigenstate of the CSCO (3.17) is thus

$$\psi_a'^{(\pm)\pm}=N'_aP_h^{(\pm)}P_a(\mathfrak{p}\pm m_aE)\exp(-ip'_a\cdot x). \tag{4.19}$$

This follows from (4.2), (4.5), (4.7), (4.10), (4.13), and

$$\begin{aligned}\mathfrak{p}\left[(\mathfrak{p}\pm m_aE)e^{-ip'_a\cdot x}\right]&=(m_a^2\pm m_a\mathfrak{p})\exp(-ip'_a\cdot x)\\&=\pm m_a\left[(\mathfrak{p}\pm m_aE)\exp(-ip'_a\cdot x)\right],\end{aligned} \tag{4.20}$$

in agreement with (4.17). The normalization constant N'_a is evaluated at the end of Sec. VIII.

When $m_a=0$, e.g., for a neutrino, (4.19) becomes

$$\psi_\nu'^{(\pm)}=N_\nu P_h^{(\pm)}P_\nu\mathfrak{p}e^{-ip'\cdot x}=0. \tag{4.21}$$

Thus there are only two neutrino states ($h=\pm\frac{1}{2}$), instead of the four states associated with the other massive fermions, namely particle, antiparticle, and $h=\pm\frac{1}{2}$. These four states collapse into two degenerate pairs for $m_\nu=0$.

To understand the reason behind this, we note from

(4.17) and (4.7) that for $m_\nu = 0$,

$$p^\mu e_\mu \psi_\nu = p'^\mu e_\mu \psi_\nu = 0. \tag{4.22}$$

Without loss of generality, we may take

$$p'^0 = p'^3 = p, \quad p'^1 = p'^2 = 0. \tag{4.23}$$

Then (4.22) and (4.23) give

$$e_3\psi_\nu = -e_0\psi_\nu.$$

In view of (3.15), this implies with the help of (2.13) that

$$F_3\psi_\nu = e_0e_1e_2e_3\psi_\nu = -e_0e_1e_2e_0\psi_\nu = -e_1e_2\psi_\nu. \tag{4.24}$$

The element F_3 corresponds to the chirality operator γ_5 in Dirac's formalism.

According to (3.13), (3.8), (3.3), and (4.23),

$$2h = ie_1e_2. \tag{4.25}$$

Combining this result with (4.24), we obtain

$$iF_3\psi_\nu = -2h\psi_\nu, \tag{4.26}$$

i.e., the eigenvalues of the chirality F_3 and helicity h become proportional when $m = 0$. If chirality is used to distinguish between particle and antiparticle for $m = 0$, then the helicity plays the same role. The negative helicity state is taken to be the neutrino, and the positive helicity state the antineutrino.

For convenience, let

$$\not{p}_a \equiv p'^\mu_a e_\mu, \tag{4.27}$$

$$\hat{\not{p}}_a = \not{p}_a/m_a, \quad \text{for } m_a \neq 0. \tag{4.28}$$

Then it follows from (3.7) and (4.12) that

$$\hat{\not{p}}_a^2\psi_a = \psi_a, \tag{4.29}$$

and hence

$$\hat{P}_a^{\pm} \equiv \tfrac{1}{2}(E \pm \hat{\not{p}}_a) \tag{4.30}$$

is the particle–antiparticle projector for $m_a \neq 0$. As in (4.2),

$$\hat{\not{p}}_a \hat{P}_a^{\pm} = \pm \hat{P}_a^{\pm}. \tag{4.31}$$

In view of (4.28), we may rewrite (4.19) in the final form

$$\psi_a^{(\pm)\pm} = N_a P_h^{(\pm)} P_a \hat{P}_a^{\pm} \exp(-ip'_a \cdot x), \quad m_a \neq 0. \tag{4.32}$$

The simultaneous eigenstate (4.32) is a product of projectors, except for the last factor $\psi_{p'}$. This factor can also be written as a projector dE_p by using von Neumann's spectral resolution operators. Since (4.8) is more commonly used, we shall continue to use it.

An interesting question is the limit of $\hat{\not{p}}_a$ defined by (4.28) as $m_a \to 0$. If this limit were nonzero, then the eigenvalues ± 1 of $\hat{\not{p}}_a$ can be used to distinguish between particle and antiparticle. We show now that

$$\lim_{m_a \to 0} \hat{\not{p}}_a \psi = 0, \tag{4.33}$$

and thus it is not possible to distinguish between particle and antiparticle, aside from helicity, when $m_a = 0$, in agreement with the previous conclusion.

Let $\lim_{m_a \to 0} \hat{\not{p}}_a \psi = \epsilon\psi$, and note that $\hat{\not{p}}_a$ commutes with h, but anticommutes with F_3. Then

$$2h\hat{\not{p}}_a\psi = \epsilon 2h\psi = -i\epsilon F_3\psi$$
$$= \hat{\not{p}}_a 2h\psi = -i\hat{\not{p}}_a F_3\psi = iF_3\hat{\not{p}}_a\psi = i\epsilon F_3\psi,$$

which implies $\epsilon = 0$.

V. INTRINSIC PROPERTIES

An intrinsic property is defined by the eigenvalues that the operator representing it has for the different eigenstates. It can easily be verified that the following quantities have the correct eigenvalues.

The *lepton* number is defined by (for $m_\nu = 0$)

$$L \equiv (\not{p}/m_e)P_e - 2hP_\nu, \quad \text{for } m_\nu = 0, \tag{5.1a}$$

$$L \equiv (\not{p}/m_e)P_e + (\not{p}/m_\nu)P_\nu, \quad \text{for } m_\nu \neq 0; \tag{5.1b}$$

the *baryon number* by

$$B \equiv \not{p}(m_p^{-1}P_p + m_n^{-1}P_n); \tag{5.2}$$

the *electric charge* by

$$Q/e \equiv \not{p}(m_p^{-1}P_p - m_e^{-1}P_e); \tag{5.3}$$

and the z component of isospin for baryons by

$$I_3 \equiv \tfrac{1}{2}\not{p}(m_p^{-1}P_p - m_n^{-1}P_n). \tag{5.4}$$

The baryon *hypercharge* is then defined by

$$Y \equiv B = 2(Q_p - I_3), \tag{5.5}$$

where $Q_p \equiv P_p \not{p}/m_p$.

The electronic charge e in (5.3) is an arbitrary parameter of the theory, which fixes the *unit* of electric charge.

From (5.3), we see that for a particle a, Q is proportional to $\hat{\not{p}}_a$ defined in (4.23). The limit of $\hat{\not{p}}_a\psi_a$ as $m_a \to 0$ was shown in (4.33) to vanish. This leads to the important conclusion, which is in agreement with all experimental facts, that the *electric charge of a massless fermion is zero.*

We now prove that if p,n form an isodoublet then

$$m_p = m_n \equiv m. \tag{5.6}$$

Moreover, e^- *and* ν_e *are isosinglets* if $m_\nu = 0$, or even if $m_\nu \neq m_e$.

Since the isospin components I_1, I_2 do not change a particle into an antiparticle, and do not change the helicity, they must commute with $\not{p}$ and h. However, since they change the charge, they must anticommute with F_5. Consequently, $I_jP_5^{\pm} = P_5^{\mp}I_j$, and, according to (4.11a),

$$I_jP_p = P_nI_j, \quad I_jP_n = P_pI_j, \quad I_jP_e = P_\nu I_j,$$
$$I_jP_\nu = P_eI_j, \tag{5.7}$$

where $j = 1,2$. Moreover,

$$iI_2 = [I_3, I_1], \quad I_3 = [iI_2, I_1]. \tag{5.8}$$

Making use of (5.8), (5.7), and (5.4), we deduce that in order for I_1, I_2 to exist for p, n, (5.6) must hold provided

$$I_1^2 = E/4. \tag{5.9}$$

If e^-, ν_e are an isodoublet, then, as in (5.6), we would have to conclude that $m_e = m_\nu$. Another way of seeing this is to assume e^-, ν_e is an isodoublet, and write, when $m_\nu = 0$,

$$-I_3 = \tfrac{1}{2}m_e^{-1}\not{p}P_e + hP_\nu.$$

Repeating the above process leads to the conclusion that

$$h = -\tfrac{1}{2}\not{p}/m_e,$$

which is false for electrons. Thus the preceeding expression of I_3 for e^-, ν_e is wrong, and e^-, ν_e must be isosinglets, if $m_\nu = 0$.

Equation (5.6) permits the definition

$$\hat{p} = p^\mu e_\mu / m, \quad \text{for bare baryons.} \tag{5.10}$$

In here, p^μ is an operator, whereas in (4.28), p^μ is a number.

With the help of (5.6) and (5.10), the expressions (5.2) and (5.4) simplify to

$$B = P_6^- \hat{p}, \tag{5.11}$$

$$I_3 = -\tfrac{1}{2} P_6^- F_5 \hat{p}. \tag{5.12}$$

Expressions for I_1, I_2 that satisfy (5.8) are

$$I_1 = \tfrac{1}{2} P_6^- F_4 E_6, \quad I_2 = \tfrac{1}{2} i P_6^- E_5 E_6 \hat{p}. \tag{5.13}$$

If we define

$$I_\pm = I_1 \pm i I_2 = \tfrac{1}{2}(E_\pm F_5 \hat{p}) P_6^- F_4 E_6, \tag{5.14}$$

then

$$[I_+, I_-] = 2 I_3, \quad [I_3, I_\pm] = \pm I_\pm. \tag{5.15}$$

From (5.14) and (4.19) it follows that

$$I_- \psi_n = 0, \quad I_- \psi_{\bar{p}} = 0, \quad I_+ \psi_p = 0, \quad I_+ \psi_{\bar{n}} = 0, \tag{5.16}$$

$$I_- \psi_p (-F_4 E_6) = \psi_n, \quad I_+ \psi_n (-F_4 E_6) = \psi_p, \tag{5.17}$$

$$I_- \psi_{\bar{n}} (-F_4 E_6) = \psi_{\bar{p}}, \quad I_+ \psi_{\bar{p}} (-F_4 E_6) = \psi_{\bar{n}}. \tag{5.18}$$

The reason for multiplying the lhs's of (5.17) and (5.18) by $(-F_4 E_6)$ is because ψ is not a vector, but an element of A_7. Thus $I_\pm$ and $(-F_4 E_6)$ are intertwining operators between ψ_p and ψ_n.

VI. REVERSION

The operation of Hermitian conjugation has meaning only for matrices. The automorphism that replaces it in a Clifford algebra is *reversion*, denoted by "$\vee$." Reversion is defined as follows:

$$i^\vee = i^* = -i, \quad E^\vee = E, \quad E_A^\vee = \beta_A E_A,$$

$$\beta_A = \pm 1, \tag{6.1}$$

$$(E_A E_B)^\vee = E_B^\vee E_A^\vee. \tag{6.2}$$

We saw in (4.32) that an eigenstate is proportional to the product of commuting projectors. Suppose $\psi \propto P_F^\pm$. If $F^\vee = F$, then $\psi^\vee \psi \propto P_F^{\pm\vee} P_F^\pm = (P_F^\pm)^2 = P_F^\pm$. If $F^\vee = -F$, then $\psi^\vee \psi \propto P_F^{\pm\vee} P_F^\pm = P_F^\mp P_F^\pm = 0$. This shows that if $\psi \propto P_F^\pm$, then F must be reversion invariant, i.e.,

$$F^\vee = F. \tag{6.3}$$

From (6.1), (6.2), (2.2), and (2.3) it follows that

$$F_6^\vee = +F_6 \text{ implies } \beta_0 \beta_1 \cdots \beta_6 = -1, \tag{6.4a}$$

$$F_5^\vee = +F_5 \text{ implies } \beta_0 \beta_1 \cdots \beta_5 = -1. \tag{6.4b}$$

To determine more of the β_A, we first note from (6.1) that

$$(p_\mu \psi)^\vee = (i \partial_\mu \psi)^\vee = i^\vee \partial_\mu{}^\vee = -i \partial_\mu \psi^\vee = \psi^\vee p_\mu^\vee. \tag{6.5}$$

Second, by partial integration we obtain as usual

$$\int \psi^\vee p_\mu \psi \, d_3x = \int \psi^\vee i \partial_\mu \psi \, d_3x = \int (-i \partial_\mu \psi^\vee) \psi \, d_3x, \tag{6.6}$$

which implies

$$\psi^\vee p_\mu = -i \partial_\mu \psi^\vee \equiv \psi^\vee (-i \overleftarrow{\partial}_\mu). \tag{6.7}$$

It follows from (6.5) and (6.6) that

$$p_\mu^\vee = p_\mu. \tag{6.8}$$

Consequently, the reversion of (4.17) gives

$$\psi_a^{\pm\vee} p_\mu^\vee e^{\mu\vee} = \psi_a^{\pm\vee} p_\mu e^{\mu\vee} = \pm m_a \psi_a^{\pm\vee}. \tag{6.9}$$

If we assume that

$$\psi_a^{\pm\vee} p^\mu e_\mu = \pm m_a \psi_a^{\pm\vee}, \tag{6.10}$$

then we must have

$$e_\mu^\vee = e_\mu. \tag{6.11}$$

According to (2.10) this implies that

$$(E_\mu E_4)^\vee = E_4^\vee E_\mu^\vee = -E_\mu^\vee E_4^\vee = -\beta_\mu \beta_4 E_\mu E_4 = E_\mu E_4,$$

or

$$\beta_\mu \beta_4 = -1. \tag{6.12}$$

Consequently, $\beta_0 \beta_1 \beta_2 \beta_3 = +1$, and we conclude from (6.4) and (6.12) that

$$\beta_\mu \beta_4 = -1, \quad \beta_4 \beta_5 = -1, \quad \beta_6 = +1. \tag{6.13}$$

The only arbitrary parameter left is β_4. We fix it by taking

$$E_\mu^\vee = E_\mu, \tag{6.14}$$

i.e., $\beta_\mu = +1$, which implies $\beta_4 = -1$. Summarizing, we have

$$\beta_0 = \beta_1 = \beta_2 = \beta_3 = +1, \quad \beta_4 = -1,$$
$$\beta_5 = \beta_6 = +1. \tag{6.15}$$

From (6.15), (6.1), (6.2), (2.3), and (2.2) it follows that

$$F_1^\vee = -F_1, \quad F_2^\vee = -F_2, \quad F_3^\vee = -F_3,$$
$$F_4^\vee = -F_4, \quad F_5^\vee = F_5, \quad F_6^\vee = F_6. \tag{6.16}$$

Moreover, according to (6.7), (6.11), (3.2) to (3.5), (3.8), and (3.13) we have

$$p_\mu, e_\mu, \hat{p}, L_{\mu\nu}, S_{\mu\nu}, J_{\mu\nu}, w^\kappa, h \text{ are reversion invariant.} \tag{6.17}$$

Thus all the elements of the CSCO (3.17) are reversion invariant.

Although $F_3^\vee = F_3$, we saw in (3.15) that $F_3^2 = -E$, i.e., $\frac{1}{2}(E \pm F_3)$ is not a projector. One can define a *chirality* projector $P_c^\pm \equiv \frac{1}{2}(E \pm i F_3)$, but then $(iF_3)^\vee = -iF_3$ and iF_3 is not an observable. This means that C_3 cannot be decomposed into $C_2^+ \oplus C_2^-$ by (2.7), i.e., *the Dirac algebra C_4 is the basic indecomposable subalgebra of C_7.*

VII. CONSERVATION LAWS

The Hamiltonian H is defined to be the energy $p_0 = p^0$. If we multiply (4.17) by e^0, we obtain

$$H \psi_a^\pm = i \partial_0 \psi_a^\pm = e^0 (\pm m_a - e^j p_j) \psi_a^\pm = e^0 (\pm m_a - e^j i \partial_j) \psi_a^\pm. \tag{7.1}$$

The reversion of (7.1) is, according to (6.7), (6.8), and (6.11),

$$\psi_a^{\pm\vee} H^\vee = i \partial_0 \psi_a^{\pm\vee} = \psi_a^{\pm\vee} (\pm m_a - p_j e^j) e^0 = \psi_a^{\pm\vee} (\pm m_a + i \overleftarrow{\partial}_j e^j) e^0. \tag{7.2}$$

From the above it follows that

$$
\begin{aligned}
i\,\partial_0(\psi_a^{\pm\vee}e^0\psi_a^{\pm}) &= \psi_a^{\pm\vee}e^0 i\,\partial_0\psi_a^{\pm} \\
&= -(-i\,\partial_0\psi_a^{\pm\vee})e^0\psi_a^{\pm} \\
&= \psi_a^{\pm\vee}(\pm m_a - e^j i\,\partial_j)\psi_a^{\pm} \\
&\quad - \psi_a^{\pm\vee}(\pm m_a + i\overleftarrow{\partial}_j e^j)\psi_a^{\pm} \\
&= -i\,\partial_j(\psi_a^{\pm\vee}e^j\psi_a^{\pm}).
\end{aligned}
$$

We thus have the continuity equation

$$
\partial_\mu J_a^{(\pm)\mu} = 0, \tag{7.3}
$$

where

$$
J_a^{(\pm)\mu} \equiv \psi_a^{\pm\vee}e^\mu\psi_a^{\pm} \tag{7.4}
$$

is a conserved current density.

If we compare (7.4) with the Dirac current $\bar{\psi}_a\gamma^\mu\psi_a$, where $\bar{\psi}_a \equiv \psi_a^\dagger\gamma^0$, we see that e^μ plays the role of γ^μ and $\psi_a^{\pm\vee}$ the role of $\bar{\gamma}_a$.

If (7.3) is integrated over a spatial volume V, and it is assumed that $\psi_a^{\pm}$ vanishes at the boundary S of V, then we obtain

$$
\begin{aligned}
\partial_0\int_V J_a^{(\pm)0}\,dV &= -\int_V \partial_k J_a^{(\pm)k}\,dV \\
&= -\oint_S J_a^{(\pm)k}n_k\,dS = 0,
\end{aligned} \tag{7.5}
$$

i.e., the quantity

$$
K_a^{\pm} \equiv \int J_a^{(\pm)0}\,dV = \int \psi_a^{\pm\vee}e^0\psi_a^{\pm}\,dV \tag{7.6}
$$

is conserved (constant in time).

To interpret $K_a^{\pm}$ it is important to note that it is not a scalar, but an element of the algebra, as can be seen from (4.19). It is the sum of a scalar, a one-element, a two-element,..., and a seven-element of C_7; each one of these elements is separately conserved. In fact, if we substitute (4.21) or (4.32) into (7.6), and note that $P_6^{\pm}$, $P_5^{\pm}$, $P_h^{\pm}$ are projectors that commute with e^0, we obtain

$$
K_a^{\pm} \propto P_6^{\pm}P_5^{\pm}P_h^{\pm}(\hat{P}_a^{\pm}e^0\hat{P}_a^{\pm}), \quad \text{for } m_a \neq 0, \tag{7.7a}
$$

$$
K_a^{\pm} \propto P_6^{\pm}P_5^{\pm}P_h^{\pm}(\not{p}_a e^0\not{p}_a), \quad \text{for } m_a = 0. \tag{7.7b}
$$

For $m_a \neq 0$, we evaluate the last factor of (7.7a) by making use of (4.31) and (2.13). Thus,

$$
\begin{aligned}
\hat{P}_a^{\pm}e^\mu\hat{P}_a^{\mu} &= \pm\hat{P}_a^{\pm}\tfrac{1}{2}(\not{p}_a e^\mu + e^\mu\not{p}_a)P^{\pm} \\
&= \pm\hat{P}_a^{\pm}\tfrac{1}{2}\{e^\mu,e^\lambda\}(p'_{a\lambda}/m_a)\hat{P}_a^{\pm} \\
&= \pm\hat{P}_a^{\pm}g^{\mu\lambda}(p'_{a\lambda}/m_a)\hat{P}_a^{\pm} \\
&= \pm(p'^{\mu}_a/m_a)(\hat{P}^{\pm})^2.
\end{aligned}
$$

Thus

$$
\hat{P}_a^{\pm}e^\mu\hat{P}_a^{\pm} = \pm\hat{P}_a^{\pm}p'^{\mu}_a/m_a, \quad \text{for } m_a \neq 0. \tag{7.8a}
$$

For $m_a = 0$, we obtain, by means of (2.13),

$$
\not{p}_a e^\mu\not{p}_a = 2p'^{\mu}_a\not{p}_a, \quad \text{for } m_a = 0. \tag{7.8b}
$$

From (7.7) and (7.8), we see that the conservation of $K_a^{\pm}$ implies the conservation of F_6, F_5, h, $\not{p}_a$, and their products. According to (5.1) to (5.5) this in turn implies the conservation of L, B, Q, and I_3, Y. The conservation of $\not{p}_a = p'^{\mu}_a e_\mu$ implies the conservation of linear momentum and energy.

Other conservation laws can be derived as follows: Let A be any element of the algebra, and define

$$
\langle A\rangle \equiv \int \psi^\vee e^0 A\psi\,dV. \tag{7.9}
$$

Note that $\psi^\vee e^0$ corresponds to $\bar{\psi}e^0 = \psi^\dagger$, and $\langle A\rangle$ corresponds to the expectation value of A. Proceeding as in the derivation of (7.3), we have

$$
\begin{aligned}
i\,\partial_0\langle A\rangle &= \int[\psi^\vee e^0 A(i\,\partial_0\psi) \\
&\quad -(-i\,\partial_0\psi^\vee)e^0 A\psi]dV + i\left\langle\frac{\partial A}{\partial t}\right\rangle \\
&= \int\psi^\vee(e^0AH - e^0e^0H^\vee e^0A)\psi\,dV + i\left\langle\frac{\partial A}{\partial t}\right\rangle.
\end{aligned}
$$

From (7.1) and (7.2), we see that

$$
e^0H^\vee e^0 = H. \tag{7.10}
$$

Thus we obtain in the Schrödinger picture

$$
\begin{aligned}
\partial_0\langle A\rangle &= -i\int\psi^\vee e^0[A,H]\psi dV + \left\langle\frac{\partial A}{\partial t}\right\rangle \\
&= \langle i[H,A] + \partial A/\partial t\rangle,
\end{aligned} \tag{7.11}
$$

which is the same result as in quantum theory.

Each term of (7.11) is an element of A_7, which is the sum of n elements of A_7. A separate conservation law is obtained for each value of $n = 1,...,7$.

Making use of (3.1) to (3.5) and

$$
H_a^{\pm} \equiv e^0(\pm m_a - e^k p_k), \quad p_k = i\,\partial_k, \tag{7.12}
$$

we obtain

$$
[p_\mu,H_a^{\pm}] = 0, \tag{7.13}
$$

$$
[\not{p},H_a^{\pm}] = 4iS_{0k}p^k(\pm m_a - \not{p}),[\not{p},H_a^{\pm}]\psi_a^{\pm} = 0. \tag{7.14}
$$

$$
i[L_{\mu\nu},H_a^{\pm}] = -e_0(e_\mu p_\nu - e_\nu p_\mu) + (g_{0\mu}p_\nu - g_{0\nu}p_\mu), \tag{7.15}
$$

$$
\begin{aligned}
i[S_{\mu\nu},H_a^{\pm}] &= +e_0(e_\mu p_\nu - e_\nu p_\mu) \\
&\quad + (g_{0\mu}e_\nu - g_{0\nu}e_\mu)(\pm m_a - \not{p}),
\end{aligned} \tag{7.16}
$$

$$
\begin{aligned}
i[J_{\mu\nu},H_a^{\pm}] &= (g_{0\mu}p_\nu - g_{0\nu}p_\mu) \\
&\quad + (g_{0\mu}e_\nu - g_{0\nu}e_\mu)(\pm m_a - \not{p}).
\end{aligned} \tag{7.17}
$$

From (7.15) to (7.17), we see that

$$
[L_{jk},H_a^{\pm}] = -[S_{jk},H_a^{\pm}] = ie_0(e_j p_k - e_k p_j), \tag{7.18}
$$

$$
[J_{jk},H_a^{\pm}] = 0. \tag{7.19}
$$

Moreover, (7.13), (7.17), (7.19), and (3.8) imply

$$
\begin{aligned}
[w^\kappa,H_a^{\pm}] &= \tfrac{1}{2}\epsilon^{\kappa\lambda\mu\nu}[J_{\lambda\mu},H_a^{\pm}]p_\nu = \epsilon^{\kappa 0jl}[J_{0j},H_a^{\pm}]p_l \\
&= i\epsilon^{\kappa 0jl}e_j p_l(\not{p} \mp m_a).
\end{aligned} \tag{7.20}
$$

Thus

$$
[w^0,H_a^{\pm}] = 0, \quad [w^\kappa,H_a^{\pm}]\psi_a^{\pm} = 0, \tag{7.21}
$$

and in view of (3.13) and (7.13),

$$
[h,H_a^{\pm}] = 0. \tag{7.22}
$$

From the above we see that although the helicity and total angular momentum J_{jk} are conserved, the spin and orbital angular momenta are not, exactly as in Dirac's theory. This is different from Greider's[2] conclusion that in C_4, spin and orbital AM are separately conserved. However, his spin operator $\not{s}$ is different than $S_{\mu\nu}$ or w^κ; it is defined by $\not{s}\not{p} = s\cdot p = 0$, and $\not{s}^2 = -1$.

VIII. ENERGY-MOMENTUM TENSOR

We now show that the energy-momentum tensor can be identified with the quantity[3]

$$T^{\mu\nu} \equiv S(e^\nu \psi^\vee e^\mu \psi) = S(e^\nu J^\mu), \tag{8.1}$$

where $S(A)$ denotes the scalar part of the element A of the algebra, and J^μ is defined by (7.4).

Since $i^\vee = i^*$, we have

$$\begin{aligned} T^{\mu\nu *} &= S(e^\nu \psi^\vee e^\mu \psi)^* = S(e^\nu \psi^\vee e^\mu \psi)^\vee \\ &= S(\psi^\vee e^\mu \psi e^\nu) = S(e^\nu \psi^\vee e^\mu \psi), \end{aligned}$$

since $S(ab) = S(ba)$. Thus

$$T^{\mu\nu *} = T^{\mu\nu}, \tag{8.2}$$

i.e., $T^{\mu\nu}$ is real.

If ψ is written explicitly in the form

$$\psi = a^{(0)}E + a^{(1)}_A e^A + a^{(2)}_{AB} e^A e^B + \cdots + a^{(7)} F_6,$$

where $a^{(n)}$ is a complex coefficient of the n element of C_7, then it can be verified by substitution into (8.1) that

$$T^{00} = |a^{(0)}|^2 + \sum_A |a^{(1)}_A|^2 + \sum_{A \neq B} |a^{(2)}_{AB}|^2 + \cdots .$$

Thus T^{00} is positive definite, i.e.,

$$T^{00} \geqslant 0, \tag{8.3}$$

as it should be for the energy component.

Since ψ is proportional to the product of projectors that are reversion invariant and mutually commuting, then $\psi^\vee$ is proportional to ψ, and it follows from the cyclic property of the scalar part that $T^{\mu\nu}$ is symmetric, i.e.,

$$T^{\mu\nu} = T^{\nu\mu}. \tag{8.4}$$

Finally, it follows from (7.3) that

$$\partial_\mu T^{\mu\nu} = \partial_\mu S(e^\nu J^\mu) = S(e^\nu \partial_\mu J^\mu) = 0. \tag{8.5}$$

Thus $T^{\mu\nu}$ defined by (8.1) has all the properties that an energy-momentum tensor should have.

The condition

$$T^{00} = p^0 \tag{8.6}$$

can be used to determine the normalization constants N in (4.21) or (4.32). Substituting (4.32) into (8.1), and making use of (7.8), we obtain for the electron

$$\begin{aligned} T^{00} &= |N_e|^2 S(P_6^+ P_5^- P_h^\pm e^0 \hat{P}_e^+ e^0 \hat{P}_e^+) \\ &= |N_e|^2 (p'^0/m) S(P_6^+ P_5^- P_h^\pm e^0 \hat{P}_e^+) \\ &= |N_e|^2 (p'^0/4m)^2 = p^0. \end{aligned}$$

Thus

$$N_e = 4m p_0'^{-1/2}, \tag{8.7}$$

and

$$\psi_e = 4m p_0'^{-1/2} P_6^+ P_5^- P_h^\pm \hat{P}_e^+ \exp(-ip'_\mu x^\mu). \tag{8.8}$$

Similarly, we obtain for the neutrino state (4.21) for $m_\nu = 0$,

$$\begin{aligned} &T^{00} = |N_\nu|^2 S(P_6^+ P_h^- e^0 \mathfrak{p}_\nu e^0 \mathfrak{p}_\nu) = |N_\nu|^2 2^{-2} p_0'^2, \\ &\psi_\nu = 2p_0'^{-1/2} P_6^+ P_5^- P_h^- \mathfrak{p} \exp(-ip'_\mu x^\mu). \end{aligned} \tag{8.9}$$

According to (4.28) and (4.30),

$$2m\hat{P}_e^+ = mE + \mathfrak{p}_e \to \mathfrak{p}_e \quad \text{as } m \to 0.$$

Thus

$$\lim_{m\to 0} \psi_e = \psi_\nu. \tag{8.10}$$

It is remarkable that the condition (8.6) specifies the normalization condition of ψ_e with the correct limit to the $m = 0$ case. In the conventional normalization of the Dirac wave function there is an ambiguity whether to take $u^\dagger u = 1$, or $u^\dagger u = E/m$, where u is defined by (4.8).

IX. MAGNETIC MOMENT

Since all states and projectors of C_7 have been interpreted, there is no room left for an independent new intrinsic property, such as the magnetic moment.

The normal magnetic moment operator is defined to express the linear response of a particle to an external electromagnetic field under minimal coupling; whereas an anomalous magnetic moment can result from the Pauli coupling. Moreover, there are nonlinear responses such as polarizabilities. In principle, these moments can be calculated by means of the wave function, but not as eigenvalues of members of the CSCO.

The action A representing the interaction of a particle of state ψ with an electromagnetic field A_μ is given by

$$A = e\int d_3x\, \bar{\psi}\gamma^\mu \psi A_\mu. \tag{9.1}$$

For a pure magnetic field $\mathbf{B}$, $A_\mu = (0, \frac{1}{2}\mathbf{B}\times\mathbf{r})$, and

$$A = \frac{1}{2} e\int d_3x\, \psi^\dagger \boldsymbol{\alpha}\cdot\mathbf{B}\times\mathbf{r}\psi = \frac{1}{2} e\delta_4(p'-p) u^\dagger \boldsymbol{\alpha}\cdot\mathbf{B}\times\mathbf{r}u. \tag{9.2}$$

The corresponding interaction operator in the Hamiltonian is

$$H_{\text{int}} = \tfrac{1}{2} e\mathbf{B}\cdot(\boldsymbol{\alpha}\times\mathbf{r}). \tag{9.3}$$

The magnetic moment $\boldsymbol{\mu}$ is defined by setting

$$H_{\text{int}} \equiv -\mathbf{B}\cdot\boldsymbol{\mu}. \tag{9.4}$$

Noting that in the Heisenberg representation ($c = 1$)

$$\mathbf{v} \equiv \frac{d\mathbf{r}}{dt} = i[H,\mathbf{r}] = \boldsymbol{\alpha}, \tag{9.5}$$

we obtain from (9.3) to (9.5),

$$\boldsymbol{\mu} = \tfrac{1}{2} e\mathbf{r}\times\mathbf{v}. \tag{9.6}$$

It has been shown[4] by means of the properties of the Dirac equation, that this operator reduces to

$$\boldsymbol{\mu} = \tfrac{1}{2} e(\mathbf{L} + 2\mathbf{S})H^{-1}, \tag{9.7}$$

which is a function of the charge, spin and orbital AM. This shows that the spin magnetic moment (second term) is not an independent intrinsic property.

The anomalous magnetic moment stems from another term in the action given by

$$A^{(a)} = a\int d_3x\, \bar{\psi} S_{\mu\nu} \psi F^{\mu\nu}, \tag{9.8}$$

where $F^{\mu\nu}$ is the electromagnetic field. For a pure magnetic

field, this contributes to the interaction Hamiltonian the term

$$a\gamma^0 S_{ij} F^{ij} = 2a\gamma^0 \mathbf{S}\cdot\mathbf{B} = -\boldsymbol{\mu}^{(a)}\cdot\mathbf{B}. \tag{9.9}$$

Here again the anomalous magnetic moment appears as a coefficient of the field in the response of the system.

Greider[2] takes an electron state which is proportional to $(1 + i\hat{p}_e)(1 + e_5\hat{s})$, where $e_5 = F_3$ corresponds to γ_5, and $\hat{s}$ is a spin vector defined by $\hat{s}\hat{p} = 0$, and $\hat{s}^2 = -1$. By substituting into (7.6), he obtains the conserved quantity corresponding to K_e^+,

$$C(e^-) = \tfrac{1}{4}(-i + \hat{p}_e + e_5\hat{p}_e\hat{s} - ie_5\hat{s}). \tag{9.10}$$

He then interprets the scalar coefficients of these four terms to be proportional to the conserved charge, four-momentum, magnetic moment, and axial spin, respectively. The magnetic moment term is proportional to $p\cdot s$, which does not agree with the standard physical quantity as measured. Moreover, it is not derived from the coupling of the particle to the electromagnetic field.

X. CONCLUSIONS

The main results of this paper are the following.

(1) The framework of Dirac's relativistic quantum theory of spin-$\frac{1}{2}$ fermions is extended to include a charge (isospin) algebra, as well as an operator that distinguishes between leptons and baryons. This is accomplished by extending the Dirac Clifford algebra C_4 of γ matrices to C_7.

(2) Since C_5 is the tensor sum of two C_4's, and C_7 is the tensor sum of two C_6's, the whole space is decomposed into four C_4 subspaces, which are interpreted as charged–neutral and lepton–baryon subspaces. Thus the eigenstates of the algebra are interpreted to be the *bare* electron, electron–neutrino, proton, neutron, and their antiparticles.

(3) The eigenstates are described mathematically by products of projection operators of the algebra, instead of the usual column matrices. The neutrino eigenstate is the zero-mass limit of the electron eigenstate.

(4) Operators are defined which can be interpreted to be the isospin components, electric charge, lepton number, and baryon number. The ultimate justification of these definitions would have to await their use in interactions in later work. Some consequences of these definitions are (a) the electric charge of a massless spin-$\frac{1}{2}$ fermion is zero, (b) the bare proton and neutron form an isodoublet if their masses are equal, and (c) the electron and electron–neutrino are isosinglets if their masses are different.

(5) A reversion operation is defined, which is essentially the reversal of order of the elements of C_7. It is shown that if a projection operator $P_F^{\pm} = \frac{1}{2}(E \pm F)$ occurs as a factor in the expression of a particle eigenstate, where E is the identity element of C_7, then the operator F must be reversion invariant. Reversion also plays the role of Hermitian conjugation.

(6) Expressions for conserved quantities are derived. Since such expressions consist of a sum of products of different number of elements of C_7, each term of the sum is separately conserved. In this way it is possible to prove simultaneously the conservation of several observables, which is not possible in the usual approach.

(7) An expression of an energy-momentum tensor is defined. The condition that $T^{00} = p^0$ serves to fix the normalization constants of the eigenstates, without having to resort to box normalization.

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A new spin-$\frac{1}{2}$ wave equation

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A su(2)⊂so(3,1)⊂so(3,3) spin Casimir operator is shown to equal a sl(2,R) Casimir operator. This sl(2,R) Casimir operator may be factored to yield a wave equation describing a massive spin-$\frac{1}{2}$ particle. This wave equation possesses only timelike momentum solutions, of both positive and negative energy. Moreover, the expectation value of the electric dipole moment, with respect to these solutions, vanishes in a rest frame of the particle.

I. INTRODUCTION

This paper is devoted to the discussion of an infinite component wave equation, which may possibly be useful in the description of a (composite) massive spin-$\frac{1}{2}$ particle. In this model, the spin degrees of freedom of the particle are carried by the functional dependence of the wave function on a real spinor independent variable u. Here, u is an element of an internal space D_4, real four-dimensional Dirac space. The wave equation itself is cast on $M_4 \times D_4$, where M_4 denotes Minkowski space-time. Solutions of the wave equation, when restricted to D_4, belong to the Hilbert space $L^2(D_4)$ of square-integrable smooth functions on D_4.

The wave equation considered in this paper is of first order in the momentum and admits only timelike momentum eigenstates. Moreover, solutions to the wave equation exist for both positive and negative energy, so that in all likelihood, minimal coupling to Yang–Mills fields is possible (but not considered in this paper). It may be worth emphasizing at the outset that the wave equation considered in this paper is not of the Majorana type,[1] viz., $(\kappa^\alpha \partial_\alpha + \kappa)\phi = 0$, where κ and κ^α commute: $[\kappa, \kappa^\alpha] = 0$. Equations of this type have been comprehensively investigated by Naimark.[2]

An important property possessed by the simultaneous eigenvectors of this wave equation, and of the operator F of Eq. (45), is that the expectation value of the intrinsic electric dipole moment, with respect to these states, vanishes in a rest frame of the particle. This, of course, is just what one demands of any acceptable model of elementary particles. The major drawback of this new equation is that it possesses the same experimentally unobserved degeneracy characteristic of infinite component wave equations.

The wave equation under consideration arises from the factorization, *à la* Dirac, of a sl(2,R) Casimir operator that equals, when evaluated in a rest frame, the su(2) spin Casimir operator. We turn now to the construction of a concrete realization of these two operators.

II. DIRAC'S UNITARY REPRESENTATION OF $\overline{\mathrm{SO}(3,3)}$

In the 1963 paper "A Remarkable Representation of the 3 + 2 de Sitter Group," Dirac constructs a unitary representation of $\overline{\mathrm{SO}(3,3)}$ [and by imposing suitable constraints, a unitary representation of $\overline{\mathrm{SO}(3,2)}$] utilizing a real four component Dirac spinor with components u^a, $a,b,\ldots = 1,2,3,4$, $u \in D_4$ (see Ref. 3). His construction may be concisely formulated, provided that we focus our attention on the restriction of $\overline{\mathrm{SO}(3,3)}$ to a $\overline{\mathrm{SO}(3,1)}$ subgroup: the generators $\Sigma^{\alpha\beta}$, $\alpha,\beta,\ldots = 1,2,3,4$ of so(3,1) acting on $L^2(D_4)$ are given by

$$\Sigma^{\alpha\beta} = \xi S^{\alpha\beta} u, \tag{1}$$

where

$$\xi = -i\frac{\partial}{\partial u}, \tag{2}$$

and

$$S^{\alpha\beta} = -\tfrac{1}{4}[\gamma^\alpha, \gamma^\beta]. \tag{3}$$

Here γ^α denotes a real 4×4 irreducible representation of Dirac's γ matrices. The γ^α verify

$$\gamma^\alpha \gamma^\beta + \gamma^\beta \gamma^\alpha = 2\gamma_0 g^{\alpha\beta}, \tag{4}$$

where

$$g^{\alpha\beta} = g_{\alpha\beta} = \mathrm{diag}(1,1,1,-1) \tag{5}$$

and γ_0 denotes the 4×4 unit matrix. The $\Sigma^{\alpha\beta}$ of Eq. (1) correspond to $-i$ times the anti-Hermitian $\chi^{\alpha\beta}$ [Eq. (12) of Ref. 3] utilized by Dirac.

In Ref. 3, Dirac proves the equivalent of

$$\tfrac{1}{2}\Sigma^{\alpha\beta}\Sigma_{\alpha\beta} = j_0^2 - c^2 - 1 \tag{6}$$

and

$$\tfrac{1}{8}\epsilon_{\alpha\beta\mu\nu}\Sigma^{\alpha\beta}\Sigma^{\mu\nu} = j_0 c, \tag{7}$$

where

$$j_0 = -\tfrac{1}{2}\xi\gamma^5 u, \tag{8}$$

with

$$\gamma^5 = -\gamma^1\gamma^2\gamma^3\gamma^4 \tag{9}$$

and

$$c = \tfrac{1}{2}\cdot\tfrac{1}{2}(\xi_a u^a + u^a \xi_a). \tag{10}$$

Equations (6) and (7) are, of course, manifestations of the well-known fact that the unitary irreducible representations of $\overline{\mathrm{SO}(3,1)}$ can be labeled by two numbers (j_0, c) (see Refs. 2–

4). In Ref. 3, Dirac shows that the unitary irrep $(j_0,c) = (\frac{1}{2},0)$ provides a representation of SO(3,2). However, we emphasize that Dirac does not work on $L^2(D_4)$. In the Appendix we show that j_0 takes on half-integer values on $L^2(D_4)$ while c is not diagonal. Here, $|j_0|$ is the so-called "minimum spin" of the representation. This nomenclature arises from the fact that $\frac{1}{2}\Sigma^{jk}\Sigma_{jk}, j,k,\ldots = 1,2,3$ has eigenvalues $s(s+1)$, where s is constrained to satisfy $s \geqslant |j_0|$ (see Refs. 2 and 4).

Since j_0 and $\Sigma^{\alpha\beta}$ are homogeneous of degree zero in u,

$$[c, j_0] = 0 \tag{11}$$

and

$$[c, \Sigma^{\alpha\beta}] = 0. \tag{12}$$

Moreover, since $[\gamma^5, S^{\alpha\beta}] = 0$, one sees that

$$[j_0, \Sigma^{\alpha\beta}] = 0. \tag{13}$$

The starting point for the calculations of this paper is Dirac's proof that

$$\tfrac{1}{2}\Sigma^{jk}\Sigma_{jk} = \tfrac{1}{4}\,\partial_a\, u^a u^b\,\partial_b - \tfrac{1}{4}\partial_a\, u^b u^b\,\partial_a, \tag{14}$$

where $\partial_a = i\xi_a$. Equation (14) is equivalent to Dirac's Eq. (24). If we put

$$u^a u^a = r^2,\ u^a\,\partial_a = r\frac{\partial}{\partial r},$$

and

$$\partial_a\,\partial_a = \frac{1}{r^3}\frac{\partial}{\partial r}r^3\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_0,$$

where Δ_0 is the restriction of the Laplacian on $\mathbb{R}^4$ to the unit three-sphere, then $\frac{1}{2}\Sigma^{jk}\Sigma_{jk}$ reduces to

$$\tfrac{1}{2}\Sigma^{jk}\Sigma_{jk} = -\tfrac{1}{4}\Delta_0. \tag{15}$$

Here, Δ_0 has eigenvalues $-l(l+2), l = 0,1,2,\ldots$ (see Ref. 5), so that $\frac{1}{2}\Sigma^{jk}\Sigma_{jk}$ has eigenvalues $s(s+1), s = 0,\frac{1}{2},1,\ldots$.

III. RECASTING THE su(2) CASIMIR OPERATOR

In this section, we rewrite the su(2) Casimir operator $\frac{1}{2}\Sigma^{jk}\Sigma_{jk}$ appearing in Eq. (15) as a sl(2,$\mathbb{R}$) Casimir operator [see Eq. (27)]. This sl(2,$\mathbb{R}$) Casimir operator can be "factored" to yield the wave equation that we seek. It is hoped that the reader will bear with us through this cacophony.

In accordance with Ref. 6, let us introduce a symplectic form on D_4 $\epsilon_{ab} = -\epsilon_{ba} \leftrightarrow \epsilon$, and its inverse $\epsilon^{-1} \leftrightarrow (\epsilon^{-1})^{ab} = \epsilon^{ba} = -\epsilon^{ab}$. One may lower (resp., raise) $\overline{\mathrm{SO}(3,1)}$ spinor indices according to $\tilde{u}\epsilon \leftrightarrow u^a\epsilon_{ab} = u_b$ (the tilde denotes transpose) (resp., $u^a = \epsilon^{ab}u_b$). Conventions are $\gamma^a \leftrightarrow \gamma^{aa}{}_b$, $\epsilon^{ab}\epsilon_{bc} = -\delta^a_c$, $\gamma^A_{ab} = \epsilon_{ca}\gamma^{Ac}{}_b = -\epsilon_{ac}\gamma^{Ac}{}_b = -\delta_{ab}$, and $\gamma^{Aab} = \gamma^{Aa}{}_c\epsilon^{bc} = \gamma^{Aa}{}_c(\epsilon^{-1})^{cb} = -\delta^{ab}$. Note that $u^a\xi_a = -u_a\xi^a$.

We may rewrite the second term appearing on the right-hand side of Eq. (14) as

$$\begin{aligned}\partial_a\, u^b u^b\,\partial_a &= 2u^a\,\partial_a + u^b u^b\,\partial_a\,\partial_a \\ &= 2u^a\,\partial_a - \tilde{u}\epsilon\gamma^A u\,\partial\gamma^A\,\epsilon^{-1}\tilde{\partial} \\ &= 2u^a\,\partial_a + \tilde{u}\epsilon\gamma^A u\xi\gamma^A\epsilon^{-1}\tilde{\xi} \\ &= 2u^a\,\partial_a + v_\alpha v_\beta\tilde{u}\epsilon\gamma^\alpha u\xi\gamma^\beta\epsilon^{-1}\tilde{\xi},\end{aligned}$$

where we have introduced a timelike unit vector $v^\alpha = \delta^\alpha_4, v_\alpha v^\alpha = -1$. Substituting this expression into Eq. (14) yields

$$\begin{aligned}4\boldsymbol{\Sigma}\cdot\boldsymbol{\Sigma} &= \partial_a u^a u^b\,\partial_b - 2u^a\,\partial_a - (v_\alpha\tilde{u}\epsilon\gamma^\alpha u)(v_\beta\xi\gamma^\beta\epsilon^{-1}\xi) \\ &= (u^a\,\partial_a)^2 + 2u^a\,\partial_a + v_\alpha n^\alpha v_\beta m^\beta,\end{aligned}$$

where we have defined

$$n^\alpha = \tilde{u}\epsilon\gamma^\alpha u \tag{16}$$

and

$$m^\alpha = -\xi\gamma^\alpha\epsilon^{-1}\tilde{\xi}. \tag{17}$$

Here n^α and m^α are future-pointing lightlike vectors. Using the identity[6]

$$\gamma_\alpha\lambda\xi\gamma^\alpha = \gamma_0\xi\lambda + \gamma^5\xi\gamma^5\lambda + \epsilon^{-1}\tilde{\xi}\tilde{\lambda}\epsilon + \gamma^5\epsilon^{-1}\tilde{\xi}\tilde{\lambda}\epsilon\gamma^5, \tag{18}$$

where $[\lambda^a, \xi_b] = 0$, one may quickly show that

$$n^\alpha n_\alpha = 0 = m_\alpha m^\alpha \tag{19}$$

and

$$\tfrac{1}{2}(n_\alpha m^\alpha + m^\alpha n_\alpha) = -8(j_0^2 + c^2 - 1). \tag{20}$$

In addition, by straightforward evaluation one finds that

$$(i/8)[n^\alpha, m^\beta] = cg^{\alpha\beta} + \Sigma^{\alpha\beta}, \tag{21}$$

$$[c, n^\alpha] = -in^\alpha, \tag{22}$$

and

$$[c, m^\alpha] = im^\alpha. \tag{23}$$

Substituting $u^a\,\partial_a = 2ic - 2$ and

$$v_\alpha n^\alpha v_\beta m^\beta = \tfrac{1}{2}(v_\alpha n^\alpha v_\beta m^\beta + v_\beta m^\beta v_\alpha n^\alpha + 8ic)$$

into the previous expression for $\boldsymbol{\Sigma}\cdot\boldsymbol{\Sigma}$ yields

$$\tfrac{1}{2}\Sigma^{jk}\Sigma_{jk} = -c^2 + \tfrac{1}{8}v_\alpha v_\beta(n^\alpha m^\beta + m^\beta n^\alpha). \tag{24}$$

This may be explicitly written as a sl(2,$\mathbb{R}$) Casimir operator as follows: define a future-pointing timelike vector $E^\alpha_{(4)}$ according to

$$E^\alpha_{(4)} = \tfrac{1}{4}(n^\alpha + m^\alpha), \tag{25}$$

and a spacelike vector $E^\alpha_{(1)}$ as

$$E^\alpha_{(1)} = \tfrac{1}{4}(m^\alpha - n^\alpha). \tag{26}$$

Clearly,

$$E^\alpha_{(4)}E^\beta_{(4)} - E^\alpha_{(1)}E^\beta_{(1)} = \tfrac{1}{8}(n^\alpha m^\beta + m^\alpha n^\beta).$$

Hence,

$$\begin{aligned}\tfrac{1}{8}v_\alpha v_\beta(n^\alpha m^\beta + m^\beta n^\alpha) &= v_\alpha v_\beta(E^\alpha_{(4)}E^\beta_{(4)} - E^\alpha_{(1)}E^\beta_{(1)}) \\ &= (-v_{(4)})^2 - (v_{(1)})^2,\end{aligned}$$

where we have put $v_{(4)} = -v_\alpha E^\alpha_{(4)}$ and $v_{(1)} = v_\alpha E^\alpha_{(1)}$. Substituting this result into Eq. (24) yields

$$\tfrac{1}{2}\Sigma^{jk}\Sigma_{jk} = v^2_{(4)} - v^2_{(1)} - c^2, \tag{27}$$

which is the expression that we seek.

We mention in passing that $E^\alpha_{(1)}$ and $E^\alpha_{(4)}$ are orthogonal in the sense that

$$g_{\alpha\beta}\{E^\alpha_{(1)}E^\beta_{(4)} + E^\beta_{(4)}E^\alpha_{(1)}\} = 0. \tag{28}$$

They verify the commutation relations

$$[E^\alpha_{(1)}, E^\beta_{(1)}] = i\Sigma^{\alpha\beta} = -[E^\alpha_{(4)}, E^\beta_{(4)}] \tag{29}$$

and

$$[E^{\alpha}_{(1)}, E^{\beta}_{(4)}] = icg^{\alpha\beta}; \tag{30}$$

these relationships are consequences of Eq. (21).

IV. THE WAVE EQUATION

We recall that D_4 denotes the real four-dimensional symplectic space coordinatized by u^a. We call D_4 Dirac space. The base space on which the wave equation is cast is $M_4 \times D_4$, where M_4 is a Minkowski space-time coordinatized by Cartesian coordinates x^α, $\alpha,\beta,\ldots = 1,2,3,4$. With respect to the canonical measure on $M_4 \times D_4$, $p_\alpha = -i\partial_\alpha$ and ξ_a are Hermitian.

Consider the scalar operators

$$p_{(1)} = p_\alpha E^{\alpha}_{(1)} \tag{31}$$

and

$$p_{(4)} = -p_\alpha E^{\alpha}_{(4)}. \tag{32}$$

They are scalar operators because they commute with the generators $J^{\alpha\beta}$ of $\overline{SO(3,1)}$ given by

$$J^{\alpha\beta} = x^\alpha p^\beta - x^\beta p^\alpha + \Sigma^{\alpha\beta}. \tag{33}$$

Setting

$$p_{(2)} = mc, \tag{34}$$

where m is a parameter with dimensions of mass, and using Eqs. (22), (23), and (30), one finds that

$$m^{-1}[p_{(1)}, p_{(2)}] = ip_{(4)}, \tag{35}$$

$$m^{-1}[p_{(2)}, p_{(4)}] = -ip_{(1)} \tag{36}$$

and

$$m^{-1}[p_{(4)}, p_{(1)}] = i(p^\alpha p_\alpha / m^2)p_{(2)}. \tag{37}$$

Therefore, when $p^\alpha p_\alpha + m^2 = 0$, $m^{-1}p_{(1)} = v_{(1)}$, $m^{-1}p_{(2)} = v_{(2)}$, and $m^{-1}p_{(4)} = v_{(4)}$ comprise a basis for the Lie algebra $sl(2,\mathbb{R}) \simeq so(2,1)$ ($v^\alpha = m^{-1}p^\alpha$). The $sl(2,\mathbb{R})$ Casimir operator is $-v^2_{(1)} - v^2_{(2)} + v^2_{(4)}$, which, from Eq. (27), is seen to equal $\mathbf{\Sigma}\cdot\mathbf{\Sigma}$ when evaluated in a rest frame. From Eqs. (35)–(37) it follows that $v_{(4)}$ is the generator of a compact SU(2) subgroup of SL(2,$\mathbb{R}$), and, hence, possesses a simple discrete spectrum and normalizable eigenfunctions. Lastly, put

$$p_{(3)} = mj_0 = mv_{(3)}. \tag{38}$$

Because $\epsilon\gamma^\alpha\gamma^5$ and $\gamma^5\gamma^\alpha\epsilon^{-1}$ are skew-symmetric matrices,[6] j_0 commutes with n^α and m^α:

$$[j_0, n^\alpha] = 0 = [j_0, m^\alpha]. \tag{39}$$

Hence, j_0 commutes with $p_{(1)}$ and $p_{(4)}$ (and, as we have seen, $c = m^{-1}p_{(2)}$).

Let $\sigma^{(j)}$, $j,h,k = 1,2,3$ denote the 2×2 Pauli matrices, with

$$\sigma^{(j)}\sigma^{(k)} = \delta^{jk}\sigma^{(4)} + i\epsilon^{jkh}\sigma^{(h)}, \tag{40}$$

where $\sigma^{(4)}$ denotes the 2×2 unit matrix. Our wave equation describing the field-free dynamical evolution of a particle with spin j_0 and rest mass m is

$$\sigma^{(\mu)}p_{(\mu)}\Psi(p,u) = 0. \tag{41}$$

Henceforth, we set $j_0 = \frac{1}{2}$ and $m > 0$.

We now show that nontrivial square-integrable (over D_4) solutions of Eq. (41) exist only if the momentum is on mass shell $p^\alpha p_\alpha + m^2 = 0$, and s [see text following Eq. (15)] is constrained to satisfy $s = j_0 = \frac{1}{2}$ in a rest frame, i.e., the particle may unambiguously be said to possess spin-$\frac{1}{2}$. For the sake of notational simplicity, the parentheses enclosing scalar indices are omitted, and $\sigma^{(4)}$ is suppressed, whenever notational confusion is unlikely.

Since $m \neq 0$, Eq. (41) is equivalent to $\sigma^\mu v_\mu \Psi = (v_4 + \sigma^j v_j)\Psi = 0$, with $v_{(\mu)} = m^{-1}p_{(\mu)}$. Left multiplication of $(v_4 + \sigma^j v_j)\Psi$ with $-v_4 + \sigma^j v_j$ yields, using Eqs. (35)–(37) and (40),

$$\begin{aligned} 0 &= (-v_4 + \sigma^j v_j)(v_4 + \sigma^k v_k)\Psi \\ &= \{-v_4^2 + v_j v_j - i(p_\alpha p^\alpha/m^2)\sigma^1 v_2 - \sigma^3(v_4 + \sigma^1 v_1)\}\Psi \\ &= \{-v_4^2 + v_1^2 + v_2^2 \\ &\quad + v_3(v_3 + 1) - (i/m^2)(p_\alpha p^\alpha + m^2)\sigma^1 v_2\}\Psi. \end{aligned}$$

Here $m^{-2}(p_\alpha p^\alpha + m^2)\sigma^1 v_2$ is a Hermitian operator and commutes with $-v_4^2 + v_1^2 + v_2^2 + v_3(v_3 + 1)$, so that this equation is of the form $(A - iB)\Psi = 0$, where $A^\dagger = A$, $B^\dagger = B$, and $[A,B] = 0$. Since Ψ is square integrable over D_4, $(A - iB)\Psi = 0$ implies that $A\Psi = 0$ and $B\Psi = 0$. Clearly, if Ψ is not square integrable over D_4, such reasoning is false (consider an equation such as $[i(\partial/\partial x) - i(i(\partial/\partial y))]f(x,y) = 0$). Therefore, one concludes that

$$(v_4^2 - v_1^2 - v_2^2)\Psi = v_3(v_3 + 1)\Psi \tag{42}$$

and

$$(p_\alpha p^\alpha + m^2)v_2\Psi = 0 \tag{43}$$

are necessary conditions for the existence of nontrivial square-integrable (over D_4) solutions of Eq. (41). To show that $p_\alpha p^\alpha + m^2 = 0$, consider the alternative $v_2\Psi = c\Psi = 0 = -i(\frac{1}{2}r(\partial/\partial r) + 1)\Psi$, where $r(\partial/\partial r) = u^a\partial_a$. This says that Ψ is positively homogeneous of degree -2 in r. However, a function homogeneous of degree -2 in r is not square integrable over the manifold D_4:

$$\int |\Psi|^2 d^4u \sim \int_0^\infty \frac{r^3\,dr}{r^4} = \int_0^\infty \frac{dr}{r},$$

and therefore does not belong to the space of physical states. Therefore

$$(p_\alpha p^\alpha + m^2)\Psi(p,u) = 0 \tag{44}$$

is a necessary condition for the existence of nontrivial square-integrable solutions of Eq. (41).

Since p^α is timelike, Eq. (42) can be evaluated in a rest frame, which, utilizing Eq. (27), yields $j_0(j_0 + 1)\Psi = \frac{1}{2}\Sigma^{jk}\Sigma_{jk}\Psi = s(s+1)\Psi$, where $j_0 = \frac{1}{2}$. Hence, $s = j_0 = \frac{1}{2}$, and moreover, the wave function contains only the spin value $s = \frac{1}{2}$ in a rest frame.

One sees from Eqs. (42) and (44) that the eigenvalue of the $sl(2,\mathbb{R})$ Casimir operator $-v^2_{(1)} - v^2_{(2)} + v^2_{(4)}$ is $s(s+1)$. Therefore, Ψ transforms under one of the discrete unitary irreducible representations of SL(2,$\mathbb{R}$) (see Ref. 7 for a discussion of these representations).

V. DISCUSSION

Equation (41) belongs to the class of so-called "infinite component" wave equations. In general, an infinite component wave equation that is covariant under a dynamical group provides a relatively simple way to model a quantum relativistic system possessing nontrivial internal degrees of freedom. Such a system may be regarded as representing a composite system.[7,8] Two fundamentally different realizations of a composite system can be found in the literature, one based on a simple physical model that possesses internal constituents, while the other, like Eq. (41), is more abstract physically. The first type,[9,10] explicit, for example, in the multilocal model of hadrons,[8,9,11] realizes a composite system as a number of *a priori* bound (by action at a distance force) pointlike constituents. Space-time degrees of freedom are assigned to each of the constituents, and these degrees of freedom are then resolved into the part that describes the "center of mass" motion of the system, and the internal degrees of freedom associated with the relative coordinates of the system. Hadrons are assumed to correspond to the eigenstates of the internal (relative) motion of the permanently bound constituents.

In the second approach,[8,12–20] a composite system is viewed as a relativistic system that transforms under a unitary representation of some noncompact group (for example, such a model[7] might exhibit each spin value once, in a rest frame of the particle). This system is endowed with internal degrees of freedom described by some SL(2,C) tensor. The internal manifold (D_4 in this paper) carrying the internal degrees of freedom has, in general, no *a priori* relationship to points (or to mass points) in space-time. Although it is not the case here, in some models[15–17] various spin states correspond to the respective eigenstates of a harmonic oscillator Hamiltonian defined on the space of internal states (the Hilbert space of square-integrable functions over the internal manifold). In most models transitions between the various Σ^2 spin states are possible in the presence of interactions.

The wave equation (41) is remarkable to the extent that the minimum spin j_0 of the representation is, in fact, also the physical spin of the particle. In addition, Eq. (41) is of first order in the momentum p_α, and possesses only timelike momentum solutions. Dirac's new positive energy wave equation[15] and Staunton's spin-$\frac{1}{2}$ positive energy wave equation[17] are two notable equations that also possess these latter two properties. However, Eq. (41) does possess both positive and negative energy solutions. Positive energy solutions correspond to the unitary irreducible ascendant discrete series $D^+(s+1)$ of SL(2,R), with $v_{(4)}$ diagonal, its spectrum being given by $s+\mu=\mu+\frac{1}{2}$, $\mu=1,2,\ldots$. Negative energy solutions correspond to the descendant discrete series $D^-(-s-1)$, $v_{(4)}$ diagonal, with spectrum $-(s+\mu)$, $\mu=1,2,\ldots$. It should be noted that $v_{(1)}$ and $v_{(2)}$ are also Hermitian, but as they generate noncompact subgroups of SL(2,R), they possess non-normalizable eigenfunctions. Hence, physically admissible solutions to Eq. (41) with either $v_{(1)}$ or $v_{(2)}$ diagonal do not exist.

Eigenstates of $v_{(4)}$ possess the property that the expectation value of the intrinsic electric dipole moment vanishes in a rest frame:

$$\begin{aligned} im^{-1}\Psi^\dagger\Sigma^{\alpha\beta}p_\beta\Psi &= -m^{-1}\Psi^\dagger[E^\alpha_{(4)}E^\beta_{(4)}-E^\beta_{(4)}E^\alpha_{(4)}]p_\beta\Psi \\ &= \Psi^\dagger[E^\alpha_{(4)}v_{(4)}-v_{(4)}E^\alpha_{(4)}]\Psi=0. \end{aligned}$$

To the author's knowledge, Eq. (41) is the only infinite component spin-$\frac{1}{2}$ wave equation that possesses this experimentally observed property.

It must be emphasized that, as it stands, Eq. (41) does not provide a satisfactory description of a massive spin-$\frac{1}{2}$ particle. Each momentum eigenstate is infinitely degenerate. The reason that this extra degeneracy exists is because the operator

$$F=v_{(4)}-\tfrac{1}{2}\sigma^{(3)} \tag{45}$$

commutes with $\sigma^{(\mu)}v_{(\mu)}$ when $p_\alpha p^\alpha+m^2=0$. Since the spectrum of $v_{(14)}$ is unbounded for both the ascendant and descendant discrete series, each momentum eigenstate is infinitely degenerate.

Here, $E^\alpha_{(4)}$ and $m^{-1}p^\alpha$ are both timelike vector operators that arise naturally in this model. The expectation value of F is a measure of their alignment. Experience indicates that one does not utilize two unrelated timelike vector operators in the physical description of a particle. This leads one to suspect that there must be some relationship between $E^\alpha_{(4)}$ and $m^{-1}p^\alpha$; perhaps some internal interaction ought to be incorporated into this model that tends to align $E^\alpha_{(4)}$ and $m^{-1}p^\alpha$ in a parallel (antiparallel) configuration in the positive (negative) energy case. It is also plausible that one should construct "effective" free particle states by summing over the eigenstates of F (with appropriate coefficients) for fixed p^α.

One should ask whether or not Eq. (41) is really a version of the SO(4,2) infinite component wave equation[8] with $j_0=\frac{1}{2}$. As is well known, the SO(4.2) wave equation, as well as the Majorana equation, the Gel'fand–Yaglom type equations, and their generalizations[12,21] all lead to constraints between mass and spin. This, of course, is a desirable feature of a theory that deals with a composite system, providing that the prediction agrees with experiment. However, even if j_0 is not set equal to $\frac{1}{2}$ in Eq. (41), we find that $-p_\alpha p^\alpha=m^2$ and $s(s+1)=j_0(j_0+1)$. Here it should be clearly understood that the mass m is simply a parameter that is inserted into the formalism in exactly the same spirit that it enters into the conventional Dirac theory of fermions. No constraints between mass and spin arise at the free-field level in our model, in contradistinction to the above-mentioned formalisms.

APPENDIX: CURSORY TREATMENT OF THE EIGENVALUE PROBLEM

Let $\psi=\psi_{j_0nss_3}\in L^2(D_4)$; consider the eigenvalue problem

$$\hat{j}_0\psi=j_0\psi, \tag{A1}$$

$$\Sigma\cdot\Sigma\psi=s(s+1)\psi, \tag{A2}$$

$$\Sigma_{12}\psi=s_3\psi, \tag{A3}$$

and

$$E^4_{(4)}\psi = n\psi. \tag{A4}$$

The treatment of Eqs. (A1)–(A4) has many formal similarities with the classic work of Biedenharn[22] concerning the Wigner coefficients for $O(4)$, and Bander and Itzykson's treatment of the hydrogen atom.[23]

The interested reader may with to show that

$$\psi_{j_0 n s s_3} = N(n,s)e^{-r^2/2}L^{2s+1}_{n-(s+1)}(r^2)D^{(s)}_{-s_3 j_0}(a) \tag{A5}$$

is the normalized solution to Eqs. (A1)–(A4). Here

$$N(n,s) = (1/\pi)[(2s+1)(n-s-1)!/(n+s!)]^{1/2} \tag{A6}$$

is a normalization factor, $r^2 = \tilde{u}u$, L^{2s+1}_{n-s-1} is a Laguerre polynomial,

$$a = u^4 I + i\boldsymbol{\sigma}\cdot\mathbf{u}, \tag{A7}$$

and $D^{(j)}_{mm'}$ denotes Wigner's function, the conventional rotation matrix element satisfying

$$D^{(j)}_{mm'}(\lambda a) = \lambda^{2j} D^{(j)}_{mm'}(a). \tag{A8}$$

We find that the allowed values for n are

$$n = s + \mu, \quad \mu = 1,2,3,..., \tag{A9}$$

which follows from the requirement that the polynomial L^{2s+1}_{n-s-1} be of finite order, so that $e^{-r^2/2}L^{2s+1}_{n-s-1}(\tilde{u}u) \in L^2(D_4)$.

In Sec. II it is stated that $c = (-i/2)(u^a \partial_a + 2) = (-i/2)(r(\partial/\partial r) + 2)$ is not diagonal on $L^2(D_4)$. This is because, if $c\psi = \lambda\psi$, then ψ is homogeneous of degree $-2 + 2i\lambda$ in r, and hence $\psi^*\psi$ is homogeneous of degree -4 in r; thus $\psi^*\psi$ is not square integrable over D_4.

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The global existence of time-dependent vortex solutions

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We study the Cauchy problem for Abelian Yang–Mills–Higgs theory in (2 + 1)-dimensional Minkowski space-time. With suitable conditions on the background fields and a suitable choice of a Sobolev space for the subtracted gauge potentials and the Higgs field, we establish local existence. We then prove global existence by showing that an appropriate norm of the solutions cannot blow up in a finite time, and discuss the topology of these solutions.

I. INTRODUCTION

In recent years the number of topologically nontrivial Yang–Mills–Higgs solutions has increased considerably. The existence of vortex solutions with arbitrary winding number has been proved for one special value of the Higgs coupling constant by using the Bogomol'nyi equations[1] and for all values of the Higgs coupling constant by using an isotropic ansatz.[2] For non-Abelian gauge theories magnetic monopoles with arbitrary magnetic charge can even be constructed explicitly in the Prasad–Sommerfield limit of vanishing Higgs potential.[3] For nonvanishing Higgs potential, the 't Hooft–Polyakov monopole[4] and its generalization to Higgs fields which do not lie in the adjoint representation of SU(2) (see Ref. 5) are still the only known solutions. All these solutions are time independent.

The natural next step is to study time-dependent topologically nontrivial solutions. This, of course, involves proving the existence of solutions first. For solitons in two dimensions[6] and CP^N instantons[7] this has been done, although most of the results only hold in local spaces and do not allow one to control the topology. To control the topology in the approach used in this paper, we introduce background fields and work with the subtracted fields. For the subtracted fields we can prove the estimates necessary to apply Segal's general theory[8] and prove local existence of time-dependent vortex solutions. The global existence is then proven by putting an upper bound on appropriately defined pseudoenergies following a similar line of argument as the one given in Ref. 9.

II. LOCAL EXISTENCE

In this paper, we study the Abelian Yang–Mills–Higgs theory in (2 + 1)-dimensional Minkowski space-time given by the Lagrangian density

$$\mathcal{L} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} - \overline{(D_\mu \Phi)}(D^\mu \Phi) - (\lambda/4)(|\Phi|^2 - 1)^2. \tag{2.1}$$

Here, the gauge fields $F_{\mu\nu}$ are defined in terms of the real gauge potentials A_μ ($\mu = 0,1,2$) as

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{2.2}$$

Here, Φ is a complex field with covariant derivative

$$D_\mu \Phi = \partial_\mu \Phi + iA_\mu \Phi, \tag{2.3}$$

the metric is diag($-1, +1, +1$), and $\bar{f}$ is the complex conjugate of f.

We want to prove that for suitable initial value data $\Phi(0,\mathbf{x})$, $\partial_t \Phi(t,\mathbf{x})|_{t=0}$, $A_\mu(0,\mathbf{x})$, and $\partial_t A_\mu(t,\mathbf{x})|_{t=0}$, time-dependent solutions to the equations of motion

$$\partial_\mu F^{\nu\mu} = i(\bar{\Phi} D^\nu \Phi - \Phi\ \overline{D^\nu \Phi}), \tag{2.4a}$$

$$D_\mu D^\mu \Phi = (\lambda/2)\Phi(|\Phi|^2 - 1) \tag{2.4b}$$

exist. To specify the conditions for the initial value data we subtract a background field

$$A_\mu = \mathring{A}_\mu + a_\mu, \tag{2.5a}$$

$$\Phi = \mathring{\Phi} + \varphi, \tag{2.5b}$$

which satisfies

$$\mathring{A}_0 = \partial_t \mathring{A}_i = \partial_t \mathring{\Phi} = 0, \quad \partial_i \mathring{A}_i = 0, \quad i = 1,2, \tag{2.6a}$$

$$\sup_{\mathbf{x}\in\mathbf{R}^2} |\underbrace{\partial_i \partial_j \cdots}_{m} \mathring{\Phi}| < \infty,$$

$$\sup_{\mathbf{x}\in\mathbf{R}^2} |\underbrace{\partial_j \partial_k \cdots}_{m-1} \mathring{A}_i| < \infty, \quad m = 0,1,2, \tag{2.6b}$$

$$(|\mathring{\Phi}|^2 - 1) \in L^2, \quad \mathring{\nabla}_i \mathring{\Phi} := \partial_i \mathring{\Phi} + i\mathring{A}_i \mathring{\Phi} \in \mathscr{H}_2,$$

$$\mathring{F}_{ij} \in \mathscr{H}_2, \quad \partial_i^2 \mathring{A}_j \in \mathscr{H}_1. \tag{2.6c}$$

In Sec. IV, where we will discuss the topology, we will impose additional conditions.

For the subtracted field

$$\psi^T = (a_0, P_0, a_1, P_1, a_2, P_2, \varphi, \pi^*), \tag{2.7a}$$

$$P_\mu := \partial_t a_\mu, \quad \pi^* := \partial_t \varphi + i a_0 \varphi, \tag{2.7b}$$

we choose initial value data which satisfy

$$\psi \in \mathscr{H}^{(s)} := (\mathscr{H}_{s+1} \times \mathscr{H}_s)^4, \quad s \geqslant 0, \tag{2.8}$$

where $\mathscr{H}_s$ is the Sobolev space of distributions f with finite norm

$$\|f\|^2_{\mathscr{H}_s} = \|f\|^2_{L^2} + \|\partial_i f\|^2_{L^2} + \cdots + \|\underbrace{\partial_i \partial_j \cdots}_{s} f\|^2_{L^2}, \tag{2.9}$$

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and $\mathscr{H}_0$ denotes L^2. Furthermore, the Lorentz condition

$$\partial_\mu a^\mu = 0 \tag{2.10}$$

and the Gauss equation

$$\Delta a_0 - \partial_t\, \partial_i a_i = i[(\mathring{\bar{\Phi}} + \varphi)(\pi - ia_0 \mathring{\bar{\Phi}}) - (\mathring{\bar{\Phi}} + \bar{\varphi})(\pi^* + ia_0 \mathring{\Phi})] \tag{2.11}$$

hold at $t = 0$ and we impose the Lorentz gauge condition for all t to achieve a unique evolution.

For the electric field

$$E_i = \partial_i a_0 - \partial_t a_i, \tag{2.12}$$

the Gauss equation reads

$$\partial_i E_i = \rho \tag{2.13}$$

and can be solved in Fourier space by

$$\tilde{E}_i = \tilde{E}_i^T + \tilde{E}_i^L, \tag{2.14}$$

$$\tilde{E}_i^T = (\delta_{ij} - k_i k_j/|k|^2)\tilde{E}_j, \quad \tilde{E}_i^L = (k_i k_j/|k|^2)\tilde{E}_j, \tag{2.15}$$

$$i\tilde{E}_i^L = (k_i/|k|^2)\tilde{\rho}. \tag{2.16}$$

Thus the initial value data satisfy[10]

$$\tilde{E}_i^T \in \mathscr{H}_s, \quad (k_i/|k|^2)\tilde{\rho} \in \mathscr{H}_s, \tag{2.17}$$

which makes

$$\pi^* = -ia_0 \mathring{\Phi}, \quad E_i^L = 0, E_i^T \in \mathscr{H}_s \tag{2.18}$$

a possible choice.

Given the initial value data, we want to solve the equation of motion

$$\frac{d}{dt}\psi = -i\tilde{A}\psi + J. \tag{2.19}$$

Here, the operator $\tilde{A}$ and the components of J read

$$\tilde{A} = i\begin{bmatrix} \Gamma & 0 & 0 & 0 \\ 0 & \Gamma & 0 & 0 \\ 0 & 0 & \Gamma & 0 \\ 0 & 0 & 0 & \Gamma \end{bmatrix}, \quad \Gamma = \begin{bmatrix} 0 & 1 \\ \Delta - m^2 & 0 \end{bmatrix} \tag{2.20}$$

$$m^2 > 0, \quad \Delta = \partial_i^2,$$

and $(\nabla_i := \partial_i + ia_i)$

$$J_1 = J_3 = J_5 = 0, \tag{2.21a}$$

$$J_2 = m^2 a_0 + i[(\mathring{\bar{\Phi}} + \bar{\varphi})\pi^* - (\mathring{\Phi} + \varphi)\pi] - a_0(\bar{\varphi}\mathring{\Phi} + 2|\mathring{\Phi}|^2 + \varphi\mathring{\bar{\Phi}}), \tag{2.21b}$$

$$\begin{aligned} J_{2+2i} = {} & m^2 a_i + \Delta \mathring{A}_i + i(\mathring{\bar{\Phi}}\mathring{\nabla}_i \mathring{\Phi} - \mathring{\Phi}\overline{\mathring{\nabla}_i \mathring{\Phi}}) \\ & + i\big[(\mathring{\bar{\Phi}} + \bar{\varphi})\nabla_i \varphi - (\mathring{\Phi} + \phi)\,\overline{\nabla_i \varphi} \\ & + \bar{\varphi}\,\mathring{\nabla}_i \mathring{\Phi} - \varphi\overline{\mathring{\nabla}_i \mathring{\Phi}}\big] \\ & - [(\mathring{\bar{\Phi}} + \bar{\varphi})(\mathring{A}_i \varphi + a_i \mathring{\Phi}) \\ & + (\mathring{\Phi} + \varphi)(\mathring{A}_i \bar{\varphi} + a_i \mathring{\bar{\Phi}})] \quad i = 1,2, \end{aligned} \tag{2.21c}$$

$$J_7 = -ia_0\varphi, \tag{2.21d}$$

$$\begin{aligned} J_8 = {} & m^2\varphi + \Delta\mathring{\Phi} + i\,\partial_i(\mathring{A}_i \mathring{\Phi}) \\ & + i\mathring{A}_i\mathring{\nabla}_i \mathring{\Phi} - (\lambda/2)\mathring{\Phi}(|\mathring{\Phi}|^2 - 1) \\ & - (\lambda/2)[\varphi(|\mathring{\Phi} + \varphi|^2 - 1) + \mathring{\Phi}(|\varphi|^2 + \varphi\mathring{\bar{\Phi}} + \bar{\varphi}\mathring{\Phi})] \\ & + i\,\partial_i(a_i \varphi) \\ & + ia_i\nabla_i \varphi - ia_0\pi^* + 2i\mathring{A}_i\nabla_i \varphi - \mathring{A}_i^2 \varphi + ia_i\mathring{\nabla}_i \mathring{\Phi} \\ & + i\mathring{\Phi}(\partial_i a_i + i\mathring{A}_i a_i) - a_\mu a^\mu \mathring{\Phi} - iP_0 \mathring{\Phi}. \end{aligned} \tag{2.21e}$$

It is well-known that $\tilde{A}$ generates a one parameter group on any $\mathscr{H}^{(s)}$ with $s \geqslant 0$. To prove local existence and uniqueness of a solution we have to show that J is a map from $\mathscr{H}^{(1)}$ to $\mathscr{H}^{(1)}$ and that the Lipschitz condition

$$\|J(\psi) - J(\eta)\|_{\mathscr{H}^{(1)}} \leqslant C(\|\psi\|_{\mathscr{H}^{(1)}}, \|\eta\|_{\mathscr{H}^{(1)}})\|\psi - \eta\|_{\mathscr{H}^{(1)}} \tag{2.22}$$

holds with a monotonically increasing, everywhere finite function C. Using the conditions (2.6b) and (2.6c), the Cauchy–Schwartz inequality, and the inequalities

$$\|f\|_{L^\infty} \leqslant K\|f\|_{\mathscr{H}_2}, \quad \|f\|_{L^4} \leqslant K\|f\|_{L^2}^{3/4}\|\partial_i f\|_{L^2}^{1/4}, \tag{2.23}$$

this can be shown.

We have therefore established the local existence and the uniqueness of solutions to the equation

$$\psi(t) = \exp\{-i\tilde{A}t\}\psi(0) + \int_0^t ds \exp\{-i\tilde{A}(t-s)\}J(\psi(s)). \tag{2.24}$$

Because J is a C^1 map also the existence and uniqueness of solutions to Eq. (2.19) is guaranteed for initial value data from the domain of $\tilde{A}$ which is $\mathscr{H}^{(2)}$. Since J is even a C^∞ map this is also true for any $\mathscr{H}^{(s)}$, $s \geqslant 2$, with solutions $\psi \in \mathscr{H}^{(s)}$, locally. All these results follow from Segal's existence and uniqueness theorem.[8]

It remains to be shown that the initial value equations (2.10) and (2.11) are propagated by the evolution equation. To show this we write

$$U = P_0 - \partial_i a_i, \tag{2.25}$$

$$V = \Delta a_0 - \partial_i P_i + i[(\mathring{\bar{\Phi}} + \bar{\varphi})(\pi^* + ia_0 \mathring{\Phi}) - (\mathring{\Phi} + \varphi)(\pi - ia_0 \mathring{\bar{\Phi}})], \tag{2.26}$$

and compute

$$\frac{d}{dt}\begin{bmatrix} U \\ V \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \Delta & 0 \end{bmatrix}\begin{bmatrix} U \\ V \end{bmatrix}, \tag{2.27}$$

for $\psi \in \mathscr{H}^{(2)}$, and therefore for $U \in \mathscr{H}_2$ and $V \in \mathscr{H}_1$. Because this equation has a unique solution, U and V vanish throughout the interval of existence of ψ. This completes the local existence proof.

III. GLOBAL EXISTENCE

To extend our local existence proof to a global one we have to show that for a solution $\psi \in \mathscr{H}^{(2)}$ the $\mathscr{H}^{(1)}$ norm does not blow up in a finite time.[8] To derive this result we first define certain pseudoenergies and prove that they do not blow up in a finite time. For $\psi \in \mathscr{H}^{(2)}$, besides the energy

$$E^0 = \int d^2x \left\{\frac{1}{2}E_i E_i + \frac{1}{4}F_{ij}F_{ij} + \overline{(D_0 \Phi)}(D_0 \Phi) + \overline{(D_i \Phi)}(D_i \Phi) + \frac{\lambda}{4}(|\Phi|^2 - 1)^2\right\}, \tag{3.1}$$

the following quantities are defined:

$$E^1 = E^0 + \int d^2x|\varphi|^2, \tag{3.2}$$

$$E^2 = E^0 + \int d^2x\, a_\mu a_\mu, \tag{3.3}$$

$$C_2 = \int d^2x\Big\{\frac{1}{2}(\partial_j E_i)(\partial_j E_i) + \frac{1}{4}(\partial_j F_{ik})(\partial_j F_{ik}) + \overline{(D_j D_0 \Phi)}(D_j D_0 \Phi) + \overline{(D_j D_i \Phi)}(D_j D_i \Phi) + \frac{\lambda}{4}(\bar{\Phi} D_j \Phi + \Phi\, \overline{D_j \Phi})^2\Big\}. \tag{3.4}$$

Their time derivatives are, respectively,

$$\frac{d}{dt}E^0 = 0, \tag{3.5}$$

$$\frac{d}{dt}E^1 = \int d^2x(\bar{\varphi}\pi^* + \varphi\pi), \tag{3.6}$$

$$\frac{d}{dt}E^2 = -2\int d^2x\, a_i E_i, \tag{3.7}$$

and

$$\begin{aligned}\frac{d}{dt}C_2 = \int d^2x\,\{&i\big[(D_j D_0 \Phi)E_j\,\overline{D_0 \Phi} - \overline{(D_j D_0 \Phi)}E_j D_0 \Phi\big] \\ &+ i(\partial_j E_i)\big[(D_j \Phi)\,\overline{(D_i \Phi)} - \overline{(D_j \Phi)}(D_i \Phi)\big] \\ &+ iE_j\big[\overline{(D_i \Phi)}(D_j D_i \Phi) - (D_i \Phi)\,\overline{(D_j D_i \Phi)}\big] \\ &+ iE_j\big[\overline{(D_i \Phi)}(D_i D_j \Phi) - (D_i \Phi)\,\overline{(D_i D_j \Phi)}\big] \\ &+ iF_{jk}\big[\overline{(D_j D_0 \Phi)}(D_k \Phi) - (D_j D_0 \Phi)\,\overline{D_k \Phi}\big] \\ &+ \tfrac{1}{2}F_{jk}F_{jk}(\Phi\,\overline{D_0 \Phi} + \bar{\Phi} D_0 \Phi) \\ &- (\lambda/2)(|\Phi|^2 - 1)\big[(D_j D_0 \Phi)\,\overline{(D_j \Phi)} \\ &+ \overline{(D_j D_0 \Phi)}(D_j \Phi)\big] \\ &+ (\lambda/2)(\bar{\Phi} D_j \Phi + \Phi\,\overline{D_j \Phi})\big[(\overline{D_0 \Phi})(D_j \Phi) \\ &+ (D_0 \Phi)\,\overline{(D_j \Phi)}\big]\}.\end{aligned} \tag{3.8}$$

To show that (3.1)–(3.4) are defined we have used the properties (2.6) of the background fields, and to calculate the time derivatives we have used the equations of motion (2.4) in Lorentz gauge. The surface terms in the time derivative of C_2 vanish because

$$\int f\,\partial_i g = \int g\,\partial_i f \tag{3.9}$$

holds for $f, g \in \mathscr{H}_1$.

From (3.6) and (3.7) we derive the inequalities

$$\frac{d}{dt}E^s \leqslant K\sqrt{E^0}\sqrt{E^s}, \quad s = 1,2. \tag{3.10}$$

Therefore, E^s is bounded from above,

$$E^s \leqslant (K_0 + \tfrac{1}{2}K\sqrt{E^0}t)^2, \tag{3.11}$$

and cannot blow up in a finite time. To put an upper bound on C_2, except for the λ terms, we can use the estimates from Ref. 9. Since all terms in (3.8) are gauge invariant we can work in the Coulomb gauge:

$$a_i^c = a_i + \partial_i\lambda, \quad \mathring{A}_i^c = \mathring{A}_i, \tag{3.12a}$$

$$\varphi^c = e^{-i\lambda}\varphi, \quad \mathring{\Phi}^c = e^{-i\lambda}\mathring{\Phi}, \tag{3.12b}$$

where

$$\|a_i^c\|_{L^\infty} \leqslant C\,\|a_i^c\|_{\mathscr{H}_2} \leqslant K\sqrt{K_0 + K_1 t^2 + C_2} \tag{3.13}$$

holds. Notice that $\mathring{A}_i$ is in Coulomb gauge and its L^∞ norm is finite because of (2.6b).

The remaining λ terms are estimated in the Coulomb gauge as follows:

$$\begin{aligned}&\Big|\int d^2x(D_j D_0 \Phi)(D_j \Phi)(|\Phi|^2 - 1)\Big| \\ &\leqslant K\Big[\int d^2x(D_j D_0 \Phi)\,\overline{(D_j D_0 \Phi)}\Big]^{1/2} \\ &\quad \times \|D_j \Phi\|_{L^4}\,\||\Phi|^2 - 1\|_{L^4} \\ &\leqslant KC_2^{3/4}\Big[\int d^2x\,\overline{(\partial_j D_i \Phi)}(\partial_j D_i \Phi)\Big]^{1/4} \\ &\leqslant KC_2^{3/4}(K_0 + K_1 t^2 + K_2 C_2)^{1/4} \\ &\leqslant K_0 + K_1 t^2 + K_2 C_2,\end{aligned} \tag{3.14}$$

$$\begin{aligned}&\Big|\int d^2x\,(\bar{\Phi} D_j \Phi + \Phi\,\overline{D_j \Phi})\,\overline{(D_0 \Phi)}(D_j \Phi)\Big| \\ &\leqslant KC_2^{1/2}\|\partial_j D_0 \Phi\|_{L^2}^{1/2}\|\partial_j D_0 \Phi\|_{L^2}^{1/2}. \\ &\leqslant K_0 + K_1 t^2 + K_2 C_2.\end{aligned} \tag{3.15}$$

The estimates of the terms in (3.8) add up to

$$\frac{d}{dt}C_2(t) \leqslant K_0 + K_1 t^2 + K_2 C_2(t). \tag{3.16}$$

Therefore, $C_2(t)$ is bounded,

$$C_2(t) \leqslant C_2(0) + K_0 t + \tfrac{1}{3}K_1 t^3 + \int_0^t ds\, K_2\Big[C_2(0) + K_0 s + \frac{1}{3}K_1 s^3\Big]e^{K_2(t-s)}, \tag{3.17}$$

and does not blow up in a finite time.

So far we have derived the gauge invariant bounds,

$$\|\varphi\|_{L^2} < \infty, \quad \|E_i\|_{\mathscr{H}_1} < \infty, \tag{3.18a}$$

$$\|D_i \Phi\|_{L^2} < \infty, \quad \|D_i D_j \Phi\|_{L^2} < \infty, \tag{3.18b}$$

$$\|D_0 \Phi\|_{L^2} < \infty, \quad \|D_i D_0 \Phi\|_{L^2} < \infty, \tag{3.18c}$$

and the bound

$$\|a_\mu\|_{L^2} < \infty \tag{3.19}$$

on a_μ in Lorentz gauge. In the Coulomb gauge,

$$\|a_i^c\|_{\mathscr{H}_2} < \infty, \tag{3.20a}$$

$$\|\partial_i \varphi^c\|_{L^2} < \infty, \tag{3.20b}$$

and

$$\|\pi^*\|_{L^2} < \infty \tag{3.20c}$$

hold. Notice that (3.19), (3.20a), and (3.12a) imply $\partial_i\lambda \in L^2$, a result we have used to derive (3.20b).

To derive $a_\mu \in \mathscr{H}_1$ in Lorentz gauge we define locally

$$\Gamma^1 = \int d^2x\,\{P_0^2 + P_i^2 + (\partial_i a_0)^2 + (\partial_i a_j)^2\}, \tag{3.21}$$

and calculate

$$\frac{d}{dt}\Gamma^1 = 2\int d^2x\{P_0 j_0 + P_i j_i\} \leqslant K\sqrt{\Gamma^1}\|j\|_{L^2}. \quad (3.22)$$

Here, the gauge-invariant j_0 and j_i read

$$j_0 = i(\bar{\Phi} D_0 \Phi - \Phi\ \overline{D_0 \Phi}), \quad (3.23a)$$

$$j_i = \Delta \mathring{A}_i + i(\bar{\Phi} D_i \Phi - \Phi\ \overline{D_i \Phi}). \quad (3.23b)$$

Their L^2 norm is finite because of (3.18) and (3.20). Thus Γ^1 does not blow up in a finite time, and $a_\mu \in \mathscr{H}_1$ and $P_\mu \in L^2$ hold globally.

Using this result we can in turn derive

$$\partial_i \lambda \in \mathscr{H}_1, \quad \varphi^c \in \mathscr{H}_2, \quad \pi^c \in \mathscr{H}_1, \quad (3.24)$$

and

$$\|j\|^2_{\mathscr{H}_1} = \|j_0\|^2_{\mathscr{H}_1} + \|j_1\|^2_{\mathscr{H}_1} + \|j_2\|^2_{\mathscr{H}_1} < \infty. \quad (3.25)$$

This shows that

$$\Gamma^2 = \int d^2x\{(\partial_i P_0)^2 + (\partial_j P_i)^2 + (\partial_i\, \partial_j a_0)^2 + (\partial_i\, \partial_j a_k)^2\} \quad (3.26)$$

satisfies

$$\frac{d}{dt}\Gamma^2 = 2\int d^2x\{(\partial_i P_0)(\partial_i j_0) + (\partial_j P_i)(\partial_j j_i)\}$$

$$\leqslant K\sqrt{\Gamma^2}\|j\|_{\mathscr{H}_1} \quad (3.27)$$

and does not blow up in a finite time.

We therefore have derived that

$$a_\mu \in \mathscr{H}_2, \quad P_\mu \in \mathscr{H}_1 \quad (3.28)$$

hold globally in Lorentz gauge. This implies $\partial_i \lambda \in \mathscr{H}_2$ and because of the bounds on φ^c and π^c,

$$\varphi \in \mathscr{H}_2, \quad \pi^* \in \mathscr{H}_1, \quad (3.29)$$

which completes our global existence proof.

IV. TOPOLOGICAL ASPECTS

To discuss topological aspects of the solutions whose existence we have just established we have to impose additional conditions on the background fields. If we assume that

$$\lim_{R\to 0}\ \sup_{|x|=R} |1 - |\mathring{\Phi}|\,| = 0 \quad (4.1)$$

and for $|x| > R_0$, $\delta > 0$,

$$|x|^{1+\delta}|\mathring{\nabla}_i \mathring{\Phi}| < \text{const} \quad (4.2)$$

hold, we can define the winding number and the magnetic flux of the background configuration.[1] The winding number is given by

$$\mathring{n} = \frac{i}{4\pi}\int_{|x|=R} dx^i(\bar{\mathring{e}}\,\partial_i \mathring{e} - \mathring{e}\ \overline{\partial_i \mathring{e}}), \quad (4.3)$$

where

$$\mathring{e} := \mathring{\Phi}/|\mathring{\Phi}| \quad (4.4)$$

is a C^1 map for $|x| > R_0$ and $R > R_0$. It is an integer independent of R as long as $R > R_0$, i.e., as long as $\mathring{e}$ is a C^1 map on the R circle.

The magnetic flux is given by the formula

$$\mathring{g} = \lim_{R\to\infty}\int_{|x|=R} dx^i \mathring{A}_i, \quad (4.5)$$

which can be cast into the form

$$\mathring{g} = \lim_{R\to\infty}\int_{|x|<R} d^2x\, \mathring{F}_{12} \quad (4.6)$$

by Stokes' theorem. Because of the condition (4.2) the winding number is proportional to the magnetic flux:

$$\mathring{g} = 2\pi\mathring{n}. \quad (4.7)$$

Before we go on we have to make sure that background fields whch satisfy the conditions (2.6), (4.1), and (4.2) exist. This is indeed the case. We can even show that the set of allowed background configurations contains vortex solutions with arbitrary winding number: Plohr[2] has proven that solutions of the form

$$\mathring{\Phi} = R(r)e^{-i\mathring{n}\theta}, \quad \mathring{A}_0 = 0, \quad \mathring{A}_i = -\epsilon_{ij}\hat{x}_j[S(r)/r] \quad (4.8)$$

exist. The functions R and S are C^∞ maps on $[0,\infty)$. Their asymptotic behavior at the origin is

$$R \sim \alpha r^{\mathring{n}}, \quad S \sim \beta r^2 + \gamma r^4. \quad (4.9)$$

At infinity, $S + \mathring{n}$, $R - 1$, and all their derivatives decay exponentially. These properties guarantee that the solutions (4.8) satisfy the conditions (2.6), (4.1), and (4.2).

For the time-dependent solutions we found in the preceding sections, $\varphi \in \mathscr{H}_2$ holds. Hence,

$$\lim_{r\to\infty} \varphi(r,\theta) = 0 \quad (4.10)$$

follows. At any time t, the Higgs field at infinity is therefore defined and equal to the background field, $\Phi(t,\mathbf{x})$ stays in the same homotopy class of $\pi_1(S^1)$, and the winding number n labels this class as time independent.

V. CONCLUSION

We have proven the global existence of time-dependent vortex solutions and by doing so established some of their properties. Our results should open the way to a study of vortex–vortex scattering. The technique used should also help us to tackle the problem of time-dependent monopole solutions and monopole–monopole scattering.

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[10]Here $\tilde{f} \in \mathscr{H}_s$ means $\int_{\mathbf{R}^2} d^2k\,(1+|k|^2)^s\,|\tilde{f}|^2 < \infty$.

On the geometric structure of gauge theories

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In the framework of the adjoint forms over the jet spaces of connections and using a canonical jet shift differential, we give a geometrical interpretation of the Yang–Mills equations both in a direct and Lagrangian formulation.

I. INTRODUCTION

As is well known, in the geometrization of gauge theories the two basic fields, the gauge field (potential) and the particle field, are identified with geometrical objects related to some fiber bundles. In particular, connections on principal bundles provide adequate geometrical models for gauge fields in classical gauge theories such as electromagnetism and Yang–Mills theory.[1,2]

In this paper, working with principal bundles, we give a geometrical interpretation of a direct approach to Yang–Mills equations and their Lagrangian formulation. We present new geometrical techniques together with new results. The work is related to some other previous papers[3–5] in which we have studied connections, curvature, and the Euler–Lagrange equation in the general framework of fibered spaces and their jet spaces. Following these papers, we devote special consideration to the affine structures of jet spaces and their possible splittings, as well as to techniques of lift, which suggest that we not work at a fixed degree of jet spaces but to go to higher degrees.

To see the things better, let $\pi : P \to M$ be a principal bundle with structure group G. In the physical interpretation of the theory, M is the space-time manifold. A key role is played by the adjoint bundle $\mathrm{Ad}\, P \to M$ which is the vector bundle of the G-invariant vertical fields on P.

First we consider the spaces $A^r(M;\mathrm{Ad}\, P)$ of the adjoint forms $\alpha : M \to \overset{r}{\wedge} T^*M \otimes \mathrm{Ad}\, P$, the differential

$$d^A : A^r(M;\mathrm{Ad}\, P) \to A^{r+1}(M;\mathrm{Ad}\, P),$$

and the codifferential

$$\delta^A : A^r(M;\mathrm{Ad}\, P) \to A^{r-1}(M;\mathrm{Ad}\, P)$$

with respect to any principal connection A.

Then we consider the affine bundle of principal connections $C = J_1P/G \to M$ (whose vector bundle is $T^*M \otimes \mathrm{Ad}\, P \to M$) and the spaces $A^r(J_kC;\mathrm{Ad}\, P)$ of the horizontal adjoint forms $\varphi : J_kC \to \overset{r}{\wedge} T^*M \otimes \mathrm{Ad}\, P$ and we introduce a canonical differential

$$d : A^r(J_kC;\mathrm{Ad}\, P) \to A^{r+1}(J_{k+1}C;\mathrm{Ad}\, P)$$

and codifferential

$$\delta : A^r(J_kC;\mathrm{Ad}\, P) \to A^{r-1}(J_{k+1}C;\mathrm{Ad}\, P)$$

which shift the degree of jet spaces by 1. This unusual shift is very important because it leads to several new and interesting differential operators. This d extends, on one hand, the canonical connection introduced by Garcia[6] and, on the other hand, the horizontal differential on jet spaces.[7]

An analogous differential d and codifferential δ can be introduced for coadjoint forms, that is for forms valued in the coadjoint bundle $\mathrm{Ad}^*\, P \to M$.

Then we introduce the canonical affine splitting of J_1C over C

$$J_1C = S \underset{C}{\otimes} (\overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P),$$

where S is an affine subbundle of $J_1C \to C$ whose vector bundle is $\overset{2}{\vee} T^*M \otimes \mathrm{Ad}\, P$. By considering the second projection of this splitting, we get the adjoint form

$$F : J_1C \to \overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P, \quad F \in A^2(J_1C;\mathrm{Ad}\, P).$$

In our formalism it is a natural thing to apply both the operators d and δ to F. We find $0 = dF \in A^3(J_2C;\mathrm{Ad}\, P)$, $\delta F \in A^1(J_2C;\mathrm{Ad}\, P)$, and $0 = \delta^2 F \in A^0(J_3C;\mathrm{Ad}\, P)$ which allow a direct and concise formulation of the Yang–Mills equations and their associated identities, with respect to *any* potential $A : M \to C$.

Then we apply the previous techniques to Lagrangian theory induced by a Lagrangian density $\Lambda : J_1C \to \overset{m}{\wedge} T^*M$ ($m = \dim M$). We observe that if the Legendre map $\Omega_\Lambda : J_1C \to \overset{m-1}{\wedge} T^*M \otimes TM \otimes \mathrm{Ad}^*\, P$ (which is canonically associated to Λ) takes its values in the subbundle $\overset{m-2}{\wedge} T^*M \otimes \mathrm{Ad}^*\, P \hookrightarrow \overset{m-1}{\wedge} T^*M \otimes TM \otimes \mathrm{Ad}^*\, P$, it is a coadjoint form, i.e., $\Omega_\Lambda \in A^{m-2}(J_1C;\mathrm{Ad}^*\, P)$. Hence we can apply the differential calculus previously introduced and then we obtain a new geometrical interpretation of the Lagrangian approach. Then to check the condition under which Ω_Λ is a coadjoint form is a valuable question. We find that the necessary and sufficient condition is that the Lagrangian density Λ be factorable through the canonical projection $J_1C \to C \underset{M}{\times} \overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$.

Furthermore, the Euler–Lagrange operator associated to Λ can always be viewed as a coadjoint form $E_\Lambda : J_2C \to \overset{m-1}{\wedge} T^*M \otimes \mathrm{Ad}^*\, P$, i.e., $E_\Lambda \in A^{m-1}(J_2C;\mathrm{Ad}^*\, P)$.

Then if the above condition on Λ is fulfilled, we can ask whether $d\Omega_\Lambda = E_\Lambda$ and we find that this holds if Λ is factorable through the projection $F : J_1C \to \overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$, i.e.,

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$\Lambda = \overline{\Lambda} \circ F, \overline{\Lambda} : \overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P \to \overset{m}{\wedge} T^*M.$

Finally if the above condition on Λ is fulfilled, then we can ask whether $d^2\Omega_\Lambda = dE = 0$ and we find that this holds if $\overline{\Lambda}$ is adjoint invariant. So we have found a new formulation of the Utiyama's theorem[8] which does not involve directly properties of invariance, but comes out naturally from the comparison of the fundamental geometrical techniques of the Lagrangian theory and the adjoint differential calculus.

We finish with a theorem that gives a new characterization of the fundamental Lagrangian (self-action density).

II. THE ADJOINT FORMS

A. The adjoint forms over the base space and their differentials

1. The adjoint forms over M

All manifolds and maps will be C^∞, and M will be a manifold of dimension m. Its local charts are denoted by (x^λ). The space of r forms $\varphi : M \to \overset{r}{\wedge} T^*M$ is denoted by $A^r(M)$.

$\pi : P \to M$ will be a (right) principal bundle with structure group G (see Ref. 9). The Lie algebra of G is denoted by g.

The tangent and vertical functors T and V induce a free (right) action of G on the tangent and vertical spaces TP and $VP \subset TP$. Then, by considering the quotient with respect to such action, we obtain the vector bundles TP/G and VP/G over M. Sections of $TP/G \to M$ are the G-invariant tangent vector fields on P, while sections of $VP/G \to M$ are the G-invariant vertical tangent vector fields on P. The adjoint bundle $\mathrm{Ad}\, P = VP/G \to M$ will play a fundamental role throughout the paper.

The Lie brackets of sections of TP and VP over P pass via the quotient to sections of TP/G and $\mathrm{Ad}\, P$ over M. These brackets will be also denoted by $[\ ,\ ]$. Clearly, $\mathrm{Ad}\, P \to M$ is a bundle of Lie algebras with each fiber being isomorphic to g. Here $\mathrm{Sec}(\mathrm{Ad}\, P)$ with the previous bracket $[\ ,\ ]$ is a Lie algebra over $C^\infty(M)$. Note that when G is Abelian (or also when P is trivial, i.e., $P = M \times G$) then $\mathrm{Ad}\, P \cong M \times g$, i.e., $\mathrm{Ad}\, P$ is canonically isomorphic with $M \times g$.

By choosing a local gauge $\pi^{-1}(U) \approx U \times G$ over a coordinate neighborhood (U, x^λ) in M and a basis (e_i) of the Lie algebra g, we get in an obvious way a local basis (∂_λ, e_i) for the sections of $TP/G \to M$. Moreover (e_i) is a local basis of $\mathrm{Sec}(\mathrm{Ad}\, P)$ and we have $[e_i, e_j] = c_{ij}^k e_k$, where $c_{ij}^k \in \mathbb{R}$ are the structure constants of G. The local expression of $[\ ,\ ]$ is

$$[\xi, \eta] = \xi^i \eta^j c_{ij}^k e_k, \tag{1}$$

for each $\xi = \xi^i e_i$, $\eta = \eta^j e_j \in \mathrm{Sec}(\mathrm{Ad}\, P)$. We will denote by (e^i) the dual basis for the local sections of $\mathrm{Ad}^* P \to M$.

We shall be concerned with the vector spaces $A^r(M; \mathrm{Ad}\, P)$ of the adjoint forms $\alpha : M \to \overset{r}{\wedge} T^*M \otimes \mathrm{Ad}\, P$. The bracket of $\mathrm{Sec}(\mathrm{Ad}\, P)$ induces naturally a graded Lie algebra structure on

$$A(M; \mathrm{Ad}\, P) = \overset{m}{\underset{r=0}{\oplus}} A^r(M; \mathrm{Ad}\, P). \tag{2}$$

This bracket is characterized by the formula

$$[\varphi \otimes \xi, \psi \otimes \eta] = (\varphi \wedge \psi) \otimes [\xi, \eta], \tag{3}$$

for each $\varphi \in A^r(M)$, $\psi \in A^s(M)$, $\xi, \eta \in \mathrm{Sec}(\mathrm{Ad}\, P)$. The local expression of the bracket is

$$[\alpha, \beta] = \alpha^i_{\lambda_1 \cdots \lambda_r} \beta^j_{\mu_1 \cdots \mu_s} c_{ij}^k\, dx^{\lambda_1} \wedge \cdots \wedge dx^{\lambda_r} \wedge dx^{\mu_1} \wedge \cdots \wedge dx^{\mu_s} \otimes e_k, \tag{4}$$

for each $\alpha = \alpha^i_{\lambda_1 \cdots \lambda_r} dx^{\lambda_1} \wedge \cdots \wedge dx^{\lambda_r} \otimes e_i$, $\beta = \beta^j_{\mu_1 \cdots \mu_s} dx^{\mu_1} \wedge \cdots \wedge dx^{\mu_s} \otimes e_j$.

Clearly, $\mathrm{Sec}(\mathrm{Ad}\, P) = A^0(M; \mathrm{Ad}\, P)$ is a subalgebra of $A(M; \mathrm{Ad}\, P)$. Then we have the maps

$$\mathrm{ad} : \mathrm{Sec}(\mathrm{Ad}\, P) \times A^r(M; \mathrm{Ad}\, P) \to A^r(M; \mathrm{Ad}\, P) \tag{5}$$

given by $\mathrm{ad}(\xi, \alpha) = \mathrm{ad}_\xi \alpha = [\xi, \alpha]$. These maps induce a $C^\infty(M)$-Lie algebra morphism of $\mathrm{Sec}(\mathrm{Ad}\, P)$ into the vertical fields over $\overset{r}{\wedge} T^*M \otimes \mathrm{Ad}\, P$. If $(x^\lambda, y^i_{\lambda_1 \cdots \lambda_r})$ is a local chart on $\overset{r}{\wedge} T^*M \otimes \mathrm{Ad}\, P$, we have

$$\mathrm{ad}_\xi = c_{ij}^k \xi^i y^j_{\lambda_1 \cdots \lambda_r} \partial_k^{\lambda_1 \cdots \lambda_r}, \tag{6}$$

for each $\xi = \xi^i e_i \in \mathrm{Sec}(\mathrm{Ad}\, P)$.

2. The principal connections

A *principal connection* is a splitting of the exact sequence[10]

$$0 \to \mathrm{Ad}\, P \to TP/G \to TM, \tag{7}$$

i.e., a one-form $A : M \to T^*M \otimes (TP/G)$ which is projectable on $\mathrm{id}_{TM} : M \to T^*M \otimes TM$. Its local expression is

$$A = dx^\lambda \otimes (\partial_\lambda - A^i_\lambda e_i), \tag{8}$$

where the A^i_λ are local functions on M. The curvature of A is the adjoint two-form $F_A \in A^2(M; \mathrm{Ad}\, P)$ given by

$$F_A(u, v) = A([u, v]) - [A(u), A(v)], \tag{9}$$

for each vector field $u, v : M \to TM$. Its local expression is

$$F_A = \tfrac{1}{2}(\partial_\lambda A^k_\mu - \partial_\mu A^k_\lambda - c_{ij}^k A^i_\lambda A^j_\mu) dx^\lambda \wedge dx^\mu \otimes e_k. \tag{10}$$

3. The adjoint covariant derivative with respect to a principal connection

Let A be a principal connection. Then the *adjoint covariant derivative* with respect to A is the map

$$\nabla^A : \mathrm{Sec}(\mathrm{Ad}\, P) \to A^1(M; \mathrm{Ad}\, P), \tag{11}$$

given by

$$\nabla^A_u \xi = u \rfloor \nabla^A \xi = [A(u), \xi], \tag{12}$$

for each $\xi \in \mathrm{Sec}(\mathrm{Ad}\, P)$ and each vector field $u : M \to TM$. Its local expression is

$$\nabla^A \xi = (\partial_\lambda \xi^k - c_{ij}^k A^i_\lambda \xi^j) dx^\lambda \otimes e_k, \tag{13}$$

for each $\xi = \xi^i e_i \in \mathrm{Sec}(\mathrm{Ad}\, P)$.

The adjoint covariant derivative is a derivation of the algebra $\mathrm{Sec}(\mathrm{Ad}\, P)$, i.e., we have

$$\nabla^A_u [\xi, \eta] = [\nabla^A_u \xi, \eta] + [\xi, \nabla^A_u \eta], \tag{14}$$

for each $\xi, \eta \in \mathrm{Sec}(\mathrm{Ad}\, P)$ and each vector field $u : M \to TM$. Then, by recalling (5) and using the induced covariant deri-

vative on $\mathrm{Ad}^* P \otimes \mathrm{Ad} P$, (14) is equivalent to

$$\nabla^A_u(\mathrm{ad}_\xi) = \mathrm{ad}_{\nabla^A_u \xi}. \tag{15}$$

4. The adjoint differential with respect to a principal connection

The adjoint covariant derivative ∇^A induces the *adjoint differential* with respect to A

$$d^A : A^r(M;\mathrm{Ad}\, P) \to A^{r+1}(M;\mathrm{Ad}\, P), \tag{16}$$

which is characterized by the formula

$$d^A(\varphi \otimes \xi) = d\varphi \otimes \xi + (-1)^r \varphi \wedge \nabla^A \xi, \tag{17}$$

for each $\varphi \in A^r(M)$, $\xi \in \mathrm{Sec}(\mathrm{Ad}\, P)$. Of course we have $d^A \xi = \nabla^A \xi$. The local expression of d^A is

$$d^A \alpha = (\partial_\lambda \alpha^k_{\lambda_1 \cdots \lambda_r} - c^k_{ij} A^i_\lambda \alpha^j_{\lambda_1 \cdots \lambda_r}) \times dx^\lambda \wedge dx^{\lambda_1} \wedge \cdots \wedge dx^{\lambda_r} \otimes e_k, \tag{18}$$

for each $\alpha = \alpha^i_{\lambda_1 \cdots \lambda_r}\, \mathrm{dx}^{\lambda_1} \wedge \cdots \wedge dx^{\lambda_r} \otimes e_i$.

The adjoint differential d^A is a derivation of the algebra $A(M;\mathrm{Ad}\, P)$, i.e., we have

$$d^A[\alpha,\beta] = [d^A\alpha,\beta] + (-1)^r[\alpha, d^A\beta], \tag{19}$$

for each $\alpha \in A^r(M;\mathrm{Ad}\, P)$, $\beta \in A^s(M;\mathrm{Ad}\, P)$.

We have the identity

$$(d^A)^2\alpha = [\alpha, F_A] \tag{20}$$

and the so-called *Bianchi identity*

$$d^A F_A = [F_A, F_A] = 0. \tag{21}$$

Note that when G is Abelian we have $d^A = d$, the ordinary differential, for any principal connection A.

5. The adjoint codifferential with respect to a principal connection

If (M,g) is an oriented Riemannian manifold, then the adjoint covariant derivative ∇^A induces the *adjoint codifferential* with respect to A

$$\delta^A : A^r(M;\mathrm{Ad}\, P) \to A^{r-1}(M;\mathrm{Ad}\, P), \tag{22}$$

which is given by $\delta^A \alpha = \pm *d^A * \alpha$, where $* : A^r(M;\mathrm{Ad}\, P) \times A^{m-r}(M;\mathrm{Ad}\, P)$ is the star isomorphism and $\alpha \in A^r(M;\mathrm{Ad}\, P)$.

From (20) we get

$$(\delta^A)^2\alpha = \pm *[*\alpha, F_A] \tag{23}$$

and, because of the formula $[\alpha,*\beta] = -[\beta,*\alpha]$ we have, in particular,

$$(\delta^A)^2 F_A = 0. \tag{24}$$

6. The coadjoint forms over M

We shall be also involved with the spaces $A^r(M;\mathrm{Ad}^* P)$ of *coadjoint forms* $\alpha : M \to \overset{r}{\wedge} T^*M \otimes \mathrm{Ad}^* P$. In a way similar to the previous one, we have the *coadjoint differential*

$$d^A : A^r(M;\mathrm{Ad}^* P) \to A^{r+1}(M;\mathrm{Ad}^* P) \tag{25}$$

and the *coadjoint codifferential*

$$\delta^A : A^r(M;\mathrm{Ad}^* P) \to A^{r-1}(M;\mathrm{Ad}^* P). \tag{26}$$

B. The adjoint forms over the space of connections and the canonical differential

1. The bundle of principal connections

The k-jet functor J_k induces a (right) free action of G over the k-jet spaces $J_k P$. Then, by considering the quotient with respect to such action, we obtain the bundles $J_k P/G$ over M. In particular, $C = J_1 P/G \to M$ is an affine bundle, whose vector bundle is $T^*M \otimes \mathrm{Ad}\, P \to M$. Then the vertical space $VC \subset TC$ is given by the fibered product over M

$$VC = C \underset{M}{\times} T^*M \otimes \mathrm{Ad}\, P. \tag{27}$$

The affine bundle $C \to M$ turns out to be the bundle of principal connections. In fact, by taking into account the canonical inclusion $J_1 P/G \hookrightarrow T^*M \otimes (TP/G)$, we can characterize the principal connections $A : M \to T^*M \otimes (TP/G)$ as the sections $A : M \to C$.

We shall also be concerned with the k-jet prolongations $J_k C$ of C. We denote by (x^λ, a^i_α) and $(x^\lambda, a^i_{\Lambda,\alpha})$ the standard charts of C and $J_k C$, where $\Lambda = (\Lambda_1, \ldots, \Lambda_m)$, with $0 \leqslant \Lambda_\lambda \leqslant k$, $1 \leqslant \lambda \leqslant m$, is a multi-index of length $|\Lambda| = \Lambda_1 + \cdots + \Lambda_m = k$. So we have

$$a^i_\alpha \circ A = -A^i_\alpha, \quad a^i_{\Lambda,\alpha} \circ j_k A = -\partial_\Lambda A^i_\alpha, \tag{28}$$

where $j_k A : M \to J_k C$ is the k-jet prolongation of $A : M \to C$. The minus sign in (28) is due to (8).

2. The adjoint forms over $J_k C$

We denote by $A^r(J_k C)$ the space of the horizontal forms $\varphi : J_k C \to \overset{r}{\wedge} T^*M$. A fundamental role will be played by the vector spaces $A^r(J_k C;\mathrm{Ad}\, P)$ of the *horizontal adjoint forms* over $J_k C$, namely $\alpha : J_k C \to \overset{r}{\wedge} T^*M \otimes \mathrm{Ad}\, P$. The local expression of such forms is

$$\alpha = \alpha^i_{\lambda_1 \cdots \lambda_r}\, dx^{\lambda_1} \wedge \cdots \wedge dx^{\lambda_r} \otimes e_i, \tag{29}$$

where $\alpha^i_{\lambda_1 \cdots \lambda_r}$ are local functions on $J_k C$.

By taking into account the pullbacks with respect to the projections $J_k C \to J_h C \to C \to M$ with $k > h > 0$, we have the linear natural inclusions

$$A^r(M;\mathrm{Ad}\, P) \subset A^r(C;\mathrm{Ad}\, P) \subset A^r(J_h C;\mathrm{Ad}\, P) \subset A^r(J_k C;\mathrm{Ad}\, P). \tag{30}$$

The bracket of $\mathrm{Sec}(\mathrm{Ad}\, P)$ induces naturally a graded Lie algebra structure on

$$A(J_k C;\mathrm{Ad}\, P) = \overset{m}{\underset{r=0}{\oplus}} A^r(J_k C;\mathrm{Ad}\, P). \tag{31}$$

This bracket is characterized by the formula

$$[\varphi \otimes \xi, \psi \otimes \eta] = (\varphi \wedge \psi) \otimes [\xi,\eta], \tag{32}$$

for each $\varphi \in A^r(J_k C)$, $\psi \in A^s(J_k C)$, $\xi,\eta \in \mathrm{Sec}(\mathrm{Ad}\, P)$. The local expression of the bracket is

$$[\alpha,\beta] = \alpha^i_{\lambda_1 \cdots \lambda_r} \beta^j_{\mu_1 \cdots \mu_s} c^k_{ij}\, dx^{\lambda_1} \wedge \cdots \wedge dx^{\lambda_r} \wedge dx^{\mu_1} \wedge \cdots \wedge dx^{\mu_s} \otimes e_k, \tag{33}$$

for each $\alpha = \alpha^i_{\lambda_1 \cdots \lambda_r}\, dx^{\lambda_1} \wedge \cdots \wedge dx^{\lambda_r} \otimes e_i$, $\beta = \beta^j_{\mu_1 \cdots \mu_s} \times dx^{\mu_1} \wedge \cdots \wedge dx^{\mu_s} \otimes e_j$.

We have the natural subalgebras

$$\mathrm{Sec}(\mathrm{Ad}\,P)\subset A\,(M;\mathrm{Ad}\,P)\subset A\,(C;\mathrm{Ad}\,P)$$
$$\subset A\,(J_hC;\mathrm{Ad}\,P)\subset A\,(J_kC;\mathrm{Ad}\,P), \tag{34}$$

with $0<h<k$. Then, as in (5), we have the maps

$$\mathrm{ad}:\mathrm{Sec}(\mathrm{Ad}\,P)\times A^r(J_kC;\mathrm{Ad}\,P)\to A^r(J_kC;\mathrm{Ad}\,P) \tag{35}$$

given by $\mathrm{ad}(\xi,\alpha)=\mathrm{ad}_\xi\alpha=[\xi,\alpha]$.

3. The canonical jet adjoint covariant derivative

Definition: The jet adjoint covariant derivative is the map

$$\nabla: A^0(J_kC;\mathrm{Ad}\,P)\to A^1(J_{k+1}C;\mathrm{Ad}\,P), \tag{36}$$

given by

$$(\nabla\xi)\circ j_{k+1}A=\nabla^A(\xi\circ j_kA), \tag{37}$$

for each (local) section $A:M\to C$ and $\xi\in A^0(J_kC;\mathrm{Ad}\,P)$.

The local expression of (36) is

$$\nabla\xi=(J_\lambda\xi^k+c^k_{ij}a^i_\lambda\xi^j)dx^\lambda\otimes e_k, \tag{38}$$

for each $\xi=\xi^ie_i$ and where

$$J_\lambda\xi^k=\partial_\lambda\xi^k+a^i_{\Lambda+\lambda,\alpha}(\partial^{\Lambda,\alpha}_i\xi^k), \tag{39}$$

with $\Lambda+\lambda=(\lambda_1,\ldots,\Lambda_\lambda+1,\ldots,\Lambda_m)$.

In the particular case when $\xi\in A^0(C;\mathrm{Ad}\,P)$, the jet adjoint covariant derivative is related to the canonical covariant derivative $\overline{\nabla}$ in the pullback vector bundle $C\underset{M}{\times}\mathrm{Ad}\,P\to C$ which has been introduced by Garcia (see Ref. 6), by means of the formula

$$(\overline{\nabla}\xi)\circ A=(\nabla\xi)\circ j_1A=\nabla^A(\xi\circ A), \tag{40}$$

for each (local) section $A:M\to C$ and $\xi\in A^0(C;\mathrm{Ad}\,P)$.

4. The canonical jet adjoint differential

The jet adjoint covariant derivative ∇ induces the *jet adjoint differential*

$$d: A^r(J_kC;\mathrm{Ad}\,P)\to A^{r+1}(J_{k+1}C;\mathrm{Ad}\,P), \tag{41}$$

which is characterized by the formula

$$d(\varphi\otimes\xi)=d_H\varphi\otimes\xi+(-1)^r\varphi\wedge\nabla\xi, \tag{42}$$

for each $\varphi\in A^r(J_kC)$, $\xi\in A^0(J_kC;\mathrm{Ad}\,P)$ and where $d_H:A^r(J_kC)\to A^{r+1}(J_{k+1}C)$ is the horizontal differential defined by $(d_H\varphi)\circ j_{k+1}A=d(\varphi\circ j_kA)$ for each (local) section $A:M\to C$ (here d is the ordinary differential). Of course we have $d\xi=\nabla\xi$.

The local expression of d is

$$d\alpha=(J_\lambda\alpha^k_{\lambda_1\cdots\lambda_r}+c^k_{ij}a^i_\lambda\alpha^j_{\lambda_1\cdots\lambda_r})dx^\lambda$$
$$\wedge dx^{\lambda_1}\wedge\cdots\wedge dx^{\lambda_r}\otimes e_k, \tag{43}$$

for each $\alpha=\alpha^i_{\lambda_1\cdots\lambda_r}dx^{\lambda_1}\wedge\cdots\wedge dx^{\lambda_r}\otimes e_i$.

Note that, by considering the inclusion $\mathrm{Sec}(\mathrm{Ad}\,P)\subset A^0(C;\mathrm{Ad}\,P)$, from (36) we obtain the map

$$d:\mathrm{Sec}(\mathrm{Ad}\,P)\to A^1(C;\mathrm{Ad}\,P)\subset A^1(J_1C;\mathrm{Ad}\,P). \tag{44}$$

Moreover, since $\mathrm{Sec}(VC)=A^1(C;\mathrm{Ad}\,P)$ as follows from (27), the map (44) becomes

$$d:\mathrm{Sec}(\mathrm{Ad}\,P)\to\mathrm{Sec}(VC). \tag{45}$$

This is an R-Lie algebra morphism whose local expression is

$$d\xi=(\partial_\lambda\xi^k+c^k_{ij}a^i_\lambda\xi^j)\partial^\lambda_k, \tag{46}$$

as we get from (38).

5. The canonical jet adjoint codifferential

If (M,g) is an oriented Riemannian manifold, then the jet adjoint covariant derivative ∇ induces the *jet adjoint codifferential*

$$\delta: A^r(J_kC;\mathrm{Ad}\,P)\to A^{r-1}(J_{k+1}C;\mathrm{Ad}\,P), \tag{47}$$

which is given by $\delta\alpha=\pm *d*\alpha$ for each $\alpha\in A^r(J_kC;\mathrm{Ad}\,P)$.

The codifferential δ is also characterized by

$$(\delta\alpha)\circ j_{k+1}A=\delta^A(\alpha\circ j_kA), \tag{48}$$

for each (local) section $A:M\to C$ and $\alpha\in A^r(J_kC;\mathrm{Ad}\,P)$.

6. The coadjoint forms over J_kC

We need also the spaces $A^r(J_kC;\mathrm{Ad}^*P)$ of the *horizontal coadjoint forms* $\alpha:J_kC\to\overset{r}{\wedge}T^*M\otimes\mathrm{Ad}^*P$. As before, we have the *jet coadjoint differential*

$$d: A^r(J_kC;\mathrm{Ad}^*P)\to A^{r+1}(J_{k+1}C;\mathrm{Ad}^*P) \tag{49}$$

and the *jet coadjoint codifferential*

$$\delta: A^r(J_kC;\mathrm{Ad}^*P)\to A^{r-1}(J_{k+1}C;\mathrm{Ad}^*P). \tag{50}$$

C. The fundamental adjoint form

1. The canonical splitting of J_1C

Theorem 1: The affine bundle $J_1C\to C$ admits the canonical splitting

$$J_1C=S\underset{C}{\oplus}(\overset{2}{\wedge}T^*M\otimes\mathrm{Ad}\,P) \tag{51}$$

into the direct sum over C of the affine subbundle $S=J_2P/G\subset J_1C$ (whose vector bundle is $\overset{2}{\vee}T^*M\otimes\mathrm{Ad}\,P$) and the linear subbundle $\overset{2}{\wedge}T^*M\otimes\mathrm{Ad}\,P$ of $T^*M\otimes T^*M\otimes\mathrm{Ad}\,P$ which is the vector bundle associated with $J_1C\to C$.

Then from the second projection of the splitting (51) we get the *fundamental form* $F\in A^2(J_1C;\mathrm{Ad}\,P)$, i.e.,

$$F:J_1C\to\overset{2}{\wedge}T^*M\otimes\mathrm{Ad}\,P. \tag{52}$$

If $A:M\to C$ is a principal connection, then its curvature is given by $F_A=F\circ j_1A$.

The local chart

$$(x^\lambda,a^k_\lambda;a^k_{\lambda,\mu}+a^k_{\mu,\lambda},a^k_{\mu,\lambda}-a^k_{\lambda,\mu}-c^k_{ij}a^i_\lambda a^j_\mu) \tag{53}$$

of J_1C is adapted to both the submanifolds S and $C\underset{M}{\times}(\overset{2}{\wedge}T^*M\otimes\mathrm{Ad}\,P)$ of J_1C. Hence the local expression of F is

$$F=\tfrac{1}{2}(a^k_{\mu,\lambda}-a^k_{\lambda,\mu}-c^k_{ij}a^i_\lambda a^j_\mu)dx^\lambda\wedge dx^\mu\otimes e_k. \tag{54}$$

Proof: We know (see Ref. 4) that the sesquiholonomic bundle $J_2P\to J_1P$ is an affine bundle whose vector bundle is (the pullback over J_1P of) $T^*M\otimes T^*M\otimes VP$ and that it admits the canonical splitting

$$\widehat{J_2P} = J_2P \underset{J_1P}{\oplus} (\overset{2}{\wedge} T^*M \otimes VP) \tag{55}$$

into the direct sum over J_1P of the affine subbundle $J_2P \subset \widehat{J_2P}$ (whose vector bundle is $\underset{2}{\vee} T^*M \otimes VP$) and the linear subbundle $\overset{2}{\wedge} T^*M \otimes VP$ of $T^*M \otimes T^*M \otimes VP$. Moreover, we know that the curvature $R_\Gamma : P \to \overset{2}{\wedge} T^*M \otimes VP$ of *any* connection $\Gamma : P \to J_1P$ is given by $R_\Gamma = d \circ J_1\Gamma \circ \Gamma$, where $d : \widehat{J_2P} \to \overset{2}{\wedge} T^*M \otimes VP$ is the second projection of the splitting (55).

Then we can prove, by means of a direct check, point by point, that all the previous structures and maps pass to the quotient with respect to the action of G. Moreover, we can prove that J_2P/G is canonically isomorphic to $J_1(J_1P/G)$. This proves the splitting (51) and the other related facts.

Remark 1: The projection F generalizes the differential of usual forms $\varphi : M \to T^*M$. Indeed, the forms $\varphi \in A^1(M)$ are nothing but the principal connections of the principal bundle $P = M \times \mathbb{R} \to M$ (as we have $C = T^*M$) and the ordinary differential is given by $d\varphi = F \circ j_1\varphi$, where $F : J_1T^*M \to \overset{2}{\wedge} T^*M$.

Remark 2: Let G_P be the *infinite Lie group* of the principal automorphisms of P over id_M (gauge group). Then $\mathrm{Sec}(\mathrm{Ad}\, P)$ can be considered as the *Lie algebra* of G_P (gauge algebra).

G_P acts naturally on the left on J_kC and also on S and $\overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$. It is easily seen that this last action is nothing but the adjoint action $G_P \times \mathrm{Ad}\, P \to \mathrm{Ad}\, P$ (with the identity on $\overset{2}{\wedge} T^*M$). The splitting (51) and the projection F are both G_P invariant.

By taking the one-jet extension (see Ref. 5) of the $\mathbb{R}$-Lie algebra morphism (45) we get precisely the derivative of the action of G_P on J_1C. In the same way, (6) is the derivative of the adjoint action of G_P on $\overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$ (with $r = 2$). Clearly these two representations of $\mathrm{Sec}(\mathrm{Ad}\, P)$ are F related.

2. Applications of the formalism of the adjoint forms to the Yang–Mills equations

Now it is a natural idea to apply the operators d and δ to $F \in A^2(J_1C; \mathrm{Ad}\, P)$. As these objects are canonical, we expect to find other important objects. In fact we obtain the following result.

Theorem 2: We have

$$0 = dF \in A^3(J_2C; \mathrm{Ad}\, P), \tag{56}$$

$$\delta F \in A^1(J_2C; \mathrm{Ad}\, P), \quad 0 = \delta^2 F \in A^0(J_3C; \mathrm{Ad}\, P). \tag{57}$$

Moreover we have the following interpretations.

(i) $dF = 0$ reduces to the Bianchi identity, with respect to *any* connection $A : M \to C$, as we have

$$0 = (dF) \circ j_2A = d^A(F \circ j_1A) = d^AF_A. \tag{58}$$

(ii) δF reduces to the Yang–Mills operator (in the direct formalism, without regard to any Lagangian formulation), which can act on *any* potential $A : M \to C$, as we have

$$(\delta F) \circ j_2A = \delta^A(F \circ j_1A) = \delta^AF_A = J_A, \tag{59}$$

where $J_A = J \circ A$ and $J \in A^1(C; \mathrm{Ad}\, P)$ is an external current.

(iii) $\delta^2 F = 0$ reduces to the charge conservation identity, with respect to *any* potential $A : M \to C$, as we have

$$0 = (\delta^2 F) \circ j_3A = (\delta^A)^2(F \circ j_1A) = (\delta^A)^2F_A = \delta^AJ_A. \tag{60}$$

Proof: It is a direct consequence of the previous definitions and results.

III. APPLICATION OF THE ADJOINT FORMS TO LAGRANGIAN THEORIES

A. The condition by which the Legendre map is a coadjoint form

Next we apply the formalism of the adjoint forms to Lagrangian theories.

Let us assume a Lagrangian density

$$\Lambda : J_1C \to \overset{m}{\wedge} T^*M, \quad \Lambda \in A^m(J_1C), \tag{61}$$

to be given. Its local expression is

$$\Lambda = \mathscr{L}\omega, \quad \omega = dx^1 \wedge \cdots \wedge dx^m, \tag{62}$$

where $\mathscr{L}$ is a local function on J_1C.

The fiber derivative of Λ, with respect to the affine bundle $J_1C \to C$, is the map

$$D\Lambda : JC \to TM \otimes V^*C \otimes \overset{m}{\wedge} T^*M$$

$$\cong \overset{m}{\wedge} T^*M \otimes TM \otimes TM \otimes \mathrm{Ad}^*\, P, \tag{63}$$

where we have used (27). Then by considering the canonical isomorphism

$$\overset{m}{\wedge} T^*M \otimes TM \xrightarrow{\langle\ ,\ \rangle} \overset{m-1}{\wedge} T^*M, \tag{64}$$

we obtain the *Legendre map* (see Ref. 5)

$$\Omega_\Lambda = \langle\ ,\ \rangle \circ D\Lambda : J_1C \to \overset{m-1}{\wedge} T^*M \otimes TM \otimes \mathrm{Ad}^*\, P. \tag{65}$$

Its local expression is

$$\Omega_\Lambda = \Pi_i^{\lambda,\alpha}\omega_\lambda \otimes \partial_\alpha \otimes e^i, \tag{66}$$

where $\Pi_i^{\lambda,\alpha} = \partial_i^{\lambda,\alpha}\mathscr{L}$ are local functions on J_1C and $\omega_\lambda = \partial_\lambda \rfloor\, \omega = (-1)^{\lambda-1} dx^1 \wedge \cdots \wedge \widehat{dx^\lambda} \wedge \cdots \wedge dx^m$.

The following remark allows us to state the condition by which Ω_Λ is a coadjoint form.

Lemma 3: We have the canonical linear isomorphism

$$\overset{m-1}{\wedge} T^*M \otimes TM \cong \overset{m-2}{\wedge} T^*M \oplus (\underset{2}{\vee} T^*M \otimes \overset{m}{\wedge} T^*M) \tag{67}$$

whose local expression is

$$\psi^{\lambda,\mu}\Omega_\lambda \otimes \partial_\mu \to \tfrac{1}{2}\psi^{\lambda,\mu}\omega_{\lambda\mu} + \tfrac{1}{2}\psi^{\lambda,\mu}\partial_\lambda \vee \partial_\mu \otimes \omega, \tag{68}$$

where $\omega_{\lambda\mu} = \partial_\mu \rfloor\, \omega_\lambda$.

Proof: Indeed, by taking any (local) volume form η: $M \to \overset{m}{\wedge} T^*M$ and by using the associated (local) star isomorphisms, that is $*$: $\overset{r}{\wedge} T^*M \to \overset{m-r}{\wedge} TM$, the (global) isomorphism (67) is given by the composition

$$\overset{m-1}{\wedge} T^*M \otimes TM \overset{*\otimes \mathrm{id}_{TM}}{\to} TM \otimes TM \cong \overset{2}{\wedge} TM \oplus \overset{2}{\vee} TM$$

$$\overset{*\oplus(*\otimes\eta)}{\to} \overset{m-2}{\wedge} T^*M \oplus (\overset{2}{\vee} TM \otimes \overset{m}{\wedge} T^*M). \quad (69)$$

Then we find the following condition.

Proposition 4 (Condition C_0): The following conditions are equivalent.

(i) $\Omega_\Lambda : J_1C \to \overset{m-2}{\wedge} T^*M \otimes \mathrm{Ad}^* P \to \overset{m-1}{\wedge} T^*M \otimes TM \otimes \mathrm{Ad}^* P$, i.e., $\Omega_\Lambda \in A^{m-2}(J_1C;\mathrm{Ad}^* P)$.

(ii) Λ is factorable through the canonical projection $J_1C \to C \underset{M}{\times} \overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$.

(iii) We have locally $\Pi_i^{\lambda,\alpha} + \Pi_i^{\alpha,\lambda} = 0$.

If one of the previous conditions is fulfilled, the local expression of Ω_Λ becomes

$$\Omega_\Lambda = \tfrac{1}{2}\Pi_i^{\lambda,\alpha}\omega_{\lambda\alpha} \otimes e^i. \quad (70)$$

Proof: For the previous Lemma we have (i)⇔(iii). Moreover, by considering the chart (53) adapted to the splitting (51) over C, we have (ii)⇔(iii).

B. The condition by which the Euler–Lagrange operator is the coadjoint differential of the Legendre map

Without any specific assumption on the Lagrangian density $\Lambda \in A^m(J_1C)$, the Euler–Lagrange operator E_Λ associated to Λ is a map (see Ref. 5)

$$E_\Lambda : J_2C \to \overset{m}{\wedge} T^*M \otimes V^*C \cong \overset{m}{\wedge} T^*M \otimes TM \otimes \mathrm{Ad}\, P. \quad (71)$$

Then, by considering the canonical isomorphism (64), E_Λ can be viewed as a coadjoint form

$$E_\Lambda : J_2C \to \overset{m-1}{\wedge} TM \otimes \mathrm{Ad}^* P, \quad E_\Lambda \in A^{m-1}(J_2C;\mathrm{Ad}^* P). \quad (72)$$

Its local expression is (see Ref. 5)

$$E_\Lambda = (\partial_i^\alpha \mathscr{L} - J_\lambda \Pi_i^{\lambda,\alpha}\omega_\alpha) \otimes e^i, \quad (73)$$

where the formal derivative J_λ has been defined in (39).

On the other hand, let us assume that the condition C_0 is fulfilled, so that $\Omega_\Lambda \in A^{m-2}(J_1C;\mathrm{Ad}^* P)$. Then we may compute $d\Omega_\Lambda \in A^{m-1}(J_2C;\mathrm{Ad}^* P)$. We find

$$d\Omega_\Lambda = E_\Lambda + (c_{ij}^k a_\lambda^i \Pi_k^{\lambda,\alpha} - \partial_j^\alpha \mathscr{L})\omega_\alpha \otimes e^j. \quad (74)$$

Now we can ask whether $d\Omega_\Lambda = E_\Lambda$. For this purpose we obtain the following result.

Proposition 5 (Condition C_1): The following conditions are equivalent.

(i) $\Omega_\Lambda \in A^{m-2}(J_1C;\mathrm{Ad}^* P)$, $d\Omega_\Lambda = E_\Lambda$.

(ii) Λ is factorable through the projection $F : J_1C \to \overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$, i.e., $\Lambda = \overline{\Lambda} \circ F$, where $\overline{\Lambda} : \overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P \to \overset{m}{\wedge} T^*M$.

(iii) We have locally

$$\Pi_i^{\lambda,\alpha} + \Pi_i^{\alpha,\lambda} = 0, \quad c_{ij}^k a_\lambda^i \Pi_k^{\lambda,\alpha} - \partial_j^\alpha \mathscr{L} = 0. \quad (75)$$

Proof: The local expressions (73) and (74) give (i)⇔(iii). Moreover, we see that the local vector fields

$$u_i^{\lambda,\alpha} = \partial_i^{\lambda,\alpha} + \partial_i^{\alpha,\lambda}, \quad u_j^\lambda = \partial_j^\lambda + c_{ij}^k a_\alpha^i \partial_k^{\lambda,\alpha} \quad (76)$$

are a local basis for the F-vertical vector fields over J_1C. Hence (ii)⇔(iii).

C. The condition by which the Euler–Lagrange operator is coadjoint closed

Now let us assume that the condition C_1 is fulfilled so that $\Omega_\Lambda \in A^{m-2}(J_1C;\mathrm{Ad}^* P)$ and $E_\Lambda = d\Omega_\Lambda \in A^{m-1}(J_2C;\mathrm{Ad}^* P)$. Then we can ask when it happens that E_Λ is coadjoint closed. For this purpose, we find the following result.

Proposition 5 (Condition C_2): The following conditions are equivalent.

(i) $\Omega_\Lambda \in A^{m-2}(J_1C;\mathrm{Ad}^* P)$, $d\Omega_\Lambda = E_\Lambda$, $dE_\Lambda = 0$.

(ii) $\Lambda = \overline{\Lambda} \circ F$ and $\overline{\Lambda}$ is (infinitesimally) adjoint invariant (see Remark 2), i.e., we have

$$L_{\mathrm{ad}_\xi}\overline{\Lambda} = 0, \quad \text{for any } \xi \in \mathrm{Sec}(\mathrm{Ad}\, P), \quad (77)$$

where L denotes the Lie derivative and ad_ξ is the vertical vector field on $\overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$ given by (6).

(iii) Locally we have the conditions (75) and the other one

$$c_{ij}^k y_{\lambda\mu}^i \partial_k^{\lambda\mu} \overline{\mathscr{L}} = 0, \quad (78)$$

where $\overline{\Lambda} = \overline{\mathscr{L}}\omega$, $\overline{\mathscr{L}}$ being a local function on $\overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$.

Proof: It is easily seen that we have the formula

$$\xi \rfloor dE_\Lambda = (L_{\mathrm{ad}_\xi}\overline{\Lambda}) \circ F, \quad (79)$$

for each $\xi \in \mathrm{Sec}(\mathrm{Ad}\, P)$. Then (i)⇔(ii). Moreover, the local expression of $L_{\mathrm{ad}_\xi}\overline{\Lambda}$ gives (ii)⇔(iii).

Remark 3: The local expressions (75) and (78) (Utiyama's conditions) are equivalent to the (infinitesimal) gauge invariance of Λ, that is the invariance of Λ by the one-jet extension of the morphism (45) (see Remark 2).

While in the direct approach (adjoint forms) we have the formulas $\delta F \in A^1(J_2C;\mathrm{Ad}\, P)$ and $\delta^2 F = 0$, in the Lagrangian approach (coadjoint forms) we have $E_\Lambda = d\Omega \in A^{m-1}(J_2C;\mathrm{Ad}^* P)$ and $d^2\Omega_\Lambda = 0$. The correspondence of the two approaches is clear.

It must be observed that a characterization of the critical sections of a gauge invariant Lagrangian density Λ by means of the Legendre map Ω_Λ (without writing the formulas $E_\Lambda = d\Omega_\Lambda$ and $d^2\Omega_\Lambda = 0$) appears in a paper of Garcia and Pérez-Rendon.[11]

D. The fundamental Lagrangian

Now let us assume (M,g) to be an oriented Riemannian manifold and also that a Riemannian metric h to be given in the adjoint bundle $\mathrm{Ad}\, P \to M$. We denote by $h : \mathrm{Ad}\, P \to \mathrm{Ad}^* P$ also the induced isomorphism.

Let $s : \overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P \to \mathbb{R}$ be the quadratic form associated to the metric on $\overset{2}{\wedge} T^*M \otimes \mathrm{Ad}\, P$ constructed by means of g and h. Put

$$\Sigma = \tfrac{1}{2}(s\eta)\circ F = S\eta : J_1C \to \overset{m}{\wedge} T^*M, \tag{80}$$

where $\eta = \sqrt{|g|}\omega$ is the canonical volume form on (M,g). The local expression of S, which follows from (54), is

$$S = \tfrac{1}{2} g^{\lambda\mu} g^{\alpha\beta} h_{ij} (a^i_{\alpha,\lambda} - a^i_{\lambda,\alpha} - c^i_{rs} a^r_\lambda a^s_\alpha) \times (a^j_{\beta,\mu} - a^j_{\mu,\beta} - c^j_{rs} a^r_\mu a^s_\beta), \tag{81}$$

where $h_{ij} = h(e_i, e_j)$.

The key property of the Lagrangian density Σ (which satisfies obviously the condition C_1) is

$$\Omega_\Sigma = \pm *h(F), \tag{82}$$

as we see by using (81).

We have the following characterization of Σ.

Theorem 6: Let $\Lambda \in A^m(J_1C)$ be a Lagrangian density. Then the following conditions are equivalent (i) $\Omega_\Lambda = \Omega_\Sigma$, $E_\Lambda = d\Omega_\Lambda$; and (ii) $\Lambda = \Sigma + \varphi$, where φ is (the pullback of) an arbitrary m form on M.

Moreover, if $\overline{\nabla} h = 0$ and if one of the previous conditions is fulfilled, then we have also

$$E_\Lambda = \pm *h(\delta F), \quad dE_\Lambda = 0. \tag{83}$$

Proof: It is clear that if $\Omega_\Lambda = \Omega_\Sigma$ then $\Lambda = \Sigma + \varphi'$, where $\varphi' : C \to \overset{m}{\wedge} TM$ is arbitrary. Furthermore, if $E_\Lambda = d\Omega_\Lambda$ it follows from the condition C_1 that φ' is the pullback of an m form on M. The converse is obvious.

If the Riemannian metric h is compatible with the canonical operator d (recall that $\overline{\nabla}$ is the canonical covariant derivative on $C \underset{M}{\times} \mathrm{Ad}\, P \to C$), then the first formula (83) follows from (82) while the second one follows from $\delta^2 F = 0$.

Remark 4: Let h be the Cartan–Killing bilinear form on Ad P, i.e.,

$$h(\xi,\eta) = \mathrm{tr}(\mathrm{ad}_\xi \circ \mathrm{ad}_\eta), \tag{84}$$

for any $\xi,\eta \in \mathrm{Sec}(\mathrm{Ad}\, P)$. Then from (15) we obtain $\overline{\nabla} h = 0$. Moreover, if G is semisimple [as is the case in which $G = \mathrm{SU}(n)$], then h is not degenerate. Hence we may apply the previous theorem. The corresponding Lagrangian density Σ is the one most used in classical gauge theories.

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Completeness relation for energy-dependent separable potentials

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We point out that the eigenfunctions of energy-dependent separable potentials, which are commonly used in the relativistic three-body problem, form a complete set of states. The completeness property is important, since it is necessary in order to satisfy the optical theorem, and consequently to conserve probability. We show that there exists a large family of energy-dependent separable potentials whose eigenfunctions form a complete set. Although the eigenfunctions of these potentials are not mutually orthogonal, it is shown that in general they are linearly independent.

I. INTRODUCTION

Many three-body calculations have been performed in the past,[1-9] using as input the two-body amplitudes obtained from energy-dependent separable potentials. Thus, in the case of the various reactions of a pion with a deuteron,[1-6] the dominant pion–nucleon amplitude, which is that of the P_{33} channel, has been derived from the energy-dependent separable potential proposed by Woloshyn, Moniz, and Aaron,[1] while in the three-body treatment of nucleon–nucleon scattering proposed by Kloet, Silbar, Aaron, and Amado,[7-9] the amplitudes for the pion–nucleon P_{11} and P_{33} channels have been derived also from this kind of interaction. In the case of the nucleon–nucleon system, energy-dependent separable potentials have been proposed[10] for the $^1S_0$ and $^3S_1$ channels, and they have been applied to study the effects of the nucleon–nucleon hard core in pion–deuteron scattering,[11] as well as in the three-nucleon bound-state problem.[12] Optimal forms for the S-wave nucleon–nucleon separable potentials have been obtained by Ahmad and Beghi,[13,14] while Sañudo has constructed a set of energy-dependent separable potentials for the kaon–nucleon system.[15]

The completeness of the eigenfunctions of the two-body interactions is important, since it is required in order to satisfy the optical theorem. Therefore, by requiring that completeness be maintained, one guarantees the conservation of probability. Let us consider, for example, the scattering of a projectile by a target which is a bound state of particles 1 and 2. The elastic scattering amplitude obeys the Lippmann–Schwinger equation

$$T = V_1 + V_2 + (V_1 + V_2)[1/(E - K_0 - H_{12} + i\epsilon)]T,$$

where V_i is the potential between the projectile and particle i, K_0 is the kinetic energy operator for the relative motion of the projectile and the target, and H_{12} is the internal Hamiltonian of the target. Since the amplitude T obeys the unitarity relation

$$T - T^\dagger = -2\pi i T\delta(E - K_0 - H_{12})T^\dagger,$$

if the eigenfunctions ψ_n of the Hamiltonian H_{12} form a complete set, we get from the unitarity relation that

$$\begin{aligned}\langle \mathbf{k}_0\psi_0|T - T^\dagger|\mathbf{k}_0\psi_0\rangle &= -2\pi i\sum_n \int d\mathbf{k}\langle \mathbf{k}_0\psi_0|T|\mathbf{k}\psi_n\rangle\delta\left(E - \frac{k^2}{2\mu} - E_n\right)\langle \mathbf{k}\psi_n|T^\dagger|\mathbf{k}_0\psi_0\rangle \\ &= -2\pi i\sum_n \int d\mathbf{k}|\langle \mathbf{k}_0\psi_0|T|\mathbf{k}\psi_n\rangle|^2\delta\left(E - \frac{k^2}{2\mu} - E_n\right) \\ &= -\frac{ik_0}{8\mu\pi^3}\sum_n \sigma_n = -\frac{ik_0}{8\mu\pi^3}\sigma^{TOT},\end{aligned}$$

which is the optical theorem. Thus, we see that in order to satisfy the optical theorem one requires not only the unitarity condition, but also the completeness of the eigenfunctions of the two-body subsystem.

II. THE EIGENFUNCTIONS OF ENERGY-DEPENDENT SEPARABLE POTENTIALS

Since we are interested in the consequences of completeness for the relativistic three-body problem, we will present in this section the solutions of the two-body problem for the case of the Blankenbecler–Sugar equation.

An energy-dependent separable potential in a given partial wave is written in momentum space as

$$V(k,k';Z) = g(k)g(k')b(Z), \tag{1}$$

where k and k' are the magnitudes of the initial and final relative momenta of the two particles in the center of mass frame, and Z is the invariant mass squared of the system. The on-shell momentum q is related to Z by

$$Z = [(m_1^2 + q^2)^{1/2} + (m_2^2 + q^2)^{1/2}]^2. \tag{2}$$

The Blankenbecler–Sugar equation for the two-body problem is

$$\begin{aligned}T(k,k';Z) = V(k,k';Z) + \int_0^\infty \frac{\omega_1(k'') + \omega_2(k'')}{\omega_1(k'')\omega_2(k'')}k''^2\,dk'' \\ \times V(k,k'';Z)[Z - S(k'') + i\epsilon]^{-1}T(k'',k';Z),\end{aligned} \tag{3}$$

where

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$$\omega_i(k) = (k^2 + m_i^2)^{1/2}, \quad i = 1,2, \tag{4}$$

$$S(k) = [\omega_1(k) + \omega_2(k)]^2. \tag{5}$$

Using Eq. (1) into Eq. (3), we find that the solution of Eq. (3) is

$$T(k, k'; Z) = g(k)g(k')/D(Z), \tag{6}$$

where

$$D(Z) = \frac{1}{b(Z)} - \int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} k^2\, dk \frac{g^2(k)}{Z - S(k) + i\epsilon}. \tag{7}$$

The continuum eigenfunctions of the potential (1) are

$$\psi_q(k) = \frac{\omega_1(k)\omega_2(k)}{\omega_1(k) + \omega_2(k)} \frac{1}{k^2} \delta(k - q) + \frac{1}{Z - S(k) + i\epsilon} \frac{g(k)g(q)}{D(Z)}, \tag{8}$$

while the wave function of a bound state of invariant mass squared S_n is

$$\psi_n(k) = N_n^{1/2} g(k)\{1/[S_n - S(k)]\}, \tag{9}$$

where $N_n^{1/2}$ is a normalization constant (see Appendix A).

III. COMPLETENESS

In order to find under which conditions the completeness property is satisfied, we will follow the same method used by Henley and Thirring to prove the completeness of the solutions of the Lippmann–Schwinger equation for an energy-independent separable potential.[16]

Let us consider first the case when the potential (1) does not have any bound state, so that $D(Z)$ has no zeros in the negative real axis. In order to prove that the continuum eigenfunctions $\psi_q(k)$ given by Eq. (8) form a complete set, we need to show that they satisfy

$$\int_0^\infty \frac{\omega_1(q) + \omega_2(q)}{\omega_1(q)\omega_2(q)} q^2\, dq\, \psi_q^*(k)\psi_q(k') = \frac{\omega_1(k)\omega_2(k)}{\omega_1(k) + \omega_2(k)} \frac{1}{k^2} \delta(k - k'). \tag{10}$$

If we substitute Eq. (8) and its complex conjugate into the left-hand side of Eq. (10), we get

$$\begin{aligned}\int_0^\infty \frac{\omega_1(q) + \omega_2(q)}{\omega_1(q)\omega_2(q)} q^2\, dq\, \psi_q^*(k)\psi_q(k') &= \frac{\omega_1(k)\omega_2(k)}{\omega_1(k) + \omega_2(k)} \frac{1}{k^2} \delta(k - k') \\ &+ \frac{1}{S(k) - S(k') + i\epsilon} \frac{g(k')g(k)}{D[S(k)]} \\ &+ \frac{1}{S(k') - S(k) - i\epsilon} \frac{g(k)g(k')}{D^*[S(k')]} \\ &+ g(k)g(k') \int_0^\infty \frac{\omega_1(q) + \omega_2(q)}{\omega_1(q)\omega_2(q)} q^2\, dq \\ &\times \frac{1}{Z - S(k) - i\epsilon} \frac{1}{Z - S(k') + i\epsilon} \frac{g^2(q)}{D^*(Z)D(Z)},\end{aligned} \tag{11}$$

so that in order for Eq. (10) to hold, we must show that the sum of the last three terms in the right-hand side of Eq. (11) is equal to zero. If we use Eq. (7), we see that

$$\frac{1}{D(Z)} - \frac{1}{D^*(Z)} = \frac{D^*(Z) - D(Z)}{D(Z)D^*(Z)} = -\pi i \frac{q}{\omega_1(q) + \omega_2(q)} \frac{g^2(q)}{D^*(Z)D(Z)}, \tag{12}$$

while

$$\frac{1}{Z - S(k) - i\epsilon} \frac{1}{z - S(k') + i\epsilon} = \frac{1}{S(k) - S(k') + i\epsilon} \left[\frac{1}{Z - S(k) - i\epsilon} - \frac{1}{Z - S(k') + i\epsilon} \right]. \tag{13}$$

Using Eqs. (12) and (13), we can write the last term of the right-hand side of Eq. (11) as

$$\begin{aligned}\text{last} &= -\frac{1}{\pi i} \frac{1}{S(k) - S(k') + i\epsilon} g(k)g(k') \\ &\times \int_0^\infty \frac{[\omega_1(q) + \omega_2(q)]^2}{\omega_1(q)\omega_2(q)} q\, dq \\ &\times \left[\frac{1}{Z - S(k) - i\epsilon} - \frac{1}{Z - S(k') + i\epsilon} \right] \\ &\times \left[\frac{1}{D(Z)} - \frac{1}{D^*(Z)} \right] \\ &= -\frac{1}{2\pi i} \frac{1}{S(k) - S(k') + i\epsilon} g(k)g(k') \\ &\times \int_{(m_1 + m_2)^2}^\infty dZ \left[\frac{1}{Z - S(k) - i\epsilon} - \frac{1}{Z - S(k') + i\epsilon} \right] \left[\frac{1}{D(Z)} - \frac{1}{D^*(Z)} \right],\end{aligned} \tag{14}$$

where we have used Eq. (2) to change the variable of integration. If we now consider the variable Z as a complex variable, then we see from Eq. (7) that for points Z not on the real axis

$$D^*(Z) = D(Z^*), \tag{15}$$

so that if the function $1/D(Z)$ is analytical everywhere except at the positive real axis and does not diverge when $|Z| \to \infty$, we can use Eq. (15) to close the contour as shown in Fig. 1, so that we can write Eq. (14) as

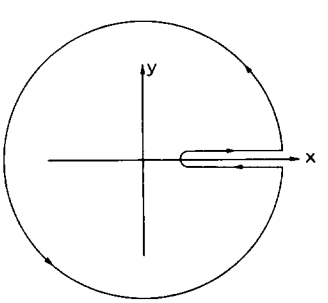

FIG. 1. Contour of integration of Eq. (16).

$$\text{last} = -\frac{1}{2\pi i} g(k)g(k') \frac{1}{S(k) - S(k') + i\epsilon}$$
$$\times \oint dZ \left[\frac{1}{Z - S(k) - i\epsilon} - \frac{1}{Z - S(k') + i\epsilon} \right] \frac{1}{D(Z)}$$
$$= -g(k)g(k') \frac{1}{S(k) - S(k') + i\epsilon}$$
$$\times \left[\frac{1}{D[S(k)]} - \frac{1}{D^*[S(k')]} \right], \tag{16}$$

where we have used Cauchy's theorem and Eq. (15). We see that Eq. (16) exactly cancels the second and third terms in the right-hand side of Eq. (11), so that Eq. (10) holds.

The result (16) is based in the assumption that $1/D(Z)$ is analytical, which means that $D(Z)$ defined by Eq. (7) must not have any zero above or below the real axis. In order to see if this is true or not, it is of course necessary to know the explicit form of the function $b(Z)$. Thus, in the next section, we will examine several forms for $b(Z)$ which satisfy the required conditions.

If the potential (1) has bound states, then the poles of $1/D(Z)$ corresponding to the bound-state energies contribute to the closed integral of Eq. (16), since from Eqs. (6) and (A16) we see that near a bound state of invariant mass squared S_n,

$$1/D(Z) \approx N_n [1/(Z - S_n)], \tag{17}$$

so that Eq. (16) becomes in this case

$$\text{last} = -g(k)g(k') \frac{1}{S(k) - S(k') + i\epsilon}$$
$$\times \left\{ \frac{1}{D[S(k)]} - \frac{1}{D^*[S(k')]} + \sum_n N_n \left[\frac{1}{S_n - S(k) - i\epsilon} - \frac{1}{S_n - S(k') + i\epsilon} \right] \right\}$$
$$= -g(k)g(k') \frac{1}{S(k) - S(k') + i\epsilon}$$
$$\times \left[\frac{1}{D[S(k)]} - \frac{1}{D^*[S(k')]} \right] - \sum_n \frac{N_n^{1/2} g(k)}{S_n - S(k) - i\epsilon} \frac{N_n^{1/2} g(k')}{S_n - S(k') + i\epsilon}$$
$$= -g(k)g(k') \frac{1}{S(k) - S(k') + i\epsilon}$$
$$\times \left[\frac{1}{D[S(k)]} - \frac{1}{D^*[S(k')]} \right] - \sum_n \psi_n^*(k)\psi_n(k'), \tag{18}$$

where we have used Eq. (A18). If we substitute Eq. (18) back into Eq. (11), we see that the completeness relation in the case where there are bound states is

$$\sum_n \psi_n^*(k)\psi_n(k') + \int_0^\infty \frac{\omega_1(q) + \omega_2(q)}{\omega_1(q)\omega_2(q)} q^2\, dq\, \psi_q^*(k)\psi_q(k')$$
$$= \frac{\omega_1(k)\omega_2(k)}{\omega_1(k) + \omega_2(k)} \frac{1}{k^2} \delta(k - k'). \tag{19}$$

IV. ACCEPTABLE MODELS OF ENERGY-DEPENDENT SEPARABLE POTENTIALS

As we mentioned in the previous section, in order to obtain Eq. (10) or Eq. (19), we had to assume that the function $1/D(Z)$ is analytical everywhere in the complex Z plane except at the real axis. This means that $D(Z)$ must not be zero above or below the real axis.

An energy-dependent separable potential of the form (1), has been proposed by Woloshyn, Moniz, and Aaron[1] for the pion–nucleon P_{33} channel, where the energy dependence was chosen of the form

$$b(Z) = 1/(Z + a), \tag{20}$$

where a is a real number, so that from Eq. (7),

$$D(Z) = Z + a - \int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} k^2\, dk \frac{g^2(k)}{Z - S(k)}. \tag{21}$$

If we write the complex variable Z as

$$Z = x + iy, \tag{22}$$

then we can write the imaginary part of Eq. (21), as

$$\text{Im}\, D(Z) = y + y \int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} k^2\, dk \frac{g^2(k)}{[x - S(k)]^2 + y^2}, \tag{23}$$

which, as we can see, never vanishes above or below the real axis, so that $1/D(Z)$ is analytical in that region, and Eq. (10) or Eq. (19) is valid, which shows that the eigenfunctions of a separable potential with the energy dependence (20) form a complete set of states.

As a second example, let us consider an energy dependence of the form

$$1/b(Z) = a - 1/(Z + c), \tag{24}$$

with a and c real numbers. This type of interaction has been used by Schwarz, Zingl, and Mathelitsch[17] to represent the pion–nucleon P_{11} channel. The imaginary part of $D(Z)$ is in this case

$$\text{Im}\, D(Z) = \frac{y}{(x + c)^2 + y^2} + y \int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} \times k^2\, dk \frac{g^2(k)}{[x - S(k)]^2 + y^2}, \tag{25}$$

which, as we can see, also never vanishes above or below the real axis, and consequently Eq. (10) or Eq. (19) is also valid in this case, so that the eigenfunctions of a separable potential with the energy dependence (24) form a complete set.

It is clear by combining Eqs. (20) and (24), that the family of separable potentials whose energy dependence is of the form

$$\frac{1}{b(Z)} = a_0^2 Z + c_0 - \sum_{i=1}^{N} \frac{a_i^2}{Z + c_i}, \tag{26}$$

where a_i and c_i are real numbers, will give rise to eigenfunctions that form a complete set.

In the case where there are bound states, the derivation of Eq. (19) requires that the poles of $1/D(Z)$ be simple, so that we need to show that $D(Z)$, as defined by Eq. (7) with the energy dependence $1/b(Z)$ given by Eq. (26), has only simple zeros. If $D(S_n) = 0$, there is a bound state of invariant mass S_n, and we can subtract $D(S_n)$ from Eq. (7), to get [using Eq. (26)]

$$\begin{aligned} D(Z) &= a_0^2(Z - S_n) - \sum_{i=1}^{N} a_i^2 \left[\frac{1}{Z + c_i} - \frac{1}{S_n + c_i} \right] \\ &\quad - \int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} k^2\, dk\, g^2 k \\ &\quad \times \left[\frac{1}{Z - S(k) + i\epsilon} - \frac{1}{S_n - S(k) + i\epsilon} \right] \\ &= (Z - S_n) \left\{ a_0^2 + \sum_{i=1}^{N} \frac{a_i^2}{(Z + c_i)(S_n + c_i)} \right. \\ &\quad + \int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} k^2\, dk\, g^2(k) \\ &\quad \left. \times \frac{1}{[Z - S(k) + i\epsilon][S_n - S(k) + i\epsilon]} \right\}, \end{aligned} \tag{27}$$

so that near $Z = S_n$,

$$\begin{aligned} D(Z) \approx (Z - S_n) &\left\{ a_0^2 + \sum_{i=1}^{N} \frac{a_i^2}{(Z + c_i)^2} \right. \\ &\left. + \int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} k^2\, dk \frac{g^2(k)}{[Z - S(k)]^2} \right\}, \end{aligned} \tag{28}$$

from which we see that the coefficient of $(Z - S_n)$ never vanishes at $Z = S_n$, and therefore the zeros of $D(Z)$ are simple.

V. LINEAR INDEPENDENCE OF THE EIGENFUNCTIONS

Although the set of eigenfunctions (8) and (9) satisfy the completeness relation (19), they are not mutually orthogonal, as we show in Appendix B. Thus, it is not clear that these eigenfunctions really span the Hilbert space, since in order to do that they must be linearly independent. Thus, we will discuss next under what conditions the set of eigenfunctions (8) and (9) are linearly independent.

As we have shown in Appendix B, the eigenfunctions (8) and (9) obey the nonorthogonality relations

$$\langle \psi_n | \psi_m \rangle = \delta_{nm} + N_n^{1/2} N_m^{1/2} \frac{1}{S_m - S_n} \times \left[\frac{1}{b(S_n)} - \frac{1}{b(S_m)} \right], \tag{29a}$$

$$\langle \psi_n | \psi_q \rangle = N_n^{1/2} \frac{g(q)}{D[S(q)]} \frac{1}{S(q) - S_n} \times \left\{ \frac{1}{b(S_n)} - \frac{1}{b[S(q)]} \right\}, \tag{29b}$$

$$\begin{aligned} \langle \psi_p | \psi_q \rangle &= \frac{\omega_1(q)\omega_2(q)}{\omega_1(q) + \omega_2(q)} \frac{1}{q^2} \delta(p - q) \\ &\quad + \frac{g(p)g(q)}{D^*[S(p)]D[S(q)]} \frac{1}{S(q) - S(p)} \\ &\quad \times \left\{ \frac{1}{b[S(p)]} - \frac{1}{b[S(q)]} \right\}, \end{aligned} \tag{29c}$$

which in the limit of an energy-independent separable potential $b(Z) = \text{const}$, reduce to the standard orthogonality relations.

Linear independence of the set of eigenfunctions (8) and (9), requires that the relation

$$\sum_m a_m |\psi_m\rangle + \int_0^\infty \frac{\omega_1(q) + \omega_2(q)}{\omega_1(q)\omega_2(q)} q^2\, dq\, a(q) |\psi_q\rangle = 0 \tag{30}$$

is possible only with $a_m = a(q) = 0$. If we multiply Eq. (30) on the left by $\langle \psi_n |$ and $\langle \psi_p |$ and use the nonorthogonality relations (29), we get

$$\begin{aligned} &\sum_m a_m N_n^{1/2} N_m^{1/2} \frac{1}{S_m - S_n} \left[\frac{1}{b(S_n)} - \frac{1}{b(S_m)} \right] \\ &\quad + \int_0^\infty \frac{\omega_1(q) + \omega_2(q)}{\omega_1(q)\omega_2(q)} q^2\, dq\, a(q) \\ &\quad \times N_n^{1/2} \frac{g(q)}{D[S(q)]} \frac{1}{S(q) - S_n} \left\{ \frac{1}{b(S_n)} - \frac{1}{b[S(q)]} \right\} \\ &\quad = -a_n, \end{aligned} \tag{31a}$$

$$\begin{aligned} &\sum_m a_m N_m^{1/2} \frac{g(p)}{D^*[S(p)]} \frac{1}{S_m - S(p)} \left\{ \frac{1}{b[S(p)]} \right. \\ &\quad \left. - \frac{1}{b(S_m)} \right\} + \int_0^\infty \frac{\omega_1(q) + \omega_2(q)}{\omega_1(q)\omega_2(q)} q^2\, dq\, a(q) \\ &\quad \times \frac{g(p)g(q)}{D^*[S(p)]D[S(q)]} \frac{1}{S(q) - S(p)} \\ &\quad \times \left\{ \frac{1}{b[S(p)]} - \frac{1}{b[S(q)]} \right\} = -a(p). \end{aligned} \tag{31b}$$

These equations represent an eigenvalue problem of the form

$$\tilde{K}\mathbf{a} = -\mathbf{a}, \tag{32}$$

where the eigenvector $\mathbf{a}$ consists of the discrete set of numbers a_m and the continuum set of numbers $a(q)$. Thus, if one solves the eigenvalue problem of the Hermitian operator $\tilde{K}$ and finds that one of its eigenvalues is -1, then the set of eigenfunctions (8) and (9) are not linearly independent. However, if the operator $\tilde{K}$, defined by Eqs. (31) and (32), does not have the eigenvalue -1, then the only vector that satisfies Eqs. (31) is $a_m = a(q) = 0$, which means that in that case the set of eigenfunctions (8) and (9) are linearly independent. Thus, we have shown that the set of eigenfunctions (8) and (9) form a complete set of states and in general are linearly independent, except in the special case when the operator $\tilde{K}$ has the eigenvalue -1.

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APPENDIX A: THE BOUND-STATE WAVE FUNCTIONS

If we introduce the plane-wave partial-wave states of relative momentum k that are normalized invariantly on the mass shell as

$$\langle k|k'\rangle = \frac{\omega_1(k)\omega_2(k)}{\omega_1(k)+\omega_2(k)}\frac{1}{k^2}\delta(k-k'), \tag{A1}$$

then they obey the completeness relation

$$1 = \int_0^\infty \frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)} k^2\, dk\, |k\rangle\langle k|. \tag{A2}$$

These states are eigenfunctions of the free Hamiltonian H_0, where

$$H_0|k\rangle = S(k)|k\rangle. \tag{A3}$$

Thus, with these definitions we can write the Blankenbecler–Sugar equation in operator form as

$$T = V + VG_0T, \tag{A4}$$

where the free Green's function G_0 is given by

$$G_0 = 1/(Z - H_0 + i\epsilon). \tag{A5}$$

If we now define the full Green's function G as

$$G = 1/(Z - H_0 - V + i\epsilon), \tag{A6}$$

then we can write the T matrix T of Eq. (A4) in terms of G as

$$T = V + VGV. \tag{A7}$$

Introducing a complete set of plane-wave states of the form (A2) into Eq. (A4), we get

$$\begin{aligned}\langle k|T|k'\rangle = \langle k|V|k'\rangle &+ \int_0^\infty \frac{\omega_1(k'')+\omega_2(k'')}{\omega_1(k'')\omega_2(k'')} k''^2\, dk'' \\ &\times \langle k|V|k''\rangle\{1/[Z - S(k'') + i\epsilon]\} \\ &\times \langle k''|T|k'\rangle,\end{aligned} \tag{A8}$$

which is the Blankenbecler–Sugar equation (3).

If the eigenfunctions of the Hamiltonian $H_0 + V$ form a complete set of states (as in the cases that we are studying in this paper), then we can write Eq. (A7) as

$$\begin{aligned}\langle k|T(Z)|k'\rangle = \langle k|V|k'\rangle &+ \sum_n \langle k|V|\psi_n\rangle \frac{1}{Z - S_n} \\ &\times \langle \psi_n|V|k'\rangle + \int_0^\infty \frac{\omega_1(k'')+\omega_2(k'')}{\omega_1(k'')\omega_2(k'')} \\ &\times k''^2\, dk''\, \langle k|V|\psi_{k''}\rangle \\ &\times \{1/[Z - S(k'') + i\epsilon]\}\langle \psi_{k''}|V|k'\rangle,\end{aligned} \tag{A9}$$

where the ψ_n are the wave functions of the bound states with invariant mass S_n (while an energy-independent separable potential can have at most only one bound state, an energy-dependent one can have several of them), and the $\psi_{k''}$ are continuum states of invariant mass $S(k'')$, that is,

$$(H_0 + V)|\psi_n\rangle = S_n|\psi_n\rangle, \tag{A10}$$

$$(H_0 + V)|\psi_{k''}\rangle = S(k'')|\psi_{k''}\rangle. \tag{A11}$$

Near a bound state of invariant mass S_n, the T matrix (A9) is given approximately by

$$\begin{aligned}\langle k|T(Z)|k'\rangle &\approx \langle k|V|\psi_n\rangle \frac{1}{Z - S_n}\langle \psi_n|V|k'\rangle \\ &= [S_n - S(k)]\langle k|\psi_n\rangle[1/(Z - S_n)] \\ &\quad\times \langle \psi_n|k'\rangle[S_n - S(k')],\end{aligned} \tag{A12}$$

where we have used Eqs. (A10) and (A3). We have, in the particular case of the potential (1), that the T matrix is given by Eqs. (6) and (7), as

$$\begin{aligned}\langle k|T(Z)|k'\rangle = g(k)g(k') &\times\left(\frac{1}{b(Z)} - \int_0^\infty \frac{\omega_1(p)+\omega_2(p)}{\omega_1(p)\omega_2(p)} p^2\, dp\right. \\ &\left.\times \frac{g^2(p)}{Z - S(p) + i\epsilon}\right)^{-1}.\end{aligned} \tag{A13}$$

Therefore, at the invariant mass S_n corresponding to a bound state, the term in large parentheses in Eq. (A13) must vanish, that is

$$\frac{1}{b(S_n)} - \int_0^\infty \frac{\omega_1(p)+\omega_2(p)}{\omega_1(p)\omega_2(p)} p^2\, dp\, \frac{g^2(p)}{S_n - S(p) + i\epsilon} = 0. \tag{A14}$$

If we subtract Eq. (A14) from the term in large parentheses in (A13), and use the Taylor expansion

$$b(Z) = b(S_n) + (Z - S_n)\left[\frac{db}{dZ}\right]_{Z=S_n} + \cdots, \tag{A15}$$

we see that for values of Z near the bound-state pole, the T matrix (A13) is given approximately by

$$\langle k|T(Z)|k'\rangle \approx N_n g(k)g(k')/(Z - S_n), \tag{A16}$$

where

$$\begin{aligned}N_n = \left(-\left[\frac{1}{b^2}\frac{db}{dZ}\right]_{Z=S_n} + \int_0^\infty \frac{\omega_1(p)+\omega_2(p)}{\omega_1(p)\omega_2(p)} p^2\, dp\right. \\ \left.\times \frac{g^2(p)}{[S_n - S(p)]^2}\right)^{-1},\end{aligned} \tag{A17}$$

so that comparing Eq. (A16) with Eq. (A12), we see that the bound-state wave function is

$$\langle k|\psi_n\rangle = N_n^{1/2} g(k)/[S_n - S(k)]. \tag{A18}$$

From Eqs. (A2), (A17), and (A18), we see that the normalization of the bound-state wave function is

$$\begin{aligned}\langle \psi_n|\psi_n\rangle &= \int_0^\infty \frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)} k^2\, dk\, \langle \psi_n|k\rangle\langle k|\psi_n\rangle \\ &= 1 + N_n\left[\frac{1}{b^2}\frac{db}{dZ}\right]_{Z=S_n}.\end{aligned} \tag{A19}$$

Thus, we see that in the case of an energy-dependent separable potential the bound-state wave functions are not normalized to unity. Of course, if the potential is energy independent, that is, if $b(Z) = \text{const}$, then we get from Eq. (A19) that, as expected,

$$\langle \psi_n|\psi_n\rangle = 1. \tag{A20}$$

APPENDIX B: NONORTHOGONALITY OF THE WAVE FUNCTIONS

We will derive in this appendix the equivalent of the orthogonality relations for the eigenfunctions (8) and (9). Let us begin with the continuum eigenfunctions. Using Eq. (8), we have that

$$\int_0^\infty \frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\,\psi_q^*(k)\psi_{q'}(k)$$
$$=\frac{\omega_1(q)\omega_2(q)}{\omega_1(q)+\omega_2(q)}\frac{1}{q^2}\delta(q-q')+\frac{1}{S(q')-S(q)+i\epsilon}\frac{g(q)g(q')}{D[S(q')]}+\frac{1}{S(q)-S(q')-i\epsilon}\frac{g(q')g(q)}{D^*[S(q)]}$$
$$+\frac{g(q)g(q')}{D^*[S(q)]D[S(q')]}\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\,\frac{g^2(k)}{[S(q)-S(k)-i\epsilon][S(q')-S(k)+i\epsilon]}, \tag{B1}$$

so that adding the second and third terms on the rhs of Eq. (B1), we get

$$\text{second}+\text{third}=\frac{g(q)g(q')}{S(q')-S(q)+i\epsilon}\left\{\frac{1}{D[S(q')]}-\frac{1}{D^*[S(q)]}\right\}=\frac{g(q)g(q')}{S(q')-S(q)+i\epsilon}\frac{D^*[S(q)]-D[S(q')]}{D[S(q')]D^*[S(q)]}$$
$$=\frac{g(q)g(q')}{S(q')-S(q)+i\epsilon}\frac{1}{D[S(q')]D^*[S(q)]}\left\{\frac{1}{b[S(q)]}-\frac{1}{b[S(q')]}\right.$$
$$\left.-\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\left[\frac{g^2(k)}{S(q)-S(k)-i\epsilon}-\frac{g^2(k)}{S(q')-S(k)+i\epsilon}\right]\right\}$$
$$=\frac{g(q)g(q')}{S(q')-S(q)+i\epsilon}\frac{1}{D[S(q')]D^*[S(q)]}\left\{\frac{1}{b[S(q)]}-\frac{1}{b[S(q')]}\right\}$$
$$-\frac{g(q)g(q')}{D[S(q')]D^*[S(q)]}\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\frac{g^2(k)}{[S(q)-S(k)-i\epsilon][S(q')-S(k)+i\epsilon]}, \tag{B2}$$

where we have used Eq. (7) in the third step. If we now use Eq. (B2) in Eq. (B1), we get the nonorthogonality relation

$$\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\,\psi_q^*(k)\psi_{q'}(k)$$
$$=\frac{\omega_1(q)\omega_2(q)}{\omega_1(q)+\omega_2(q)}\frac{1}{q^2}\delta(q-q')+\frac{g(q)g(q')}{S(q')-S(q)}\frac{1}{D[S(q')]D^*[S(q)]}\left\{\frac{1}{b[S(q)]}-\frac{1}{b[S(q')]}\right\}. \tag{B3}$$

For energy-independent separable potentials, $b(Z)=\text{const}$, and the second term of Eq. (B3) vanishes as expected.

We will obtain now the nonorthogonality relation between continuum and bound-state wave functions. Using Eqs. (8) and (9), we have that

$$\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\,\psi_n^*(k)\psi_q(k)$$
$$=N_n^{1/2}\frac{g(q)}{S_n-S(q)}+N_n^{1/2}\frac{g(q)}{D[S(q)]}\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\,\frac{g^2(k)}{[S_n-S(k)][S(q)-S(k)+i\epsilon]}$$
$$=N_n^{1/2}\frac{g(q)}{S_n-S(q)}+N_n^{1/2}\frac{g(q)}{D[S(q)]}\frac{1}{S(q)-S_n}\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\,g^2(k)$$
$$\times\left[\frac{1}{S_n-S(k)}-\frac{1}{S(q)-S(k)+i\epsilon}\right]$$
$$=N_n^{1/2}\frac{g(q)}{S_n-S(q)}+N_n^{1/2}\frac{g(q)}{D[S(q)]}\frac{1}{S(q)-S_n}\left\{\frac{1}{b(S_n)}+D[S(q)]-\frac{1}{b[S(q)]}\right\}$$
$$=N_n^{1/2}\frac{g(q)}{D[S(q)]}\frac{1}{S(q)-S_n}\left\{\frac{1}{b(S_n)}-\frac{1}{b[S(q)]}\right\}, \tag{B4}$$

where we have used in the third step the bound-state condition $D(S_n)=0$, as well as Eq. (7). Of course, for an energy-independent separable potential, $b(Z)=\text{const}$, and the rhs of Eq. (B4) is equal to zero as expected.

Finally, we will obtain the nonorthogonality relation between two different bound-state wave functions. Using Eq. (9), we have that

$$\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\,\psi_n^*(k)\psi_m(k)$$
$$=N_n^{1/2}N_m^{1/2}\int_0^\infty\frac{\omega_1(k)+\omega_2(k)}{\omega_1(k)\omega_2(k)}\,k^2\,dk\,\frac{g^2(k)}{[S_n-S(k)][S_m-S(k)]}$$

$$= N_n^{1/2} N_m^{1/2} \frac{1}{S_m - S_n} \int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} k^2 dk \left[\frac{g^2(k)}{S_n - S(k)} - \frac{g^2(k)}{S_m - S(k)} \right]$$

$$= N_n^{1/2} N_m^{1/2} \frac{1}{S_m - S_n} \left[\frac{1}{b(S_n)} - \frac{1}{b(S_m)} \right]. \tag{B5}$$

As expected, the rhs of Eq. (B5) is equal to zero if $b(Z) = \text{const}$. If we now combine Eq. (B5) with Eq. (A19), we see that the non-orthogonality relation for n and m arbitrary is

$$\int_0^\infty \frac{\omega_1(k) + \omega_2(k)}{\omega_1(k)\omega_2(k)} k^2 dk \, \psi_n^*(k)\psi_m(k) = \delta_{nm} + N_n^{1/2} N_m^{1/2} \frac{1}{S_m - S_n} \left[\frac{1}{b(S_n)} - \frac{1}{b(S_m)} \right]. \tag{B6}$$

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Multiply connected universes and inequivalent fields

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Multiply connected universes with nice physical properties can be obtained from a standard model through identifications under discrete groups. We classify the possible transformation properties of matter and gauge fields under these groups. The example of zero-curvature models is analyzed giving the number of inequivalent fields.

I. INTRODUCTION

It is now generally recognized that the mathematical framework of fiber bundles provides precise definitions of the concepts used in classical gauge theories. In particular, gauge fields are best described by connections on a principal bundle over a manifold and particle fields are considered as sections of vector bundles or spinor bundles associated to the principal fibration. Therefore an exciting possibility which arises in this picture is that a theory might contain distinct topological sectors, i.e., different fields that could be represented, at a classical level, by sections of topologically inequivalent bundles with structure group G over a four-dimensional space-time M (see, e.g., Avis and Isham[1]). In this approach it is known that the problem of the classification will depend crucially on the properties of the group G and of the base manifold M that have been chosen.

As far as the topology of G is concerned, physical and mathematical considerations indicate that one can restrict the study mainly to compact groups. On the other hand, it is well known that Einstein's field equations describe the local geometry of the space-time but do not specify completely its topology. In fact, given any space-time (M, g) there exists a universal covering space-time $(\tilde{M},\tilde{g})$ such that $\tilde{M}$ is simply connected and $M = \tilde{M}/H$, where H is a properly discontinuous, discrete group of isometries without fixed points.[2] Therefore, given a solution of the field equations one can first take the universal covering space-time $(\tilde{M},\tilde{g})$ and then determine the possible identifications by H. The space-times obtained in this way exhibit topological properties which, in general, are different from those of $\tilde{M}$. For example,[2,3] when it is applied to the standard Friedmann models this procedure leads to multiply connected universes which have a number of promising features. In fact, through suitable identifications, one can produce compact spacelike sections corresponding to a present spatial radius of some fraction of the Hubble radius. In this "small universe" picture, the space-time is assumed to be topologically of the form $\tilde{M}/H = (\Sigma/H)\times R$ where Σ is a three-space of constant curvature K. This provides a natural explanation of the apparent homogeneity of the universe and good reasons for the microwave background isotropy.[3]

As observed by Ellis,[2] this description is fully equivalent to a situation in which we would see a large universe built up out of many repetitions of a small elementary building cell. That is, H acts as a symmetry group on the universe $\tilde{M}$.

However, if one adopts this point of view, it is no longer obvious that fields could be described as before by sections of vector bundles over $\tilde{M}/H$. Rather, if the above equivalence had to be reflected also on the possible field configurations, one should require that the physical fields "correctly" transform under the group H previously used to form the elementary cell.

In this paper, we address ourselves to the study of these laws of transformation. Given a properly discontinuous and free action of a group H on $\tilde{M}$, we classify the possible lifts to the bundle space of this action. For any lift, we define a field to be a section invariant under the action of H, and show that invariant sections may be viewed as sections of an appropriate bundle over $M = \tilde{M}/H$. Having established the desired equivalence, we observe, however, that this result allows one to obtain twisted fields even by starting with a trivial bundle. In the following we shall sometimes understand the difference between our description and the usual picture of fields as sections over a nontrivial base manifolds. In the following we will consider trivial vector bundles over a contractible base manifold. Although the extensions of our results to a more general case is still problematic, we observe that this last assumption does not seem to be very restrictive. For instance in the "small universe" picture it turns out[3] that a transition from a Rees-type chaotic cosmology to a homogeneous and isotropic cosmology is possible only when $K = 0, -1$, i.e., when $\tilde{M} = R^4$.

In Sec. II we show that the lifts to a vector bundle over a manifold M of an action of H on M are classified by the isomorphism classes of vector bundles over M/H. In Sec. III we shall give some examples of this classification for cosmological models constructed from the $K = 0$ standard Friedmann solution.

II. LIFTS OF GROUP ACTIONS

As we have seen in the Introduction, we have to consider sections of a vector bundle which transform appropriately under the group H, i.e., h-invariant sections.

In order to define what is an h-invariant section and how it is related to a section of a bundle over M/H, we need a

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lift to the bundle space of the h action on the base manifold M. Given a lift $\tilde{h}$, an h-invariant section will be a section σ such that $\sigma(hx) = \tilde{h}\sigma(x)$. As we shall see, any h-invariant section of a bundle over M can be viewed as a section of an appropriate bundle over M/H and vice versa.

In the following we shall consider the trivial vector bundle E over M with group G and fiber V. Given a trivialization $E \to M \times V$ of E and an h action of H on M we define a lift of the h action as a map $\tilde{h}: M \times V \to M \times V$ such that it is fiber preserving (i.e., it commutes with the projection $\pi: M \times V \to M$) and is associative [i.e., $\widetilde{(h_1 h_2)}\ (x,v) = \tilde{h}_1(\tilde{h}_2(x,v))$, $h_1, h_2 \in H$, $(x,v) \in M \times V$]. From these two requirements we see that any $\tilde{h}$ action can be obtained from a map $\psi: M \times H \to G$ such that

$$\psi(x,h_1h_2) = \psi(h_2x,h_1)\psi(x,h_2) \tag{1}$$

as

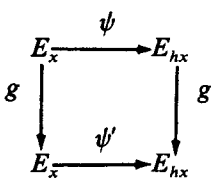
$$\tilde{h}(x,v) = (hx,\psi(x,h)v).$$

In the following we will denote by ψ also the action $\tilde{h}$ on $M \times V$. Two actions are defined to be equivalent if they coincide up to a vertical automorphism of E. Then two maps ψ and ψ' will give equivalent actions if there exists a map g: $M \to G$ such that

$$\psi'(x,h) = g(hx)^{-1}\psi(x,h)g(x). \tag{2}$$

We shall write $\psi \approx \psi'$ or $\psi' \in [\psi]$.

In fact, $g(x)$ gives an automorphism of the fiber E_x over x, and Eq. (2) means that the diagram



is commutative.

Our problem will be classification on the maps $\psi: M \times H \to G$ that satisfy (1) up to the equivalence (2).

We will show the following proposition.

Proposition: The lifts to E of an h action on M are classified by the isomorphism classes of vector bundles over M/H with group G.

Proof: Let ψ be any lift and $(M \times V)/\psi$ be the orbit space of H in $M \times V$ under the action ψ. It is easy to see that $(M \times V)/\psi$ is a vector bundle over M/H with projection π. If α: $M \to M/H$ is the canonical projection and $[x,v]_\psi = \{(hx,\psi(x,h)v),\ h \in H\}$ is the orbit that contains (x,v), the projection π is

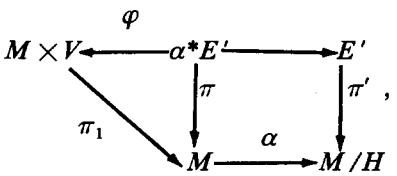
$$\pi[x,v]_\psi = \alpha(x).$$

The local triviality follows from the fact that H is properly discontinuous: any $\alpha(x) \in M/H$ have a neighborhood W such that α is a homeomorphism of each connected component of $\alpha^{-1}(W)$ onto W. Let U be a connected component of $\alpha^{-1}(W)$, then there exists a one to one map β: $W \to U$ and a homeomorphism $f: W \times V \to \pi^{-1}(W)$ that maps (p,v) into the orbit that contains $(\beta(p),v)$. Now, if $\psi \approx \psi'$ then $(M \times V)/\psi$ is isomorphic to $(M \times V)/\psi'$. In fact, let $\psi'(x,h)$ be defined by Eq. (2) and φ: $E \to E$ be an isomorphism given by

$$\varphi(x,v) = (x,g(x)^{-1}v).$$

Then, if $p \in [x,v]_\psi$, $\varphi(p) \in [x,g(x)^{-1}v]_\psi$. Therefore there exists an isomorphism $\tilde{\varphi}$: $E/\psi \to E/\psi'$, locally given by $\tilde{\varphi}(p,v) = (p,g^{-1}(\beta(p))v)$, $v \in V$, $p \in M/H$. Vice versa, we must show that a vector bundle over M/H with group G and fiber V gives an action ψ.

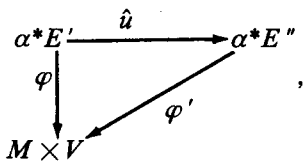
Let E' be such a bundle and $\alpha^*E' = \{(x,e') \in M \times E'/\alpha(x) = \pi'(e')\}$ the pullback bundle over M. As M is contractible, α^*E' is trivial and we have a trivialization φ: $\alpha^*E' \to M \times V$:



where $\pi(x,e') = \pi_1(\varphi(x,e')) = x$.

We define a natural action ν_h of H on α^*E' as $\nu_h(x,e') = (hx,e')$ and then an action of H on $M \times V$: $\tilde{h}(x,v) = \varphi\nu_h\varphi^{-1}(x,v)$.

$\tilde{h}$ is an action because it commutes with π_1 and it is associative: $\pi_1\varphi\nu_h\varphi^{-1} = \pi\nu_h\varphi^{-1} = h\pi\varphi^{-1} = h\pi_1$ and $\varphi\nu_{h_1}\nu_{h_2}\varphi^{-1} = \varphi\nu_{h_1}\varphi^{-1}\varphi\nu_{h_2}\varphi^{-1}$. If we now take another isomorphism φ': $\alpha^*E' \to M \times V$ it follows easily that $\psi = \varphi\nu_h\varphi^{-1}$ and $\psi' = \varphi'\nu_h\varphi'^{-1}$ are equivalent. In fact, if $\beta = \varphi\varphi'^{-1}$ we have $\beta\psi'\beta^{-1} = \psi$ and hence, putting $\beta(x,v) = (x,g(x)v)$, $\beta\psi'\beta^{-1}(x,v) = (hx,g(hx)\psi'(x,h)g(x)^{-1}v) = (hx,\psi(x,h)v)$, i.e., $\psi \approx \psi'$. Moreover, any automorphism of E' gives an automorphism of α^*E', and if $[\psi_{E'}]$ is the equivalence class of the actions given by E', we have that if E'' is isomorphic to E' then $[\psi_{E'}] = [\psi_{E''}]$. In fact, if $u: E' \to E''$ is an isomorphism, $\hat{u}(x,e') = (x,u(e'))$ is an isomorphism between $(\alpha^*E')_x$ and $(\alpha^*E'')_x$. This can be interpreted as a change of trivialization



and we apply the same argument as before.

Summing up, we have shown that any bundle E' over M/H gives an action of H on E and that isomorphic bundles give equivalent actions. This completes the proof of the proposition.

It is clear that any h-invariant section can be considered as a section of E/ψ over M/H and, vice versa, given a section $\hat{\sigma}$ of E' over M/H we can find a section σ of E over M invariant under the action determined by E'. In fact, we define

$$\sigma(x) = \varphi(x,\hat{\sigma}(\alpha(x))),$$

where φ is a trivialization of α^*E'. Here σ is invariant under the action $\varphi\nu_h\varphi^{-1}$:

$$\sigma(hx) = \varphi(hx,\hat{\sigma}(\alpha(hx)) = \varphi(hx,\hat{\sigma}(\alpha(x))$$
$$= \varphi\nu_h(x,\hat{\sigma}(\alpha(x))) = \varphi\nu_h\varphi^{-1}\sigma(x).$$

Therefore, as we assumed that any field must be an invariant section, we have that there might exist a classification of fields based on their transformation properties under H.

III. EXAMPLES FROM COSMOLOGY

In the following we shall consider some examples of universes that can be constructed from Friedmann models by making identifications under an appropriate discrete subgroup H of the complete isometry group of $\tilde{M}$.

If the space-time $M = \tilde{M}/H$ is to be time orientable, H must map each three-space ($t = \text{const}$) into itself. In this case the problem reduces to the Clifford–Klein space-form problem[2] of finding all the complete connected Riemann three-spaces Σ of constant curvature K. As usual[2,3] Σ is assumed to be compact and orientable.

As was said in the Introduction, multiply connected universes offer a very simple way to realize the specific initial conditions required by a chaotic cosmology. The model looks chaotic up until the epoch at which the entire finite volume of the universe (or of the elementary cell) becomes visible. At later epochs uniformity prevails since the observers see multiple images of the same fundamental cell. In Ref. 3, it is shown that thermalization of the background radiation is possible only for $K = 0, -1$ models.

We shall restrict to the $K = 0$ case in which a complete classification of the groups H is available.

There are only ten groups producing compact $\Sigma = R^3/H$. If orientability of Σ is required then the number of admissible groups reduces further to 6. The six groups $H_i (i = 1\text{–}6)$ are explicitly described by Wolf[4] who, moreover, computes the first (singular) homology module with integer coefficients $H_1(\Sigma_i, Z)$ of the resulting quotients $\Sigma_i = R^3/H_i$:

$$H_1(\Sigma_1,Z) = Z \oplus Z \oplus Z, \quad H_1(\Sigma_2,Z) = Z \oplus Z_2 \oplus Z_2,$$
$$H_1(\Sigma_3,Z) = Z \oplus Z_3, \quad H_1(\Sigma_4,Z) = Z \oplus Z_2,$$
$$H_1(\Sigma_5,Z) = Z, \quad H_1(\Sigma_6,Z) = Z_4 \oplus Z_4,$$

where Z_p is the Abelian group Z/pZ.

We can now apply the results on the classification of bundles[1] in order to classify the lifts of the H_i actions, i.e., the H_i-inequivalent fields. In the following $M_i = \Sigma_i \times R$ are noncompact, space- and time-orientable, four-dimensional manifolds.

The inequivalent scalar real fields and spinor structures are classified by $H^1(M_i,Z_2)$, the first (singular) cohomology module with values in Z_2. In our case the Kunneth formula in cohomology (see, e.g., Greenberg[5]) gives $H^1(M_i,Z_2) = H^1(\Sigma_i,Z_2)$. Moreover, $H^1(\Sigma_i,Z_2) = H_1(\Sigma_i,Z_2)$ because Z_2 is a field, and the universal coefficient formula gives $H_1(\Sigma_i,Z_2) = H_1(\Sigma_i,Z) \otimes Z_2$. We obtain

$$H_1(\Sigma_1,Z_2) = Z_2 \oplus Z_2 \oplus Z_2, \quad H_1(\Sigma_2,Z_2) = Z_2 \oplus Z_2 \oplus Z_2,$$
$$H_1(\Sigma_3,Z_2) = Z_2, \quad H_1(\Sigma_4,Z_2) = Z_2 \oplus Z_2,$$
$$H_1(\Sigma_5,Z_2) = Z_2, \quad H_1(\Sigma_6,Z_2) = Z_2 \oplus Z_2.$$

When G is simply connected [e.g., Su(n)] the inequivalent fields are classified by $H^4(M_i,Z)$, which in our case is the zero module.

U(n) fields are classified by $H^2(M_i,Z) \oplus H^4(M_i,Z)$, i.e., by $H^2(M_i,Z)$. Again $H^2(M_i,Z) = H^2(\Sigma_i,Z)$. Now Poincaré duality applies, giving $H^2(\Sigma_i,Z) = H_1(\Sigma_i,Z)$. In particular for $n = 1$ the same formula give us a classification of inequivalent scalar complex fields.

SO(n) fields are classified by $H^2(M_i,Z_2) = H^2(\Sigma_i,Z_2)$. Poincaré duality gives $H^2(\Sigma_i,Z_2) = H_1(\Sigma_i,Z_2)$, which was previously computed.

Another interesting case is $SU(3)/Z_3$ (see 't Hooft[6]). The classification is in term of $H^2(M_i,Z_3)$. We have $H^2(M_i,Z_3) = H^2(\Sigma_i,Z_3) = H_1(\Sigma_i,Z_3) \otimes Z_3$:

$$H_1(\Sigma_1,Z_3) = Z_3 \oplus Z_3 \oplus Z_3, \quad H_1(\Sigma_2,Z_3) = Z_3,$$
$$H_1(\Sigma_3,Z_3) = Z_3 \oplus Z_3, \quad H_1(\Sigma_4,Z_3) = Z_3,$$
$$H_1(\Sigma_5,Z_3) = Z_3, \quad H_1(\Sigma_6,Z_3) = 0.$$

We see that in some cases the classification gives a finite number of topologically inequivalent fields.

This leads to the possibility that the different members of a family of particles might be represented through topologically inequivalent structures.[7]

We have seen that such structures in fact can arise by taking into account at the same time the structure group of the bundle and the isometry group of the base manifold.

We note that the identification of points in $\tilde{M}$ via H to produce M usually lowers the dimension of the group of isometries of the space-time.[2]

This means that the existence of a set of distinct inequivalent sectors in general is consistent only with some particular cosmological models.

Therefore, although only a complete field theory could substantiate these considerations, our simple examples may be considered also as an indication of possible connections between gauge groups and symmetries of the space-times.

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Bound states, resonances, and symmetries of a neutral Dirac particle with anomalous magnetic moment, coupled to a fixed monopole

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For the system consisting of a neutral Dirac particle with anomalous magnetic moment, interacting with a fixed magnetic monopole, zero-energy bound states are constructed for each possible value of the total angular momentum. Results of Kazama and Yang for the charge–monopole system are used to deduce the existence of other bound states for this system, when the mass of the bound particle is nonzero. In the zero-mass case, there are no other bound states, but there are resonant states, and these are determined exactly. A noncompact, so(3,2) symmetry algebra of the zero-energy bound states is given for the finite-mass case and for the zero-mass case. In each case the infinite number of such states is associated with an irreducible Majorana representation of the algebra.

I. INTRODUCTION

This work continues the study of bound states and resonances of relativistic two-body problems involving magnetic interactions. Earlier related works have discussed a relativistic charged particle in a monopole field,[1] a Dirac particle with anomalous magnetic moment in a Coulomb field,[2] a neutrino with anomalous moment in a Coulomb field,[3] a Dirac particle in the field of a magnetic dipole,[4] and various other charge–dipole models.[5] The general forms of relativistic potentials describing the interactions between charges, magnetic monopoles, and magnetic dipoles (i.e., anomalous magnetic moments) have been derived from field theory.[6] Some of the techniques necessary to handle the singular potentials which can arise in such problems have been developed.[7]

The problem considered here is that of a neutral spin-$\frac{1}{2}$ particle having mass m and anomalous magnetic moment a, interacting with a fixed monopole having magnetic charge g. It is assumed that a relativistic description of the particle in an external electromagnetic field $F^{\mu\nu}$ is provided by Dirac's equation with a Pauli coupling term $ia\gamma_\mu\gamma_\nu F^{\mu\nu}$, in the usual notation, so that the Hamiltonian for the system under discussion is

$$H = \boldsymbol{\alpha}\cdot\mathbf{p} + \beta(m + \theta\boldsymbol{\sigma}\cdot\mathbf{r}/r^3), \tag{1.1}$$

where $\theta = 2ag$ and the remaining symbols have their usual meanings. [We use $\boldsymbol{\sigma}$ to denote the Pauli matrices and also the 4×4 matrices

$$\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix},$$

relying on context to fix the meaning of a particular usuage.]

Concerning physical applications, it is questionable to what extent the study of this H gives realistic information about the bound states and resonances of a *neutron* interacting with a fixed monopole. In particular, at the short distances which characterize the strongly bound (zero-energy) states of H discussed below (if m and a are given the values appropriate to the neutron, and $|eg| = \frac{1}{2}$, where e is the electronic charge), the strong field of the monopole would certainly detect the extended structure of the neutron, so that H might define a poor approximation to the true dynamics. However, the problem may be of interest at the substructure level of particles. Furthermore, the problem is of considerable indirect interest because H is sufficiently simple to permit an exact determination of some (though not all) bound states when $m > 0$; and of bound states and resonances in the limiting case $m = 0$. (If it should be found that one or more of the neutrinos has a magnetic moment, this latter limit could become physically relevant.) The Hamiltonian H therefore defines a simple relativistic model, in which some of the characteristic features of magnetic interactions[5] can be determined exactly. The mathematical interest of the system is increased by the remarkable appearance of a noncompact Lie algebra so(3,2) as an invariance algebra of the infinite set of bound states associated with the eigenvalue $E = 0$ of H. This occurs whether or not $m = 0$.

The system with Hamiltonian H may be regarded as the special case $Z = 0$ of the charge–monopole system considered by Kazama, Yang, and Goldhaber,[8–11] who took

$$H' = \boldsymbol{\alpha}\cdot(\mathbf{p} - Ze\mathbf{A}) + \beta(m + \theta\boldsymbol{\sigma}\cdot\mathbf{r}/r^3), \tag{1.2}$$

where $\mathbf{A}$ is the monopole potential. However, it must be noted that the structure of the conserved angular momentum vector, and indeed the possible values of the total angular momentum quantum number j, are quite different in cases with $eg \neq 0$ ($j = |eg| - \frac{1}{2}, |eg| + \frac{1}{2}, \ldots$) and $eg = 0$ ($j = \frac{1}{2}, \frac{3}{2}, \ldots$). In the latter case, which is the one of interest here, the singular monopole potential does not appear in H and the angular momentum therefore has the familiar form

$$\mathbf{J} = \mathbf{r}\wedge\mathbf{p} + \tfrac{1}{2}\boldsymbol{\sigma} = \mathbf{L} + \tfrac{1}{2}\boldsymbol{\sigma}. \tag{1.3}$$

Kazama and Yang[9,10] found bound states of two types for H'. Type A occur for $j \geqslant |eg| + \frac{1}{2}$, and type B for $j = |eg| - \frac{1}{2}$. They found eigenfunctions of H' corresponding to eigenvalue $E = 0$, and hence to binding energies equal to m, for every j (types A and B). They also showed that there are infinitely many other bound states of type B for $|\theta|$ sufficiently large, and found numerical estimates of some of the corresponding eigenvalues. Later Olaussen *et al.*[12] found approximate analytic expressions for these type B eigenfunctions and eigenvalues. In the meantime, Yang[11] showed that there exists an

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infinite number of bound states of type A for each j value, such that

$$|eg| + \tfrac{1}{2} \leqslant j < (|eg|^2 + 2m|\theta| + \tfrac{1}{4})^{1/2} - \tfrac{1}{2}. \tag{1.4}$$

The type B bound states do not occur for the Hamiltonian H. However, the "radial part" of the eigenvalue problem for H has the same structure as that for the type A bound states of H', so we are able to adapt relevant results of Kazama and Yang to the case we consider.

The problem of determining resonant states of H in the case $m > 0$ remains intractable, but in the limit $m = 0$ we find that the radial problem reduces to one of the cases described by Barut *et al.*[7] for which exact solutions can be given, corresponding to bound states and resonances.

The coupling of a spin-$\frac{1}{2}$ particle (with magnetic moment) to a fixed monopole has been considered in various nonrelativistic approximations.[13] The variety of results obtained for binding energies reflects the fact that the nonrelativistic Hamiltonian with attractive $\boldsymbol{\sigma}\cdot\mathbf{r}/r^3$ potential is not essentially self-adjoint, and an *ad hoc* repulsive core or cutoff has to be introduced to regularize the eigenvalue problem. In contrast, the relativistic problem, whether for a charged or uncharged particle, has an effective potential which already has a repulsive $1/r^4$ core, and needs no regularization. The nonrelativistic approaches typically miss the strongly bound, zero-energy states found by Kazama *et al.* and ourselves, which are characterized by distances at which the nature of the core is critical.

II. BOUND STATES WHEN $m > 0$

Introducing the Hermitian matrix γ_5 ($= i\alpha_1\alpha_2\alpha_3$), we note that $i\beta\gamma_5$ anticommutes with H. It is therefore convenient to adopt a representation of the Dirac matrices in which this matrix is diagonal. We take

$$\beta = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \boldsymbol{\alpha} = \begin{pmatrix} 0 & -i\boldsymbol{\sigma} \\ i\boldsymbol{\sigma} & 0 \end{pmatrix}, \tag{2.1}$$

where I is the 2×2 unit matrix, so that

$$i\beta\gamma_5 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{2.2}$$

The bispinor Ψ is now written as

$$\psi = \begin{pmatrix} f \\ g \end{pmatrix}, \tag{2.3}$$

where f and g have two components each and the eigenvalue equation $H\psi = E\psi$ becomes

$$\begin{aligned} (-i\boldsymbol{\sigma}\cdot\mathbf{p} + \theta\sigma_r/r^2 + m)g &= Ef, \\ (i\boldsymbol{\sigma}\cdot\mathbf{p} + \theta(\sigma_r/r^2) + m)f &= Eg, \end{aligned} \tag{2.4}$$

where $\sigma_r = \boldsymbol{\sigma}\cdot\mathbf{r}/r$.

Introducing

$$R = \mathbf{L}\cdot\boldsymbol{\sigma} + 1, \tag{2.5}$$

so that, on f or g,

$$R^2 = \mathbf{J}^2 + \tfrac{1}{4}, \quad \{R, \sigma_r\} = 0, \tag{2.6}$$

we suppose now that ψ is also an eigenvector of $\mathbf{J}^2$ with eigenvalue $j(j+1)$, where $2j$ is a positive integer. Then we can write, in the coordinate representation,

$$\begin{aligned} rf &= f_k(r)\chi_k + f_{-k}(r)\chi_{-k}, \\ rg &= g_k(r)\chi_k + g_{-k}(r)\chi_{-k}, \end{aligned} \tag{2.7}$$

where $f_{\pm k}, g_{\pm k}$ are one-component functions, which vanish at $r = 0$ and are square integrable on $[0, \infty)$; and $\chi_{\pm k}$ are two-component vectors which do not depend on the radial variable r, and which satisfy

$$R\chi_{\pm k} = k\chi_{\pm k}, \quad k = j + \tfrac{1}{2}. \tag{2.8}$$

(Each $\chi_{\pm k}$ can also be labeled by an eigenvalue of J_3; we suppress these labels.) With a suitable choice of phases, we also have

$$\sigma_r\chi_{\pm k} = \pm i\chi_{\mp k}. \tag{2.9}$$

Now

$$\boldsymbol{\sigma}\cdot\mathbf{p} = \sigma_r(p_r + (i/r)R), \tag{2.10}$$

where

$$p_r = \tfrac{1}{2}(r^{-1}\mathbf{r}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{r}r^{-1}). \tag{2.11}$$

On $f_{\pm k}$ and $g_{\pm k}$, p_r equals $-i(d/dr)$, so that Eqs. (2.4) give

$$\begin{aligned} (d_r + k/r - \theta/r^2)g_{-k} &= img_k - iEf_k, \\ (d_r - k/r - \theta/r^2)g_k &= -img_{-k} + iEf_{-k}, \\ (d_r + k/r + \theta/r^2)f_{-k} &= -imf_k + iEg_k, \\ (d_r - k/r + \theta/r^2)f_k &= imf_{-k} - iEg_{-k}, \end{aligned} \tag{2.12}$$

where $d_r = d/dr$.

Suppose for definiteness that $\theta > 0$; the treatment when $\theta < 0$ is quite similar and the corresponding results are obtained by interchanging the roles of f_k and g_k, and of f_{-k} and $-g_{-k}$. Consider first the case $E = 0$. Then Eqs. (2.12) fall into two uncoupled pairs.

The first pair is

$$\begin{aligned} (d_r + k/r - \theta/r^2)g_{-k} &= img_k, \\ (d_r + k/r - \theta/r^2)g_k &= -img_{-k}, \end{aligned} \tag{2.13}$$

and implies

$$\left(d_r^2 - \frac{2\theta}{r^2} - \frac{k(k-1)}{r^2} + \frac{2\theta}{r^3} + \frac{\theta^2}{r^4}\right)g_k = m^2 g_k. \tag{2.14}$$

This has the acceptable solution (square integrable, and vanishing at $r = 0$)

$$\begin{aligned} g_k &= A_k \sum_{l=0}^{k-1} \frac{(k+l-1)!}{l!(k-l-1)!}(2mr)^{-l}e^{-\theta/r - mr} \\ &= A_k(2mr/\pi)^{1/2}K_{k-1/2}(mr)e^{-\theta/r}, \end{aligned} \tag{2.15}$$

where A_k is a constant to be determined by normalization, and K_j is a modified Bessel function.[14] The second of Eqs. (2.13) then gives[14]

$$g_{-k} = -iA_k(2mr/\pi)^{1/2}K_{k+1/2}(mr)e^{-\theta/r}. \tag{2.16}$$

The second pair of Eqs. (2.12) implies

$$\left(d_r^2 + \frac{2\theta}{r^2}d_r - \frac{k(k-1)}{r^2} - \frac{2\theta}{r^3} + \frac{\theta^2}{r^4}\right)f_k = m^2 f_k, \tag{2.17}$$

which is also solvable in terms of Bessel functions, but has no acceptable nontrivial solutions. Thus f_k and from the last of Eqs. (2.12), f_{-k}, must vanish.

The (unnormalized) eigenfunctions of H and $\mathbf{J}^2$, with eigenvalues 0 and $j(j+1)=k^2-\frac{1}{4}$, now follow from Eqs. (2.3) and (2.7). Because $f_{\pm k}=0$, it follows from Eqs. (2.2) and (2.3) that these eigenfunctions are also eigenvectors of $i\beta\gamma_5$, with eigenvalue -1. (When $\theta<0$, the corresponding eigenfunctions have $i\beta\gamma_5=+1$.) They are of essentially the zame form as the zero-energy eigenfunctions found by Kazama and Yang,[9,10]

The determination of the nonzero eigenvalues of H is much more difficult, and exact solutions have not been found. We have to deal with all four coupled equations (2.12). However, if we put (for the case $\theta>0$)

$$\begin{aligned} &r=\theta\rho, \quad A_0=\theta m, \quad B_0=\theta E, \\ &h_1=\tfrac{1}{2}(f_k+g_k), \quad h_2=-\tfrac{1}{2}i(f_{-k}+g_{-k}), \\ &h_3=\tfrac{1}{2}(f_k-g_k), \quad h_4=-\tfrac{1}{2}i(f_{-k}-g_{-k}), \end{aligned} \tag{2.18}$$

we obtain precisely the equations considered by Kazama and Yang (with their μ replaced by our k). We may then adapt the qualitative results obtained by Yang.[11]

Thus, for any value of j such that $j(j+1)<2m\theta$, there is an infinite sequence of eigenvalues of H, which is bounded below, and bounded above by m; and there is an image set which is bounded above, and bounded below by $-m$. No estimates of the eigenvalues are available, and the forms of the corresponding eigenfunctions are unknown. For any value of j such that $j(j+1)>2m\theta$, there are no nonzero eigenvalues of H. If it should happen that $2m\theta$ equals $j(j+1)$ for some j, then $+m$ and $-m$ are the only nonzero eigenvalues of H for that value of j.

It may be expected that, as in the $m=0$ case (see Section III), the Hamiltonian H with $m>0$ also exhibits resonances in Gamow's sense.[15] These would correspond to complex values of E for which Eqs. (2.12) admit a solution in which $f_{\pm k}$ $g_{\pm k}$ vanish at $r=0$ and behave like $\exp(i\lambda r)$ as $r\to\infty$, where $\lambda^2=E^2-m^2$. The problem of finding these resonance values E, and the corresponding functions, has not been solved. In fact it is difficult to see how the analysis sketched by Yang, for (real) nonzero eigenvalues, could be extended to give even qualitative results about the existence of resonances.

III. BOUND STATES AND RESONANCES WHEN $m=0$

In this case Eqs. (2.12) reduce to two uncoupled pairs of coupled equations. Taking $\theta>0$, and setting $r=\theta\rho$, we have

$$\begin{aligned} &(d_\rho+k/\rho-1/\rho^2)g_{-k}=-i\lambda f_k, \\ &(d_\rho-k/\rho+1/\rho^2)f_k=-i\lambda g_{-k}, \\ &(d_\rho-k/\rho-1/\rho^2)g_k=i\lambda f_{-k}, \\ &(d_\rho+k/\rho+1/\rho^2)f_{-k}=i\lambda g_k, \end{aligned} \tag{3.1}$$

where $d_\rho=d/d\rho$ and $\lambda=\theta E$.

Consider first the zero-energy bound states ($\lambda=0$), which are seen to be associated now with uncoupled first-order equations. These integrate to give

$$\begin{aligned} &g_{-k}=A\rho^{-k}e^{-1/\rho}, \quad f_k=B\rho^k e^{1/\rho}, \\ &g_k=C\rho^k e^{-1/\rho}, \quad f_{-k}=D\rho^{-k}e^{-1/\rho}, \end{aligned} \tag{3.2}$$

where A, B, C, and D are constants. Solutions which behave acceptably at $\rho=0$ and $\rho=\infty$ are obtained only if $B=C=D=0$. It follows from Eqs. (2.3) and (2.7) that the resulting eigenfunctions of H and J^2 are also eigenfunctions of R and $i\beta\gamma_5$, with eigenvalues $-k$ and -1, respectively. (When $\theta<0$, these eigenvalues become $-k$ and $+1$.) It may be noted that with increasing angular momentum (increasing k), these eigenfunctions become more and more concentrated near $r=0$.

Are there any nonzero eigenvalues of H? If λ is real and nonzero, then it can be seen from Eqs. (3.1) that for large ρ, each of $g_{\pm k}, f_{\pm k}$ behaves like

$$ce^{i\lambda\rho}+de^{-i\lambda\rho}, \tag{3.3}$$

with c and d constant, and is therefore not normalizable. The answer is therefore no.

We now seek solutions corresponding to resonant states, by allowing λ complex in Eqs. (3.1) and requiring that $g_{\pm k}, f_{\pm k}$ vanish at $\rho=0$ and behave like $\exp(i\lambda\rho)$ as $\rho\to\infty$. We can suppose $\lambda\neq 0$, since that case has been discussed. The first pair of Eqs. (3.1) gives

$$\begin{aligned} &\left(d_\rho^2-\frac{k(k+1)}{\rho^2}+\frac{2(k+1)}{\rho^3}-\frac{1}{\rho^4}\right)g_{-k}=-\lambda g_{-k}, \\ &\left(d_\rho^2-\frac{k(k-1)}{\rho^2}+\frac{2(k-1)}{\rho^3}-\frac{1}{\rho^4}\right)f_k=-\lambda^2 f_k, \end{aligned} \tag{3.4}$$

while the second pair gives

$$\begin{aligned} &\left(d_\rho^2-\frac{k(k-1)}{\rho^2}-\frac{2(k-1)}{\rho^3}-\frac{1}{\rho^4}\right)g_k=-\lambda^2 g_k, \\ &\left(d_\rho^2-\frac{k(k-1)}{\rho^2}-\frac{2(k+1)}{\rho^3}-\frac{1}{\rho^4}\right)f_k=-\lambda^2 f_{-k}. \end{aligned} \tag{3.5}$$

Consider the last equation. It is the same as the radial equation we would obtain for a nonrelativistic spinless particle with total angular momentum k, mass $\frac{1}{2}$ and energy λ^2, moving in the purely repulsive central potential

$$V(\rho)=2(k+1)/\rho^3+1/\rho^4, \tag{3.6}$$

which decreases monotonically for $\rho>0$. It is evident that there are no resonances for such a potential, and so f_{-k} must vanish. It then follows from the last of Eqs. (3.1) that $g_k=0$.

Now consider the first of Eqs. (3.4), which is of the form considered by Barut *et al.*[7] Following their analysis, we seek a solution which behaves like $\exp(-1/\rho)$ as $\rho\to 0$, and like $\exp(i\lambda\rho)$ as $\rho\to\infty$. Setting

$$g_{-k}=G(\rho)\rho^{-k}\exp(-1/\rho+i\lambda\rho), \tag{3.7}$$

we find

$$\left[d_\rho^2+\left(\frac{2}{\rho^2}-\frac{2k}{\rho}+2i\lambda\right)d_\rho+\left(\frac{2i\lambda}{\rho^2}-\frac{2ik\lambda}{\rho}\right)\right]G=0. \tag{3.8}$$

We now seek a solution of this equation which is a polynomial in ρ of finite degree. [This is a sufficient, though possibly not necessary, condition that g_{-k} as in Eq. (3.7) will have the right behavior as $\rho\to\infty$.] Then we find that this degree must equal k, that is,

$$G(\rho)=\sum_{n=0}^{k}A_n\rho^n. \tag{3.9}$$

Substitution of this expression in Eq. (3.8) leads to the condition

$$W\begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ \cdot \\ \cdot \\ \cdot \\ A_{k-1} \\ A_k \end{pmatrix} \equiv \begin{pmatrix} i\lambda & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -i\lambda k & i\lambda - k & 2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -i\lambda(k-1) & i\lambda + 1 - 2k & 3 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdots & -2i\lambda & i\lambda - \tfrac{1}{2}(k-1)(k+2) & k \\ 0 & 0 & 0 & 0 & \cdots & 0 & -i\lambda & i\lambda - \tfrac{1}{2}k(k+1) \end{pmatrix} \begin{pmatrix} A_0 \\ A_1 \\ A_2 \\ \cdot \\ \cdot \\ \cdot \\ A_{k-1} \\ A_k \end{pmatrix} = 0, \tag{3.10}$$

for the coefficients A_n, and hence to the condition

$$\det W = 0, \tag{3.11}$$

for λ. Equation (3.11) is a polynomial equation of the $(k+1)$th degree in λ. The polynomial always has λ^2 as a factor, corresponding to the zero-energy case already discussed, where g_{-k} takes the form in Eqs. (3.2) and only A_0 in Eq. (3.9) is nonzero. The complex roots always appear in pairs λ, $-\lambda^*$, each such pair corresponding to a single resonance at the energy value $E \sim \mathrm{Re}\,\lambda$, with width $\sim \mathrm{Im}\,\lambda$.

For example, when $k = 1$,

$$\det W = -\lambda^2, \tag{3.12}$$

so there are no resonances in this case—only the zero-energy bound state.

When $k = 2$,

$$\det W = -\lambda^2(i\lambda - 1), \tag{3.13}$$

and there is a resonance (antibound state) with $\lambda = -i$.

When $k = 3$,

$$\det W = -\lambda^2(-\lambda^2 - 4i\lambda + 6), \tag{3.14}$$

and there is a resonance with $\lambda = \pm\sqrt{2} - 2i$.

For $k = 4$ and 5, calculation of exact values for the roots of Eq. (3.11) is possible but increasingly complicated. For $k \geqslant 6$, we are faced with a polynomial equation of degree greater than or equal to five, and must resort to numerical methods to find the roots to any desired accuracy.

Once a nonzero root λ has been determined, the corresponding coefficents A_n can be found from Eq. (3.10), and hence g_{-k} determined from Eqs. (3.7) and (3.9). Then f_k is given by the first of Eqs. (3.1); it has the form

$$f_k = F(\rho)\rho^{-(k-1)} \exp(-1/\rho + i\lambda\rho), \tag{3.15}$$

where F is a polynomial of degree $(k-1)$. We could alternatively find f_k by applying the analysis of Barut *et al.*[7] directly to the second of Eqs. (3.4).

Because f_{-k} and g_k vanish for all these resonances, the latter correspond, according to Eqs. (2.3) and (2.7), to eigenfunctions of $i\beta\gamma_5 R$ with eigenvalue $+1$. (For $\theta < 0$, the corresponding eigenvalue is -1.) It may be noted that $i\beta\gamma_5 R$ is a constant of the motion when $m = 0$ but not when $m > 0$.

IV. ZERO-ENERGY BOUND STATES AND so(3,2) SYMMETRY

It is convenient to introduce the Hermitian operators

$$\mathbf{n} = \mathbf{r}/r, \quad \mathbf{e} = \tfrac{1}{2}(\mathbf{n}\wedge\mathbf{L} - \mathbf{L}\wedge\mathbf{n}), \tag{4.1}$$

which satisfy

$$\begin{aligned} &[n_i, n_j] = 0, \quad [e_i, e_j] = -i\epsilon_{ijk}L_k, \\ &[e_i, n_j] = i(\delta_{ij} - n_i n_j), \\ &e_i n_j - e_j n_i = \epsilon_{ijk}L_k, \\ &\mathbf{e}\cdot\mathbf{n} = i = -\mathbf{n}\cdot\mathbf{e}, \end{aligned} \tag{4.2}$$

and then to define

$$\begin{aligned} &\mathbf{u} = R\mathbf{n} + i\mathbf{e} = \mathbf{n}R + i\mathbf{e} - i\boldsymbol{\sigma}\wedge\mathbf{n}, \\ &\mathbf{d} = \mathbf{u}^\dagger = \mathbf{n}R - i\mathbf{e} = R\mathbf{n} - i\mathbf{e} + i\boldsymbol{\sigma}\wedge\mathbf{n}. \end{aligned} \tag{4.3}$$

It is then straightforward to check that

$$\begin{aligned} &R\mathbf{u} = \mathbf{u}(R+1), \quad R\,\mathbf{d} = \mathbf{d}(R-1), \\ &[u_i, u_j] = 0 = [d_i, d_j], \quad [u_i, d_j] = -2R\,\delta_{ij} - 2i\,\epsilon_{ijk}J_k. \end{aligned} \tag{4.4}$$

In addition, we have, of course,

$$[u_i, J_j] = i\,\epsilon_{ijk}u_k, \quad [d_i, J_j] = i\,\epsilon_{ijk}d_k, \quad [R, J_i] = 0. \tag{4.5}$$

If we set, for $i, j = 1, 2, 3$,

$$\begin{aligned} &l_{ij} = \epsilon_{ijk}J_k, \quad l_{45} = R, \\ &l_{i4} = -l_{4i} = \tfrac{1}{2}(u_i + d_i), \\ &l_{i5} = -l_{5i} = \tfrac{1}{2}i(u_i - d_i), \end{aligned} \tag{4.6}$$

then relations (4.4) and (4.5) can be written in a standard form for so(3,2),

$$[l_{AB},l_{CD}] = i(g_{AC}l_{BD} + g_{BD}l_{AC} - g_{BC}l_{AD} - g_{AD}l_{BC}), \tag{4.7}$$

where A, B, C, D run over 1 to 5, and the metric tensor $g_{AB} = \text{diag}(1,1,1,-1,-1)$. Note that each l_{AB} is Hermitian.

These operators all commute with the radial variables r and ρ_r, and can be thought of as acting in the vector space spanned by the χ_k and χ_{-k}, $k = 1, 2, \ldots$. In fact, they leave invariant separately the subspaces S_+ and S_- spanned by the χ_k and χ_{-k}, respectively, since none of the l_{AB} change the sign of R. (Because R does not have zero as an eigenvalue, it follows that the lowering operator $\mathbf{d}$ annihilates χ_1, and the raising operator $\mathbf{u}$ annihilates χ_{-1}.) On each of S_+ and S_- the l_{AB} span an irreducible Majorana representation of so(3,2) which remains irreducible when restricted to so(3,1). To see this, take as so(3,1) basis operators the l_{ij} and l_{i4}, and note that the two so(3,1) invariants have the form

$$\begin{aligned} C_1 &\equiv \tfrac{1}{2}l_{ij}l_{ij} - l_{i4}l_{i4} \\ &= \mathbf{J}^2 - \tfrac{1}{4}(\mathbf{u}^2 + \mathbf{d}^2 + \mathbf{u}\cdot\mathbf{d} + \mathbf{d}\cdot\mathbf{u}), \\ C_2 &\equiv \epsilon_{ijk}l_{ij}l_{k4} = \mathbf{J}\cdot\mathbf{u} + \mathbf{J}\cdot\mathbf{d}. \end{aligned} \tag{4.8}$$

It follows from the definitions (4.3) that

$$\begin{aligned} &\mathbf{u}^2 = 0 = \mathbf{d}^2, \quad \mathbf{u}\cdot\mathbf{d} = (2R-1)(R-1), \\ &\mathbf{d}\cdot\mathbf{u} = (2R+1)(R+1), \quad \mathbf{j}\cdot\mathbf{u} = 0 = \mathbf{j}\cdot\mathbf{d}. \end{aligned} \tag{4.9}$$

Therefore, noting the first of Eqs. (2.6), we have

$$C_1 = -\tfrac{3}{4}, \quad C_2 = 0. \tag{4.10}$$

In the infinite-dimensional irreducible representation $[k_0,c]$ of so(3,1), where j takes values $k_0, k_0+1, \ldots$, these two invariants equal[16] $(k_0^2 + c^2 - 1)$ and $2ik_0c$, respectively, and it follows that we are dealing with the representation $[\frac{1}{2},0]$. It is well known[17] that this extends in two different ways to irreducible Majorana representations of so(3,2). In one of these, say R_+, l_{45} takes positive eigenvalues; in the other, say R_-, it takes negative eigenvalues. We see that we have the representation $R\pm$ on $S\pm$. Note that the operator σ_r intertwines these two representations, according to the second of Eqs. (2.6), and that

$$\mathbf{u}\,\sigma_r = -\sigma_r\mathbf{d}, \quad \mathbf{d}\,\sigma_r = -\sigma_r\mathbf{u}. \tag{4.11}$$

The Casimir operator of so(3,2) has the same value on $R_\pm$. In fact, it is given in each case by

$$\begin{aligned} &\tfrac{1}{2}l_{ij}l_{ij} - l_{i4}l_{i4} - l_{i5}l_{i5} + (l_{45})^2 \\ &\quad = -\tfrac{3}{4} + \tfrac{1}{4}(\mathbf{u}^2 + \mathbf{d}^2 - \mathbf{u}\cdot\mathbf{d} - \mathbf{d}\cdot\mathbf{u}) + R^2 = -\tfrac{5}{4}, \end{aligned} \tag{4.12}$$

using Eqs. (4.9).

Because this so(3,2) algebra is independent of the radial variables, it underlies all problems involving Dirac's equation (or even the Schrödinger–Pauli equation for a spin-$\frac{1}{2}$ particle) with a centrally symmetric potential or external field. However, it is not an invariance algebra of any Hamiltonian of such an equation, in general, and indeed it is not the invariance algebra of the zero-energy eigenspace of the Hamiltonian H of Eq. (1.1), whether or not $m = 0$.

To define the latter invariance algebra, consider first the case $m = 0$. Introduce (with $\theta > 0$ and $r = \theta\rho$ as before)

$$\mathbf{U} = \rho\mathbf{u}, \quad \mathbf{D} = \rho^{-1}\mathbf{d}, \tag{4.13}$$

which can be seen to satisfy the same relations among themselves, and with R and $\mathbf{J}$, as the $\mathbf{u}$ and $\mathbf{d}$. [See Eqs. (4.4), (4.5), and (4.9).] Then the generators L_{AB}, defined in terms of $\mathbf{U}$, $\mathbf{D}$, R, and $\mathbf{J}$ just as the l_{AB} were defined in terms of $\mathbf{u}$, $\mathbf{d}$, R, and $\mathbf{J}$, also span a representation of so(3,2). The L_{AB} can be seen to leave invariant the vector space P_0 spanned by vectors of the form

$$\psi_k = \begin{pmatrix} 0 \\ \rho^{-(k+1)}e^{-1/\rho}\chi_{-k} \end{pmatrix}, \tag{4.14}$$

which is just the zero-energy eigenspace of H in the case $m = 0$, $\theta > 0$ [cf. Eqs. (2.3) and (2.2)]. The invariance of this subspace can also be seen from the relations

$$\begin{aligned} &\{H,R\} = 0, \quad [H,\mathbf{J}] = 0, \\ &H\mathbf{U} = -\rho^2\mathbf{D}H, \quad H\mathbf{D} = -\rho^{-2}\mathbf{U}H, \end{aligned} \tag{4.15}$$

which hold when $m = 0$, and which are established with the help of Eqs. (4.4) and (4.11).

Note that $\mathbf{U}$ is not a Hermitian conjugate to $\mathbf{D}$ as defined, so the L_{AB} are not Hermitian. Nevertheless, they satisfy on P_0 exactly the same relations as do the l_{AB} on S_-, spanning an irreducible Majorana representation R_- there. They are related by a complicated similarity transformation to Hermitian operators on P_0.

In the case $m > 0$, the zero-energy eigenfunctions of H are not eigenfunctions of R, but rather of

$$|R| = \epsilon R, \tag{4.16}$$

where ϵ is the operator with eigenvalue ± 1 on each $\chi_{\pm k}$, and hence on $S_\pm$. With $\theta > 0$, we define

$$\begin{aligned} \mathbf{U}' &= \frac{1}{m}\mathbf{u}\left(ip_r - \frac{R}{r} - \frac{\theta}{r^2}\right)\frac{1}{2}(1+\epsilon) + \frac{1}{m}\mathbf{d}\left(ip_r + \frac{R-1}{r} - \frac{\theta}{r^2}\right)\frac{1}{2}(1-\phi), \\ \mathbf{D}' &= \frac{1}{m}\mathbf{d}\left(ip_r + \frac{R-1}{r} - \frac{\theta}{r^2}\right)\frac{1}{2}(1+\epsilon) + \frac{1}{m}\mathbf{u}\left(ip_r - \frac{R}{r} - \frac{\theta}{r^2}\right)\frac{1}{2}(1-\epsilon). \end{aligned} \tag{4.17}$$

Then

$$\begin{aligned} [U_i',U_j'] &= \frac{1}{m^2}[u_i,u_j]\frac{1}{2}(1+\epsilon)\left(ip_r - \frac{R+1}{r} - \frac{\theta}{r^2}\right)\left(ip_r - \frac{R}{r} - \frac{\theta}{r^2}\right) + \frac{1}{m^2}[d_i,d_j] \\ &\quad \times\frac{1}{2}(1-\epsilon)\left(ip_r + \frac{R-2}{r} - \frac{\theta}{r^2}\right)\left(ip_r + \frac{R-1}{r} - \frac{\theta}{r^2}\right) = 0, \end{aligned} \tag{4.18}$$

and similarly

$$[D_i',D_j'] = 0. \tag{4.19}$$

Also,

$$m^2U_i'D_j' = u_id_j\frac{1}{2}(1+\epsilon)\left(ip_r - \frac{R-1}{r} - \frac{\theta}{r^2}\right)\left(ip_r + \frac{R-1}{r} - \frac{\theta}{r^2}\right) + d_iu_j\frac{1}{2}(1-\epsilon)$$
$$\times\left(ip_r + \frac{R}{r} - \frac{\theta}{r^2}\right)\left(ip_r - \frac{R}{r} - \frac{\theta}{r^2}\right). \tag{4.20}$$

With $g_k(r)$ as in Eq. (2.15), we have on $g_k\chi_k$,

$$\left(ip_r - \frac{R-1}{r} - \frac{\theta}{r^2}\right)\left(ip_r - \frac{R-1}{r} - \frac{\theta}{r^2}\right) = \left(d_r^2 - \frac{2\theta}{r^2}d_r - \frac{k(k-1)}{r^2} + \frac{2\theta}{r^3} + \frac{\theta^2}{r^4}\right) = m^2, \tag{4.21}$$

so that the first term on the right-hand side of Eq. (4.20) reduces to

$$m^2d_iu_j\tfrac{1}{2}(1+\epsilon). \tag{4.22}$$

In a similar way, the second term reduces on $g_{-k}\chi_{-k}$ [with g_{-k} as in Eq. (2.16)], to

$$m^2d_iu_j\tfrac{1}{2}(1-\epsilon). \tag{4.23}$$

Then, on

$$\psi = \begin{pmatrix} 0 \\ r^{-1}(g_k\chi_k + g_{-k}\chi_{-k}) \end{pmatrix}, \tag{4.24}$$

we have

$$U_i'D_j' = u_id_j\tfrac{1}{2}(1+\epsilon) + d_iu_j\tfrac{1}{2}(1-\epsilon), \tag{4.25}$$

and similarly

$$D_j'U_i' = d_ju_i\tfrac{1}{2}(1+\epsilon) + u_jd_i\tfrac{1}{2}(1-\epsilon), \tag{4.26}$$

so that

$$[U_i',D_j'] = [u_i,d_j]\tfrac{1}{2}(1+\epsilon) - [u_j,d_i]\tfrac{1}{2}(1-\epsilon)$$
$$= -2|R|\delta_{ij} - 2i\epsilon_{ijk}J_k. \tag{4.27}$$

Using the same kind of manipulations we check that on such functions ψ, **U**, **D**, R, and **J** also satisfy the remaining relations (4.4), (4.5), and (4.9) satisfied by **u**, **d**, R, and **J**.

Defining L'_{AB} by analogy with L_{AB}, we have, on the space P_0' of vectors spanned by ψ of the form (4.24), an irreducible R_+ Majorana representation of so(3,2).

Like L_{AB}, the operators L'_{AB} are not Hermitian, but in a similar way they are related by a similarity transformation to Hermitian operators on the zero-energy eigenspace P_0'.

In closing this section, we remark that the irreducible Majorana representations of SO(3,2) are known to be integrable to unitary representations of the group SO(3,2) (or more accurately, of its double-covering group.)

V. CONCLUDING REMARKS

The appearance of zero-energy bound states for this system, as for the charge–monopole system considered by Kazama *et al.*, is remarkable. Such zero-energy modes are also found for Dirac particles interacting with non-Abelian, su(2) monopoles,[18] suggesting that their occurrence may have a topological interpretation. The operator $i\beta\gamma_5$ is diagonal on all the zero-energy states found by Kazama *et al.* and ourselves. The corresponding solutions $\psi(\mathbf{x})$ of Dirac's equation are necessarily static, and it can be seen that they are therefore eigenstates of CT, where C and T are the usual charge conjugation and time-reversal operators, acting on a general spinor [for our representation (2.1) of Dirac matrices] as

$$C\psi(\mathbf{x},t) = \alpha_2\psi^*(\mathbf{x},t),$$
$$T\psi(\mathbf{x},t) = i\alpha_2\beta\gamma_5\psi^*(\mathbf{x},-t),$$

so that

$$CT\,\psi(\mathbf{x}) = i\beta\gamma_5\psi(\mathbf{x}).$$

The other bound states ($m>0$) and resonant states ($m=0$) of H are not eigenstates of CT. Moreover, neither these states nor the zero-energy states are eigenstates of the parity operator

$$P\psi(\mathbf{x},t) = \beta\psi(-\mathbf{x},t),$$

because of the presence of the pseudoscalar σ_r in H.

It is also remarkable that the zero-energy states are associated with a Majorana representation of so(3,2), whether or not $m=0$. We are familiar with accidental symmetries in bound-state problems, associated with finite degeneracies and compact invariance algebras, but the appearance in such problems of infinite degeneracies associated with noncompact algebras is quite unusual. It seems likely that noncompact invariance algebras can also be found for the zero-energy bound states of the charge–monopole system, but we have not pursued that here.

For the Hamiltonian H with $m=0$, we have been able to determine the form of resonant states, occurring at all possible values of the total angular momentum except $j=\frac{1}{2}(k=1)$. Although this system may turn out to be unphysical, it is nevertheless satisfying to have found a relativistic model in which such states can be determined exactly.

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Kinematics of the two-angle-dependent reactive infinite-order sudden approximation

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The so-called "matching problem" in the earlier formulations of the reactive infinite-order sudden approximation (RIOSA) is analyzed in detail. The kinematics of a new, two-angle-dependent RIOSA scheme, which is based on an independent selection of the "frozen" angles in the reactants and products channels, is derived. It is shown that the only pairs of these angles to be excluded from consideration are those which violate the "collinearity conservation rule." The new scheme does not invoke any additional assumption which is not an inherent part of the RIOSA approach. It is free from the matching problem and treats the different arrangement channels in a completely symmetrical fashion.

I. INTRODUCTION

New theories, in general, and approximate schemes, in particular, rarely escape a number of revisions, modifications, and generalizations before they acquire the "status of acceptability." The infinite-order sudden approximation for reactive scattering (RIOSA) does not constitute an exception in this respect.

The value of a theoretical construction can be defined in simplified terms by its "external" and "internal" merits. The external merits characterize the ability of a theory to be in accord with the existing body of knowledge (both theoretical and experimental), on the one hand, and to produce new results and predict new phenomena, on the other. The internal merits depend on the severity of the assumptions used and the degree of their generality and justifiability.

Results of RIOSA studies on several atom–diatomic molecule reactive systems were evaluated in a number of studies.[1-11] Here we shall address the question about the internal qualifications of the RIOSA scheme. More specifically, we shall examine in detail the so-called "matching problem," which undoubtedly is a weak point of all the previous formulations. We shall show how the theory can be reformulated in a form which is free from this problem. A preliminary account of elements of the new formulation was presented by us earlier.[12]

The essence of the infinite-order sudden approximation is in assuming that the angle γ between the collision vector $\mathbf{R}'$ and the axis $\mathbf{r}'$ of the target diatomic molecule (the primes denote physical coordinates) does not change in the course of the collision event. In the case of reactive scattering one should consider simultaneously at least two fixed ("frozen") angles γ_α; $\alpha = \lambda, \nu$, where λ and ν label different arrangement channels. The main question which arises in this respect can be formulated as follows: How should the frozen angles in the reactants channel be correlated with those in the products channel, if at all?

In all previous RIOSA treatments an *a priori* one-to-one correlation between the fixed γ_λ and γ_ν was assumed. Barg and Drolshagen[3] considered the specific case of a light–heavy–light system for which $\gamma_\lambda = \gamma_\nu$ in the limit $H \to \infty$, where H stands for "heavy." Bowman and Lee[1] associated with each angle γ_λ the angle $\gamma_\nu = \pi - \gamma_\lambda$. Adopting the presumption about the one-to-one correlation between the frozen angles, one effectively introduces into the theory an additional parameter, the so-called "matching" constant $B_{\nu\lambda}$ (see Sec. II). Selection of γ_λ and $B_{\nu\lambda}$ defines the value of γ_ν (Ref. 13) (see also Sec. III). In the formulation of Bowman and Lee the value $B_{\nu\lambda} = 1$ was chosen for all γ_λ's. In the scheme of Khare, Kouri, and Baer[13] $B_{\nu\lambda}$ could acquire, in principle, any positive value. But once selected, it again remained the same for all γ_λ's.

It should be clearly understood that the fixing of $B_{\nu\lambda}$ is not a necessary requirement inherent in the RIOSA theory. The RIOSA dynamics does not determine the actual value (or set of values) of $B_{\nu\lambda}$. Moreover, since the matching constant does not have any special physical meaning the very possibility of such a determination is questionable. Though in actual calculations[1-11] the value of $B_{\nu\lambda}$ was selected using considerations of symmetry and those of numerical convenience, the choice, in general, remains arbitrary. The related ambiguity is usually called the matching problem. This problem may become a major drawback of the theory since nothing, in principle, precludes the final results from being $B_{\nu\lambda}$ dependent. The main conclusion to be drawn is that a fixed matching constant should not appear in the theory as a basic parameter.

In general, different $B_{\nu\lambda}$ values may and should be chosen for different γ_λ values; moreover, a whole range of $B_{\nu\lambda}$'s may correspond to each value of γ_λ. Shapiro and Zeiri[14] suggested correlating the frozen angles via a turning point model. Effectively, this model assigns to each value of γ_λ its "own" (single) value of $B_{\nu\lambda}$. Yet the restriction of the one-to-one correspondence between the angles remains.

As will be shown below, the problem of the correlation between the frozen angles [i.e., of the selection of the value(s) of $B_{\nu\lambda}$] is equivalent to the question about the extent of the arrangement channels or about the border between them. In the RIOSA formalism the different arrangement channels are separated by a line (rather than by a surface, as in the exact 3-D treatment[15]) which passes through the strong interaction region. In case of a quantum mechanical treatment the approximate so-called channel wave functions and their first derivatives (with respect to the propagation coordinate) are to be matched on this line. This gives rise to the term

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matching problem. It should, however, be noted that this term is quite misleading, since the task of matching is that of solving a system of linear equations, and as such does not constitute any problem. Moreover, in the classical mechanical RIOSA scheme[5,7,12] one avoids the matching completely, propagating the trajectory across the borderline in a continuous fashion. The problem, however, remains. It concerns the borderline (we shall denote it $\Gamma_{\lambda\nu}$) itself. The principal importance of defining the borderline lies in that on $\Gamma_{\lambda\nu}$ a collinear-type problem corresponding to a fixed γ_λ should be converted to that corresponding to a fixed γ_ν and vice versa. Each pair $(\gamma_\lambda, \gamma_\nu)$ defines $\Gamma_{\lambda\nu}$ uniquely, and thus a one-to-one correlation between the frozen angles implies that one and only one borderline is associated with each fixed γ_λ and/or γ_ν. Selection of a particular borderline, however, lacks any general physical justification, and the very perception about its uniqueness is nothing more than an *a priori* assumption. In principle, one should consider all the possible borderlines for each fixed γ_λ (or γ_ν). The possible "shrinkage" of the (continuous) manifold of all $\Gamma_{\lambda\nu}$'s in certain particular cases should then be substantiated by the specificity of the system at hand, i.e., by the energy and masses of the interacting particles and the "shape" of the potential. Inclusion of a manifold of different $\Gamma_{\lambda\nu}$'s for each fixed γ_λ (or γ_ν) means removal from the theory of the one-to-one correspondence between the frozen angles or of a "privileged" value of $B_{\nu\lambda}$. We shall refer to the RIOSA theory based on an independent selection of the fixed values of γ_λ and γ_ν as the two-angle-dependent RIOSA.

The classical and quantal two-angle-dependent RIOSA dynamics is presented in Refs. 12 and 16, respectively (a refinement of the classical RIOSA is given in Ref. 17). Here we shall deal with the two-angle-dependent RIOSA kinematics, which is common for both classical and quantal schemes. In Sec. II the arrangement channel representation and the RIOSA configuration space are defined. In Sec. III general kinematical relations valid for any pair $(\gamma_\lambda, \gamma_\nu)$ are derived and analyzed. A brief summary is given in Sec. IV.

II. THE RIOSA ARRANGEMENT CHANNELS

The configuration of a three-atom system *A-B-C* in the center-of-mass body fixed frame may be described in each arrangement channel by a set of three coordinates R'_α, r'_α, and γ_α, where $\alpha = \lambda, \nu, \kappa$ denotes the arrangement channel (see Fig. 1). Here, $\mathbf{R}'_\alpha$ and $\mathbf{r}'_\alpha$ are the α-channel (space-fixed) collision and diatomic separation vectors, respectively, and γ_α is the angle between them.

It is convenient to perform the following scaling[18] of the physical coordinates:

$$\mathbf{R}_\lambda = a_\lambda \mathbf{R}'_\lambda, \quad \mathbf{r}_\lambda = a_\lambda^{-1}\mathbf{r}'_\lambda, \qquad (1)$$

where $a_\lambda = (\mu_{\lambda,\nu\kappa}/\mu_{\nu\kappa})^{1/4}$.

Here, $\mu_{\lambda,\nu\kappa}$ and $\mu_{\nu\kappa}$ are the reduced masses of the λ-channel projectile-diatomic target and the diatomic molecule, respectively. The ν- and κ-channel scalings are obtained from (1) by combining cyclically the λ, ν, and κ indices. Note that the scaling procedure does not alter the γ_α angles, but it attributes to the system a unique effective mass

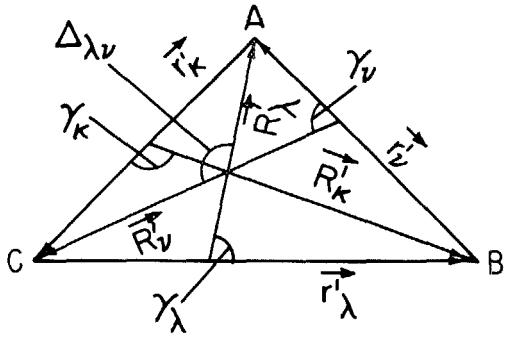

FIG. 1. Arrangement channel coordinates of a three-atom system.

$$\mu = [m_\lambda \cdot m_\nu \cdot m_\kappa/(m_\lambda + m_\nu + m_\kappa)]^{1/2}, \qquad (2)$$

the same in all the arrangements[18]; m_α is the mass of the α-channel projectile atom.

It can be readily verified[13,15] that the interchannel relation between the scaled vector coordinates $(\mathbf{R}_\lambda, \mathbf{r}_\lambda)$ and $(\mathbf{R}_\nu, \mathbf{r}_\nu)$ gives rise to an orthogonal transformation M

$$\begin{pmatrix}\mathbf{R}_\nu \\ \mathbf{r}_\nu\end{pmatrix} = \mathsf{M}\begin{pmatrix}\mathbf{R}_\lambda \\ \mathbf{r}_\lambda\end{pmatrix}, \qquad (3)$$

where

$$\mathsf{M} = \begin{pmatrix}\cos\beta_{\nu\lambda} & -\sin\beta_{\nu\lambda} \\ \sin\beta_{\nu\lambda} & \cos\beta_{\nu\lambda}\end{pmatrix} \qquad (4)$$

and

$$\cos\beta_{\nu\lambda} = -[m_\lambda m_\nu/(m_\lambda + m_\kappa)(m_\nu + m_\kappa)]^{1/2},$$
$$\sin\beta_{\nu\lambda} = \sqrt{1 - \cos^2\beta_{\nu\lambda}}. \qquad (5)$$

The relations between the magnitudes of the vectors implied by (3) and (4) are

$$r_\nu^2 = R_\lambda^2 \sin^2\beta_{\nu\lambda} + r_\lambda^2 \cos^2\beta_{\nu\lambda} + r_\lambda R_\lambda \cos\gamma_\lambda \sin 2\beta_{\nu\lambda}, \qquad (6)$$

$$r_\lambda^2 = R_\nu^2 \sin^2\beta_{\nu\lambda} + r_\nu^2 \cos^2\beta_{\nu\lambda} - r_\nu R_\nu \cos\gamma_\nu \sin 2\beta_{\nu\lambda}, \qquad (7)$$

and

$$R_\lambda^2 + r_\lambda^2 = R_\nu^2 + r_\nu^2. \qquad (8)$$

Again, combining cyclically the λ, ν, and κ indices one easily obtains the $\lambda \leftrightarrow \kappa$ and $\nu \leftrightarrow \kappa$ analogs of Eqs. (3)–(8).

A transparent description of the arrangement channels is obtained by the use of cylindrical coordinates. Each channel $\alpha(=\lambda, \nu, \kappa)$ is represented by a cylinder, the axis of which coincides with the R_α axis. The case $\alpha = \lambda, \nu$ is depicted in Fig. 2. Note that all the axes have a common origin and the angle between the R_λ and R_ν axes is chosen to be $\pi - \beta_{\nu\lambda}$ (the reason for this choice will become clear below).

As already mentioned, the RIOSA scheme implies freezing the angles $\gamma_\alpha(\alpha = \lambda, \nu, \kappa)$. In what follows we shall consider two channels at a time. The frozen angles define a fixed-γ_λ plane and a fixed-γ_ν plane (see Fig. 2) which represent the RIOSA λ-arrangement and ν-arrangement configuration spaces, respectively. The two planes intersect along a

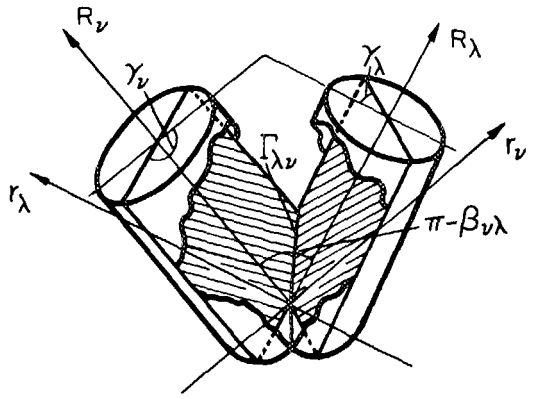

FIG. 2. The λ- and ν-arrangement channels represented in cylindrical coordinates. The fixed-γ_λ and fixed-γ_ν planes (the RIOSA configuration spaces) intersect along the borderline $\Gamma_{\lambda\nu}$.

straight line $\Gamma_{\lambda\nu}$ passing through the origin. This line separates the RIOSA λ and ν configuration spaces and will be called "borderline." Each pair of fixed γ_λ and γ_ν defines a borderline. Each borderline represents a continuous set of similar triangles formed by the three atoms. These triangles are the RIOSA $\lambda \leftrightarrow \nu$ transition configurations. All the triangles belonging to the same set (represented by the same borderline) are characterized by the same values of five parameters γ_λ, γ_ν, $B_{\nu\lambda}$, $\eta_{0\lambda}$, and $\eta_{0\nu}$, where $B_{\nu\lambda}$, $\eta_{0\lambda}$, and $\eta_{0\nu}$ are introduced as follows:

$$B_{\nu\lambda} = (r_\nu/r_\lambda)|_{\Gamma_{\lambda\nu}}, \tag{9}$$

$$\cot \eta_{0\alpha} = (R_\alpha/r_\alpha)|_{\Gamma_{\lambda\nu}}, \quad \alpha = \lambda, \nu. \tag{10}$$

Since Eqs. (9) and (10) define, in fact, the borderline $\Gamma_{\lambda\nu}$ ($\eta_{0\alpha}$ is the angle between $\Gamma_{\lambda\nu}$ and the R_α axis; $\alpha = \lambda, \nu$) we shall refer to $B_{\nu\lambda}$, $\eta_{0\lambda}$, and $\eta_{0\nu}$ as borderline parameters. Fixing any two of the five parameters defines the remaining three and thus the borderline. This general statement is easily proved by noting that exclusion of the coordinates from Eqs. (6)–(8) gives

$$B_{\nu\lambda}^2 - \cot^2 \eta_{0\lambda} \sin^2 \beta_{\nu\lambda} - \cos^2 \beta_{\nu\lambda} - \cot \eta_{0\lambda} \cos \gamma_\lambda \sin 2\beta_{\nu\lambda} = 0, \tag{11}$$

$$B_{\nu\lambda}^{-2} - \cot^2 \eta_{0\nu} \sin^2 \beta_{\nu\lambda} - \cos^2 \beta_{\nu\lambda} + \cot \eta_{0\nu} \cos \gamma_\nu \sin 2\beta_{\nu\lambda} = 0, \tag{12}$$

$$\cos \gamma_\lambda \cot \eta_{0\lambda} + B_{\nu\lambda}^2 \cos \gamma_\nu \cot \eta_{0\nu} + (1 - B_{\nu\lambda}^2) \cot \beta_{\nu\lambda} = 0. \tag{13}$$

This system of three nonlinear equations (11)–(13) with respect to three unknowns (two of the five parameters are fixed) has, in general, more than one solution. From pure geometrical considerations it follows, however, that in most of the cases only one solution will have physically meaningful values (see Sec. III). Note that Eq. (13) may be replaced by the equality

$$B_{\nu\lambda}^2 = (\cot^2 \eta_{0\lambda} + 1)/(\cot^2 \eta_{0\nu} + 1) \tag{14}$$

or

$$B_{\nu\lambda} = \sin \eta_{0\nu}/\sin \eta_{0\lambda}, \tag{15}$$

which is easily obtained through dividing both sides of Eq. (8) by r_λ^2 and taking into account Eqs. (9) and (10).

III. THE TWO-ANGLE-DEPENDENT RIOSA KINEMATICS

In all the earlier RIOSA theories γ_λ and $B_{\nu\lambda}$ were effectively chosen as basic parameters subject to initial selection. Those then defined the values of γ_ν, $\eta_{0\lambda}$, and $\eta_{0\nu}$, and thus the borderline $\Gamma_{\lambda\nu}$. While γ_λ assumed different fixed values from the range $[0, \pi]$, $B_{\nu\lambda}$ was kept constant. The drawbacks of such an approach were pointed out in Sec. I.

Here we shall single out for initial selection the angles γ_λ and γ_ν. "Equal rights" will be granted to each of the angles, and no correlation whatsoever between them will be assumed. This means that all the possible pairs of values of γ_λ and γ_ν are allowed and should be considered. The advantages of this approach are that (1) parameters (γ_λ and γ_ν) subjected to initial selection have clear physical meaning; (2) the reactants and the products channels are treated in a completely symmetrical fashion; and (3) since no *a priori* restriction on the choice of the pairs (γ_λ, γ_ν) is imposed, no particular value(s) of $B_{\nu\lambda}$ enter the theory as basic parameter(s) and the matching problem does not appear at all. As a convenient auxiliary quantity $B_{\nu\lambda}$ can be retained in the theory, but in each case its numerical value will be defined by the selected values of γ_λ and γ_ν. In what follows we show how γ_λ and γ_ν actually define the borderline $\Gamma_{\lambda\nu}$.

Once the values of the angles are fixed one calculates the borderline parameters $B_{\nu\lambda}$, $\eta_{0\lambda}$, and $\eta_{0\nu}$ from Eqs. (11)–(13) [(14)]. The solutions of Eqs. (11) and (12) with respect to $\cot \eta_{0\lambda}$ and $\cot \eta_{0\nu}$ are

$$\cot \eta_{0\lambda} = \frac{-\cos \gamma_\lambda \cos \beta_{\nu\lambda} \pm (B_{\nu\lambda}^2 - \sin^2 \gamma_\lambda \cos^2 \beta_{\nu\lambda})^{1/2}}{\sin \beta_{\nu\lambda}}, \tag{16}$$

$$\cot \eta_{0\nu} = \frac{\cos \gamma_\nu \cos \beta_{\nu\lambda} \pm (B_{\nu\lambda}^{-2} - \sin^2 \gamma_\nu \cos^2 \beta_{\nu\lambda})^{1/2}}{\sin \beta_{\nu\lambda}}. \tag{17}$$

An immediate consequence of Eqs. (16) and (17) is that the range of definition of $B_{\nu\lambda}$ for a fixed γ_λ is

$$\sin \gamma_\lambda |\cos \beta_{\nu\lambda}| < B_{\nu\lambda} < \infty, \tag{18}$$

while that for a fixed γ_ν is

$$0 < B_{\nu\lambda} < 1/\sin \gamma_\nu |\cos \beta_{\nu\lambda}|. \tag{19}$$

If both γ_λ and γ_ν are fixed then the value of $B_{\nu\lambda}$ is (uniquely, provided $\gamma_\lambda \neq 0, \pi$ and $\gamma_\nu \neq 0, \pi$—see below) defined and it satisfies the inequality

$$\sin \gamma_\lambda |\cos \beta_{\nu\lambda}| \leqslant B_{\nu\lambda} \leqslant 1/\sin \gamma_\nu |\cos \beta_{\nu\lambda}|. \tag{20}$$

[For $\gamma_\lambda = 0, \pi$ and $\gamma_\nu = 0, \pi$ the " $=$ " signs should be omitted in Eq. (20)]. In fact, more restrictive inequalities can be obtained for the value of $B_{\nu\lambda}$ defined by specific pairs of the frozen γ_λ and γ_ν. These inequalities follow from the requirement of positiveness of $\cot \eta_{0\lambda}$ and $\cot \eta_{0\nu}$ in Eqs. (16) and (17) [see definition (10)].

The fixed γ_λ and fixed γ_ν assume, in general, values from 0 to π. We analyze separately four cases.

(a) $\pi/2 \leqslant \gamma_\lambda \leqslant \pi$, $0 \leqslant \gamma_\nu \leqslant \pi/2$. Then the first terms in the numerators of Eqs. (16) and (17) are negative or zero and

thus only the " + " sign in front of the square roots together with the inequality

$$|\cos\beta_{\nu\lambda}| < B_{\nu\lambda} < 1/|\cos\beta_{\nu\lambda}| \tag{21}$$

can guarantee the positiveness of cot $\eta_{0\lambda}$ and cot $\eta_{0\nu}$. Note that only one pair of $\eta_{0\lambda}$ and $\eta_{0\nu}$ and, thus, only one borderline $\Gamma_{\lambda\nu}$, correspond to $B_{\nu\lambda}$ in this case.

(b) $0 \leqslant \gamma_\lambda < \pi/2$, $0 \leqslant \gamma_\nu \leqslant \pi/2$. Now the first term in the numerator of Eq. (16) is positive and thus both choices " + " and " − " in front of the square root can lead to physical cot $\eta_{0\lambda}$. Concerning Eq. (17) the situation is the same as in the previous case: only the positive value of the square root should be considered. The $B_{\nu\lambda}$, thus, satisfies in general the inequality

$$\sin\gamma_\lambda\,|\cos\beta_{\nu\lambda}| \leqslant B_{\nu\lambda} < 1/|\cos\beta_{\nu\lambda}|. \tag{22}$$

[If $\gamma_\lambda = 0$ the " = " sign should be omitted in Eq. (22).] If the actual value of $B_{\nu\lambda}$ implied by the fixed γ_λ and γ_ν is such that in addition the inequality (21) is valid for it or

$$B_{\nu\lambda} = |\cos\beta_{\nu\lambda}|, \tag{23}$$

then, as in case (a), only the positive value of the square root in Eq. (16) should be kept. If, however,

$$\sin\gamma_\lambda\,|\cos\beta_{\nu\lambda}| < B_{\nu\lambda} < |\cos\beta_{\nu\lambda}|, \tag{24}$$

then Eq. (16) gives two physical values of cot $\eta_{0\lambda}$, while only one such value of cot $\eta_{0\nu}$ is defined by Eq. (17). The physical implication of this can easily be understood by taking into account that each of Eqs. (16) and (17) depends only on one of the angles γ_λ or γ_ν and on the same $B_{\nu\lambda}$. The conclusion to be drawn is the following: The same value of $B_{\nu\lambda}$, which satisfies the inequality (24), can be obtained by fixing two different pairs $(\gamma_\lambda, \gamma_{\nu 1})$ and $(\gamma_\lambda, \gamma_{\nu 2})$ with the same γ_λ and $\gamma_{\nu 1} \neq \gamma_{\nu 2}$ [note that not necessarily both $\gamma_{\nu 1}$ and $\gamma_{\nu 2}$ are from the range $[0, \pi/2]$—see case (d) below]. This situation is illustrated in Fig. 3: $\gamma_{\nu 1} \neq \gamma_{\nu 2}$ but $r'_{\nu 1} = r'_{\nu 2}$ and thus [see definition (9)] $(\gamma_\lambda, \gamma_{\nu 1})$ and $(\gamma_\lambda, \gamma_{\nu 2})$ define the same $B_{\nu\lambda}$. Though the value of $B_{\nu\lambda}$ is the same the corresponding borderlines $\Gamma_{\lambda\nu 1}(\gamma_\lambda, \gamma_{\nu 1})$ and $\Gamma_{\lambda\nu 2}(\gamma_\lambda, \gamma_{\nu 2})$ are different. They are defined by different pairs $(\eta_{0\lambda 1}, \eta_{0\nu 1})$ and $(\eta_{0\lambda 2}, \eta_{0\nu 2})$. The fact that $B_{\nu\lambda}$ defines (for a fixed γ_λ) the borderline not always uniquely is an additional argument against the matching constant as a basic parameter. If $B_{\nu\lambda} = \sin\gamma_\lambda\,|\cos\beta_{\nu\lambda}|$ for $\gamma_\lambda \neq 0$ then the two physical values of cot $\eta_{0\lambda}$ coalesce to one, giving a single borderline corresponding to $B_{\nu\lambda}$.

(c) $\pi/2 \leqslant \gamma_\lambda \leqslant \pi$, $\pi/2 < \gamma_\nu \leqslant \pi$. In this case the first term in the numerator of Eq. (16) is negative or zero while that in Eq. (17) is positive. The general inequality for $B_{\nu\lambda}$ is

$$|\cos\beta_{\nu\lambda}| < B_{\nu\lambda} \leqslant 1/\sin\gamma_\nu\,|\cos\beta_{\nu\lambda}|. \tag{25}$$

[If $\gamma_\nu = \pi$ the " = " sign should be omitted in Eq. (25).] If the value of $B_{\nu\lambda}$ satisfies actually the more restrictive inequality (21) or

$$B_{\nu\lambda} = 1/|\cos\beta_{\nu\lambda}|, \tag{26}$$

then only the " + " sign in front of the square roots in Eqs. (16) and (17) will lead to physical cot $\eta_{0\lambda}$ and cot $\eta_{0\nu}$. If, however,

$$1/|\cos\beta_{\nu\lambda}| < B_{\nu\lambda} < 1/\sin\gamma_\nu\,|\cos\beta_{\nu\lambda}|, \tag{27}$$

both the " + " and the " − " signs in Eq. (17), but still only the " + " sign in Eq. (16), are acceptable. Then again two different borderlines correspond to the same $B_{\nu\lambda}$ for which condition (27) is valid. This $B_{\nu\lambda}$ can be defined by two different pairs of frozen angles $(\gamma_{\lambda 1}, \gamma_\nu)$ and $(\gamma_{\lambda 2}, \gamma_\nu)$ with the same γ_ν and $\gamma_{\lambda 1} \neq \gamma_{\lambda 2}$ (not necessarily both $\gamma_{\lambda 1}$ and $\gamma_{\lambda 2}$ are from the range $[\pi/2, \pi]$—see the next case (d)). And again if $B_{\nu\lambda} = (\sin\gamma_\nu\,|\cos\beta_{\nu\lambda}|)^{-1}$ for $\gamma_\nu \neq \pi$ the two physical values of cot $\eta_{0\nu}$ coalesce, giving rise to only one borderline.

(d) $0 \leqslant \gamma_\lambda < \pi/2$, $\pi/2 < \gamma_\nu \leqslant \pi$. Then the first terms in the numerators of Eqs. (16) and (17) are positive and $B_{\nu\lambda}$ satisifes in general the inequality (20) with the " = " signs omitted for $\gamma_\lambda = 0$ and $\gamma_\nu = \pi$. All the three distinct possibilities encountered in cases (a)–(c) for the signs in front of the square roots in Eqs. (16) and (17) can be realized here depending on which of the three conditions [(21) + (23) + (26)], (24), or (27) is actually satisfied by $B_{\nu\lambda}$.

In order to obtain an equation for $B_{\nu\lambda}$ for selected values of γ_λ and γ_ν, substitute expressions (16) and (17) into Eq. (13). In accordance with the three possibilities mentioned above we arrive at three equations rather than at one:

$$\begin{aligned} &F_1(B_{\nu\lambda}; \gamma_\lambda, \gamma_\nu) \\ &\quad \equiv G(B_{\nu\lambda}; \gamma_\lambda)\cos\gamma_\lambda + B_{\nu\lambda} H(B_{\nu\lambda}; \gamma_\nu)\cos\gamma_\nu \\ &\qquad + (\sin^2\gamma_\lambda - B^2_{\nu\lambda}\sin^2\gamma_\nu)\cos\beta_{\nu\lambda} = 0, \end{aligned} \tag{28}$$

$$\begin{aligned} &F_2(B_{\nu\lambda}; \gamma_\lambda, \gamma_\nu) \\ &\quad \equiv -G(B_{\nu\lambda}; \gamma_\lambda)\cos\gamma_\lambda + B_{\nu\lambda} H(B_{\nu\lambda}; \gamma_\nu)\cos\gamma_\nu \\ &\qquad + (\sin^2\gamma_\lambda - B^2_{\nu\lambda}\sin^2\gamma_\nu)\cos\beta_{\nu\lambda} = 0, \end{aligned} \tag{29}$$

$$\begin{aligned} &F_3(B_{\nu\lambda}; \gamma_\lambda, \gamma_\nu) \\ &\quad \equiv G(B_{\nu\lambda}; \gamma_\lambda)\cos\gamma_\lambda - B_{\nu\lambda} H(B_{\nu\lambda}; \gamma_\nu)\cos\gamma_\nu \\ &\qquad + (\sin^2\gamma_\lambda - B^2_{\nu\lambda}\sin^2\gamma_\nu)\cos\beta_{\nu\lambda} = 0, \end{aligned} \tag{30}$$

where

$$G(B_{\nu\lambda}; \gamma_\lambda) \equiv (B^2_{\nu\lambda} - \cos^2\beta_{\nu\lambda}\sin^2\gamma_\lambda)^{1/2} \tag{31}$$

and

$$H(B_{\nu\lambda}; \gamma_\nu) \equiv (1 - B^2_{\nu\lambda}\cos^2\beta_{\nu\lambda}\sin^2\gamma_\nu)^{1/2}. \tag{32}$$

One or more of Eqs. (28)–(30) correspond to each of the cases (a)–(d). From geometrical considerations it follows that one and only one $B_{\nu\lambda}$ value is defined by any pair of selected $\gamma_\lambda \neq 0, \pi$ and $\gamma_\nu \neq 0, \pi$. In the cases characterized by more than one equation for $B_{\nu\lambda}$ these equations should be solved successively until the physically meaningful value for $B_{\nu\lambda}$ is obtained. As criteria for selecting the physical value of $B_{\nu\lambda}$ the inequalities presented above should be used. Thus, in

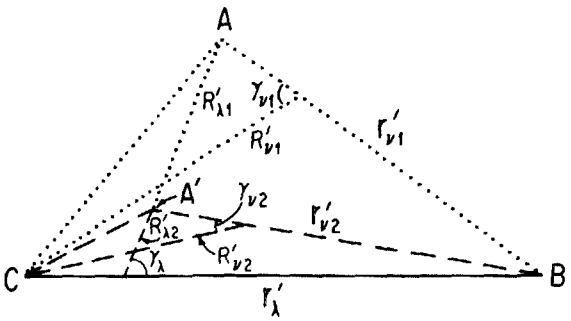

FIG. 3. Illustration of a situation when two different $\lambda \leftrightarrow \nu$ transition configurations (ABC and $A'BC$) of three atoms, defined by the same γ_λ and $\gamma_{\nu 1} \neq \gamma_{\nu 2}$, correspond to the same value of $B_{\nu\lambda}$ ($r'_{\nu 1} = r'_{\nu 2}$).

case (a) only Eq. (28) should be solved. Its physical solution will satisfy the inequality (21). Two equations for $B_{\nu\lambda}$ correspond to case (b): Equation (28) with the inequality criterion (22) and Eq. (29) with the criterion (24). If the selected γ_λ and γ_ν belong to case (c) again two equations should, in principle, be considered: Equation (28) with the inequality (25) and Eq. (30) with the condition (27). In case (d) one of the three equations (28)–(30) with the criteria (20), (24), and (27), respectively, will furnish the physical value of $B_{\nu\lambda}$. The four cases (a)–(d) for the fixed γ_λ and γ_ν and the "regions of validity" of Eqs. (28)–(30) are shown in Fig. 4.

Once $B_{\nu\lambda}$ is found [e.g., by numerically solving Eqs. (28)–(30)] the values of η_λ and η_ν are calculated from Eqs. (16) and (17), respectively. The signs that should be used in front of the square roots will be prescribed by that one of Eqs. (28)–(30), which actually provides the physical value of $B_{\nu\lambda}$. Equation (28) implies that the positive value of the square roots should be used in both Eqs. (16) and (17). Equation (29) dictates the " + " sign in Eq. (16) and the " − " sign in Eq. (17). Finally, the " − " sign in Eq. (16) and the " + " sign in Eq. (17) should be used if the physical value of $B_{\nu\lambda}$ is the solution of Eq. (30).

Note that $B_{\nu\lambda}$, $\eta_{0\lambda}$, and $\eta_{0\nu}$, found in accordance with the prescription given above, will depend on $\beta_{\nu\lambda}$, which is defined by the masses of the interacting atoms [Eq. (5)]. This reflects the fact that the borderlines are parametrically system dependent.

Analysis of Eqs. (28)–(30) together with the corresponding inequality criteria leads to a number of interesting conclusions. Consider first Eq. (28). Let $\gamma_\lambda = 0$ and $\gamma_\nu = \pi$ (one of the "RIOSA collinear" cases). Then taking into account expressions (31) and (32) we immediately arrive at the equation

$$F_1(B_{\nu\lambda}; \gamma_\lambda = 0, \gamma_\nu = \pi) = B_{\nu\lambda} - B_{\nu\lambda} = 0, \tag{33}$$

which together with the inequality (20) implies that any finite positive $B_{\nu\lambda}$ is a physical solution. The case $\gamma_\lambda = \pi$, $\gamma_\nu = 0$ leads to the same Eq. (33). But the range of all physical $B_{\nu\lambda}$'s is defined now by the inequality (21). The existence of whole (continuous) manifolds of acceptable $B_{\nu\lambda}$'s and thus of different collinear configurations, each of which can serve as a transition configuration, is reminiscent of the situation in the true collinear collisions ($l_\alpha = 0, j_\alpha = 0$; $\alpha = \lambda, \nu$), for which any finite positive value of $B_{\nu\lambda}$ can be chosen since the final results, e.g., transition probabilities and vibrational distribution, are independent of this value.

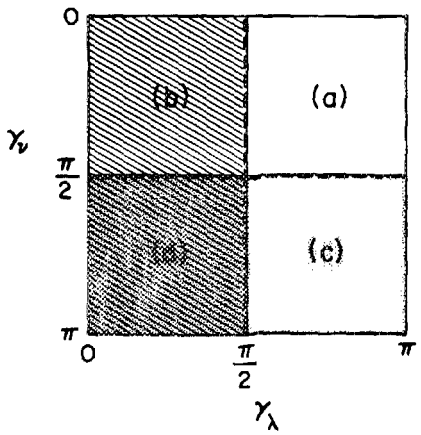

FIG. 4. The four cases (a)–(d) for the fixed γ_λ and γ_ν. Equation (28) corresponds to the entire large square. The overlapping "regions of validity" of Eqs. (29) and (30) are depicted by oblique lines and dots, respectively.

Choose now $\gamma_\lambda = 0$ or π and $\gamma_\nu \neq 0$ or π. It is easy to verify that Eq. (28) does not have physically acceptable solutions for these cases at all. The conclusion to be extracted is that three atoms initially in a collinear configuration conserve their collinear alignment for the whole duration of the reactive scattering event, if γ_λ and γ_ν are kept fixed. Selecting $\gamma_\nu = 0$ or π and $\gamma_\lambda \neq 0$ or π, we again obtain that Eq. (28) has only nonphysical solutions. Thus a reactive collision initiated in a noncollinear arrangement of the reactants cannot end up with collinear alignment of the products, if γ_λ and γ_ν are frozen. The two last conclusions can be referred to as the "collinearity conservation rule." This rule was, of course, known for true collinear collisions, for which, in the case of absence of force fields, it is a trivial consequence of the conservation of the total linear momentum of the system. In contrast to the true collinear case the RIOSA version of the collinearity conservation rule is derived here on the basis of pure kinematical arguments only.

It can readily be verified that if $B_{\nu\lambda}$ is a solution of the equation

$$F_1(B_{\nu\lambda}; \gamma_\lambda, \gamma_\nu) = 0, \tag{34}$$

where $\gamma_\lambda \neq 0, \pi$, $\gamma_\nu \neq 0, \pi$, and F_1 is defined by (28), then $B_{\nu\lambda}^{-1}$ satisfies the equation

$$F_1(B_{\nu\lambda}^{-1}; \pi - \gamma_\nu, \pi - \gamma_\lambda) = 0. \tag{35}$$

Note that if $B_{\nu\lambda}$ is the physical solution of Eq. (34), i.e., it satisfies the proper inequality criterion, then the inequality related to Eq. (35) will automatically be valid for $B_{\nu\lambda}^{-1}$ and thus $B_{\nu\lambda}^{-1}$ is the physical solution of Eq. (35). Choosing $\gamma_\nu = \pi - \gamma_\lambda$ we conclude that both $B_{\nu\lambda}$ and $B_{\nu\lambda}^{-1}$ satisfy the same equation

$$F_1(X; \gamma_\lambda, \pi - \gamma_\lambda) = 0, \quad X = B_{\nu\lambda}, B_{\nu\lambda}^{-1}. \tag{36}$$

But Eq. (36) has only one physical solution. This can be if and only if $B_{\nu\lambda} = 1$.

While considering the RIOSA collinear cases we omitted the analysis of two possibilities: $\gamma_\lambda = 0, \gamma_\nu = 0$ and $\gamma_\lambda = \pi, \gamma_\nu = \pi$. Equation (28) does not provide physical values of $B_{\nu\lambda}$ for these possibilities. But their "legality" (from a kinematical point of view) is guaranteed by Eqs. (29) and (30). It follows immediately from Eq. (29) and the corresponding criterion (24) that any $B_{\nu\lambda}$ satisfying the inequality

$$0 < B_{\nu\lambda} < |\cos\beta_{\nu\lambda}| \tag{37}$$

is a physical solution for $\gamma_\lambda = 0$ and $\gamma_\nu = 0$. Analogously, Eq. (30) together with the condition (27) gives that all $B_{\nu\lambda}$'s from the range

$$1/|\cos\beta_{\nu\lambda}| < B_{\nu\lambda} < \infty \tag{38}$$

are acceptable for $\gamma_\lambda = \pi$ and $\gamma_\nu = \pi$. Both Eqs. (29) and (30) obey the collinearity conservation rule, i.e., they do not have physical solutions when $\gamma_\lambda = 0, \pi$ but $\gamma_\nu \neq 0, \pi$ or $\gamma_\nu = 0, \pi$ but $\gamma_\lambda \neq 0, \pi$. It is easy to verify that if $B_{\nu\lambda}$ is the physical solution of the equation

$$F_2(B_{\nu\lambda}; \gamma_\lambda, \gamma_\nu) = 0, \tag{39}$$

where F_2 is defined by Eq. (29), then $B_{\nu\lambda}^{-1}$ is the physical solution of the equation

$$F_3(B_{\nu\lambda}^{-1}, \pi - \gamma_\nu, \pi - \gamma_\lambda) = 0, \tag{40}$$

with F_3 defined by Eq. (30).

The kinematical relations obtained above are those to be employed in actual numerical calculations. These calculations should, in principle, take into account all the possible pairs of values of γ_λ and γ_ν which do not violate the collinearity conservation rule.

Calculate now the angle between the R_λ and R_ν axes in Fig. 2. Note that the fixed $\gamma_\lambda = 0$ and fixed $\gamma_\nu = \pi$ planes, corresponding to collinear collision, merge to one plane containing both the R_λ and R_ν axes. The so-called "skewed" angle between the two axes in this plane is equal to the sum $\eta_{0\lambda} + \eta_{0\nu}$ for any borderline $\Gamma_{\lambda\nu}$, i.e., any finite positive $B_{\nu\lambda}$. Choosing $B_{\nu\lambda} = 1$ and substituting it together with $\gamma_\lambda = 0$ into Eq. (16), in which the positive value of the square root should be used, we obtain

$$\cot \eta_{0\lambda} = (1 - \cos \beta_{\nu\lambda})/\sin \beta_{\nu\lambda} = \tan(\beta_{\nu\lambda}/2), \tag{41}$$

or

$$\eta_{0\lambda} = \pi/2 - \beta_{\nu\lambda}/2. \tag{42}$$

Since $\eta_{0\nu} = \eta_{0\lambda}$ for $B_{\nu\lambda} = 1$ [see Eq. (14)] we conclude that the angle between the R_λ and R_ν axes is $\pi - \beta_{\nu\lambda}$.

Finally, we present alternative, more convenient forms of two expressions obtained earlier in the framework of a fixed-$B_{\nu\lambda}$ RIOSA formalism.[13] Calculate first the value of the angle $\Delta_{\lambda\nu}$ between the $\mathbf{R}_\lambda$ and $\mathbf{R}_\nu$ vectors (see Fig. 1) in the transition configuration. By definition

$$\cos \Delta_{\lambda\nu} = (\mathbf{R}_\lambda \cdot \mathbf{R}_\nu)/R_\lambda R_\nu. \tag{43}$$

Expressing $\mathbf{R}_\nu$ in (43) through $\mathbf{R}_\lambda$ and $\mathbf{r}_\lambda$ [Eqs. (3) and (4)] we obtain

$$\cos \Delta_{\lambda\nu} = (R_\lambda/R_\nu) \cos \beta_{\nu\lambda} - (r_\lambda/R_\nu) \cos \gamma_\lambda \sin \beta_{\nu\lambda}. \tag{44}$$

Equation (44) defines $\Delta_{\lambda\nu}$ in any configuration of the three atoms. The transition configuration expression for $\cos \Delta_{\lambda\nu}$ follows from (44) by application of Eqs. (9) and (10), which yields

$$\cos \Delta_{\lambda\nu}|_{\Gamma_{\lambda\nu}} = (1/B_{\nu\lambda} \cot\eta_{0\nu})(\cot \eta_{0\lambda} \cos \beta_{\nu\lambda} - \cos \gamma_\lambda \sin \beta_{\nu\lambda}). \tag{45}$$

Show now how to obtain the value of the angle γ_ν for given values of $\gamma_\lambda (\neq 0, \pi)$ and $B_{\nu\lambda}$. Stress once more that only a $B_{\nu\lambda}$ which satisfies one of the conditions

$$|\cos \beta_{\nu\lambda}| \leq B_{\nu\lambda} < \infty \tag{46}$$

or

$$B_{\nu\lambda} = \sin \gamma_\lambda |\cos \beta_{\nu\lambda}|, \tag{46'}$$

if $0 < \gamma_\lambda < \pi/2$, or the condition (46) with the " = " sign omitted if $\pi/2 \leq \gamma_\lambda < \pi$, leads to a unique definition of the value of γ_ν. If such a $B_{\nu\lambda}$ is chosen one calculates $\cot \eta_{0\lambda}$ from Eq. (16) with the " + " sign in front of the square root and then $\cot \eta_{0\nu}$ from Eq. (14). Once $\cot \eta_{0\lambda}$ and $\cot \eta_{0\nu}$ are known the value of $\cos \gamma_\nu$ can be obtained from Eq. (13):

$$\cos \gamma_\nu = \frac{(B_{\nu\lambda}^2 - 1) \cot \beta_{\nu\lambda} - \cos \gamma_\lambda \cot \eta_{0\lambda}}{B_{\nu\lambda}^2 \cot \eta_{0\nu}}. \tag{47}$$

IV. SUMMARY

In this communication we gave a detailed analysis of the so-called matching problem in the RIOSA theory, and have shown that the problem concerns the question about the correlation between the frozen angles or about the borderline between the RIOSA arrangement channel configuration spaces, rather than the matching itself. We removed this problem from the theory by considering the angle parameters γ_λ and γ_ν on equal basis and presuming no correlation whatsoever between them. Elimination of the angle-correlation requirement, which is an external, additional assumption and not a necessary, inherent condition of the RIOSA approach, considerably consolidates the physical foundations of this scheme.

Initial selection of the pairs of values $(\gamma_\lambda, \gamma_\nu)$ and inclusion into consideration of all the pairs which do not violate the collinearity conservation rule results in the change of the status of quantity $B_{\nu\lambda}$: from a basic fixed-value matching constant of earlier formulations it converts to an auxiliary borderline parameter with no preselected value(s) in the two-angle-dependent RIOSA approach. An additional advantage of the new scheme is in that it treats the reagents and products channels in complete symmetry.

The kinematical relations derived in Sec. III complement the classical and quantal dynamics parts of the two-angle-dependent RIOSA presented in Refs. 12, 17, and 16, respectively. The expressions for physical quantities calculated from the two-angle-dependent RIOSA transition probabilities[12,7] or S-(R-) matrix elements[16] involve double integrals over γ_λ and γ_ν. This means that, in general, the RIOSA quantities should be calculated on a double grid of $\gamma_\lambda, \gamma_\nu \in [0, \pi]$. In certain particular cases, however, the specificity of the system (masses of the particles, interaction potential, total energy) may justify considering instead of the complete double grid only the "important" part of it, i.e., only those pairs $(\gamma_\lambda, \gamma_\nu)$ which give non-negligible contributions. This may be taken into account via multiplication of the integrand by a weighting function $Q(\cos \gamma_\lambda, \cos \gamma_\nu)$ of the proper form. The only general requirement on this function is

$$\int_{-1}^{1} \int_{-1}^{1} Q(\cos \gamma_\lambda, \cos \gamma_\nu) d \cos \gamma_\lambda \, d \cos \gamma_\nu = 1. \tag{48}$$

In contrast to all earlier formulations of the RIOSA theory the new scheme furnishes approximate physical quantities which are independent of additional assumptions, such as, e.g., a fixed numerical value of $B_{\nu\lambda}$. As a consequence, these quantities should be viewed as the true RIOSA results and may be used to make ultimate inferences about the validity of the RIOSA approach for different reactive systems. Preliminary results of the application of the two-angle-dependent RIOSA theory to the $F + H_2 \rightarrow HF + H$ reaction are presented in Ref. 7. Further work on numerical implementation of the new scheme is under way, and the results will be reported in future publications.

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Vector fields near caustics

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The modified Lagrange manifold technique enables determination of the asymptotic series solution of linear scalar wave equations near caustics of simple geometries. Here the technique is extended to include vector field considerations and more complicated caustic geometries.

I. INTRODUCTION

A commonly used approach for studying high-frequency wave propagation in spatially inhomogeneous media is the geometrical optics or asymptotic series technique introduced by Friedlander[1] and extended by Keller and his coworkers (cf. Felsen and Marcuvitz[2] for a comprehensive treatment and bibliography). For illustration, we consider the time harmonic electric field equation from Felsen and Marcuvitz in R^3

$$\nabla^2\mathscr{E}(\mathbf{r}) + \tau^2 f(\mathbf{r})\mathscr{E}(\mathbf{r}) + 2\nabla(\mathscr{E}(\mathbf{r})\cdot\nabla g(\mathbf{r})) = 0. \tag{1}$$

In Eq. (1), $\mathscr{E}(\mathbf{r})$ is the field, τ is the frequency, $f(\mathbf{r})$ is the index of refraction, and $g(\mathbf{r}) = \ln[f(\mathbf{r})]^{1/2}$. An asymptotic series solution of the form

$$\mathscr{E}(\mathbf{r}) \sim \exp\{i\tau\phi(\mathbf{r})\}\sum_{k=0}^{\infty}\mathbf{E}_k(\mathbf{r})\tau^{-k} \tag{2}$$

is assumed. In Eq. (2), $\phi(\mathbf{r})$ may be considered a phase and $\mathbf{E}_k(\mathbf{r})$ amplitudes. Substituting Eq. (2) into Eq. (1) and regrouping by powers of τ leads to the eikonal equation for the phase and the transport equation for the amplitudes, Eqs. (3) and (4), respectively,

$$\nabla\phi\cdot\nabla\phi - f(\mathbf{r}) = 0, \tag{3}$$

$$\mathbf{E}_k\nabla^2\phi + 2\nabla\phi(\mathbf{E}_k\cdot\nabla g(\mathbf{r})) + 2\nabla\phi(\nabla\cdot\mathbf{E}_k) + 2\nabla(\mathbf{E}_{k-1}\cdot\nabla g(\mathbf{r})) + \nabla^2\mathbf{E}_{k-1} = 0, \quad k\geqslant 0, \quad \mathbf{E}_{-1} = 0. \tag{4}$$

The phase may be determined using the classical method of characteristics; the $\mathbf{E}_k$ follow from Eq. (4). At caustic (turning) points, this procedure leads to unbounded field amplitudes.[3]

An alternate approach, leading to bounded field amplitudes at caustic points, is the Lagrange manifold formalism introduced by Maslov[4] and developed by Arnold,[5] among others. In this approach, the electric (vector) field is represented by a generalized Fourier integral of the form

$$\mathscr{E} = \int \mathbf{E}(\mathbf{r},\mathbf{p},\tau)\exp\{i\tau\phi(\mathbf{r},\mathbf{p})\}d\mathbf{p},$$

where

$$\mathbf{E}(\mathbf{r},\mathbf{p},\tau)\sim\sum_{k=0}^{\infty}\mathbf{E}_k(\mathbf{r},\mathbf{p})\tau^{-k}$$

and

$$\phi(\mathbf{r},\mathbf{p}) = \mathbf{r}\cdot\mathbf{p} - S(\mathbf{p}).$$

In the above, $\mathbf{p}$ may be regarded as a wave vector and $S(\mathbf{p})$ is analytic and the generating function of a canonical transformation. This technique has been applied to study caustics associated with acoustic (scalar) fields in stratified media in R^2 ($f(x,y) = f(x)$) (Ref. 6). Substituting a scalar integral analogous to that above into the reduced Helmholtz equation obtains an eikonal equation similar to Eq. (3). The corresponding transport equation for the amplitudes determines the field on the caustic in terms of oscillatory integrals. On the caustic the Hessian determinant of the eikonal phase, i.e., (in R^2) $\det(\partial^2\phi/\partial p_i\,\partial p_j)$, vanishes. After the phase is transformed to a canonical form, the transformed integrals may be evaluated asymptotically using a modified stationary phase technique. The appropriate canonical form corresponding to a given eikonal phase is determined from the Hessian matrix of $\phi(\mathbf{r})$. Caustics whose geometry corresponds to the Hessian matrix having one zero-eigenvalue have been considered for the acoustic field. In this note, we illustrate how the algorithm extends to those caustic geometries corresponding to the Hessian matrix having two zero-eigenvalues using the context of electric field propagation—to parallel some off-caustic considerations included in Felsen and Marcuvitz. For brevity and coherence of exposition, some involved calculational details (and considerations regarding structural stability) have been left to more extensive references.[6–8] To facilitate comparison with these references, we consider axial propagation, $f(x,y,z) = f(x,y)$. Although the extension to R^3 is primarily algebraic, the principal considerations involved in this extension are also discussed.

II. FORMALISM

We assume Eq. (1) has an asymptotic solution of the form

$$\mathscr{E}(\mathbf{r}) - \int\mathbf{E}(\mathbf{r},\mathbf{p},\tau)\exp\{i\tau(\mathbf{r}\cdot\mathbf{p} - S(\mathbf{p}))\}d\mathbf{p} = O(\tau^{-\infty}), \tag{5}$$

where here $\mathbf{r} = (x,y)$, $\mathbf{p} = (p_x,p_y)$. The algorithm proceeds by carrying the differentiation in Eq. (1) across the integral in Eq. (5), followed by a regrouping by powers of $i\tau$ to obtain

$$\int d\mathbf{p}\exp\{i\tau\phi\}\{(i\tau)^2[\mathbf{p}\cdot\mathbf{p} - f(\mathbf{r})]\mathbf{E} + (i\tau)[2\mathbf{p}(\nabla\cdot\mathbf{E} + \mathbf{E}\cdot\nabla\ln g(\mathbf{r}))] + (i\tau)^0[\nabla^2\mathbf{E} + 2\nabla(\mathbf{E}\cdot\nabla\ln g(\mathbf{r}))]\} = O(\tau^{-\infty}). \tag{6}$$

The coefficient of the $(i\tau)^2$ term is Maslov's Hamiltonian. Then by invoking the stationary phase condition ($\nabla_p\phi = 0$), Maslov's Hamiltonian becomes an eikonal equation on the Lagrange manifold [$\mathbf{r} = \nabla_p S(\mathbf{p})$]

$$\mathbf{p}\cdot\mathbf{p} - f(\mathbf{r}) = 0, \tag{7}$$

which may be used to find the phase.[3] For example, analogous to the classical case, using Hamilton's equations

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$$\dot{x} = 2p_x, \quad \dot{p}_x = -\frac{\partial H}{\partial x}, \quad \dot{y} = 2p_y, \quad \dot{p}_y = -\frac{\partial H}{\partial y}, \tag{8}$$

leads to

$$x = x(t,\theta), \quad p_x = p_x(t,\theta),$$
$$y = y(t,\theta), \quad p_y = p_y(t,\theta), \tag{9}$$

where t is the time and θ a parametrized initial condition. But on the caustic the map $(t,\theta) \to (x,y)$ is singular. Consequently, we may determine the phase by inverting the wave vector (**p**) map, yielding

$$t = t(p_x,p_y), \quad \theta = \theta(p_x,p_y).$$

Then a direct substitution in the configuration space equations explicitly determines the Lagrange manifold

$$x = x[t(p_x,p_y),\theta(p_x,p_y)] = X(p_x,p_y) = \frac{\partial S}{\partial p_x},$$
$$y = y[t(p_x,p_y),\theta(p_x,p_y)] = Y(p_x,p_y) = \frac{\partial S}{\partial p_y}. \tag{10}$$

An integration leads to the phase

$$\theta(x,y,p_x,p_y) = xp_x + yp_y - S(p_x,p_y). \tag{11}$$

If $f(x,y)$ is cyclic in either variable, e.g., $f(x,y) = f(x)$, a simpler procedure applies for $f(x)$ analytic. In this case the eikonal equation becomes

$$\mathbf{p}\cdot\mathbf{p} - f(x) = 0,$$

leading to the Lagrange manifold

$$x = f^{-1}(p_x^2 + p_y^2) = \frac{\partial S}{\partial p_x},$$
$$y = \int \frac{\partial^2 S}{\partial p_x\,\partial p_y}\,dp_x = \frac{\partial S}{\partial p_y} + \theta(p_y) = \frac{\partial S}{\partial p_y}, \tag{12}$$

where $\theta(p_y)$ can be made explicit from the initial conditions.[6]

In either case, the equation of the caustic can be determined by setting

$$\det\left\{\frac{\partial^2 \phi}{\partial p_x\,\partial p_y}\right\} = 0. \tag{13}$$

Each (p_x,p_y) satisfying Eq. (13) corresponds to a point on the caustic in configuration space obtained by substituting into the appropriate Lagrange manifold. The locus of these points specifies the caustic in configuration space.

To obtain the transport equation for the amplitudes, we may proceed as with acoustic propagation. Briefly, the Hamiltonian is Taylor expanded near the Lagrange manifold, resulting in

$$\begin{aligned}\mathbf{p}\cdot\mathbf{p} - f(\mathbf{r}) &= \mathbf{p}\cdot\mathbf{p} - f(\nabla_p S(\mathbf{p})) + (\mathbf{r} - \nabla_p S(\mathbf{p}))\cdot\mathbf{D}(\mathbf{r},\mathbf{p}) \\ &= (\mathbf{r} - \nabla_p S(\mathbf{p}))\cdot\mathbf{D}(\mathbf{r},\mathbf{p}),\end{aligned} \tag{14}$$

where

$$\mathbf{D}(\mathbf{r},\mathbf{p}) = \mathbf{D} = -\int_0^1 \nabla_r f[t(\mathbf{r} - \nabla_p S(\mathbf{p})) + \nabla_p S(\mathbf{p})]\,dt.$$

Substituting into Eq. (5) leads to

$$\begin{aligned}\int d\mathbf{p}\,\exp\{i\tau(\mathbf{r}\cdot\mathbf{p} - S(\mathbf{p}))\}\{ &- [(\nabla_p\cdot\mathbf{D})\mathbf{E} + \mathbf{D}\nabla_p\cdot\mathbf{E}] \\ &+ 2\mathbf{p}[\nabla\cdot\mathbf{E} + \mathbf{E}\cdot\nabla\ln g(\mathbf{r})] \\ &+ (1/i\tau)[\nabla^2\mathbf{E} + 2\nabla(\mathbf{E}\cdot\nabla\ln g(\mathbf{r}))]\} = O(\tau^{-\infty}).\end{aligned}$$

Then, requiring

$$\begin{aligned}&- [(\nabla_p\cdot\mathbf{D})\mathbf{E} + \mathbf{D}\nabla_p\cdot\mathbf{E}] + 2\mathbf{p}[\nabla\cdot\mathbf{E} + \mathbf{E}\cdot\nabla\ln g(\mathbf{r})] \\ &\quad + (1/i\tau)[\nabla^2\mathbf{E} + 2\nabla((\mathbf{E}\cdot\nabla\ln g(\mathbf{r}))] = 0\end{aligned} \tag{15}$$

in a neighborhood of the Lagrange manifold leads to a transport equation if we introduce the flow

$$\dot{\mathbf{r}} = 2\mathbf{p}, \quad \dot{\mathbf{p}} = -\mathbf{D}(\mathbf{r},\mathbf{p}), \tag{16}$$

where the dots indicate time differentiation. That is, Eq. (15) holds—and consequently Eq. (5) is an asymptotic solution—if we allow the asymptotic series

$$\mathbf{E} = \sum_{k=0} \mathbf{E}_k(\mathbf{r},\mathbf{p})\tau^{-k}$$

to evolve along the transport equation

$$\begin{aligned}\dot{\mathbf{E}}_k &+ [2\mathbf{p}\cdot(\nabla\ln g(\mathbf{r})) - \nabla_p\cdot\mathbf{D}\hat{\mathbf{I}}]\mathbf{E}_k + \nabla_r^2\,\mathbf{E}_{k-1} \\ &+ 2\nabla(\mathbf{E}_{k-1}\cdot\nabla\ln g(\mathbf{r})) = 0,\end{aligned} \tag{17}$$

where $\hat{\mathbf{I}}$ is the unit dyadic. Corresponding equations for $\mathscr{H}$, the magnetic field, follow either from duality or Maxwell's equations.

As with the field away from the caustic, the first approximation to the time-averaged Poynting vector (power density) $\mathscr{S}$ on the caustic (or, equivalently, the magnitude of the field vector E_0^2)

$$\mathscr{S} = \mathrm{Re}(\mathscr{E}\times\mathscr{H}^*) \sim \sqrt{\epsilon_0/\mu_0}E_0^2\,\mathbf{p},$$

where ϵ_0 and μ_0 are the permittivity and permeability, respectively, of vacuum, proceeds from the $k = 0$ term of Eq. (15), i.e.,

$$\begin{aligned}&- (\nabla_p\cdot\mathbf{D})\mathbf{E}_0 - \mathbf{D}\nabla_p\cdot\mathbf{E}_0 + 2\mathbf{p}(\mathbf{E}\cdot\nabla\ln g(\mathbf{r})) + 2\mathbf{p}(\nabla\cdot\mathbf{E}_0) \\ &\quad = 0.\end{aligned} \tag{18}$$

Multiplying Eq. (18) scalarly by $\mathbf{E}_0^*$ and the complex conjugate of Eq. (18) by $\mathbf{E}_0$, adding and introducing the flow in Eq. (16), leads to

$$\frac{dE_0^2}{dt^2} - 2E_0^2\,(\nabla_p\cdot\mathbf{D}) = 0 \tag{19}$$

and thus

$$E_0^2(t) = E_0^2(0)\exp\left\{-2\int(\nabla_p\cdot\mathbf{D})dt\right\}, \tag{20}$$

where here t assumes its more standard role as a position parameter [via Eq. (9)] on the caustic (analogous to arclength along a ray in the classical technique). A similar consideration leads to a transport equation for the polarization

$$\mathscr{P} = \mathbf{E}_0/(\mathbf{E}_0\cdot E_0^*)^{1/2}.$$

Substituting for $\nabla_p\cdot\mathbf{D}$ from Eq. (19) in Eq. (18) and regrouping obtains

$$\frac{d\mathscr{P}}{dt} + 2\mathbf{p}[\mathscr{P}\cdot\nabla\ln g(\mathbf{r})] = 0, \tag{21}$$

analogous to the off-caustic transport equation. Finally, we note that propagation in a conductor adds a (dissipative) term proportional to $\partial\mathscr{E}/\partial t$ in Eq. (1). As would be expected,

this term affects the transport equation for the field amplitudes [Eq. (17)], but the basic algorithm proceeds as above.

III. COMPUTATIONAL CONSIDERATIONS

The asymptotic evaluation of the field integrals

$$\int \mathbf{E}_k(\mathbf{r},\mathbf{p})\exp\{i\tau\phi(\mathbf{r},\mathbf{p})\}d\mathbf{p},$$

where $\phi(\mathbf{r},\mathbf{p})$ and $\mathbf{E}_k(\mathbf{r},\mathbf{p})$ follow from Eqs. (11) and (17), at any field point [for definiteness taken at $(\mathbf{r}_0,\mathbf{p}_0)$] proceeds by transforming the phase to its canonical form. If the Hessian determinant of $\phi(\mathbf{r},\mathbf{p})$ at $\mathbf{r}_0$ is nonzero or the Hessian matrix has one zero-eigenvalue, the canonical form for the phase is

$$\tilde{\phi}(\mathbf{r}_0,\beta) = \phi(\mathbf{r}_0,\mathbf{p}_0) \pm \beta_1^2 \pm \beta_2^n.$$

If the Hessian determinant is nonzero, $\mathbf{r}_0$ is not on the caustic and $n = 2$. If the Hessian determinant vanishes, the exponent "n" may be obtained by forming

$$F(t) = \phi(\mathbf{r}_0, p_{x0} + te_1, p_{y0} + te_2),$$

where e_1 and e_2 are the components of the zero-eigenvalue eigenvector. The first nonvanishing term in the Taylor series determines the value of n. The sign of β_2 corresponds to the sign of this Taylor coefficient and the sign of β_1 to the sign of the nonzero eigenvalue. If $n = 2$, 3, or 4, the coordinate transformations carrying the eikonal phase to the canonical form may be determined algebraically. If $n \geqslant 5$, an application of the implicit function theorem is required.[6] The resulting integral is

$$\int \mathbf{E}(\mathbf{r}_0,\mathbf{p},\tau)\exp\{i\tau\phi(\mathbf{r},\mathbf{p})\}d\mathbf{p}$$
$$= \exp\{i\tau\phi(\mathbf{r}_0,\mathbf{p}_0)\}\int\int \mathsf{E}(\mathbf{r}_0,\beta_1,\beta_2,\tau)$$
$$\times\exp\{i\tau(\pm\beta_1^2 \pm \beta_2^n)\}d\beta_1\, d\beta_2, \tag{22}$$

where

$$\mathsf{E}(\mathbf{r}_0,\beta_1,\beta_2,\tau) = \mathbf{E}(\mathbf{r}_0,p_x(\beta_1,\beta_2),p_y(\beta_1,\beta_2),\tau)\left(\frac{\partial(p_x,p_y)}{\partial(\beta_1,\beta_2)}\right).$$

If the Hessian matrix of $\phi(\mathbf{r},\mathbf{p})$ at $\mathbf{p}_0$ has two zero-eigenvalues and the cubic terms in the Taylor series are not all zero, the eikonal phase (and hence the integral) may still be put into a form suitable for asymptotic analysis.[9] To determine the form appropriate to a particular case, let the phase be represented as

$$\phi(\mathbf{r},\mathbf{p}) = \phi(\mathbf{r}_0,\mathbf{p}_0) + t_{30}p_x^3 + t_{21}p_x^2p_y + t_{12}p_xp_y^2 + t_{03}p_y^3 + \text{higher-order terms},$$

where the t_{ij} are constants. If $t_{30} \neq 0$, equating the cubic terms to zero and dividing by p_y^3 obtains

$$t_{30}u^3 + t_{21}u^2 + t_{12}u + t_{03} = 0,$$

where $u = p_x/p_y$. (If $t_{30} = 0$ and $t_{03} \neq 0$, interchanging p_x and p_y yields an analogous cubic). The cubic may have four possible root combinations, each corresponding to a specific canonical form:

(a) three real equal roots	β^3	fold,
(b) three real unequal roots	$\beta_1^3 - \beta_1\beta_2^2$	elliptic umbilic,
(c) three real roots, two equal	$\beta_1^2\beta^2 + \beta_2^4$	parabolic umbilic,
(d) one real root, one complex conjugate pair	$\beta_1^3 + \beta_1\beta_2^2$ (or $\beta_1^3 + \beta_2^3$)	hyperbolic umbilic.

If $t_{30} = t_{03} = 0$ and both $t_{21}, t_{12} \neq 0$ the corresponding form is the parabolic umbilic. If $t_{30} = t_{03} = 0$ and one of t_{21} or $t_{12} = 0$, there is no corresponding canonical form.

The case corresponding to three real equal roots represents a symmetry where the two-dimensional propagation may be modeled as one dimensional and is not considered here. To determine the coordinate transformations carrying the eikonal phase to either the elliptic or hyperbolic umbilic (for clarity, represented as $\xi_1^2\xi_2 + b\xi_2^3$, $b = \pm 1$), a linear transformation

$$\begin{bmatrix}\xi_1\\ \xi_2\end{bmatrix} = \begin{bmatrix}\alpha & \beta\\ \sigma & \delta\end{bmatrix}\begin{bmatrix}p_x\\ p_y\end{bmatrix}$$

is first introduced. Then $\xi_1^2\xi_2 + b\xi_2^3$ is compared with the cubic terms in $\phi(\mathbf{r},\mathbf{p})$, obtaining a system of equations which can be solved for $\alpha,\beta,\sigma,\delta$ and putting $\phi(\mathbf{r}_0,\mathbf{p})$ in the form

$$\tilde{\phi}(r_0,p) = \phi(r_0,p_0) + \xi_1^2\xi_2 + b\xi_2^3 + t_{40}\xi_1^4 + t_{31}\xi_1^3\xi_2 + t_{22}\xi_1^2\xi_2^2 + t_{13}\xi_1\xi_2^3 + t_{04}\xi_2^4 + \text{higher}.$$

The fourth-order terms may be removed by inserting the nonlinear transformation

$$\beta_1 = \xi_1 + \sum_{m+n>2} A_{mn}\xi_1^m\xi_2^n,$$
$$\beta_2 = \xi_2 + \sum_{m+n>2} B_{mn}\xi_1^m\xi_2^n$$

into the canonical form $\beta_1^2\beta_2 + b\beta_2^3$, expanding, and making a term-by-term comparison. The result is a series of equations for the A_{mn} and B_{mn}, specifying the transformation; this argument extends to the removal of higher-order terms as well.[7] The coordinate transformation carrying the eikonal phase to the parabolic umbilic proceeds similary. First the linear transformation is introduced into the form $\xi_1^2\xi_2$ and the result is compared with the cubic terms in $\phi(\mathbf{r}_0,\mathbf{p})$, obtaining a system of equations for $\alpha,\beta,\sigma,\delta$ and putting $\phi(\mathbf{r}_0,\mathbf{p})$ into the form

$$\tilde{\phi}(\mathbf{r}_0,\mathbf{p}) = \phi(\mathbf{r}_0,\mathbf{p}_0) + \xi_1^2\xi_2 + t_{40}\xi_1^4 + t_{31}\xi_1^3\xi_2 + t_{22}\xi_1^2\xi_2^2 + t_{13}\xi_1\xi_2^3 + t_{04}\xi_2^4 + \text{higher}.$$

The fourth-order terms may be removed by inserting the nonlinear transformation

$$\beta_1|t_{04}|^{-1/8}\left(\xi_1+\sum_{m+n>2}A_{mn}\xi_1^m\xi_2^n\right),$$
$$\beta_2|t_{04}|^{1/4}(\xi_2+t_{40}\xi_1^2)$$

into the parabolic umbilic form $\beta_1^2\beta_2+\beta_2^4$, expanding, and making a term-by-term comparison. This leads to equations for the A_{mn} and specifies the transformation. As with the other umbilics, this argument extends to remove other higher-degree terms. (More complete treatments are given by Gilmore[7] and Poston and Stewart.[9]) The transformed integrals are of the form

$$\int \mathbf{E}(\mathbf{r}_0,\mathbf{p},\tau)\exp\{i\tau\phi(\mathbf{r},\mathbf{p})\}d\mathbf{p}$$
$$=\exp\{i\tau\phi(\mathbf{r}_0,\mathbf{p}_0)\}\int\int \mathbf{E}(\mathbf{r}_0,\beta_1,\beta_2,\tau)$$
$$\times\exp\{i\tau\hat{\Phi}(\beta_1,\beta_2)\}d\beta_1\,d\beta_2, \tag{23}$$

where

$$\mathbf{E}(\mathbf{r}_0,\beta_1,\beta_2,\tau)=\mathbf{E}(\mathbf{r}_0,p_x(\beta_1,\beta_2),p_y(\beta_1,\beta_2),\tau)\left(\frac{\partial(p_x,p_y)}{\partial(\beta_1,\beta_2)}\right),$$

and $\hat{\Phi}(\beta_1,\beta_2)$ is the appropriate umbilic. The asymptotic evaluation of the field integrals, Eqs. (22) and (23), has been detailed elsewhere[6,8]; for brevity we do not repeat it here.

The extension of the basic algorithm to three dimensions is straightfoward, when Hessian has no more than two zero-eigenvalues. For these cases the formalism is as above and the principal considerations are algebraic. If the Hessian determinant of the eikonal phase at $\mathbf{r}_0$ is nonzero or the Hessian matrix has one zero-eigenvalue, the canonical form of the transformed phase is

$$\phi(\mathbf{r}_0,\beta)=\phi(\mathbf{r}_0,\mathbf{p}_0)\pm\beta_1^2\pm\beta_2^2\pm\beta_3^n.$$

Obtaining this form basically requires "completing the square" twice in the procedure leading to Eq. (22). If the Hessian matrix has two zero-eigenvalues, the canonical form is

$$\phi(\mathbf{r}_0,\beta)=\phi(\mathbf{r}_0,\mathbf{p}_0)\pm\beta_1^2+\hat{\Phi}(\beta_2,\beta_3),$$

where $\hat{\Phi}$ is the appropriate umbilic. Obtaining this form from the eikonal phase follows from the splitting lemma.[7,9] First, the square is completed in the naturally occurring quadratic. Then the appropriate umbilic is identified by considering the cubic in the remaining variables and coordinate transformations carrying the cubic (and higher) terms to the umbilic are obtained as above. The evaluation of the transformed integrals (using an integral with an umbilic in the phase as an example) proceeds by noting these integrals may be factored into the form

$$\exp\{i\tau\phi(\mathbf{r}_0,\mathbf{p}_0)\}\int\int\exp\{i\tau\hat{\Phi}(\beta_2,\beta_3)\}d\beta_2\,d\beta_3$$
$$\times\int \mathbf{E}_k(\mathbf{r}_0,\beta_1,\beta_2,\beta_3,)\exp\{\pm i\tau\beta_1^2\}d\beta_1.$$

The classical stationary phase technique applies to the integral over $d\beta_1$. Each term in the resulting series is multiplied by an integral having the umbric as the phase. The asymptotic evaluation of the "umbilic integrals" has been discussed elsewhere.[8] The full asymptotic series of the above integral then consists of the terms in the asymptotic series due to the β_1 integration, each of which is multiplied by an asymptotic series due to the asymptotic evaluation of the umbilic integral. If the Hessian matrix has three zero-eigenvalues, the canonical forms for the transformed phase have been specified by Arnol'd.[10] This case is not considered here.

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Scattering by a spherical inhomogeneity in a fluid-saturated porous medium

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A fast compressional wave incident on an inhomogeneity in a fluid-saturated porous medium will produce three scattered elastic waves: a fast compressional wave, a slow compressional wave, and a shear wave. This problem is formulated as a multipole expansion using Biot's equations of poroelasticity. The solution for the first term ($n = 0$) in the multipole series involves a 4×4 system which is solved analytically in the long-wavelength limit. All higher-order terms ($n \geqslant 1$) require the solution of a 6×6 system. A procedure for solving these equations by splitting the problem into a 4×4 system and a 2×2 system and then iterating is introduced. The first iterate is just the solution of the elastic wave scattering problem in the absence of fluid effects. Higher iterates include the successive perturbation effects of fluid/solid interaction.

I. INTRODUCTION

The scattering of elastic waves by a spherical inhomogeneity in an elastic medium has been investigated by Yamakawa,[1-3] by Ying and Truell,[4] and by Einspruch, Witterholt, and Truell.[5] A review of the literature and a comprehensive presentation of the analysis was also given later by Yamakawa.[6] In addition to the insight that these results provide for both scattering and attenuation of elastic waves in inhomogeneous materials,[6] the formulas may also be used in developing approximate theories[7,8] and rigorous bounds[9] for effective elastic constants of composite materials.

Biot[10-12] has developed equations for elastic wave propagation in fluid-saturated porous media. Although some approximate studies of wave speeds and attenuation in liquid-saturated porous media containing spherical regions with liquid replaced by gas have been presented by White[13] and by Dutta and Ode,[14] no comprehensive analysis of scattering from spherical inhomogeneities in porous media has yet appeared. For poroelasticity as well as for elasticity, the results of the single-inclusion scattering analysis will prove to be of importance for studies of attenuation of waves and also for theories of effective constants of composite porous materials.

One major difficulty with the analysis of a single scatterer in poroelasticity is the fact that the solution of a 6×6 system of equations is required in general. Although a 6×6 system is easily solved numerically, the main goal of the present study is to derive analytical results for the scattering coefficients which may then be used to provide some insight, especially into the coupling between fast and slow compressional waves in the presence of inhomogeneities. Since the slow compressional mode is highly damped at low frequencies, we expect the coupling between fast and slow waves due to mode conversion at interfaces may provide an efficient method of attenuating an incident fast wave. To study the attenuation in detail, it will be most helpful to possess an analytical expression for the scattering coefficients. Unfortunately, solution of the 6×6 system of equations requires on the order of 6! operations per coefficient. Furthermore, as in the elastic scattering problem, the lowest-order determinants are degenerate (numerator and denominator vanish to lowest order in the long-wavelength limit) which makes the analysis still more tedious. Thus, the analytical problem is essentially intractable unless we enlist the aid of an automatic symbolic manipulator—which we will not do here.

We solve this problem approximately by splitting the 6×6 system into a 4×4 system and a 2×2 system with coupling terms. The chosen 4×4 system reduces exactly to the elastic scattering problem in the absence of fluid coupling terms. Treating the fluid effects as perturbations to the elastic scattering problem, the equations may be solved iteratively to obtain the scattering coefficients to the desired order of accuracy.

Section II introduces the equations of poroelasticity and the general form of their solution. Section III presents the exact form of the multipole expansions for the scattering of a fast compressional wave from a spherical inhomogeneity. Section IV solves the equations exactly for the lowest-order multipole terms since this problem only requires solution of a 4×4. Section V presents the general form of our perturbation-iteration scheme and applies it to the problem solved in Section IV to provide some insight into the method and the solution. Section VI presents the results for the higher-order multipole expansion coefficients.

II. EQUATIONS OF POROELASTICITY

Before proceeding to analyze the scattering of elastic waves from spherical inhomogeneities, we must first introduce Biot's equations of poroelasticity. Consider a porous medium whose connected pore space is saturated with a single-phase viscous fluid. The fraction of the total volume occupied by the fluid is the porosity ϕ, which is assumed uniform within each constituent but which may vary between host and inclusion. The bulk modulus and density of the fluid are K_f and ρ_f, respectively, in the host. The bulk and shear moduli of the (dry) porous frame for the host are K and μ. For simplicity we assume the frame of the host is composed of a single constituent whose bulk and shear moduli and density are K_m, μ_m, and ρ_m. Inclusion parameters will be distinguished from host parameters by adding a prime superscript. The frame moduli may be measured directly or

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they may be estimated using a general theory of elastic composites which has been developed recently.[8]

For long-wavelength disturbances ($\lambda > h$, where h is a typical pore size) propagating through such a porous medium, we define average values of the (local) displacements in the solid and also in the saturating fluid. The average displacement vector for the solid frame is $\mathbf{u}$ while that for the pore fluids is $\mathbf{u}_f$. The average displacement of the fluid relative to the frame is $\mathbf{w} = \phi(\mathbf{u}_f - \mathbf{u})$. For small strains, the frame dilatation is

$$e = e_x + e_y + e_z = \nabla \cdot \mathbf{u}, \tag{1}$$

where e_x, e_y, e_z are the Cartesian strain components. Similarly, the average fluid dilatation is

$$e_f = \nabla \cdot \mathbf{u}_f \tag{2}$$

(e_f also includes flow terms as well as dilatation) and the increment of fluid content is defined by

$$\zeta = \nabla \cdot \mathbf{w} = \phi(e - e_f). \tag{3}$$

With these definitions, Biot[10–12] shows that the strain-energy functional for an isotropic, linear medium is a quadratic function of the strain invariants[15] $I_1 = e, I_2$, and of ζ having the form

$$2E = He^2 - 2Ce\zeta + M\zeta^2 - 4\mu I_2, \tag{4}$$

where

$$I_2 = e_x e_y + e_y e_z + e_z e_x - \tfrac{1}{4}(\gamma_x^2 + \gamma_y^2 + \gamma_z^2), \tag{5}$$

and $\gamma_x, \gamma_y, \gamma_z$ are the shear strain components.

With time dependence of the form $\exp(-i\omega t)$, the coupled wave equations of poroelasticity in the presence of dissipation are

$$\begin{aligned} &\mu\nabla^2 u + (H-\mu)\nabla e - C\nabla\zeta + \omega^2(\rho\mathbf{u} + \rho_f \mathbf{w}) = 0, \\ &C\nabla e - M\nabla\zeta + \omega^2(\rho_f \mathbf{u} + q\mathbf{w}) = 0, \end{aligned} \tag{6}$$

where

$$\rho = \phi\rho_f + (1-\phi)\rho_m \tag{7}$$

and

$$q = \rho_f[\alpha/\beta + iF(\xi)\eta/\kappa\omega]. \tag{8}$$

The kinematic viscosity of the liquid is η, the permeability of the porous frame is κ, and the dynamic viscosity factor is given, for our choice of sign for the frequency dependence, by

$$F(\xi) = \tfrac{1}{4}\{\xi T(\xi)/[1 + 2T(\xi)/i\xi]\}, \tag{9}$$

where

$$T(\xi) = \frac{\mathrm{ber}'(\xi) - i\,\mathrm{bei}'(\xi)}{\mathrm{ber}(\xi) - i\,\mathrm{bei}(\xi)} \tag{10}$$

and

$$\xi = (\omega h^2/\eta)^{1/2}. \tag{11}$$

The functions $\mathrm{ber}(\xi)$ and $\mathrm{bei}(\xi)$ are the real and imaginary parts of the Kelvin function. The dynamic parameter h is a characteristic length generally associated with and comparable in magnitude to the steady-flow hydraulic radius. The tortuosity $\alpha \geq 1$ is a pure number related to the frame inertia which has been measured recently[16] and has also been estimated theoretically.[17,18]

The coefficients H, C, and M are given by[19,20]

$$H = K + \tfrac{4}{3}\mu + \sigma C, \tag{12}$$

$$C = [((\sigma - \phi)/K_m + \phi/K_f)/\sigma]^{-1}, \tag{13}$$

$$M = C/\sigma, \tag{14}$$

where

$$\sigma = 1 - K^*/K_m. \tag{15}$$

To decouple the wave equations (6) into Helmholtz equations for the three modes of propagation, we note that the displacements $\mathbf{u}$ and $\mathbf{w}$ can be decomposed as

$$\mathbf{u} = \nabla\Upsilon + \nabla\times\boldsymbol{\beta}, \quad \mathbf{w} = \nabla\psi + \nabla\times\boldsymbol{\chi}, \tag{16}$$

where Υ, ψ are scalar potentials and $\boldsymbol{\beta}, \boldsymbol{\chi}$ are vector potentials. Substituting (16) into (6), we find (6) is satisfied if two pairs of equations are satisfied:

$$(\nabla^2 + k_s^2)\boldsymbol{\beta} = 0, \quad \boldsymbol{\chi} = -\Gamma_s \boldsymbol{\beta}, \tag{17}$$

where $\Gamma_s = \rho_f/q$ and

$$(\nabla^2 + k_\pm^2) A_\pm = 0. \tag{18}$$

The wave vectors in (17) and (18) are defined by

$$k_s^2 = \omega^2(\rho - \rho_f^2/q)\mu \tag{19}$$

and

$$k_\pm^2 = (\omega^2/2\Delta)\{b + f \mp [(b-f)^2 + 4cd]^{1/2}\}, \tag{20}$$

where

$$\begin{aligned} &b = \rho M - \rho_f C, \quad c = \rho_f M - qC, \\ &d = \rho_f H - \rho C, \quad f = qH - \rho_f C, \end{aligned} \tag{21}$$

with

$$\Delta = MH - C^2. \tag{22}$$

The linear combination of scalar potentials has been chosen to be

$$A_\pm = \Gamma_\pm \Upsilon + \psi, \tag{23}$$

where

$$\Gamma_\pm = d/[(k_\pm \Delta/\omega^2)^2 - b] = [(k_\pm \Delta/\omega^2)^2 - f]/c. \tag{24}$$

With the identification (24), the decoupling is complete.

Since (17) and (18) are valid for any choice of coordinate system, they may be applied to boundary value problems with arbitrary symmetry. Biot's theory will therefore be applied to scattering of elastic waves for a spherical inhomogeneity in Sec. III.

III. SCATTERING FROM A SPHERICAL INHOMOGENEITY

The analysis which follows will closely parallel Yamakawa's analysis of scattering by a general elastic spherical obstacle.[6]

The boundary conditions[21] which must be satisfied at the surface of the spherical inhomogeneity are continuity of the normal and tangential stresses

$$\tau_{rr} = (H - 2\mu)e + 2\mu e_r - C\zeta \tag{25}$$

and

$$\tau_{r\theta} = \mu\left(\frac{1}{r}\frac{\partial u_r}{\partial \theta} + \frac{\partial u_r}{\partial r} - \frac{u_r}{r}\right), \tag{26}$$

continuity of fluid pressure

$$p = M\zeta - Ce, \tag{27}$$

and continuity of solid displacement $\mathbf{u}$ and of the normal component of the relative fluid/solid displacement w_r. For convenience, the displacements (16) are separated into compressional and shear components as

$$\hat{\mathbf{u}} = \nabla\Upsilon, \quad \tilde{\mathbf{u}} = \nabla\times\boldsymbol{\beta},$$
$$\hat{\mathbf{w}} = \nabla\psi, \quad \tilde{\mathbf{w}} = \nabla\times\boldsymbol{\chi} = -\Gamma_s\mathbf{u}. \tag{28}$$

Then, for a plane-wave incident on a spherical obstacle, we need only consider

$$e = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\hat{u}_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\,\hat{u}_\theta), \tag{29}$$

$$e_r = \frac{\partial u_r}{\partial r}, \tag{30}$$

and

$$-\zeta = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\hat{w}_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\hat{w}_\theta). \tag{31}$$

The vector potential $\boldsymbol{\beta}$ is most conveniently defined as

$$\boldsymbol{\beta} = \hat{r}\beta_1 + \nabla\times(\hat{r}\beta_2), \tag{32}$$

where both β_1 and β_2 satisfy (17). Then, if we choose the gauge so that $\nabla\cdot\boldsymbol{\beta} = 0$ as we are free to do in the present problem, we find $\beta_1 = 0$ and

$$\boldsymbol{\beta} = -\frac{1}{r}\frac{\partial\beta_2}{\partial\theta}\hat{\phi}, \tag{33}$$

which relates $\boldsymbol{\beta}$ to the scalar solution of (17). The scalar potentials are related to the solutions of (18) by

$$\Upsilon = (A_+ - A_-)/(\Gamma_+ - \Gamma_-), \tag{34}$$

$$\psi = -(A_+\Gamma_- - A_-\Gamma_+)/(\Gamma_+ - \Gamma_-). \tag{35}$$

The solution of (17) and (18) in terms of spherical Bessel functions j_n and $h_n^{(1)}$ and Legendre polynomials P_n is well known.

Following Yamakawa,[6] the incident plane fast compressional waves for the solid satisfy

$$e_0 = A_0 e^{ik_+ r\cos\theta}$$
$$= A_0\sum_{n=0}^{\infty}(2n+1)i^n j_n(k_+r)P_n(\cos\theta), \tag{36}$$

$$\hat{u}_{0r} = -\frac{A_0}{k_+^2}\sum_{n=0}^{\infty}(2n+1)i^n\frac{d}{dr}j_n(k_+r)P_n(\cos\theta), \tag{37}$$

$$\hat{u}_{0\theta} = -\frac{A_0}{k_+^2}\sum_{n=1}^{\infty}(2n+1)i^n\frac{1}{r}j_n(k_+r)\frac{d}{d\theta}P_n(\cos\theta), \tag{38}$$

and for the relative fluid/solid displacement

$$\zeta_0 = A_0\Gamma_-\sum_{n=0}^{\infty}(2n+1)i^n j_n(k_+r)P_n(\cos\theta), \tag{39}$$

$$\hat{w}_{1r} = \frac{A_0\Gamma_-}{k_+^2}\sum_{n=0}^{\infty}(2n+1)i^n\frac{d}{dr}j_n(k_+r)P_n(\cos\theta), \tag{40}$$

$$\hat{w}_{1\theta} = \frac{A_0\Gamma_-}{k_+^2}\sum_{n=1}^{\infty}(2n+1)i^n\frac{1}{r}j_n(k_+r)\frac{d}{d\theta}P_n(\cos\theta). \tag{41}$$

The time dependence $e^{-i\omega t}$ is implicit.

The reflected compressional waves are given for the solid by

$$e_1 = \sum_{n=0}^{\infty}[B_n^{(+)}h_n^{(1)}(k_+r) - B_n^{(-)}h_n^{(1)}(k_-r)]P_n(\cos\theta), \tag{42}$$

$$\hat{u}_{1r} = -\sum_{n=0}^{\infty}\left[\frac{B_n^{(+)}}{k_+^2}\frac{d}{dr}h_n^{(1)}(k_+r) - \frac{B_n^{(-)}}{k_-^2}\frac{d}{dr}h_n^{(1)}(k_-r)\right] \times P_n(\cos\theta), \tag{43}$$

$$\hat{u}_{1\theta} = -\sum_{n=1}^{\infty}\left[\frac{B_n^{(+)}}{k_+^2}h_n^{(1)}(k_+r) - \frac{B_n^{(-)}}{k_-^2}h_n^{(1)}(k_-r)\right] \times\frac{d}{r\,d\theta}P_n(\cos\theta), \tag{44}$$

and for the relative fluid/solid displacement by

$$\zeta_1 = \sum_{n=0}^{\infty}[B_n^{(+)}\Gamma_-h_n^{(1)}(k_+r) - B_n^{(-)}\Gamma_+h_n^{(1)}(k_-r)] \times P_n(\cos\theta), \tag{45}$$

$$\hat{w}_{1r} = \sum_{n=0}^{\infty}\left[\frac{B_n^{(+)}\Gamma_-}{k_+^2}\frac{d}{dr}h_n^{(1)}(k_+r) - \frac{B_n^{(-)}\Gamma_+}{k_-^2}\frac{d}{dr}h_n^{(1)}(k_-r)\right]P_n(\cos\theta), \tag{46}$$

$$\hat{w}_{1\theta} = \sum_{n=1}^{\infty}\left[\frac{B_n^{(+)}\Gamma_-}{k_+^2}h_n^{(1)}(k_+r) - \frac{B_n^{(-)}\Gamma_+}{k_-^2}\frac{d}{dr}h_n^{(1)}(k_-r)\right] \times\frac{1}{r}\frac{d}{d\theta}P_n(\cos\theta). \tag{47}$$

The reflected shear waves for the solid are

$$\hat{\phi}\cdot\nabla\times\mathbf{u}_2 = \sum_{n=0}^{\infty}C_n h_n^{(1)}(k_s r)\frac{d}{d\theta}P_n(\cos\theta), \tag{48}$$

$$\tilde{u}_{2r} = -\frac{1}{k_s^2}\sum_{n=1}^{\infty}C_n n(n+1)\frac{1}{r}h_n^{(1)}(k_s r)P_n(\cos\theta), \tag{49}$$

$$\tilde{u}_{2\theta} = -\frac{1}{k_s^2}\sum_{n=1}^{\infty}C_n\frac{1}{r}\frac{d}{dr}[rh_n^{(1)}(k_s r)]\frac{d}{d\theta}P_n(\cos\theta), \tag{50}$$

and for the relative fluid/solid displacement by (28) together with (48)–(50).

The refracted compressional waves are given for the solid by

$$e_3 = \sum_{n=0}^{\infty}[D_n^{(+)}j_n(k'_+r) - D_n^{(-)}j_n(k'_-r)]P_n(\cos\theta), \tag{51}$$

$$\hat{u}_{3r} = \sum_{n=0}^{\infty}\left[\frac{D_n^{(+)}}{(k'_+)^2}\frac{d}{dr}j_n(k'_+r) - \frac{D_n^{(-)}}{(k'_-)^2}\frac{d}{dr}j_n(k'_-r)\right] \times P_n(\cos\theta), \tag{52}$$

$$\hat{u}_{3\theta} = -\sum_{n=1}^{\infty}\left[\frac{D_n^{(+)}}{(k'_1)^2} j_n(k'_+ r) - \frac{D_n^{(-)}}{(k'_-)^2} j_n(k'_- r)\right] \times \frac{1}{r}\frac{d}{d\theta} P_n(\cos\theta), \tag{53}$$

and for the relative fluid/solid displacement by

$$\zeta_3 = \sum_{n=0}^{\infty}\left[D_n^{(+)}\Gamma_- j_n(k'_+ r) - D_n^{(-)}\Gamma_+ j_n(k'_- r)\right] \times P_n(\cos\theta), \tag{54}$$

$$\hat{w}_{3r} = \sum_{n=0}^{\infty}\left[\frac{D_n^{(+)}\Gamma_-}{(k'_+)^2}\frac{d}{dr} j_n(k'_+ r) - \frac{D_n^{(-)}\Gamma_+}{(k'_-)^2}\frac{d}{dr} j_n(k'_- r)\right] P_n(\cos\theta), \tag{55}$$

$$\hat{w}_{3\theta} = \sum_{n=1}^{\infty}\left[\frac{D_n^{(+)}\Gamma_-}{(k'_+)^2} j_n(k'_1 r) - \frac{D_n^{(-)}\Gamma_+}{(k'_-)^2} j_n(k'_- r)\right]\frac{1}{r}\frac{d}{d\theta} P_n(\cos\theta). \tag{56}$$

The refracted shear waves for the solid are

$$\hat{\phi}\cdot\nabla\times\mathbf{u}_4 = \sum_{n=1}^{\infty} E_n\, j_n(k'_s r)\, P_n(\cos\theta), \tag{57}$$

$$\tilde{u}_{4r} = -\frac{1}{(k'_s)^2}\sum_{n=1}^{\infty} E_n\, n(n+1)\frac{1}{r} j_n(k'_s r)\, P_n(\cos\theta), \tag{58}$$

$$\tilde{u}_{4\theta} = -\frac{1}{(k'_s)^2}\sum_{n=1}^{\infty} E_n\,\frac{1}{r}\frac{d}{dr}\left[\, r j_n(k'_s r)\right]\frac{d}{d\theta} P_n(\cos\theta), \tag{59}$$

and for the relative fluid/solid displacement by (28) together with (57)–(59).

Let the spherical inhomogeneity have radius a. Then the boundary conditions are given for $r = a$ by

$$(H-2\mu)(e_0+e_1) + 2\mu\frac{\partial}{\partial r}(u_{0r}+u_{1r}+u_{2r}) - C(\zeta_0+\zeta_1) = (H'-2\mu')e_3 + 2\mu'\frac{\partial}{\partial r}(u_{3r}+u_{4r}) - C\zeta_3, \tag{60}$$

$$\mu\left[\frac{1}{r}\frac{\partial}{\partial\theta}(u_{0r}+u_{1r}+u_{2r}) + \frac{\partial}{\partial r}(u_{0\theta}+u_{1\theta}+u_{2\theta}) - \frac{1}{r}(u_{0\theta}+u_{1\theta}+u_{2\theta})\right] = \mu'\left[\frac{1}{r}\frac{\partial}{\partial\theta}(u_{3r}+u_{4r}) + \frac{\partial}{\partial r}(u_{3\theta}+u_{4\theta}) - \frac{1}{r}(u_{3\theta}+u_{4\theta})\right], \tag{61}$$

$$\hat{u}_{0r}+\hat{u}_{1r}+\tilde{u}_{2r} = \hat{u}_{3r}+\tilde{u}_{4r}, \tag{62}$$

$$\hat{u}_{0\theta}+\hat{u}_{1\theta}+\tilde{u}_{2\theta} = \hat{u}_{3\theta}+\tilde{u}_{4\theta}, \tag{63}$$

$$C(e_0+e_1) - M(\zeta_0+\zeta_1) = C'e_3 - M'\zeta_3, \tag{64}$$

and

$$\hat{w}_{0r}+\hat{w}_{1r}+\tilde{w}_{2r} = \hat{w}_{3r}+\tilde{w}_{4r}. \tag{65}$$

The first four equations (60)–(63) reduce to the usual boundary conditions for elastic wave scattering from an elastic sphere when fluid effects are neglected. The last two equations (64) and (65) determine the relative fluid/solid motion, but they are also coupled to the first four equations. The orthogonality properties of the Legendre polynomials assure the independence of the coefficients for different values of n. For $n = 0$, the boundary conditions give four equations in the four unknowns $B_0^{(\pm)}, D_0^{(\pm)}$. For $n \geq 1$, the boundary conditions give six equations in the six unknowns $B_n^{(\pm)}$, C_n, $D_n^{(\pm)}$, E_n.

In general, we may write the equations for the coefficients in the form

$$\beta_{nm}^{(+)}B_n^{(+)} + \beta_{nm}^{(-)}B_n^{(-)} + \gamma_{nm}C_n + \delta_{nm}^{(+)}D_n^{(+)} + \delta_{nm}^{(-)}D_n^{(-)} + \epsilon_{nm}E_n = i^n(2n+1)\alpha_{nm}A_0, \tag{66}$$

where $m = 1, \ldots, 6$ corresponding to (60)–(65), respectively. Defining $\xi_\pm = k_\pm a$ and $\eta = k_s a$, the coefficients in (66) become

$$\alpha_{n1} = -\left\{\left[(H - C\Gamma_-) - \frac{2\mu(n+1)(n+2)}{\xi_+^2}\right] \times j_n(\xi_+) + \frac{4\mu}{\xi_+} j_{n-1}(\xi_+)\right\}, \tag{67}$$

$$\beta_{n1}^{(\pm)} = \pm\left\{\left[(H - C\Gamma_\mp) - \frac{2\mu(n+1)(n+2)}{\xi_\pm^2}\right] \times h_n^{(1)}(\xi_\pm) + \frac{4\mu}{\xi_\pm} h_{n-1}^{(1)}(\xi_\pm)\right\}, \tag{68}$$

$$\gamma_{n1} = -[2\mu n(n+1)/\eta^2]\,[\eta h_{n-1}^{(1)}(\eta) - (n+2)h_n^{(1)}(\eta)], \tag{69}$$

$$\delta_{n1}^{(\pm)} = \mp\{[(H' - C\Gamma'_\mp) - 2\mu'(n+1)(n+2)/(\xi'_\pm)^2] \times j_n(\xi'_\pm) + (4\mu'/\xi'_\pm) j_n(\xi'_\pm)\}, \tag{70}$$

$$\epsilon_{n1} = [2\mu' n(n+1)/\eta'^2]\,[\eta' j_{n-1}(\eta') - (n+2) j_n(\eta')], \tag{71}$$

$$\alpha_{n2} = -(2\mu/\xi_+^2)[(n+2) j_n(\xi_+) - \xi_+ j_{n-1}(\xi_+)], \tag{72}$$

$$\beta_{n2}^{(\pm)} = \pm(2\mu/\xi_\pm^2)[(n+2)h_n^{(1)}(\xi_\pm) - \xi_\pm h_{n-1}^{(1)}(\xi_\pm)], \tag{73}$$

$$\gamma_{n2} = (\mu/\eta^2)\{2\eta h_{n-1}^{(1)}(\eta) + [\eta^2 - 2n(n+2)]h_n^{(1)}(\eta)\}, \tag{74}$$

$$\delta_{n2}^{(\pm)} = \mp[2\mu'/(\xi'_\pm)^2][(n+2) j_n(\xi'_\pm) - \xi'_\pm j_{n-1}(\xi'_\pm)], \tag{75}$$

$$\epsilon_{n2} = -(\mu'/\eta'^2)\{2\eta' j_{n-1}(\eta') + [\eta'^2 - 2n(n+2)] j_n(\eta')\}, \tag{76}$$

$$\alpha_{n3} = (1/\xi_+)[j_{n-1}(\xi_+) - [(n+1)/\xi_+] j_n(\xi_+)], \tag{77}$$

$$\beta_{n3}^{(\pm)} = \mp(1/\xi_\pm)[h_{n-1}^{(1)}(\xi_\pm) - [(n+1)/\xi_\pm]h_n^{(1)}(\xi_\pm)], \tag{78}$$

$$\gamma_{n3} = -[n(n+1)/\eta^2]h_n^{(1)}(\eta), \tag{79}$$

$$\delta_{n3}^{(\pm)} = \pm(1/\xi'_\pm)[j_{n-1}(\xi') - [(n+1)/\xi'_\pm] j_n(\xi'_\pm)], \tag{80}$$

$$\epsilon_{n3} = [n(n+1)/(\eta')^2] j_n(\eta'), \tag{81}$$

$$\alpha_{n4} = (1/\xi_+^2) j_n(\xi_+), \tag{82}$$

$$\beta_{n4}^{(\pm)} = \mp(1/\xi_\pm^2)h_n^{(1)}(\xi_\pm), \tag{83}$$

$$\gamma_{n4} = -(1/\eta^2)[\eta h^{(1)}_{n-1}(\eta) - n h^{(1)}_n(\eta)], \tag{84}$$

$$\delta^{(\pm)}_{n4} = \pm [1/(\xi'_\pm)^2] j_n(\xi'_\pm), \tag{85}$$

$$\epsilon_{n4} = [1/(\eta')^2][\eta' j_{n-1}(\eta') - n j_n(\eta')], \tag{86}$$

$$\alpha_{n5} = -(C - M\Gamma_-) j_n(\xi_+), \tag{87}$$

$$\beta^{(\pm)}_{n5} = \pm (C - M\Gamma_\mp) h^{(1)}_n(\xi_\pm), \tag{88}$$

$$\gamma_{n5} = 0, \tag{89}$$

$$\delta^{(\pm)}_{n5} = \mp (C' - M'\Gamma'_\mp) j_n(\xi'_\pm), \tag{90}$$

$$\epsilon_{n5} = 0, \tag{91}$$

and, finally,

$$\alpha_{n6} = (\Gamma_-/\xi_+)[j_{n-1}(\xi_+) - [(n+1)/\xi_+] j_n(\xi_+)], \tag{92}$$

$$\beta^{(\pm)}_{n6} = \mp (\Gamma_\mp/\xi_\pm)[h^{(1)}_{n-1}(\xi_\pm) - [(n+1)/\xi_\pm] h^{(1)}_n(\xi_\pm)], \tag{93}$$

$$\gamma_{n6} = -\Gamma_s [n(n+1)/\eta^2] h^{(1)}_n(\eta), \tag{94}$$

$$\delta^{(\pm)}_{n6} = \pm (\Gamma'_\mp/\xi'_\pm)[j_{n-1}(\xi'_\pm) - [(n+1)/\xi'_\pm] j_n(\xi'_\pm)], \tag{95}$$

$$\epsilon_{n6} = \Gamma'_s [n(n+1)/(\eta')^2] j_n(\eta'). \tag{96}$$

Equations (67) – (96) are valid for all $n \geqslant 1$. For $n = 0$, Eq. (66) is replaced by

$$\beta^{(+)}_{0m} B^{(+)}_0 + \beta^{(-)}_{0m} B^{(-)}_0 + \delta^{(+)}_{0m} D^{(+)}_0 + \delta^{(-)}_{0m} D^{(-)}_0 = \alpha_{0m} A_0, \tag{97}$$

for $m = 1,3,5,6$—corresponding to boundary conditions (60), (62), (64), and (65). The coefficients become

$$\alpha_{01} = -[(H - C\Gamma_-) j_0(\xi_+) - (4\mu/\xi_+) j_1(\xi_+)], \tag{98}$$

$$\beta^{(\pm)}_{01} = \pm [(H - C\Gamma) h^{(1)}_0(\xi_\pm) - (4\mu/\xi_\pm) h^{(1)}_1(\xi_\pm)], \tag{99}$$

$$\delta^{(\pm)}_{01} = \mp [(H' - C'\Gamma'_\mp) j_0(\xi'_\pm) - (4\mu'/\xi'_\pm) j_1(\xi'_\pm)], \tag{100}$$

$$\alpha_{03} = -(1/\xi_+) j_1(\xi_+), \tag{101}$$

$$\beta^{(\pm)}_{03} = \pm (1/\xi_\pm) h^{(1)}_1(\xi_\pm), \tag{102}$$

$$\delta^{(\pm)}_{03} = \mp (1/\xi'_\pm) j_1(\xi'_\pm), \tag{103}$$

$$\alpha_{05} = -(C - M\Gamma_-) j_0(\xi_+), \tag{104}$$

$$\beta^{(\pm)}_{05} = \pm (C - M\Gamma_\mp) h^{(1)}_0(\xi_\pm), \tag{105}$$

$$\delta^{(\pm)}_{05} = \mp (C' - M'\Gamma'_\mp) j_0(\xi'_\pm), \tag{106}$$

and

$$\alpha_{06} = (\Gamma_-/\xi_+) j_1(\xi_+), \tag{107}$$

$$\beta^{(\pm)}_{06} = \mp (\Gamma_\mp/\xi_\pm) h^{(1)}_1(\xi_\pm), \tag{108}$$

$$\delta^{(\pm)}_{06} = \pm (\Gamma'_\mp/\xi'_\pm) j_1(\xi'_\pm). \tag{109}$$

These equations give the complete solution to the problem of scattering from a spherical inhomogeneity in a fluid-saturated porous medium. The system of equations may be solved numerically without much difficulty for any value of n and any choice of ω. In the following sections, the equations will be analyzed in more detail for $n = 0, 1, 2$ and in the long-wavelength limit.

IV. EXACT LONG-WAVELENGTH SOLUTION FOR $n = 0$

In the long-wavelength limit ($\xi_\pm, \eta \ll 1$) we may use the asymptotic formulas for j_n and $h^{(1)}_n$ with small arguments[22] to simplify the coefficients in Sec. III. For $n = 0$, the system to be solved is only 4×4 and, therefore, may be treated analytically. We find the coefficients to lowest order become

$$\alpha_{01} = -(H - \tfrac{4}{3}\mu - C\Gamma_-), \tag{110}$$

$$\beta^{(\pm)}_{01} = \pm i4\mu/\xi^3_\pm, \tag{111}$$

$$\delta^{(\pm)}_{01} = \mp (H' - \tfrac{4}{3}\mu' - C'\Gamma'_\mp), \tag{112}$$

$$\alpha_{03} = -\tfrac{1}{3}, \tag{113}$$

$$\beta^{(\pm)}_{03} = \mp i/\xi^3_\pm, \tag{114}$$

$$\delta^{(\pm)}_{03} = \mp \tfrac{1}{3}, \tag{115}$$

$$\alpha_{05} = -(C - M\Gamma_-), \tag{116}$$

$$\beta^{(\pm)}_{05} = \mp (i/\xi_\pm)(C - M\Gamma_\mp), \tag{117}$$

$$\delta^{(\pm)}_{05} = \mp (C' - M'\Gamma'_\mp), \tag{118}$$

and

$$\alpha_{06} = \Gamma_-/3, \tag{119}$$

$$\beta^{(\pm)}_{06} = \pm i(\Gamma_\mp/\xi^3_\pm), \tag{120}$$

$$\delta^{(\pm)}_{06} = \pm \Gamma'_\mp/3. \tag{121}$$

The solution of (97) with the coefficients (110)–(121) may be found using Cramer's rule for inverting a matrix. If the exterior scattering coefficients are written as $B^{(\pm)}_0/A_0 = N^\pm/D$, then the relevant determinants are

$$D = \frac{(\Gamma_+ - \Gamma_-)(\Gamma'_+ - \Gamma'_-)}{\xi^3_+ \xi^3_-}\left[M'\left(H' - \frac{(C')^2}{M'} - \frac{4}{3}\mu' + \frac{4}{3}\mu\right) + O(\xi^2_\pm)\right], \tag{122}$$

$$N^+ = \frac{-i(\Gamma'_+ - \Gamma'_-)}{3\xi^3_-}\left[(\Gamma_+ - \Gamma_-)M'\left(H' - \frac{(C')^2}{M'} - \frac{4}{3}\mu' + \frac{4}{3}\mu\right) + (H - C\Gamma_-)(C' - M'\Gamma_+) - (C - M\Gamma_-)(H' - C'\Gamma_+ - \frac{4}{3}\mu' + \frac{4}{3}\mu) + O(\xi^2_\pm)\right], \tag{123}$$

$$N^- = \frac{i(\Gamma'_+ - \Gamma'_-)}{3\xi^3_+}\left[(C - M\Gamma_-)\left(H' - C'\Gamma_- - \frac{4}{3}\mu' + \frac{4}{3}\mu\right) - (C' - M\Gamma_-)(H - C\Gamma_-) + O(\xi^2_\pm)\right]. \tag{124}$$

Recalling that $H = K + \frac{4}{3}\mu + C^2/M$, the scattering coefficients may be written as

$$B^{(+)}_0 = -\frac{i\xi^3_+ A_0}{3}\frac{[K' - K + (C - M\Gamma_-)(C'/M' - C/M)]}{K' + \frac{4}{3}\mu} + (\xi_+/\xi_-)^3 B^{(-)}_0 \tag{125}$$

and

$$B_0^{(-)}=\frac{i\xi_-^3 A_0}{3M'(\Gamma_+-\Gamma_-)(K'+\frac{4}{3}\mu)}\left[(C-M\Gamma_-)\left(K'+\frac{4}{3}\mu\right)\right.$$
$$\left.-(C'-M'\Gamma_-)\left(K+\frac{4}{3}\mu\right)+(C-M\Gamma_-)(C'-M'\Gamma_-)\left(\frac{C'}{M'}-\frac{C}{M}\right)\right]. \quad (126)$$

To check the result, consider the elastic limit of the equations: $C\to 0$, $M\to 0$, $\xi_-\to 0$, $\Gamma_-\to 0$. Then, Eqs. (125) and (126) reduce to

$$B_0^{(+)}=-i\xi_+^3(K'-K)/3(K'+\tfrac{4}{3}\mu) \quad (127)$$

and

$$B_0^{(-)}=0. \quad (128)$$

Equation (127) is the standard result for elastic scattering from a spherical inhomogeneity. Equation (128) shows that slow compressional waves do not propagate in the absence of a pore fluid.

V. PERTURBATION METHOD FOR $n=0$

Since solution of the 6×6 system of equations (66) for $n\geqslant 1$ requires on the order of $6!(=720)$ multiplications per determinant, a complete analytical solution will not be attempted here. The aid of an automatic symbolic manipulator could be enlisted for solving this problem. However, we propose instead to solve the problem approximately by introducing an iterative perturbation method. Since the scattering coefficients reduce to those for purely elastic scattering when no fluid is in the pores, the pore-fluid effects may be treated as perturbations to the elastic scattering. In particular, the constants C and M $(=C/\sigma)$ in Biot's equations are small compared to K and μ if the porous frame is well consolidated, the porosity is not too great, and the bulk modulus of the pore fluid is comparable to (or less than) that of water.

A formal perturbation method may be constructed with $\epsilon=C/K$ as the small parameter. Thus, the elastic constants C, M, C', and M' will all be treated as $O(\epsilon K)$. At low frequencies, $\Gamma_+=H/C$ so $\Gamma_+=O(1/\epsilon)$. Also at low frequencies, $\Gamma_-\to 0$.

The details of the perturbation method for $n\geqslant 1$ will be presented in the next section. In this section, we will apply the method to the case $n=0$. Since the exact solution was found in Sec. IV, this application will help to illustrate the strengths and weaknesses of the perturbation method.

We will expand the scattering coefficients as

$$B_0^{(+)}\equiv\xi_+^3\sum_{p=0}^{\infty}\epsilon^p b_{0p}^{(+)},\quad B_0^{(-)}\equiv\xi_-^3\sum_{p=1}^{\infty}\epsilon^p b_{0p}^{(-)}, \quad (129)$$
$$D_0^{(+)}\equiv\sum_{p=0}^{\infty}\epsilon^p d_{0p}^{(+)},\quad D_0^{(-)}\equiv\sum_{p=1}^{\infty}\epsilon^p d_{0p}^{(-)},$$

and rewrite the affected coefficients of Eq. (97) as

$$\alpha_{01}=-K-\epsilon K(C/M-\Gamma_-)\equiv\bar{\alpha}_{01}+\epsilon\bar{\bar{\alpha}}_{01}, \quad (130)$$
$$\delta_{01}^{(+)}=-K'-\epsilon(C'/C)K(C'/M'-\Gamma'_-)$$
$$\equiv\bar{\delta}_{01}^{(+)}+\epsilon\bar{\bar{\delta}}_{01}^{(+)}, \quad (131)$$
$$\delta_{01}^{(-)}=(K'-C'\Gamma'_+)+\epsilon[(C')^2/CM']K$$
$$\equiv\bar{\delta}_{01}^{(-)}+\epsilon\bar{\bar{\delta}}_{01}^{(-)}, \quad (132)$$
$$\alpha_{05}=-\epsilon K(1-(M/C)\Gamma_-)\equiv\epsilon\bar{\bar{\alpha}}_{05}, \quad (133)$$
$$\beta_{05}^{(+)}=-\epsilon K(i/\xi_+)(1-(M/C)\Gamma_-)\equiv\epsilon\bar{\bar{\beta}}_{05}^{(+)}/\xi_+^3, \quad (134)$$
$$\beta_{05}^{(-)}=(-i/\xi_-)(M\Gamma_+-\epsilon K)\equiv\epsilon\bar{\bar{\beta}}_{05}^{(-)}/\xi_-^3, \quad (135)$$
$$\delta_{05}^{(+)}=-\epsilon(C'/C)K(1-(M'/C')\Gamma'_-)\equiv\epsilon\bar{\bar{\delta}}_{05}^{(+)}, \quad (136)$$
$$\delta_{05}^{(-)}=-M'\Gamma'_+ +\epsilon(C'K/C)\equiv\bar{\delta}_{05}^{(-)}+\epsilon\bar{\bar{\delta}}_{05}^{(-)}, \quad (137)$$
$$\beta_{06}^{(-)}=-\frac{1}{\epsilon}\frac{i}{\xi_-^3}\frac{C\Gamma_+}{K}\equiv\frac{1}{\epsilon}\frac{\dot{\beta}_{06}^{(-)}}{\xi_-^3}, \quad (138)$$
$$\delta_{06}^{(-)}=-\frac{1}{\epsilon}\frac{C\Gamma'_+}{3K}\equiv\frac{1}{\epsilon}\dot{\delta}_{06}^{(-)}. \quad (139)$$

In addition to (130)–(139), we define $\bar{\beta}_{0m}^{(\pm)}\equiv\xi_\pm^3\beta_{0m}^{(\pm)}$ for those values of m not mentioned explicitly.

Substituting (129)–(137) into (97) and collecting terms which multiply the same power of ϵ, we find the sets of equations

$$\bar{\beta}_{01}^{(+)}b_{00}^{(+)}+\bar{\delta}_{01}^{(+)}d_{00}^{(+)}=\bar{\alpha}_{01}A_0, \quad (140)$$
$$\bar{\beta}_{03}^{(+)}b_{00}^{(+)}+\bar{\delta}_{03}^{(+)}d_{00}^{(+)}=\bar{\alpha}_{03}A_0,$$
$$\bar{\delta}_{05}^{(-)}d_{01}^{(-)}=\bar{\bar{\alpha}}_{05}A_0-\bar{\bar{\beta}}_{05}^{(+)}b_{00}^{(+)}-\bar{\bar{\delta}}_{05}^{(+)}d_{00}^{(+)}, \quad (141)$$
$$\dot{\beta}_{00}^{(-)}b_{01}^{(-)}+\dot{\delta}_{06}^{(-)}d_{01}^{(-)}=\alpha_{06}A_0-\bar{\beta}_{06}^{(+)}b_{00}^{(+)}-\delta_{06}^{(+)}d_{00}^{(+)},$$

and

$$\bar{\beta}_{01}^{(+)}b_{01}^{(+)}+\delta_{01}^{(+)}d_{01}^{(+)}$$
$$=\bar{\bar{\alpha}}_{01}A_0-\bar{\beta}_{01}^{(-)}b_{01}^{(-)}-\bar{\delta}_{01}^{(+)}d_{00}^{(+)}-\bar{\delta}_{01}^{(-)}d_{01}^{(-)}, \quad (142)$$
$$\bar{\beta}_{03}^{(+)}b_{01}^{(+)}+\delta_{03}^{(+)}d_{01}^{(+)}=-\bar{\beta}_{03}^{(-)}b_{01}^{(-)}-\delta_{03}^{(-)}d_{01}^{(-)}.$$

Each of these three pairs of equations is a 2×2 system which is easily solved analytically. The equations have been written with the unknowns on the left and the knowns on the right—assuming that the pairs are solved successively. Higher-order terms may be found using this procedure but in this paper we will stop calculating after the first nontrivial corrections to the elastic scattering results.

Solving the first pair of equations, we find

$$b_{00}^{(+)}=(-i/3)[(K'-K)/(K'+\tfrac{4}{3}\mu)]A_0, \quad (143)$$
$$d_{00}^{(+)}=[(K+\tfrac{4}{3}\mu)/(K'+\tfrac{4}{3}\mu)]A_0, \quad (144)$$

which are the exact results for scattering from an elastic inhomogeneity.

Solving the second pair of equations gives

$$b_{01}^{(-)}=\left(\frac{K}{C}\right)\frac{iA_0}{3M'\Gamma_+(K'+\frac{4}{3}\mu)}[(C-M\Gamma_-)(K'+\tfrac{4}{3}\mu)$$
$$-(C'-M'\Gamma_-)(K+\tfrac{4}{3}\mu)], \quad (145)$$

and

$$d_{01}^{(-)}=\left(\frac{K}{C}\right)\frac{A_0}{M'\Gamma'_+(K'+\frac{4}{3}\mu)}\times[(C-M\Gamma_-)(K'+\tfrac{4}{3}\mu)-(C'-M'\Gamma'_-)(K+\tfrac{4}{3}\mu)]\,. \tag{146}$$

Comparing (145) to the exact result for $B_0^{(-)}$ in (126) shows that the approximate result is the same as the first two terms of the exact result except for the factor of $(\Gamma_+-\Gamma_-)$ in the denominator of (126). This difference is expected since $\Gamma_+=O(1/\epsilon)$ while $\Gamma_-=O(1)$. Furthermore, this difference is inconsequential at low frequencies since $\Gamma_-\to 0$ in this limit.

Solving the third pair of equations produces

$$b_{01}^{(+)}=-\left(\frac{K}{C}\right)\frac{iA_0}{3(K'+\frac{4}{3}\mu)}(C-M\Gamma_-)\times\left(\frac{C'}{M'}-\frac{C}{M}\right)+b_{01}^{(-)}. \tag{147}$$

The corresponding result for $d_{01}^{(+)}$ is not of direct interest. Again we see that (147) agrees with the first-order corrections contained in (125) as anticipated.

We conclude that this perturbation method works very well for determining the fluid-dependent corrections to the elastic scattering coefficients.

VI. PERTURBATION METHOD FOR $n\geq 1$

For $n=0$, we have split the 4×4 system of equations into two coupled 2×2 systems using the perturbation method. Applying the same idea to the 6×6 systems for $n\geq 1$, we will split each of these problems into one 4×4 system and one 2×2 system. The 4×4 system to lowest order gives the elastic scattering in the absence of fluid effects.

As in (129), we will expand the scattering coefficients as

$$B_n^{(+)}=\frac{\xi_+^{n+3}}{iG_n}\sum_{p=0}^{\infty}\epsilon^p b_{np}^{(+)},\quad B_n^{(-)}=\frac{\xi_-^{n+3}}{iG_n}\sum_{p=1}^{\infty}\epsilon^p b_{np}^{(-)},$$
$$C_n=\frac{\eta^{n+3}}{inG_n}\sum_{p=0}^{\infty}\epsilon^p c_{np}, \tag{148}$$
$$D_n^{(+)}=\frac{(\xi'_+)^{2-n}}{F_n}\sum_{p=0}^{\infty}\epsilon^p d_{np}^{(+)},$$
$$D_n^{(-)}=\frac{(\xi'_+)^{2-n}}{F_n}\sum_{p=1}^{\infty}\epsilon^p d_{np}^{(-)},$$
$$E_n=\frac{(\eta')^{2-n}}{(n+1)F_n}\sum_{p=0}^{\infty}\epsilon^p e_{np},$$

where the numerical coefficients are

$$F_n\equiv 2^n n!/(2n+1)!,\quad G_n=(2n)!/2^n n!\,. \tag{149}$$

Now we need to expand the spherical Bessel functions in (67)–(96) for small arguments and also keep track of the $O(\epsilon)$ contributions to these coefficients. For convenience, we define the special elastic constants

$$\lambda_+\equiv K-\tfrac{2}{3}\mu,\quad \lambda_-\equiv H-2\mu-C\Gamma_+\,. \tag{150}$$

Then, the results become

$$\alpha_{n1}=\mu F_n\xi_+^{n-2}\left\{2(n-1)n-\left[\frac{(n+1)(n+2)}{(2n+3)}+\frac{\lambda_+}{\mu}\right]\xi_+^2\right\}-\epsilon F_n\xi_+^n K(C/M-\Gamma_-)\equiv\bar{\alpha}_{n1}+\epsilon\bar{\bar{\alpha}}_{n1}, \tag{151}$$

$$\beta_{n1}^{(+)}=\pm\frac{\mu iG_n}{\xi_\pm^{n+3}}\left\{2(n+1)(n+2)+\left[\frac{(n-1)n}{(2n-1)}-\frac{\lambda_\pm}{\mu}\right]\xi_\pm^2\right\}-\epsilon\frac{iG_n}{\xi_+^{n+1}}K\left(\frac{C}{M}-\Gamma_-\right)\equiv(\bar{\beta}_{n1}^{(\pm)}+\epsilon\bar{\bar{\beta}}_{n1}^{(+)})\frac{iG_n}{\xi_\pm^{n+3}}, \tag{152}$$

$$\gamma_{n1}=-\mu(n+1)\frac{inG_n}{\eta^{n+3}}\left[2(n+2)+\frac{n}{2n-1}\eta^2\right]\equiv\bar{\gamma}_{n1}\frac{inG_n}{\eta^{n+3}}, \tag{153}$$

$$\delta_{n1}^{(\pm)}=\pm\mu' F_n(\xi'_\pm)^{n-2}\left\{2(n-1)n-\left[\frac{(n+1)(n+2)}{(2n+3)}+\frac{\lambda'_\pm}{\mu'}\right](\xi'_\pm)^2+\left[\frac{(n+3)(n+4)}{4(2n+3)(2n+5)}+\frac{\lambda'_\pm}{2\mu'(2n+3)}\right](\xi'_\pm)^4\right\}$$
$$-\epsilon F_n(\xi'_+)^n\left(\frac{C'}{C}\right)K\left(\frac{C'}{M'}-\Gamma'_-\right)\left[1-\frac{(\xi'_+)^2}{2(2n+3)}\right]\equiv\bar{\delta}_{n1}^{(\pm)}F_n(\xi'_\pm)^{n-2}+\epsilon\bar{\bar{\delta}}_{n1}^{(+)}F_n(\xi'_+)^{n-2}, \tag{154}$$

$$\epsilon_{n1}=\mu' n(n+1)F_n(\eta')^{n-2}\left[2(n-1)-\frac{(n+1)}{(2n+3)}(n')^2+\frac{(n+3)}{4(2n+3)(2n+5)}(\eta')^4\right]\equiv\bar{\epsilon}_{n1}(n+1)F_n(\eta')^{n-2}, \tag{155}$$

$$\alpha_{n2}=\mu F_n\xi_+^{n-2}\left[2(n-1)-\frac{(n+1)}{(2n+3)}\xi_+^2\right], \tag{156}$$

$$\beta_{n2}^{(\pm)}=\mp\frac{\mu iG_n}{\xi_\pm^{n+3}}\left[2(n+2)+\frac{n}{(2n-1)}\xi_\pm^2\right]\equiv\bar{\beta}_{n2}^{(\pm)}\frac{iG_n}{\xi_\pm^{n+3}}, \tag{157}$$

$$\gamma_{n2}=\frac{\mu iG_n}{\eta^{n+3}}\left[2n(n+2)+\frac{(n-1)(n+1)}{(2n-1)}\eta^2\right]\equiv\bar{\gamma}_{n2}\frac{inG_n}{\eta^{n+3}}, \tag{158}$$

$$\delta_{n2}^{(\pm)}=\pm\mu' F_n(\xi'_\pm)^{n-2}\left[2(n-1)-\frac{(n+1)}{(2n+3)}(\xi'_\pm)^2+\frac{(n+3)}{4(2n+3)(2n+5)}(\xi'_\pm)^4\right]\equiv\bar{\delta}_{n2}^{(\pm)}F_n(\xi'_\pm)^{n-2}, \tag{159}$$

$$\epsilon_{n2}=\mu' F_n(\eta')^{n-2}\left[2(n-1)(n+1)-\frac{n(n+2)}{(2n+3)}(\eta')^2+\frac{4n^2+10n+5}{4(2n+3)(2n+5)}(\eta')^4\right]\equiv\bar{\epsilon}_{n2}(n+1)F_n(\eta')^{n-2}, \tag{160}$$

$$\alpha_{n3} = F_n \xi_+^{n-2}\left[n - \frac{(n+2)}{2(2n+3)}\xi_+^2\right], \tag{161}$$

$$\beta_{n3}^{(\pm)} = \mp \frac{iG_n}{\xi_\pm^{n+3}}\left[(n+1) + \frac{(n-1)}{2(2n-1)}\xi_\pm^2\right] \equiv \bar{\beta}_{n3}^{(\pm)} \frac{iG_n}{\xi_\pm^{n+3}}, \tag{162}$$

$$\gamma_{n3} = (n+1)\frac{inG_n}{\eta^{n+3}}\left[1 + \frac{\eta^2}{2(2n-1)}\right] \equiv \bar{\gamma}_{n3}\frac{inG_n}{\eta^{n+3}}, \tag{163}$$

$$\delta_{n3}^{(\pm)} = \pm F_n(\xi'_\pm)^{n-2}\left[n - \frac{(n+2)}{2(2n+3)}(\xi'_\pm)^2 + \frac{(n+4)}{8(2n+3)(2n+5)}(\xi'_\pm)^4\right] \equiv \bar{\delta}_{n3}^{(\pm)} F_n(\xi'_\pm)^{n-2}, \tag{164}$$

$$\epsilon_{n3} = n(n+1)F_n(\eta')^{n-2}\left[1 - \frac{(\eta')^2}{2(2n+3)} + \frac{(\eta')^4}{8(2n+3)(2n+5)}\right] \equiv \bar{\epsilon}_{n3}(n+1)F_n(\eta')^{n-2}, \tag{165}$$

$$\alpha_{n4} = F_n \xi_+^{n-2}[1 - \xi_+^2/2(2n+3)], \tag{166}$$

$$\beta_{n4}^{(\pm)} = \pm \frac{iG_n}{\xi_\pm^{n+3}}\left[1 + \frac{\xi_\pm^2}{2(2n-1)}\right] \equiv \bar{\beta}_{n4}^{(\pm)}\frac{iG_n}{\xi_\pm^{n+3}}, \tag{167}$$

$$\gamma_{n4} = -\frac{iG_n}{\eta^{n+3}}\left[n + \frac{(n-2)}{2(2n-1)}\eta^2\right] \equiv \bar{\gamma}_{n4}\frac{inG_n}{\eta^{n+3}}, \tag{168}$$

$$\delta_{n4}^{(\pm)} = \pm F_n(\xi'_\pm)^{n-2}\left[1 - \frac{(\xi'_\pm)^2}{2(2n+3)} + \frac{(\xi'_\pm)^4}{8(2n+3)(2n+5)}\right] \equiv \bar{\delta}_{n4}^{(\pm)} F_n(\xi'_\pm)^{n-2}, \tag{169}$$

$$\epsilon_{n4} = F_n(\eta')^{n-2}\left[(n+1) - \frac{(n+3)}{2(2n+3)}(\eta')^2 + \frac{(n+5)}{8(2n+3)(2n+5)}(\eta')^4\right] \equiv \bar{\epsilon}_{n4}(n+1)F_n(\eta')^{n-2}, \tag{170}$$

$$\alpha_{n5} = -\epsilon K(1 - (M/C)\Gamma_-)\xi_+^2 \alpha_{n4} \equiv \epsilon\bar{\alpha}_{n5}, \tag{171}$$

$$\beta_{n5}^{(+)} = -\epsilon K(1 - (M/C)\Gamma_-)\xi_+^2 \beta_{n4}^{(+)} \equiv \epsilon\bar{\beta}_{n5}^{(+)} iG_n/\xi_+^{n+3}, \tag{172}$$

$$\beta_{n5}^{(-)} = (M\Gamma_+ - \epsilon K)\xi_-^2 \beta_{n4}^{(-)} \equiv (\bar{\beta}_{n5}^{(-)} + \epsilon\bar{\beta}_{n5}^{(-)}) iG_n/\xi_-^{n+3}, \tag{173}$$

$$\delta_{n5}^{(+)} = -\epsilon(C'/C)K(1 - (M'/C')\Gamma'_-)(\xi'_+)^2\delta_{n4}^{(+)} \equiv \epsilon\bar{\delta}_{n5}^{(+)} F_n(\xi'_+)^{n-2}, \tag{174}$$

$$\delta_{n5}^{(-)} = [M'\Gamma'_+ - \epsilon(C'/C)K](\xi'_-)^2\delta_{n4}^{(-)} \equiv (\bar{\delta}_{n5}^{(-)} + \epsilon\bar{\delta}_{n5}^{(-)}) F_n(\xi'_-)^{n-2}, \tag{175}$$

and

$$\alpha_{n6} = \Gamma_-\alpha_{n3}, \tag{176}$$

$$\beta_{n6}^{(+)} = \Gamma_-\beta_{n3}^{(+)} \equiv \bar{\beta}_{n6}^{(+)} iG_n/\xi_+^{n+3}, \tag{177}$$

$$\beta_{n6}^{(-)} = \frac{1}{\epsilon}\left(\frac{C}{K}\right)\Gamma_+\beta_{n3}^{(-)} \equiv \frac{1}{\epsilon}\dot{\beta}_{n6}^{(-)}\frac{iG_n}{\xi_-^{n+3}}, \tag{178}$$

$$\gamma_{n6} = \Gamma_s\gamma_{n3} \equiv \bar{\gamma}_{n6}\, inG_n/\eta^{n+3}, \tag{179}$$

$$\delta_{n6}^{(+)} = \Gamma'_-\delta_{n3}^{(+)} \equiv \bar{\delta}_{n6}^{(+)} F_n(\xi'_+)^{n-2}, \tag{180}$$

$$\delta_{n6}^{(-)} = \frac{1}{\epsilon}\left(\frac{C}{K}\right)\Gamma'_+\delta_{n3}^{(-)} \equiv \frac{1}{\epsilon}\dot{\delta}_{n6}^{(-)} F_n(\xi'_\pm)^{n-2}, \tag{181}$$

$$\epsilon_{n6} = \Gamma'_s\epsilon_{n3} \equiv \bar{\epsilon}_{n6}(n+1)F_n(\eta')^{n-2}. \tag{182}$$

Substituting (148)–(182) into (66) and collecting terms which multiply the same power of ϵ, we first find the set of equations

$$\begin{aligned}
&\bar{\beta}_{n1}^{(+)}b_{n0}^{(+)} + \bar{\gamma}_{n1}c_{n0} + \bar{\delta}_{n1}^{(+)}d_{n0}^{(+)} + \bar{\epsilon}_{n1}e_{n0} = i^n(2n+1)\bar{\alpha}_{n1}A_0,\\
&\bar{\beta}_{n2}^{(+)}b_{n0}^{(+)} + \bar{\gamma}_{n2}c_{n0} + \bar{\delta}_{n2}^{(+)}d_{n0}^{(+)} + \bar{\epsilon}_{n2}e_{n0} = i^n(2n+1)\bar{\alpha}_{n2}A_0,\\
&\bar{\beta}_{n3}^{(+)}b_{n0}^{(+)} + \bar{\gamma}_{n3}c_{n0} + \bar{\delta}_{n3}^{(+)}d_{n0}^{(+)} + \bar{\epsilon}_{n3}e_{n0} = i^n(2n+1)\bar{\alpha}_{n3}A_0,\\
&\bar{\beta}_{n4}^{(+)}b_{n0}^{(+)} + \bar{\gamma}_{n4}c_{n0} + \bar{\delta}_{n4}^{(+)}d_{n0}^{(+)} + \bar{\epsilon}_{n4}e_{n0} = i^n(2n+1)\bar{\alpha}_{n4}A_0,
\end{aligned} \tag{183}$$

which is exactly the set for elastic scattering from a spherical inhomogeneity. The next set of equations we find is

$$\begin{aligned}
&\bar{\beta}_{n5}^{(-)}b_{n0}^{(-)} + \bar{\delta}_{n5}^{(-)}d_{n0}^{(-)} = i^n(2n+1)\bar{\alpha}_{n5}A_0 - \bar{\beta}_{n5}^{(+)}b_{n0}^{(+)} - \bar{\delta}_{n5}^{(+)}d_{n0}^{(+)}\\
&\dot{\beta}_{n6}^{(-)}b_{n0}^{(-)} + \dot{\delta}_{n6}^{(-)}d_{n0}^{(-)} = i^n(2n+1)\alpha_{n6}A_0 - \bar{\beta}_{n6}^{(+)}b_{n0}^{(+)} - \bar{\gamma}_{n6}c_{n0} - \bar{\delta}_{n6}^{(+)}d_{n0}^{(+)} - \bar{\epsilon}_{n6}e_{n0},
\end{aligned} \tag{184}$$

which determines the lowest-order contributions to the scattered slow compressional wave. The final set of equations we will consider is given by

$$\begin{aligned}
&\bar{\beta}_{n1}^{(+)}b_{n1}^{(+)} + \bar{\gamma}_{n1}c_{n1} + \bar{\delta}_{n1}^{(+)}d_{n1}^{(+)} + \bar{\epsilon}_{n1}e_{n1} = i^n(2n+1)\bar{\alpha}_{n1}A_0 - \bar{\beta}_{n1}^{(+)}b_{n0}^{(+)} - \bar{\beta}_{n1}^{(-)}b_{n1}^{(-)} - \bar{\delta}_{n1}^{(+)}d_{n0}^{(+)} - \bar{\delta}_{n1}^{(-)}d_{n1}^{(-)},\\
&\bar{\beta}_{n2}^{(+)}b_{n1}^{(+)} + \bar{\gamma}_{n2}c_{n1} + \bar{\delta}_{n2}^{(+)}d_{n1}^{(+)} + \bar{\epsilon}_{n2}e_{n1} = -\bar{\beta}_{n2}^{(-)}b_{n1}^{(-)} - \bar{\delta}_{n2}^{(-)}d_{n1}^{(-)},\\
&\bar{\beta}_{n3}^{(+)}b_{n1}^{(+)} + \bar{\gamma}_{n3}c_{n1} + \bar{\delta}_{n3}^{(+)}d_{n1}^{(+)} + \bar{\epsilon}_{n3}e_{n1} = -\bar{\beta}_{n3}^{(-)}b_{n1}^{(-)} - \bar{\delta}_{n3}^{(-)}d_{n1}^{(-)},\\
&\bar{\beta}_{n4}^{(+)}b_{n1}^{(+)} + \bar{\gamma}_{n4}c_{n1} + \bar{\delta}_{n4}^{(+)}d_{n1}^{(+)} + \bar{\epsilon}_{n4}e_{n1} = -\bar{\beta}_{n4}^{(-)}b_{n1}^{(-)} - \bar{\delta}_{n4}^{(-)}d_{n1}^{(-)},
\end{aligned} \tag{185}$$

which determines the first corrections to the ordinary elastic scattering coefficients.

To analyze the solution to (183), it is convenient to introduce column vectors defined by

$$(v_0+\delta v_0)_j \equiv \bar{\alpha}^{(-)}_{nj}/F_n\,\xi_+^{n-2}, \quad (v_1+\delta v_1)_j \equiv \bar{\beta}^{(+)}_{nj},$$
$$(v_2+\delta v_2)_j \equiv \bar{\gamma}_{nj}, \quad (v_3+\delta v_3)_j \equiv \bar{\delta}^{(+)}_{nj}, \tag{186}$$
$$(v_4+\delta v_4)_j \equiv \bar{\epsilon}^{(+)}_{nj}, \quad \text{for } j=1,\ldots,4.$$

The first term on the left-hand side of each expression in (186) is the value of the right-hand side at $\omega=0$. The second term on the left-hand side contains the remaining finite frequency contributions.

The first important observation about (186) is that

$$v_2 \equiv -v_1 \quad \text{and} \quad v_4 \equiv v_3. \tag{187}$$

Then, applying Cramer's rule to (183), we find, for example, that

$$b^{(+)}_{n0} = (N_b/D_n)F_n\xi_+^{n-2}i^n(2n+1)A_0, \tag{188}$$

where

$$D_n = \det(v_1+\delta v_1, -v_1+\delta v_2, v_3+\delta v_3, v_3+\delta v_4) \tag{189}$$

and

$$N_b = \det(v_0+\delta v_0, -v_1+\delta v_2, v_3+\delta v_3, v_3+\delta v_4). \tag{190}$$

Using the properties of determinants,[23] the denominator of (188) becomes

$$D_n = \det(v_1, \delta v_1+\delta v_2, \delta v_3-\delta v_4, v_3)+O(\delta^3), \tag{191}$$

indicating that the lowest-order contributions to D_n are at least $O(\delta^2)=O(\omega^4)$. Similarly, the numerator is given by

$$N_b = \det(v_0, -v_1, \delta v_3-\delta v_4, v_3)+O(\delta^2), \tag{192}$$

for $n\geq 2$ and, furthermore,

$$N_b = \det(v_1, \delta v_0-\delta v_3, \delta v_3-\delta v_4, v_3)+O(\delta^3), \tag{193}$$

for $n=1$, since $v_0 \equiv v_3$ in this case.

Repeating the analysis for c_{n0}, we find

$$N_c = \det(v_1+\delta v_1, v_0+\delta v_0, v_3+\delta v_3, v_3+\delta v_4) = N_b+\cdots, \tag{194}$$

to lowest order in the frequency-dependent corrections for all $n\geq 1$. [See Eqs. (214) and (223) for further discussion of $n\geq 2$.] Thus, we have derived very simply the well-known but important result that

$$c_{n0} = b^{(+)}_{n0}, \quad \text{for } n\geq 1. \tag{195}$$

Another general result for (183), which will be needed in the subsequent calculations, is the value of (191) which may be shown to be

$$D_n = R_n \cdot S_n, \tag{196}$$

where

$$\begin{aligned} R_n &= \{(\bar{\beta}^{(+)}_{n1}+\bar{\gamma}^{(+)}_{n1}) + (n+1)(\bar{\beta}^{(+)}_{n2}+\bar{\gamma}^{(+)}_{n2}) \\ &\quad -2\mu'(n-1)[(\bar{\beta}^{(+)}_{n3}+\bar{\gamma}^{(+)}_{n3}) \\ &\quad +(n+1)(\bar{\beta}^{(+)}_{n4}+\bar{\gamma}^{(+)}_{n4})]\} \\ &= -[\xi^2_+/n(2n-1)\mu] \\ &\quad \times\{\mu[(2n^2+1)\lambda_+ + 2(n^2+n+1)\mu] \\ &\quad +2\mu'(n-1)[(n+1)\lambda_+ + (3n+2)\mu]\} \end{aligned} \tag{197}$$

and

$$\begin{aligned} S_n &= \{(\bar{\delta}^{(+)}_{n1}-\bar{\epsilon}^{(+)}_{n1}) - n(\bar{\delta}^{(+)}_{n2}-\bar{\epsilon}^{(+)}_{n2}) + 2\mu(n+2) \\ &\quad \times[(\bar{\delta}^{(+)}_{n3}-\bar{\epsilon}^{(+)}_{n3}) - n(\bar{\delta}^{(+)}_{n4}-\bar{\epsilon}^{(+)}_{n4})]\} \\ &= -[(\xi'_+)^2/(n+1)(2n+3)\mu] \\ &\quad \times\{\mu'[(2n^2+4n+3)\lambda'_+ + 2(n^2+n+1)\mu'] \\ &\quad +2\mu(n+2)[n\lambda'_+ + (3n+1)\mu']\}, \end{aligned} \tag{198}$$

to the lowest order in frequency. The relatively simple result (196) follows from (191) after some manipulation and noting the interesting intermediate results that

$$\begin{aligned} &\{(\bar{\beta}^{(+)}_{n1}+\bar{\gamma}^{(+)}_{n1}) - n(\bar{\beta}^{(+)}_{n2}+\bar{\gamma}^{(+)}_{n2}) \\ &\quad +2\mu(n+2)[\bar{\beta}^{(+)}_{n3}+\bar{\gamma}^{(+)}_{n3} - n(\bar{\beta}^{(+)}_{n4}+\bar{\gamma}^{(+)}_{n4})]\} = 0, \end{aligned} \tag{199}$$

$$\begin{aligned} &\{(\bar{\delta}^{(+)}_{n1}-\bar{\epsilon}^{(+)}_{n1}) + (n+1)(\bar{\delta}^{(+)}_{n2}-\bar{\epsilon}^{(+)}_{n2}) \\ &\quad -2\mu'(n-1)[\bar{\delta}^{(+)}_{n3}-\bar{\epsilon}^{(+)}_{n3} \\ &\quad +(n+1)(\bar{\delta}^{(+)}_{n4}-\bar{\epsilon}^{(+)}_{n4})]\} = 0, \end{aligned}$$

to the order at which we are working.

It is also convenient to analyze (184) for all $n\geq 1$ before proceeding to the special cases. The 2×2 system is easily solved. The important elements of the solution are the determinant of the coefficients

$$\bar{\beta}^{(-)}_{n5}\dot{\bar{\delta}}^{(-)}_{n6} - \dot{\bar{\beta}}^{(-)}_{n6}\bar{\delta}^{(-)}_{n5} = (C/K)\Gamma_+\Gamma'_+[nM\xi^2_- + (n+1)M'(\xi'_-)^2] + O(\xi^4_-) \tag{200}$$

and the various combinations relevant to $b^{(-)}_{n0}$,

$$\begin{aligned} &\dot{\bar{\delta}}^{(-)}_{n6}\bar{\alpha}_{n5} - \bar{\delta}^{(-)}_{n5}\alpha_{n6} \\ &\quad = F_n\xi_+^{n-2}\{n\Gamma'_+[(C-M\Gamma_-)\xi^2_+ \\ &\qquad + M'\Gamma_-(\xi'_-)^2] + O((\xi'_-)^4)\}, \end{aligned} \tag{201}$$

$$\begin{aligned} &\bar{\delta}^{(-)}_{n5}(\bar{\beta}^{(+)}_{n6}+\gamma_{n6}) - \dot{\bar{\delta}}^{(-)}_{n6}\bar{\beta}^{(+)}_{n5} \\ &\quad = -\Gamma'_+[n(C-M\Gamma_-)\xi^2_+ + (n+1)M' \\ &\qquad \times(\Gamma_- - \Gamma_s)(\xi'_-)^2] + O((\xi'_-)^4), \end{aligned} \tag{202}$$

$$\begin{aligned} &\bar{\delta}^{(-)}_{n5}\bar{\delta}^{(+)}_{n6} - \dot{\delta}_{n6}\bar{\delta}^{(+)}_{n5} \\ &\quad = -n\Gamma'_+[(C'-M'\Gamma'_-)(\xi'_+)^2 \\ &\qquad + M'\Gamma'_-(\xi'_-)^2] + O((\xi'_-)^4), \end{aligned} \tag{203}$$

and

$$\bar{\delta}^{(-)}_{n5}\bar{\epsilon}_{n6} = -n\Gamma'_+ M'\Gamma'_s(\xi'_-)^2 + O((\xi'_-)^4). \tag{204}$$

Equations (201)–(204) may be simplified somewhat in the long-wavelength limit. The frequency dependence as $\omega\to 0$ of the various terms may be shown to be

$$\xi^2_+ = O(\omega^2), \quad \xi^2_- = O(\omega), \quad \Gamma_- = O(\omega),$$
$$\Gamma_s = O(\omega), \quad \Gamma_- - \Gamma_s = O(\omega^{3/2}). \tag{205}$$

These relations will be used in our final results.

We now proceed to a more detailed analysis of the special cases.

A. $n=1$

For $n=1$, the relevant determinants are

$$D_1 = \tfrac{8}{10}\left[\mu\eta^2(\xi'_+)^2/\mu'\right]\left[\mu'(3\lambda'+2\mu')+2\mu(\lambda'+4\mu')\right], \tag{206}$$

$$\begin{aligned} N_b = N_c &= -3\left[v_{01}-\bar{\delta}_{11}^{(+)}+2(v_{02}-\bar{\delta}_{12}^{(+)})\right]\{\bar{\delta}_{12}^{(+)}-\bar{\epsilon}_{12}^{(+)} \\ &\quad -2\mu\left[(\bar{\delta}_{13}^{(+)}-\epsilon_{13})-(\bar{\delta}_{14}^{(+)}-\epsilon_{14})\right]\} \\ &= -\tfrac{3}{10}\left[\mu\eta^2(\xi'_+)^2/\mu'\right](\rho'/\rho-1) \\ &\quad \times\left[\mu'(3\lambda'+2\mu')+2\mu(\lambda'+4\mu')\right], \end{aligned} \tag{207}$$

$$\begin{aligned} N_d &= \det(v_1,\delta v_1+\delta v_2,\delta v_0-\delta v_4,v_3) \\ &= -3\{\left[\bar{\beta}_{11}^{(+)}+\bar{\gamma}_{11}^{(+)}+2(\bar{\beta}_{12}^{(+)}+\bar{\gamma}_{12}^{(+)})\right] \\ &\quad \times\left[v_{02}-\bar{\epsilon}_{12}^{(+)}-2\mu(v_{03}-\bar{\epsilon}_{13}^{(+)}-(v_{04}-\bar{\epsilon}_{14}^{(+)}))\right] \\ &\quad -\left[v_{01}-\bar{\epsilon}_{11}^{(+)}+2(v_{02}-\bar{\epsilon}_{12}^{(+)})\right]\left[\bar{\beta}_{12}^{(+)}+\bar{\gamma}_{12}^{(+)}\right. \\ &\quad \left.-2\mu(\bar{\beta}_{13}^{(+)}+\bar{\gamma}_{13}^{(+)}-(\bar{\beta}_{14}^{(+)}+\bar{\gamma}_{14}^{(+)}))\right]\} \\ &= -3\mu\eta^2\left[(\rho'/\rho-1)\eta^2\mu-\tfrac{3}{10}(\eta')^2(2\mu+3\mu')\right], \end{aligned} \tag{208}$$

and

$$\begin{aligned} N_e &= \det(v_1,\delta v_1+\delta v_2,\delta v_3-\delta v_0,v_3) \\ &= -3\{\left[\bar{\beta}_{11}^{(+)}+\bar{\gamma}_{11}^{(+)}+2(\bar{\beta}_{12}^{(+)}+\bar{\gamma}_{12}^{(+)})\right] \\ &\quad \times\left[\bar{\delta}_{12}^{(+)}-\bar{v}_{02}^{(+)}-2\mu(\bar{\delta}_{13}^{(+)}-\bar{v}_{03}^{(+)}-(\bar{\delta}_{14}^{(+)}-\bar{v}_{04}^{(+)}))\right] \\ &\quad -\left[\bar{\delta}_{11}^{(+)}-v_{01}+2(\bar{\delta}_{12}^{(+)}-v_{02})\right]\left[\bar{\beta}_{12}^{(+)}+\bar{\gamma}_{12}^{(+)}\right. \\ &\quad \left.-2\mu(\bar{\beta}_{13}^{(+)}+\bar{\gamma}_{13}^{(+)}-(\bar{\beta}_{14}^{(+)}+\bar{\gamma}_{14}^{(+)}))\right] \\ &= 3\mu\eta^2\left[(\rho'/\rho-1)\eta^2\mu+\tfrac{6}{5}(\xi'_+)^2(\mu-\mu')\right]. \end{aligned} \tag{209}$$

The scattering coefficients for $n=1$ to lowest order are therefore

$$\begin{aligned} b_{10}^{(+)} &= c_{10} = (N_b/D_1)\,\xi_+^{-1}3iF_1A_0 \\ &= (i/3\xi_+)(1-\rho'/\rho)A_0, \end{aligned} \tag{210}$$

$$\begin{aligned} d_{10}^{(+)} &= (N_d/D_1)\,\xi_+^{-1}3iF_1A_0 \\ &= (i/\xi_+)(\lambda'_+ + 2\mu') \\ &\quad \times\frac{\left[\frac{10}{3}(\rho/\rho'-1)\mu'+(2\mu+3\mu')\right]}{\left[\mu'(3\lambda'+2\mu')+2\mu(\lambda'_+ + 4\mu')\right]}A_0, \end{aligned} \tag{211}$$

and

$$\begin{aligned} e_{10} &= (N_e/D_1)\xi_+^{-1}3iF_1A_0 \\ &= \frac{i\mu'}{\xi_+}\frac{\left[\frac{10}{3}(1-\rho/\rho')(\lambda'_+ + 2\mu')+4(\mu-\mu')\right]}{\left[\mu'(3\lambda'+2\mu')+2\mu(\lambda'+4\mu')\right]}A_0. \end{aligned} \tag{212}$$

The result (210) is well known but the other results (211) and (212) are usually not needed in analyzing the scattering from an elastic inhomogeneity. It is interesting to note that (210) and (212) vanish identically if the spherical inclusion has the same elastic properties as the host medium. Equation (211) does not vanish in this case since $d_{n0}^{(+)}$ determines the coupling of the exterior compressional wave to the interior one. Then (211) reduces to iA_0/ξ_+ as expected.

Using (200)–(204) and (210)–(212) in the solution of (184), we find

$$\begin{aligned} b_{11}^{(-)} &= \left(\frac{K}{C}\right)\frac{iA_0}{\xi_+}\frac{1}{\left[M\xi_-^2+2M'(\xi'_-)^2\right]} \\ &\quad \times\left\{C\xi_+^2\,\frac{1}{3}\left(4-\frac{\rho'}{\rho}\right)+M'(\Gamma_- - \Gamma'_-)(\xi'_-)^2\right. \\ &\quad -C'(\xi'_+)^2(\lambda'_+ + 2\mu') \\ &\quad \left.\times\frac{\left[\frac{10}{3}(\rho/\rho'-1)+(2\mu+3\mu')\right]}{\left[\mu'(3\lambda'_+ + 2\mu')+2\mu(\lambda'_+ + 4\mu')\right]}\right\}. \end{aligned} \tag{213}$$

We have used (205) in simplifying (213). Also notice that, if the spherical inclusion has the same properties as the host medium, (213) vanishes identically as expected.

B. $n\geqslant 2$

For $n\geqslant 2$, the relevant determinants are (196) and

$$\begin{aligned} N_b = N_c &= \det(v_0,-v_1,\delta v_3-\delta v_4,v_3) \\ &= 2(2n+1)(\mu-\mu')(n-1)\{(\delta_{n1}-\epsilon_{n1})-n(\delta_{n2}-\epsilon_{n2}) \\ &\quad +2\mu(n+2)\left[(\delta_{n3}-\epsilon_{n3})-n(\delta_{n4}-\epsilon_{n4})\right]\} \\ &= \frac{2(n-1)(2n+1)(\mu'-\mu)(\xi'_+)^2}{(n+1)(2n+3)\mu'} \\ &\quad \times\{\mu'\left[(2n^2+4n+3)\lambda'_+\right. \\ &\quad \left.+2(n^2+n+1)\mu'\right] \\ &\quad +2(n+2)\mu\left[n\lambda'_+ + (3n+1)\mu'\right]\}, \end{aligned} \tag{214}$$

$$\begin{aligned} N_d &= \det(v_1,\delta v_1+\delta v_2,v_0,v_s)+O(\delta^2) \\ &= 2(n-1)(2n+1)(\mu'-\mu)\{\left[\beta_{n1}^{(+)}+\bar{\gamma}_{n1}^{(+)}\right. \\ &\quad \left.-n(\bar{\beta}_{n2}^{(+)}+\bar{\gamma}_{n2}^{(+)})\right]+2(n+2)\mu\left[\bar{\beta}_{n3}^{(+)}+\bar{\gamma}_{n3}^{(+)}\right. \\ &\quad \left.-n(\bar{\beta}_{n4}^{(+)}+\bar{\gamma}_{n4}^{(+)})\right]\}+O(\delta^2)=0+O(\delta^2), \end{aligned} \tag{215}$$

using (199) and similarly

$$\begin{aligned} N_e &= -\det(v_1,\delta v_1+\delta v_2,v_0,v_3)+O(\delta^2) \\ &= 0+O(\delta^2). \end{aligned} \tag{216}$$

The scattering coefficients for $n\geqslant 2$ to lowest order are therefore

$$\begin{aligned} b_{n0}^{(+)} &= c_{n0}(N_b/D_n)\,F_n\xi_+^{n-2}i^n(2n+1)A_0 \\ &= 2(n-1)n(2n-1)(2n+1)^2F_n\,\mu(\mu-\mu')\xi_+^{n-4}i^nA_0 \\ &\quad \times\{\mu\left[(2n^2+1)\lambda_+ + 2(n^2+n+1)\mu\right] \\ &\quad +2\mu'(n-1)\left[(n+1)\lambda_+ + (3n+2)\mu\right]\}^{-1} \end{aligned} \tag{217}$$

and

$$d_{n0}^{(+)} = e_{n0} = 0+O(b_{n0}^{(+)}\delta). \tag{218}$$

In particular, we find that

$$b_{20}^{(+)} = c_{20} = \frac{20\mu(\mu'-\mu)A_0}{\xi_+^2\left[\mu(9\lambda_+ + 14\mu)+2\mu'(3\lambda_+ + 8\mu)\right]} \tag{219}$$

and

$$d_{20}^{(+)} = e_{20} = 0. \tag{220}$$

Using (200) – (204), (217), and (218) to solve (184), we find to lowest order in frequency that

$$b_{n1}^{(-)} = -\left(\frac{K}{C}\right)\frac{n(C-M\Gamma_-)\xi_+^2\, b_{n0}^{(+)}}{[nM\xi_-^2 + (n+1)M'(\xi'_-)^2]} + \text{higher-order terms}. \quad (221)$$

In particular, we find that

$$b_{21}^{(+)} = -(K/C)\,40\mu(\mu'-\mu) \times CA_0\{[2M\xi_-^2 + 3M'(\xi'_-)^2] \times [\mu(9\lambda_+ + 14\mu) + 2\mu'(3\lambda_+ + 8\mu)]\}^{-1}, \quad (222)$$

using (205) again to simplify the final result.

Although (221) is the dominant term in many situations, it vanishes identically when $\mu' = \mu$. Since the case $\mu' = \mu$ is important in applications of these results, we must reconsider the analysis for $n \geqslant 2$ when the host and inclusion shear moduli are the same. First, note that $v_0 = v_3$ for $n \geqslant 2$ if $\mu = \mu'$. Then, we find

$$\begin{aligned} N_b &= N_c = \det(v_1, \delta v_0 - \delta v_4, \delta v_3 - \delta v_4, v_3) \\ &= S_n\{v_{01} - \bar{\epsilon}_{n1}^{(+)} + (n+1)(v_{02} - \bar{\epsilon}_{n2}^{(+)}) \\ &\quad - 2\mu(n-1)[v_{03} - \bar{\epsilon}_{n3}^{(+)} + (n+1)(v_{04} - \bar{\epsilon}_{n4}^{(+)})]\} \\ &= \eta^2\mu(\rho'/\rho - 1)S_n, \end{aligned} \quad (223)$$

$$\begin{aligned} N_d &= \det(v_1, \delta v_1 + \delta v_2, \delta v_0 - \delta v_4, v_3) \\ &= R_n\{v_{01} - \bar{\epsilon}_{n1}^{(+)} - n(v_{02} - \bar{\epsilon}_{n2}^{(+)}) \\ &\quad + 2\mu(n+2)[v_{03} - \bar{\epsilon}_{n3}^{(+)} - n(v_{04} - \bar{\epsilon}_{n4}^{(+)})]\} \\ &= -\eta^2\mu(1 + [n/(n+1)](\rho'/\rho))R_n, \end{aligned} \quad (224)$$

and

$$\begin{aligned} N_e &= \det(v_1, \delta v_1 + \delta v_2, \delta v_3 - \delta v_0, v_3) \\ &= R_n\{\bar{\delta}_{n1}^{(+)} - v_{01} - n(\bar{\delta}_{n2}^{(+)} - v_{02}) \\ &\quad + 2\mu(n+2)[\bar{\delta}_{n3}^{(+)} - v_{03} - n(\bar{\delta}_{n4}^{(+)} - v_{04})]\} \\ &= \eta^2\mu(1 - \rho'/\rho)R_n, \end{aligned} \quad (225)$$

where R_n and S_n are defined in (197) and (198).

Thus, when $\mu' = \mu$,

$$b_{n0}^{(+)} = c_{n0} = \frac{\eta^2\mu(\rho'/\rho - 1)}{R_n} F_n\, \xi_+^{n-2}\, i^n(2n+1)A_0, \quad (226)$$

$$d_{n0}^{(+)} = -\frac{\eta^2\mu(1 + [n/(n+1)](\rho'/\rho))}{S_n} \times F_n\, \xi_+^{n-2} i^n(2n+1)A_0 \quad (227)$$

and

$$e_{n0} = [\eta^2\mu(1 - \rho'/\rho)/S_n]\, F_n\, \xi_+^{n-2} i^n(2n+1)A_0, \quad (228)$$

where R_n and S_n simplify to become

$$R_n = -[(2n+1)/n]\,\eta^2\mu, \quad (229)$$

$$S_n = -[(2n+1)/(n+1)](\eta')^2\mu. \quad (230)$$

Thus, we find

$$b_{n0}^{(+)} = c_{n0} = (1 - \rho'/\rho)\, F_n\, \xi_+^{n-2} i^n n\, A_0, \quad (231)$$

$$d_{n0}^{(+)} = [\rho/\rho' + n/(n+1)]\, F_n\, \xi_+^{(n-2)}\, i^n(n+1)A_0, \quad (232)$$

$$e_{n0} = (1 - \rho/\rho')\, F_n\, \xi_+^{n-2}\, i^n(n+1)A_0. \quad (233)$$

Using (200)–(204) and (231)–(233) to solve (184), we find

$$b_{n1}^{(-)} = \left(\frac{K}{C}\right)\frac{nF_n\xi_+^{n-2} i^n A_0}{\Gamma_+[nM\xi_-^2 + (n+1)M'(\xi'_-)^2]} \times \left\{(n+1)\left[C\xi_+^2\left(1 + \frac{n}{n+1}\frac{\rho'}{\rho}\right)\right] - \left[C'(\xi'_+)^2\left(\frac{\rho}{\rho'} + \frac{n}{n+1}\right) + (2n+1)M'(\Gamma_- - \Gamma'_-)(\xi'_-)^2\right\}, \quad (234)$$

which is valid only for inhomogeneities that satisfy $\mu' = \mu$.

The analysis of the leading terms in the expansion for the slow-wave scattering coefficients is now complete. To obtain the first corrections to the elastic scattering coefficients due to pore-fluid effects, we must solve (185). To do so, we would need $d_{n1}^{(-)}$ in addition to the coefficients $b_{n0}^{(+)}$, $d_{n0}^{(+)}$, and $b_{n1}^{(-)}$ which we have already obtained. Since the analysis needed to derive $d_{n1}^{(-)}$ is straightforward but tedious and since these correction terms are of doubtful importance, we will not calculate $d_{n1}^{(-)}$ here. We will, however, present the general form of the solution for $b_{n1}^{(+)}$ since it follows quite easily from the algorithm developed for solving (183).

The denominator in Cramer's rule for (185) is the same as for (183) and is given by (196). The determinant in the numerator of $b_{n1}^{(+)}$ is

$$N_b = \det(v_5 + \delta v_5, -v_1 + \delta v_1, \delta v_3 - \delta v_4, v_3 + \delta v_4), \quad (235)$$

where the new column vector is chosen to be

$$(v_5 + \delta v_5)_1 = [\, i^n(2n+1)\bar{\alpha}_{n1}\, A_0 - \bar{\beta}_{n1}^{(+)} b_{n0}^{(+)} - \bar{\beta}_{n1}^{(-)} b_{n1}^{(-)} - \bar{\delta}_{n1}^{(+)} d_{n0}^{(+)} - \bar{\delta}_{n1}^{(-)} d_{n1}^{(-)}]/b_{n1}^{(-)}, \quad (236)$$

$$(v_5 + \delta v_5)_j = -[\,\bar{\beta}_{nj}^{(-)} b_{n1}^{(-)} + \bar{\delta}_{nj}^{(-)} d_{n1}^{(-)}]/b_{n1}^{(-)}, \text{ for } j = 2-4.$$

To lowest order in frequency,

$$N_b = \det(v_5, -v_1, \delta v_3 - \delta v_4, v_3) = -S_n\{v_{51} + (n+1)v_{52} - 2\mu'(n-1)[v_{53} + (n+1)v_{54}]\}, \quad (237)$$

where S_n is again given by (198). Furthermore, using the fact that $\lambda_- = -2\mu$ at low frequencies, we have

$$\{\bar{\beta}_{n1}^{(-)} + (n+1)\bar{\beta}_{n2}^{(-)} - 2\mu'(n-1)[\bar{\beta}_{n3}^{(-)} + (n+1)\bar{\beta}_{n4}^{(-)}]\} = -[2(n-1)/(2n-1)]\,\xi_-^2(\mu - \mu') \quad (238)$$

and

$$\{\bar{\delta}_{n1}^{(-)} + (n+1)\bar{\delta}_{n2}^{(-)} - 2\mu'(n-1)[\bar{\delta}_{n3}^{(-)} + (n+1)\bar{\delta}_{n4}^{(-)}]\} = [n(n-1)/(2n+3)](\xi'_-)^2\mu'. \quad (239)$$

Equations (238) and (239) may be used to simplify (237) and the result is then substituted into

$$b_{n1}^{(+)} = (N_b/D_n)b_{n1}^{(-)}. \quad (240)$$

Once $d_{n1}^{(-)}$ is known, (236)–(240) may be used to find $b_{n1}^{(+)}$.

The analysis of all first-order corrections to the elastic scattering coefficients is now complete.

VII. DISCUSSION

In this paper, we have derived the multipole scattering coefficients in a fluid-saturated porous medium. In the long-

wavelength limit, the exact analytical expressions were obtained for $n = 0$ and approximate expressions were obtained for $n \gg 1$. A small parameter expansion was presented which treats all pore-fluid effects as perturbations to the elastic scattering in the dry porous frame. The first terms in the slow-wave multipole expansion were calculated explicitly. The general formula for obtaining the lowest-order fluid-dependent corrections to the usual elastic scattering coefficients was also presented.

These results have a multitude of possible applications. One straightforward application is the calculation of energy loss from elastic waves due to scattering by randomly distributed particles.[6] The attenuation of elastic waves may be estimated directly from the results of such an analysis. A second important application is to the estimation of (low-frequency) effective constants for composite porous media containing multiple pore fluids. In fact, it is not difficult to show by using techniques already established for elastic materials[8] that (126) leads to the Reuss average[24] (or Woods formula) for the effective low-frequency bulk modulus of a composite fluid and that (213) leads to known effective medium results for the permeability of a composite porous medium.[25]

Detailed discussion of the applications of these results will be presented elsewhere.

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A mean-field solution of the reflection of a spherical acoustic wave from a rough interface

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We use mean-field methods to calculate the reflection by a rough interface of incident acoustic waves emanating from a point source. The calculation is accurate to second order in roughness height. For the special cases of very long and very short roughness wavelengths, we find closed-form expressions for the reflected field. We give special attention to the head-wave arrival and find the roughness can attenuate *or* enhance head-wave arrival amplitude depending on the velocities and densities of the media. The roughness can also cause a delay of the head-wave arrival though the apparent velocity is not changed (to second-order accuracy). As a prerequisite to the rough-interface calculation, we consider a smooth interface and find an asymptotic method of calculating the reflected field which avoids severe distortions of the path of integration.

I. INTRODUCTION

Head-wave arrivals are essentially a diffraction phenomenon arising from waves which graze an interface at near-critical angles. We expect that small roughness in the shape of the interface can alter significantly the interaction of these waves with the interface. This paper addresses this question by examining the reflection from a rough interface of acoustic waves generated by a point source.

We assume that the roughness is small on the scale of the acoustical wavelength being considered. Rather than use standard perturbative methods, however, we use mean-field techniques.[1-5] These methods allow a description of the repeated scattering of waves as they graze along the rough interface. For the special cases of very long and very short roughness wavelengths, we are able to arrive at closed-form expressions which show that the roughness can alter both the amplitude and arrival time of the head wave, though to second order in the roughness height there is no change in the apparent velocity of the arrival. In particular, for the very rough case, the analysis shows that it is possible for the roughness to cause an *increase* in the amplitude of the head-wave arrival.

Before considering a rough interface we consider the flat case. Well-known methods of asymptotically evaluating the reflection of spherical waves from plane boundaries[6] resort to severe distortions of paths of integration. We present a method where only small distortions are necessary. Not only does this method allow one to study the more complex problem where roughness is present, it also gives a more accurate value of the overall amplitude of the smooth boundary head-wave arrival.

II. A SMOOTH INTERFACE

The acoustic waves are governed by the equation

$$\rho\nabla\cdot(\rho^{-1}\nabla p)+\omega^2 s^2 p=0, \tag{1}$$

where p is the pressure field while ρ and s are the position-dependent density and slowness. We wish to put a smooth boundary at $z=0$ so that ρ and s take on the values ρ_1 and s_1 (ρ_2 and s_2) for $z>0$ ($z<0$).

We will use the convention of representing a three-dimensional vector by lowercase letters and its projection in the x–y plane by uppercase letters; for example, a three-dimensional position vector is written $\mathbf{r}=(\mathbf{R},z)$ with $\mathbf{R}=(x,y)$. Wave vectors are denoted in a similar fashion. In medium 1, a plane-wave component satisfying Eq. (1) has a three-dimensional wave vector $(\mathbf{K},k_1)$ with the z component

$$k_1=(\omega^2 s_1^2-K^2)^{1/2}. \tag{2}$$

The root in Eq. (2) is always taken such that $\mathrm{Im}\{k_1\}\geqslant 0$. Likewise, in medium 2, we have the three-dimensional wave vector $(\mathbf{K},k_2)$ with the z component

$$k_2=(\omega^2 s_2^2-K^2)^{1/2}, \tag{3}$$

with $\mathrm{Im}\,(k_2)\leqslant 0$.

A point source is located on the positive z axis at z_0. The incident field is

$$P_{\mathrm{inc}}(\mathbf{r})=\frac{i}{2\pi}\int d\mathbf{K}\,\frac{e^{i\mathbf{K}\cdot\mathbf{R}+ik_1|z-z_0|}}{k_1} \tag{4a}$$

$$=i\int_0^\infty J_0(KR)k_1^{-1}e^{ik_1|z-z_0|}K\,dk. \tag{4b}$$

Inspection of Eq. (1) shows that p and the normal derivative $\rho^{-1}\,\partial p/\partial n$ must be continuous across the boundary. Thus, the reflection coefficient for an incident plane-wave component of the source field is

$$B=\frac{\rho_2 k_1-\rho_1 k_2}{\rho_2 k_1+\rho_1 k_2}. \tag{5}$$

Since (4a) is an integral over plane waves, we have the reflected field

$$P_{\mathrm{refl}}=i\int_0^\infty\left\{\frac{\omega^2\rho_1^2(s_2^2-s_1^2)+(\rho_1^2+\rho_2^2)k_1^2-2\rho_1\rho_2 k_1 k_2}{\omega^2(\rho_2^2 s_1^2-\rho_1^2 s_2^2)+K^2(\rho_1^2-\rho_2^2)}\right\}\times\frac{J_0(KR)e^{ik_1(z+z_0)}}{k_1}K\,dK. \tag{6}$$

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The factor in braces is B after rationalizing the denominator. The rationalization causes an apparent pole; the residue is zero, however, so it does not contribute to the total response of the system. Defining $z_* = |z + z_0|$, (6) can be expressed as

$$P_{\text{refl}} = i\left[\omega^2\rho_1^2(s_2^2 - s_1^2)I_1 - (\rho_1^2 + \rho_2^2)\frac{\partial^2 I_1}{\partial z_*^2} - 2\rho_1\rho_2 I_2\right], \tag{7}$$

where

$$I_1 = \int_0^\infty \frac{K\,dK\,J_0(KR)e^{ik_1 z_*}}{k_1[\omega^2(\rho_2^2 s_1^2 - \rho_1^2 s_2^2) + K^2(\rho_1^2 - \rho_2^2)]} \tag{8}$$

and

$$I_2 = \int_0^\infty \frac{K\,dK\,k_2 J_0(KR)e^{ik_1 z_*}}{[\omega^2(\rho_2^2 s_1^2 - \rho_1^2 s_2^2) + K^2(\rho_1^2 - \rho_2^2)]}. \tag{9}$$

We are interested in propagating disturbances at large distances from the source. Hence in (8) and (9), we can restrict the range of integration to $0 \leqslant K \leqslant \omega s_1$ and use the asymptotic representation for the Bessel function

$$J_0(KR) \sim (2/\pi KR)^{1/2}\cos(KR - \pi/4). \tag{10}$$

When using (10) in (8) and (9), stationary points occur only for the component of the cosine in (10) varying as $\frac{1}{2}\exp[i(KR - \pi/4)]$. Thus, retaining this term in each of the integrals and making the variable changes

$$K = \omega s_1 \sin\theta \tag{11}$$

and

$$z_* = \mu\cos\phi \quad \text{and} \quad R = \mu\sin\phi, \tag{12}$$

we obtain

$$I_1 \simeq e^{-i\pi/4}(\omega s_1)^{-2}\left(\frac{\omega s_1}{2\pi R}\right)^{1/2}\int_0^{\pi/2}\frac{d\theta(\sin\theta)^{1/2}}{a + b\sin^2\theta} \times e^{i\omega s_1\mu\cos(\theta-\phi)}, \tag{13}$$

$$I_2 \simeq e^{-i\pi/4}\left(\frac{\omega s_1}{2\pi R}\right)^{1/2}\int_0^{\pi/2}\frac{d\theta\cos\theta(\sin\theta)^{1/2}}{a + b\sin^2\theta} \times (s_2^2/s_1^2 - \sin^2\theta)^{1/2} e^{i\omega s_1\mu\cos(\theta-\phi)}, \tag{14}$$

where

$$a = \rho_2^2 - \rho_1^2(s_2^2/s_1^2) \quad \text{and} \quad b = \rho_1^2 - \rho_2^2. \tag{15}$$

Evaluation of (13) and (14) by the method of steepest descents is then in line with the asymptotic development of the far field. The factor $(\sin\theta)^{1/2}$ in (13) and (14) is caused by the asymptotic expansion of $J_0(KR)$. Thus stationary points near $\theta = 0$ caused by this factor are only apparent and we can see from (8), (9), and (11) that actually there are no stationary phase contributions near $\theta = K = 0$.

The phase in (13) has a stationary point at $\theta = \phi$. A steepest descents evaluation then gives

$$I_1 \simeq -i(\omega s_1)^2\frac{\mu}{a\mu^2 + bR^2}e^{i\omega s_1\mu}. \tag{16}$$

To evaluate (14), we recognize that the factor $(s_2^2/s_1^2 - \sin^2\theta)^{1/2}$ is rapidly varying when $s_2/s_1 < 1$ and θ approaches the critical angle θ_c,

$$\sin\theta_c = s_2/s_1. \tag{17}$$

This variation is most easily handled by including the factor $(\sin^2\theta_c - \sin^2\theta)^{1/2}$ in the phase

$$I_2 \simeq e^{-i\pi/4}\left(\frac{\omega s_1}{2\pi R}\right)^{1/2}\int_0^{\pi/2}\frac{d\theta\cos\theta(\sin\theta)^{1/2}}{a + b\sin^2\theta} \times \exp[iN\cos(\theta - \phi) + \tfrac{1}{2}\ln(s_2^2/s_1^2 - \sin^2\theta)], \tag{18}$$

where

$$N = \omega s_1\mu \gg 1. \tag{19}$$

Let the exponent in (18) be ψ. The stationary points of ψ are at the roots of

$$\sin(\theta - \phi)(\sin^2\theta_c - \sin^2\theta) = (i/2N)\sin 2\theta. \tag{20}$$

We shall concentrate on evaluating the head-wave contribution from the I_2 integral in the regime $\phi \geqslant \theta_c$ as have others.[6–10]

Only in the case $\phi \geqslant \theta_c$ does the head wave arrive, so that, despite having a much smaller amplitude than the direct wave, the head wave can be cleanly and clearly recognized. Therefore, throughout the remainder of this paper we discuss the head wave only in the regime $\phi \geqslant \theta_c$. See Fig. 1.

Case (a) Separate stationary points: If $|\phi - \theta_c| \gtrsim O(N^{-1/2})$, and $\phi > \theta_c$, one root occurs at

$$\theta_1 = \phi + O(N^{-1}) \tag{21}$$

and another at

$$\theta_2 = \theta_c + (i/2N)[1/\sin(\phi - \theta_c)] + O(N^{-2}). \tag{22}$$

The steepest descents evaluation of the contribution at θ_1 is

$$I_2|_{\theta_1} = -i\frac{z_*}{a\mu^2 + bR^2}\left(\frac{s_2^2}{s_1^2} - \frac{R^2}{\mu^2}\right)^{1/2}e^{i\omega s_1\mu}. \tag{23}$$

When contributions (23) and (16) are substituted into (7), one obtains the specularly reflected contribution to the reflected field

$$B\mu^{-1}\exp(i\omega s_1\mu), \tag{24}$$

where B is evaluated at $K = \omega s_1\sin\theta$.

The steepest descents evaluation at θ_2 gives the head-wave contribution. The values of the exponent and its second derivative at the stationary point are

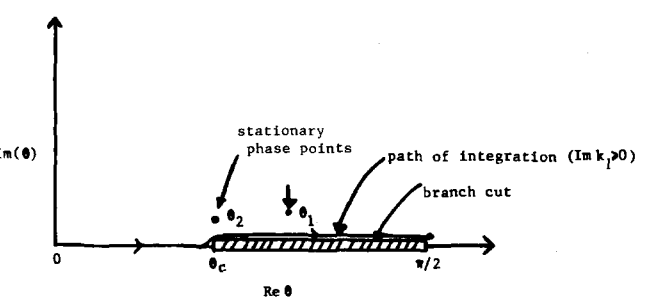

FIG. 1. A sketch of the asymptotic ($s,\omega r \gg 1$) path of integration in θ space. The stationary phase points θ_1 and θ_2, corresponding to Eq. (21) and (22), are marked. This path of integration should be compared and contrasted with that given by Fig. 6.9 of Aki and Richards[6] for general integration of the reflected wave amplitude, not just in the asymptotic regime. The simplification afforded by asymptotic evaluation (this figure) of the head-wave integral is apparent.

$$\psi = iN\cos(\theta_c - \phi) - \frac{1}{2} + \frac{1}{2}\ln\left(\frac{-i\sin 2\theta_c}{2N\sin(\phi-\theta_c)}\right) + O(N^{-1}), \tag{25}$$

$$\psi'' = -iN\left(\frac{(1+\sin^2\theta_c)\sin\phi}{\sin\theta_c} + \frac{(1+\cos^2\theta_c)\cos\phi}{\cos\theta_c}\right) + 2N^2\sin^2(\theta_c - \phi) + O(1). \tag{26}$$

The first term in (26) determines the sign on the phase factor coming from the stationary phase evaluation of the integral. We obtain

$$I_2|_{\theta_2} = \frac{1}{\omega s_1}\frac{\sin\theta_c}{(2eR)^{1/2}}\left(\frac{\cos\theta_c}{\mu|\sin(\phi-\theta_c)|}\right)^{3/2} \times \frac{\exp[i\omega s_1\mu\cos(\theta_c-\phi)]}{a+b\sin^2\theta_c}. \tag{27}$$

Define the head-wave arrival time

$$\tau_h = s_1\mu\cos(\theta_c - \phi) = s_1 z_* \sec\theta_c + s_2(R - z_*\tan\theta_c). \tag{28}$$

The length of the ray path through medium 2 is

$$L = R - z_*\tan\theta_c. \tag{29}$$

See Fig. 2. Use (27)–(29) in (7) to obtain the head-wave contribution

$$P_{\text{head}} = \frac{i}{\omega}\left(\frac{2}{e}\right)^{1/2}\frac{\rho_1}{\rho_2}\frac{s_2}{s_1^2 - s_2^2}\frac{\exp(i\omega\tau_h)}{R^{1/2}L^{3/2}}. \tag{30}$$

Equation (30) differs from the expression in Aki and Richards[6] by a factor of $(2/e)^{1/2}$. Their derivation involves distorting the path of integration and identifying the head-wave contribution as being due to a region where the phase is slowly varying. Their evaluation of the contribution due to the slowly varying phase involves further approximations whereby the factor $(2/e)^{1/2}$ is lost.

Case (b) Comingled stationary phase points: If $|\phi - \theta_c| \leqslant O(N^{-1/2})$, and $\phi > \theta_c$, the roots of (20) merge with the root at

$$\theta_3 = \theta_c + e^{3i\pi/4}/(2N)^{1/2} + O(N^{-1}). \tag{31}$$

The values of the exponent and its second derivative in (18) are then

$$\psi = iN\cos(\theta_3 - \phi) + \frac{1}{2}\ln\left(-\frac{\sin(2\theta_c)e^{3i\pi/4}}{(2N)^{1/2}}\right) \tag{32}$$

and

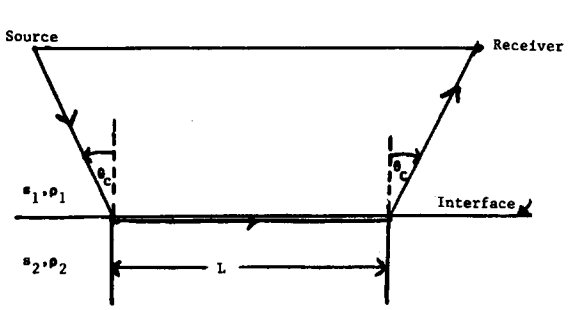

FIG. 2. Sketch of the geometrical configuration. The surface marked "Interface" is flat in Sec. II of the paper, but rough in Sec. III.

$$\psi'' = -i2N + \cot(2\theta_c)(2N)^{1/2}e^{-3i\pi/4}, \tag{33}$$

so that

$$\left(\frac{R}{\omega s_1}\right)^{1/2} I_2 \cong \frac{e^{-i\pi/8}}{2^{3/4}}\frac{\sin\theta_c}{N^{3/4}}\frac{(\cos\theta_c)^{3/2}e^{iN}}{(a+b\sin^2\theta_c)}, \tag{34}$$

for $|\phi - \theta_c| < O(N^{-1/2})$.

We are by no means the first to discuss the behavior of head-wave reflection from a planar interface nor are we the first to investigate the behavior of head-wave amplitude for observation angles far away from the critical angle θ_c or in the neighborhood of the critical angle.

Using a uniform asymptotic scheme of approximation, after considerable effort Brekhovskikh[7] obtained results for the head-wave amplitude which differ from ours by a factor of 1.02 (representing our numerical evaluation of an infinite product obtained by Brekhovskikh[7]).

We regard the present section, then, as a uniform notation for the rest of the paper and as providing confirmation (vis-a-vis Berkhovskikh's[7] results as a template) of the essential soundness of the asymptotic method we use for evaluation of the head-wave integrals. The 2% difference from the lead term in an asymptotic evaluation (ours) versus the more precise, but much more involved, result based on a method of uniform asymptotic approximation a là Brekhovskikh,[7] we do not regard as significant. Further, in the rough surface case (to be addressed in the next section of the paper) the general complexity of the resulting head-wave integrals would seem to preclude use of a uniform asymptotic approximation beyond lowest order. Recourse to numerical evaluation of the relevant integrals would seem to be the only avenue open except in special cases—two of which we address to illustrate the diversity of behaviors possible for head waves reflected from a rough surface.

III. A ROUGH INTERFACE

Now we examine the interaction of an acoustic wave with a rough boundary described by

$$Z = F(\mathbf{R}). \tag{35}$$

The magnitude of F is small compared to the acoustic wavelength and the average value of F is zero. The density and slowness are ρ_1 and s_1 (ρ_2 and s_2) above (below) the boundary.

Again, a point source is located on the z axis at z_0 and radiates the incident field given by (4a). The total field in medium 1 expressed in plane-wave components is

$$P_1(\mathbf{r}) = \int d\mathbf{K}\{P_i(\mathbf{K})e^{ik_1|z-z_0|} + P_R(\mathbf{K})e^{ik_1 z}\}e^{i\mathbf{K}\cdot\mathbf{R}} \tag{36}$$

and in medium 2 is

$$P_2 = \int d\mathbf{K}\, P_T(\mathbf{K})e^{-ik_2 z + i\mathbf{K}\cdot\mathbf{R}} \tag{37}$$

The plane-wave coefficients of the incident field $P_i(\mathbf{K})$ are given by (4a), while the coefficients of the reflected and transmitted fields $P_R(\mathbf{K})$ and $P_T(\mathbf{K})$ are found by satisfying the boundary conditions at the rough interface.

Again, p and the normal derivative $\rho^{-1}\,\partial p/\partial n$ must be

continuous across the rough boundary. The first condition gives

$$\int d\mathbf{K}\{\pi_i(\mathbf{K})e^{-ik_1F} + P_R(\mathbf{K})e^{ik_1F} - P_T(\mathbf{K})e^{-ik_2F}\}e^{i\mathbf{K}\cdot\mathbf{R}} = 0, \tag{38}$$

where

$$\pi_i(\mathbf{K}) = P_i(\mathbf{K})e^{ik_1z_0}. \tag{39}$$

A vector in the normal direction is $\mathbf{n} = \hat{z} - \partial F/\partial\mathbf{R}$, where the derivative denotes a gradient operation with respect to x and y. Thus the second boundary condition gives

$$\int d\mathbf{K}\left\{\pi_i(\mathbf{K})\left[k_1 + \mathbf{K}\cdot\frac{\partial F}{\partial\mathbf{R}}\right]e^{-ik_1F} - P_R(\mathbf{K})\left[k_1 - \mathbf{K}\cdot\frac{\partial F}{\partial\mathbf{R}}\right]e^{ik_1F} - \frac{\rho_1}{\rho_2}P_T(\mathbf{K})\left[k_2 + \mathbf{K}\cdot\frac{\partial F}{\partial\mathbf{R}}\right]e^{-ik_2F}\right\}e^{i\mathbf{K}\cdot\mathbf{R}} = 0. \tag{40}$$

Take the $\mathbf{K}'$ Fourier components of (38) and (40). Also, to remove the derivative term in the second equation we write

$$\frac{\partial F}{\partial\mathbf{R}}e^{ikF} = \frac{1}{ik}\frac{\partial}{\partial\mathbf{R}}(e^{ikF}) \tag{41}$$

and integrate by parts. We then have the equations

$$\int d\mathbf{K}\int d\mathbf{R}\{\pi_i(\mathbf{K})e^{-ik_1F} + P_R(\mathbf{K})e^{ik_1F} - P_T(\mathbf{K})e^{-ik_2F}\}e^{i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{R}} = 0 \tag{42}$$

and

$$\int d\mathbf{K}\int d\mathbf{R}\left\{\pi_i(\mathbf{K})\left[k_1 + \frac{\mathbf{K}\cdot(\mathbf{K}-\mathbf{K}')}{k_1}\right]e^{-ik_1F} - P_R(\mathbf{K})\times\left[k_1 + \frac{\mathbf{K}\cdot(\mathbf{K}-\mathbf{K}')}{k_1}\right]e^{ik_1F} - \frac{\rho_1}{\rho_2}P_T(\mathbf{K})\left[k_2 + \frac{\mathbf{K}\cdot(\mathbf{K}-\mathbf{K}')}{k_2}\right]e^{-ik_2F}\right\}e^{i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{R}} = 0. \tag{43}$$

Questions have been raised regarding the validity of extending the expansions into outgoing plane waves (36) and (37) up to the boundary $F(\mathbf{R})$ (Ref. 11). In fact, it has been shown that sometimes the plane-wave coefficients can be divergent.[12] Nevertheless, plane-wave expansions (the so-called Rayleigh ansatz) can be used in a convergent manner by truncating the limits of integration in (36) and (37), finding plane-wave coefficients which minimize the error in the resulting equation, and then letting the limits of integration increase[13] (see, for example, Ref. 14). We will assume that (42) and (43) can be solved as they stand, which is true for a large class of surfaces.[15]

To find a mean-field solution of (42) and (43), we break the transmitted and reflected plane-wave coefficients into statistically sharp and fluctuating components

$$P_R(\mathbf{K}) = \langle P_R(\mathbf{K})\rangle + \delta P_R(\mathbf{K}), \tag{44}$$

$$P_T(\mathbf{K}) = \langle P_T(\mathbf{K})\rangle + \delta P_T(\mathbf{K}), \tag{45}$$

where angular brackets are reserved throughout to denote an ensemble averaging operation.

Taking $F(\mathbf{R})$ to be described by a random Gaussian process, we can then write

$$\langle e^{ikF}\rangle = \exp(-\tfrac{1}{2}k^2\langle F^2\rangle). \tag{46}$$

Substituting (44) and (45) into (42) and taking an ensemble average gives the exact equation

$$[\pi_i(\mathbf{K}) + \langle P_R(\mathbf{K})\rangle]\exp(-\tfrac{1}{2}k_1^2\langle F^2\rangle) - \langle P_T(\mathbf{K})\rangle \times\exp(-\tfrac{1}{2}k_2^2\langle F^2\rangle) + (2\pi)^{-2}\int d\mathbf{K}'\int d\mathbf{R}\left\{\langle\delta P_R(\mathbf{K}')e^{ik_2'F}\rangle - \langle\delta P_T(\mathbf{K})e^{ik_2'F}\rangle\right\}e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}} = 0. \tag{47}$$

The primed wave-vector components k_1' and k_2' are (2) and (3) evaluated at K'. Subtracting (47) from (42) gives an equation satisfied by the fluctuating parts of the fields

$$\left[\delta P_R(\mathbf{K})\exp\left(-\frac{1}{2}k_1^2\langle F^2\rangle\right) - \delta P_T(\mathbf{K})\exp\left(-\frac{1}{2}k_2^2\langle F^2\rangle\right) + (2\pi)^{-2}\int d\mathbf{K}'\int d\mathbf{R}\left\{\langle P_R(K')\rangle\left[e^{ik_1'F} - \exp\left(-\frac{1}{2}(k_1')^2\langle F^2\rangle\right)\right] - \langle P_T(\mathbf{K}')\rangle\left[e^{-ik_2'F} - \exp\left(-\frac{1}{2}(k_2')^2\langle F^2\rangle\right)\right] + \pi_i(\mathbf{K}')\left[e^{-ik_1'F} - \exp\left(-\frac{1}{2}(k_1')^2\langle F^2\rangle\right)\right]\right\}e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}} = -(2\pi)^{-2}\int d\mathbf{K}'\int d\mathbf{R}\left\{\delta P_R(\mathbf{K}')\left[e^{ik_1'F} - \exp\left(-\frac{1}{2}(k_1')^2\langle F^2\rangle\right)\right] - \delta P(\mathbf{K}_T')\left[e^{-ik_2'F} - \exp\left(-\frac{1}{2}(k_2')^2\langle F^2\rangle\right)\right] + \langle\delta P(\mathbf{K}_R')e^{ik_1'F}\rangle - \langle\delta P(\mathbf{K}_T')e^{-ik_2'F}\rangle\right\}e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}}. \tag{48}$$

Likewise, substituting (44) and (45) into (43) and taking an ensemble average gives the exact equation

$$[\pi_i(\mathbf{K}) - \langle P_R(\mathbf{K})\rangle]k_1\exp(-\tfrac{1}{2}k_1^2\langle F^2\rangle) - \rho_1/\rho_2\langle P_T(\mathbf{K})\rangle k_2\exp(-\tfrac{1}{2}k_2^2\langle F^2\rangle) - (2\pi)^{-2}\times\int d\mathbf{K}'\int d\mathbf{R}\left\{\left[k_1' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_1'}\right]\langle\delta P_R(\mathbf{K}')e^{ik_1'F}\rangle + \frac{\rho_1}{\rho_2}\left[k_2' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_2'}\right]\times\langle\delta P_T(\mathbf{K}')e^{-ik_2'F}\rangle\right\}e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}} = 0. \tag{49}$$

Subtracting (49) from (43) gives the second equation satisfied by the fluctuating components

$$\delta P_R(\mathbf{K})k_1 \exp\left(-\frac{1}{2}k_1^2\langle F^2\rangle\right) + \delta P_T(\mathbf{K})\frac{k_2\rho_1}{\rho_2}\exp\left(-\frac{1}{2}k_2^2\langle F^2\rangle\right) + (2\pi)^{-2}\int d\mathbf{K}'\int d\mathbf{R}\Big\{\langle P_R(\mathbf{K}')\rangle$$
$$\times\left[e^{ik_1'F} - \exp\left(-\frac{1}{2}(k_1')^2\langle F^2\rangle\right)\right]\left[k_1' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_1'}\right] + \langle P_T(\mathbf{K}')\rangle\left[e^{-ik_2'F} - \exp\left(-\frac{1}{2}(k_2')^2\langle F^2\rangle\right)\right]\frac{\rho_1}{\rho_2}$$
$$\times\left[k_2' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_2'}\right] - \pi_i(\mathbf{K}')\left[e^{ik_1'F} - \exp\left(-\frac{1}{2}(k_1')^2\langle F^2\rangle\right)\right]\left[k_1' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_1'}\right]\Big\}e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}}$$
$$= (2\pi)^{-2}\int d\mathbf{K}'\int d\mathbf{R}\Big\{\delta P_R(\mathbf{K}')\left[e^{ik_1'F} - \exp\left(-\frac{1}{2}(k_1')^2\langle F^2\rangle\right)\right]\left[k_1' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_1'}\right]$$
$$+ \delta P_T(\mathbf{K}')\left[e^{-ik_2'F} - \exp\left(-\frac{1}{2}(k_2')^2\langle F^2\rangle\right)\right]\frac{\rho_1}{\rho_2}\left[k_2' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_2'}\right]\Big\}e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}}. \tag{50}$$

The basic mean-field method is to ignore the right-hand sides of (48) and (50). The justification of this stems from the fact that the quantities $\langle \delta P_R(\mathbf{K}')e^{ik_1'F}\rangle$ and $\langle \delta P_T(\mathbf{K}')e^{ik_2'F}\rangle$ are required in the mean-field equations (47) and (49). Hence, as far as the mean field is concerned, neglect of the right-hand sides of (48) and (50) is tantamount to ignoring the irreducible statistically sharp components of triple correlations of δP_R and δP_T with two phase factors, each of the form $\exp(ikF)$. Furthermore, we will later expand the exponentials in the equations, keeping only terms to order $\langle F^2\rangle$. When (48) and (50) are used to evaluate the terms $\langle \delta P_R(\mathbf{K}')e^{ik_1'F}\rangle$ and $\langle \delta P_T(\mathbf{K}')e^{ik_2'F}\rangle$ required in the mean-field equations, the right-hand sides of (48) and (50) give no contribution to order $\langle F^2\rangle$.

Choosing $F(\mathbf{R})$ as a random Gaussian process with homogeneous stationary statistics, we have

$$\langle F(\mathbf{R})F(\mathbf{R}')\rangle = \langle F^2\rangle A(\mathbf{R}-\mathbf{R}'), \qquad \text{with } A(0)=1 \quad \text{and} \quad A(\mathbf{R}) = A(-\mathbf{R}). \tag{51}$$

Equations (48) and (50) can now be solved for δP_R and δP_T and the quantities $\langle \delta P_R(\mathbf{K}')e^{ik_1'F}\rangle$ and $\langle \delta P_T(\mathbf{K}')e^{-ik_2'F}\rangle$ needed in the mean-field equations (47) and (49) can be evaluated. Making the variable change $\boldsymbol{\xi} = \mathbf{R}' - \mathbf{R}$, we then find

$$4\pi^2\left(k_1 + \frac{\rho_1}{\rho_2}k_2\right)\langle \delta P_R(\mathbf{K})e^{ik_2F(\mathbf{R})}\rangle$$
$$= \int d\mathbf{K}'\, e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}}\int d\boldsymbol{\xi}\Big\{\pi_i(\mathbf{K}')\left[-\frac{k_2\rho_1}{\rho_2} + k_1' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_1'}\right]$$
$$\times e^{-(1/2)(k_1')^2\langle F^2\rangle}\left[e^{k_1k_1'\langle F^2\rangle A(\xi)} - 1\right] - \langle P_R(\mathbf{K}')\rangle\left[\frac{k_2\rho_1}{\rho_2} + k_1' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_1'}\right]$$
$$\times e^{-(1/2)(k_1')^2\langle F^2\rangle}\left[e^{-k_1k_1'\langle F^2\rangle A(\xi)} - 1\right] + \langle P_T(\mathbf{K})\rangle\frac{\rho_1}{\rho_2}\left[k_2 - k_2' - \frac{\mathbf{K}'\cdot(\mathbf{K}-\mathbf{K})}{k_2'}\right]$$
$$\times e^{-(1/2)(k_2')^2\langle F^2\rangle}\left[e^{k_1k_2'\langle F^2\rangle A(\xi)} - 1\right]\Big\}e^{i(\mathbf{K}'-\mathbf{K})\cdot\boldsymbol{\xi}} \tag{52}$$

and

$$4\pi^2\left(k_1 + \frac{\rho_1}{\rho_2}k_2\right)\langle \delta P_T(\mathbf{K})e^{-ik_2F(\mathbf{R})}\rangle = \int d\mathbf{K}'\, e^{i(\mathbf{K}'-\mathbf{K})\cdot\mathbf{R}}\int d\boldsymbol{\xi}\Big\{\pi_i(\mathbf{K}')\left[k_1 + k_1' + \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_1'}\right]$$
$$\times e^{-(1/2)(k_1')^2\langle F^2\rangle}\left[e^{-k_1'k_2\langle F^2\rangle A(\xi)} - 1\right] + \langle P_R(\mathbf{K}')\rangle\left[k_1 - k_1' - \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_1'}\right]$$
$$\times e^{-(1/2)(k_1')^2\langle F^2\rangle}\left[e^{k_1'k_2\langle F^2\rangle A(\xi)} - 1\right] + \langle P_T(\mathbf{K}')\rangle\Big[-k_1 - k_2'\frac{\rho_1}{\rho_2}$$
$$- \frac{\mathbf{K}'\cdot(\mathbf{K}'-\mathbf{K})}{k_2'}\frac{\rho_1}{\rho_2}\Big]e^{-(1/2)(k_2')^2\langle F^2\rangle}\left[e^{-k_2k_2'\langle F^2\rangle A(\xi)} - 1\right]\Big\}e^{i(\mathbf{K}'-\mathbf{K})\cdot\boldsymbol{\xi}}. \tag{53}$$

We can expand exponents to order $\langle F^2\rangle$ and substitute (52) and (53) into (47) and (49) to obtain equations for the mean-field $\langle P_R(\mathbf{K})\rangle$ and $\langle P_T(\mathbf{K})\rangle$, obtaining

$$\pi_i(\mathbf{K})(1+a_1) + \langle P_R(\mathbf{K})\rangle(1+b_1) - \langle P_T(\mathbf{K})\rangle(1+c_1) = 0, \tag{54a}$$

$$k_1\pi_i(\mathbf{K})(1+a_2) - k_1\langle P_R(\mathbf{K})\rangle(1+b_2) - (\rho_1/\rho_2)k_2\langle P_T(\mathbf{K})\rangle(1+c_2) = 0, \tag{54b}$$

with

$$a_1 = -\frac{1}{2}k_1^2\langle F^2\rangle + \langle F^2\rangle\int d\mathbf{K}'\left(k_1' + \frac{\rho_1}{\rho_2}k_2'\right)^{-1}A(\mathbf{K}-\mathbf{K}')\Big\{(k_1'+k_2')\left[k_1^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}\right] + k_1k_1'k_2'\left(1-\frac{\rho_1}{\rho_2}\right)\Big\}, \tag{55a}$$

$$b_1 = -\frac{1}{2}k_1^2\langle F^2\rangle + \langle F^2\rangle \int d\mathbf{K}' \left(k_1' + \frac{\rho_1}{\rho_2}k_2'\right)^{-1} A(\mathbf{K}-\mathbf{K}')\left\{(k_1'+k_2')[k_1^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}'] - k_1k_1'k_2'\left(1-\frac{\rho_1}{\rho_2}\right)\right\}, \tag{55b}$$

$$c_1 = -\frac{1}{2}k_2^2\langle F^2\rangle + \langle F^2\rangle \int d\mathbf{K}' \left(k_1' + \frac{\rho_1}{\rho_2}k_2'\right)^{-1} A(\mathbf{K}-\mathbf{K}')\left\{\frac{\rho_1}{\rho_2}(k_1'+k_2')[k_2^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}] + k_1'k_2k_2'\left(1-\frac{\rho_1}{\rho_2}\right)\right\}, \tag{55c}$$

$$a_2 = -\frac{1}{2}k_1^2\langle F^2\rangle + \langle F^2\rangle \int d\mathbf{K}' \left(k_1' + \frac{\rho_1}{\rho_2}k_2'\right)^{-1} A(\mathbf{K}-\mathbf{K}')\left\{[k_1^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}]\right.$$
$$\left.\times\left[k_2'\frac{\rho_1}{\rho_2} - k_1 - \frac{(\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}}{k_1}\right] + \frac{\rho_1}{\rho_2}[k_2^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}]\left[k_1' + k_1 + \frac{(\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}}{k_1}\right]\right\}, \tag{55d}$$

$$b_2 = -\frac{1}{2}k_1^2\langle F^2\rangle + \langle F^2\rangle \int d\mathbf{K}' \left(k_1' + \frac{\rho_1}{\rho_2}k_2'\right)^{-1} A(\mathbf{K}-\mathbf{K}')\left\{[k_1^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}]\right.$$
$$\left.\times\left[k_2'\frac{\rho_1}{\rho_2} + k_1 + \frac{(\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}}{k_1}\right] + \frac{\rho_1}{\rho_2}[k_2^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}]\left[k_1' - k_1 - \frac{(\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}}{k_1}\right]\right\}, \tag{55e}$$

$$c_2 = -\frac{1}{2}k_2^2\langle F^2\rangle + \langle F^2\rangle \int d\mathbf{K}' \left(k_1' + \frac{\rho_1}{\rho_2}k_2'\right)^{-1} A(\mathbf{K}-\mathbf{K}')\left\{[k_1^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}]\right.$$
$$\left.\times\left[k_2' - k_2 - \frac{(\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}}{k_1}\right] + [k_2^2 + (\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}]\left[k_1' + k_2\frac{\rho_1}{\rho_2} + \frac{(\mathbf{K}-\mathbf{K}')\cdot\mathbf{K}}{k_2}\frac{\rho_1}{\rho_2}\right]\right\}. \tag{55f}$$

Notice that to do the expansions, exponents like $k_1k_1'\langle F^2\rangle A(\xi)$ must be small. Wave vector k_1 is on the scale of the reciprocal wavelength of the acoustic energy while the range of k_1' is prescribed by the wavelength of the surface roughness. Therefore, the condition necessary for small exponents is that the maximum slope of the surface profile times the ratio of roughness height to wavelength must be small.

The solution of (54) for the mean reflected wave is

$$\langle P_R(\mathbf{K})\rangle = -\pi_i(\mathbf{K})\frac{k_2\rho_1(1+c_2)(1+a_1) - k_1(1+a_2)(1+c_1)\rho_2}{k_2\rho_1(1+c_2)(1+b_1) + k_1(1+b_2)(1+c_1)\rho_2}. \tag{56}$$

We recognize that Eqs. (55) are all of quadratic order in F, which is the degree of accuracy of the overall mathematical formulation. Hence, to this same order, we have

$$\langle P_R(\mathbf{K}) = \pi_i(\mathbf{K})\frac{k_1 - k_2\rho_1/\rho_2}{k_1 + k_2\rho_1/\rho_2}\left\{1 + \left(k_1^2 - k_2^2\frac{\rho_1^2}{\rho_2^2}\right)^{-1}\left[\frac{\rho_1}{\rho_2}k_1k_2[2(c_1-c_2)\right.\right.$$
$$\left.\left. + (a_2-a_1) + (b_2-b_1)] + k_1^2(a_2-b_2) - k_2^2\frac{\rho_1}{\rho_2}(a_1-b_1)\right]\right\}. \tag{57}$$

Inspection of Eqs. (55) reveals rather complex functions involving quite sophisticated integrals over the power spectrum of the surface roughness fluctuations. While amenable to numerical procedures, they are too complicated for much physical insight to be gained as they stand. Fortunately, two limiting cases provide a great deal of insight into the effect of surface roughness on head-wave propagation. They are (a) if the roughness power spectrum can be approximated by a δ function, $A(\mathbf{K}) = \delta(\mathbf{K})$—corresponding to a variation of roughness on a spatial scale much longer than the wavelength of interest, and (b) if the roughness power spectrum can be approximated by a constant A_0 out to a very large wave number G and zero beyond G—corresponding to a variation of roughness on a spatial scale much smaller than the wavelength of interest.

A. Roughness on a spatial scale much longer than the wavelength of interest

With $A(\mathbf{K}) = \delta(\mathbf{K})$, we can evaluate (55) to find

$$a_1 = \frac{1}{2}k_1\langle F^2\rangle\left[\frac{k_1^2 + 4k_1k_2 - 3k_1k_2\rho_1/\rho_2}{k_1 + k_2\rho_1/\rho_2}\right], \tag{58a}$$

$$a_2 = \frac{1}{2}k_1\langle F^2\rangle\left[\frac{-3k_1^2 + k_1k_2\rho_1/\rho_2 + 4k_2^2\rho_1/\rho_2}{k_1 + k_2\rho_1/\rho_2}\right], \tag{58b}$$

$$b_1 = b_2 = \tfrac{1}{2}k_1^2\langle F^2\rangle, \tag{58c}$$

$$c_1 = c_2 = \tfrac{1}{2}k_2^2\langle F^2\rangle. \tag{58d}$$

We then evaluate (57) to obtain

$$\langle P_R(\mathbf{K})\rangle = \pi_i\frac{k_1 - k_2\rho_1/\rho_2}{k_1 + k_2\rho_1/\rho_2}\{1 - 2\langle F^2\rangle k_1^2\}. \tag{59}$$

Hence, for the nearly smooth surface, the effect is to cut the amplitude of the coherent component of the reflected field. This simple result serves as a check on the long calculation by which it was derived. Since the acoustic wavelength is much smaller than the wavelength, the roughness of the ensemble members is simply that of flat surfaces shifted from $z = 0$ by a random Gaussian distribution. The reflection amplitude for each member is

$$P_R = \pi_i(\mathbf{K})\frac{k_1 - k_2\rho_1/\rho_2}{k_1 + k_2\rho_1/\rho_2}e^{ik_1 2F}. \tag{60}$$

Then by (46) ensemble averaging gives (59) to second order.

B. Roughness on a spatial scale much smaller than the wavelength of interest

In this case, we take the correlation function to be

$$A(\mathbf{K}) = 1/\pi G^2, \quad \text{for} |\mathbf{K}| < G,$$
$$= 0, \quad \text{for} |\mathbf{K}| > G. \tag{61}$$

Notice that this preserves

$$\int d\mathbf{K}\, A(\mathbf{K}) = 1. \tag{62}$$

We evaluate (55) to find

$$a_1 = -\frac{1}{2}k_1^2\langle F^2\rangle + \frac{2\langle F^2\rangle}{(1+\rho_1/\rho_2)}\left[\omega^2 s_1^2 + i\frac{k_1 G}{3}\left(1-\frac{\rho_1}{\rho_2}\right)\right] + O(G^{-1}), \tag{63a}$$

$$b_1 = -\frac{1}{2}k_1^2\langle F^2\rangle + \frac{2\langle F^2\rangle}{(1+\rho_1/\rho_2)}\left[\omega^2 s_1^2 - i\frac{k_1 G}{3}\left(1-\frac{\rho_1}{\rho_2}\right)\right] + O(G^{-1}), \tag{63b}$$

$$c_1 = -\frac{1}{2}k_2^2\langle F^2\rangle + \frac{2\langle F^2\rangle}{(1+\rho_1/\rho_2)}\left[\frac{\rho_1}{\rho_2}\omega^2 s_2^2 + i\frac{k_2 G}{3}\left(1-\frac{\rho_1}{\rho_2}\right)\right] + O(G^{-1}), \tag{63c}$$

$$a_2 = -\frac{1}{2}k_1^2\langle F^2\rangle + \frac{2\langle F^2\rangle}{(1+\rho_1/\rho_2)}\left[\frac{\rho_1}{\rho_2}\omega^2\frac{(s_1^2+s_2^2)}{2} + i\frac{K^2 G}{6k_1}\left(1-\frac{\rho_1}{\rho_2}\right)\right] + O(G^{-1}), \tag{63d}$$

$$b_2 = -\frac{1}{2}k_1^2\langle F^2\rangle + \frac{2\langle F^2\rangle}{(1+\rho_1/\rho_2)}\left[\frac{\rho_1}{\rho_2}\omega^2\frac{(s_1^2+s_2^2)}{2} - \frac{iK^2 G}{6k_1}\left(1-\frac{\rho_1}{\rho_2}\right)\right] + O(G^{-1}), \tag{63e}$$

$$c_2 = -\frac{1}{2}k_2^2\langle F^2\rangle + \frac{2\langle F^2\rangle}{(1+\rho_1/\rho_2)}\left[\omega^2\frac{(s_1^2+s_2^2)}{2} + \frac{iK^2 G}{6k_2}\left(1-\frac{\rho_1}{\rho_2}\right)\right] + O(G^{-1}). \tag{63f}$$

Substitution of (63) into (57) gives

$$\langle P_R(\mathbf{K})\rangle = \pi_i(\mathbf{K})\frac{k_1 - k_2\rho_1/\rho_2}{k_1 + k_2\rho_1/\rho_2}\left\{1 + \frac{2\langle F^2\rangle k_1}{1+\rho_1/\rho_2}\left(k_1^2 - \frac{k_2^2\rho_1^2}{\rho_2^2}\right)^{-1}\right.$$
$$\left.\times\left[\frac{\rho_1}{\rho_2}k_2\omega^2\left[s_2^2\left(3\frac{\rho_1}{\rho_2}-1\right) + s_1^2\left(\frac{\rho_1}{\rho_2}-3\right)\right] + \frac{iG}{3}\left(1-\frac{\rho_1}{\rho_2}\right)^2\left[k_2^2\left(2\frac{\rho_1}{\rho_2}-1\right) + \omega^2 s_2^2\right]\right]\right\}. \tag{64}$$

The result for the slightly rough or the very rough surfaces, Eq. (59) or Eq. (64), respectively, can be used in the ensemble average of Eq. (36) to obtain the statistically sharp component of the reflected field for a point source. The quantity in braces in (59) or (64) is of the form $1+\sigma$ and can be expressed as e^{σ} to second order. The evaluation of the specularly reflected contribution proceeds as in Sec. II with e^{σ} regarded as a slowly varying factor. Thus the specular reflection is altered by the factor e^{σ} evaluated at the stationary point.

The evaluation of the head-wave contribution requires more care since the roughness modifies both the original head wave and causes scattering into and out of the head-wave region. The contributions to (59) or (64) which provide input to the head wave are those in which k_2 occurs to an odd power, for then we have a square root branch integral to do in the far field. Further, the head-wave contribution arises from those places in the integral over K where $k_2 \simeq 0$ $(s_2 < s_1)$. Hence, in attempting to extract those factors in (36) which contribute to the head wave, we can be guided by the techniques of Sec. II and use them in the following way.

(1) Extract those factors in (59) or (64) which have a single power of k_2 multiplying them.

(2) Since the dominant variation as far as the integral over K is concerned is from $k_2 \simeq 0$, i.e., $k_2 \simeq \omega^2 s_2^2$, in the resulting expression set $k_1 = \omega(s_1^2 - s_2^2)^{1/2}$.

Equation (59) shows that for a slightly rough surface, the single powers of k_2 are the same as in the smooth case. Hence, the head wave is merely altered by the attenuating amplitude factor $\exp[-2\langle F^2\rangle\omega^2(s_1^2 - s_2^2)]$.

For a very rough surface, identifying the single powers of k_2 in (64) shows that the head wave is altered by the factor

$$\exp\left\{-\frac{\langle F^2\rangle}{1+\rho_1/\rho_2}\left\{\omega^2\left[s_2^2\left(\frac{3\rho_1}{\rho_2}-1\right) + s_1^2\left(\frac{\rho_1}{\rho_2}-3\right)\right]\right.\right.$$
$$\left.\left. - \frac{i2G}{3}\left(1-\frac{\rho_1}{\rho_2}\right)^2\frac{\omega s_2}{(s_1^2/s_2^2 - 1)^{1/2}}\right\}\right\}. \tag{65}$$

While others (e.g., Refs. 16 and 17) have also examined the behavior of scattering of waves from rough and random surfaces, we believe that our results extend upon those previous works in that we provide an explicit result for the mean reflected field and go further in deriving the head-wave arrival times with additional effects due to path variations. In addition we believe the possible enhancement of the head-wave amplitude, which we obtain, is a completely new effect of potentially great significance to seismic exploration of the Earth.

IV. DISCUSSION AND CONCLUSIONS

Several interesting facts are evident. First, in the very rough case (65), it is possible for the roughness to enhance the head-wave amplitude. For example, when there is no density contrast ($\rho_1 = \rho_2$) Eq. (65) becomes

$$\exp[\langle F^2\rangle\omega^2(s_1^2 - s_2^2)], \tag{66}$$

showing an enhancement of the amplitude since $s_1 > s_2$.

More generally, amplitude enhancement occurs whenever

$$\rho_1(s_1^2 - 3s_2^2) < \rho_2(3s_1^2 - s_2^2). \tag{67}$$

If $\rho_2 > \rho_1$, Eq. (67) predicts that the amplitude is always enhanced, while if $\rho_2 < \rho_1$ the amplitude is enhanced only if $(\rho_1 - \rho_2)/(\rho_1 + \rho_2) < 2\,(s_1^2/s_2^2 - 1)^{-1}$.

Second, Eq. (65) also shows that roughness causes a time delay (if $\rho_1 \neq \rho_2$) and that the magnitude of this delay is quadratically dependent upon the density contrast.

Indeed the head-wave arrival time T is then given by

$$T = \tau_h + \tfrac{2}{3}(1 - s_2^2/s_1^2)^{-1/2}(1 + \rho_1/\rho_2)^{-1} \times (1 - \rho_1/\rho_2)^2 \langle F^2 \rangle G s_1, \tag{68}$$

representing a delay $\Delta\tau$ relative to the smooth surface head-wave arrival time τ_h with $\Delta\tau$ quadratically dependent on both the density contrast across the rough surface and on the roof-mean-square (rms) height of the roughness, and linearly dependent on the wave number G characterizing the spatial scale of the roughness. For instance, with a density contrast of 30%, a slowness contrast of 1%, a wave number G, ten times the typical seismic wave number (corresponding to a roughness scale of about 20 feet), and a rms height of 0.1 of a typical seismic wavelength ($\sim$200 ft), we have a delay of about 16 msec. The point to be made here is that under the right set of conditions, the time delay produced by the roughness is a measurable quantity.

Finally note that the roughness does not alter the apparent velocity of head-wave arrivals to second order in roughness height. This can be seen by expressing the quantity of the form $1 + \sigma$ in the braces in (64) as e^{σ} to second order and carrying through the analysis of Sec. II with this added phase factor. The position of the stationary point in the asymptotic evaluation of the integral is not significantly altered. The angles of the upgoing and downgoing legs of the head-wave paths are not altered. Thus the analysis of this paper shows that small-scale interface roughness does not change standard interpretation of head-wave arrivals. In a future paper we will explore the influence of a curved interface in modifying the arrival time and amplitude.

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Lie transformation group solutions of the nonlinear one-dimensional Vlasov equation

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The solution of the exact, nonlinear one-dimensional Vlasov equation with a space- and time-dependent electric field is reduced to the solution of a nonlinear, first-order ordinary differential equation with two subsidiary equations. The reduction holds for any electric field nonlinear in the spatial coordinate or for a subclass of electric fields linear in the spatial coordinate and is equivalent to the solution of a generalized Bernstein–Greene–Kruskal (BGK) Vlasov equation with a velocity-dependent Lorentz force. The Lie method for the solution of differential equations invariant under a transformation group has been used to calculate the group generator, the canonical variables, and the generalized BGK Vlasov equation. Analytical forms for the functional dependence of the Vlasov equation one-particle distribution function are given.

I. INTRODUCTION

Exact, time-dependent solutions of the Vlasov or Liouville equation have recently been reported.[1–7] The Vlasov one-particle distribution function is a functional of the Liouville invariant. This distribution function under certain conditions has been shown to produce self-consistent solutions of the Vlasov–Poisson equations[8] and Vlasov–Maxwell equations.[9] These solutions are much more general in structure than the uniformly translated solutions[10] of the nonlinear, equilibrium Vlasov–Maxwell equations which are usually called the BGK (Bernstein–Greene–Kruskal)[11] solutions. In this article the time-dependent solutions of the nonlinear Vlasov equation for a one-dimensional plasma in a time- and space-dependent longitudinal electric field are treated.

Lewis and Leach derived a time-dependent Liouville invariant I for a system quadratic in the momenta.[3,4] This invariant was then used by Lewis and Symon[8] to find an exact solution of the Vlasov–Poisson equations where the one-particle distribution function, a functional of the invariant I, was used to calculate the charge density integral in Poisson's equation. In an earlier paper[9] we generalized their formalism for the Vlasov–Poisson model to include all of Maxwell's equations for the one-dimensional plasma. We found the same invariant as Lewis and Leach had by a coordinate transformation for the BGK spatial coordinate, a function of laboratory space and time coordinates.

The generalization of their results to include a more general momentum dependence of the invariant has been a goal as the quadratic momentum dependence is too restrictive in certain applications. Lewis and Leach[6] have introduced the resonance formulation for invariants in an effort to find a new momentum dependence of the invariant of the Liouville or Vlasov equation.

The one-particle distribution function of the Vlasov equation is found here by the Lie theory that determines solutions of differential equations invariant under one-parameter Lie groups.[12–17] These Lie groups are transformation groups and the invariance is tested by infinitesimal transformations. The infinitesimal transformation of a function $g(t,x)$ is represented by a group generator $Ug = \xi(t,x)(\partial g/\partial t) + \eta(t,x)(\partial g/\partial x)$ and is itself sometimes called the infinitesimal transformation. We derive U for the exact, nonlinear one-dimensional Vlasov equation with a time- and space-dependent longitudinal electric field. Once the group as represented by Ug is determined where the time-dependent functions in Ug obey subsidiary conditions, we can in principle, at least, find a set of canonical coordinates. The Vlasov equation in these canonical coordinates is stationary as the electric field is independent of the new time; it is in the BGK form even though the force term may be velocity dependent. Hence, we present a method by which general exact, time-dependent solutions of the nonlinear, one-dimensional Vlasov equation that are transformed generalized BGK solutions can be found analytically or numerically.

Another approach to the solutions of the Vlasov–Maxwell equations involves the invariance under Lie point transformations of the complete Vlasov–Maxwell equations. This has been done by Baranov[18] for a single-species plasma in an immobile, neutralizing background of constant density by an indirect method and by Axford[19] in lecture notes. Subsequent to the submission of the present paper Roberts[20] has analyzed the invariance of the one-dimensional Vlasov–Maxwell equations of a multispecies plasma with a time- and space-varying neutralizing background that includes results of Baranov and Axford, and some of the results of this paper.

In Sec. II the infinitesimal transformation for the Lie group under which the one-dimensional Vlasov equation is invariant is derived. In Sec. III the generalized BGK Vlasov equation is found for a coordinate function ξ, a function of time only, by use of a complete solution. The characteristic equation for this generalized BGK Vlasov equation is a nonlinear, first-order ordinary equation. In Sec. IV the functional dependence of the generalized BGK distribution function is calculated analytically for several cases.

II. INFINITESIMAL TRANSFORMATION OF THE 1-D VLASOV EQUATION GROUP

The Vlasov equation for the one-particle distribution function $f(t,x,v)$ is

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + \frac{q}{m}E(t,x)\frac{\partial f}{\partial v} = 0. \tag{1}$$

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The velocity component v is used here rather than the particle momentum $p = mv$ because it seems a more natural coordinate for Lie groups. The time t, the spatial coordiate x, the charge q, the mass m, and the electric field E complete the variables. The solution of the Vlasov equation for the one-particle distribution function together with Maxwell's equations specifies the state of the plasma.

The Vlasov equation as written here is a linear partial differential equation where the coefficients depend on the independent variables (t,x,v). Actually the electric field $E(t,x)$ is a functional of the one-particle distribution function $f(t,x,v)$ which can be found through Maxwell's equations by Green's functions. However, the usual procedure for collisionless plasmas is to solve for the distribution function from the Vlasov equation and then to substitute the distribution function into the charge density and current density integrals in Maxwell's equations. The electric field and the distribution function are then found self-consistently since they both obey the Vlasov–Maxwell equations. Several special cases of the time-dependent solutions have been found by these means: the uniformly translated BGK solutions,[10,11] the one-dimensional solutions with the distribution functions functionals of an invariant quadratic in the momenta,[8,9] and a temporally damped sinusoidal electric field for a multispecies plasma in a related paper presented elsewhere.[21] Although the electric field is treated as a function of (x,t) in this paper, the constraints imposed by Maxwell's equations should be added later.

A linear partial differential equation of the Vlasov form can be invariant under a group and is equivalent to the invariance of the equation of motion of a single particle, a second-order nonlinear ordinary differential equation,

$$\frac{d^2x}{dt^2} - \frac{q}{m}E(t,x) = 0, \quad \frac{dx}{dt} = v, \tag{2}$$

which is invariant under a twice-extended group transformation with the group generator U'',

$$U''\tilde{F}(t,x,\dot{x},\ddot{x}) = 0,$$

$$U'' = \xi(t,x)\frac{\partial}{\partial t} + \eta(t,x)\frac{\partial}{\partial x} + \eta'(t,x,\dot{x})\frac{\partial}{\partial \dot{x}} + \eta''(t,x,\dot{x}\ddot{x})\frac{\partial}{\partial \ddot{x}}, \tag{3}$$

for $\dot{x} = dx/dt, \ddot{x} = d^2x/dt^2$, and $\tilde{F} = 0$, is a second-order differential equation here. The time derivatives of x are treated as additional variables. Conventionally the differential equation is said to be invariant under a group Ug. The functions η' and η'' can be calculated and are given in Cohen[12]:

$$\eta' = \frac{\partial \eta}{\partial t} + \left(\frac{\partial \eta}{\partial x} - \frac{\partial \xi}{\partial t}\right)\dot{x} - \frac{\partial \xi}{\partial x}\dot{x}^2, \tag{4a}$$

$$\eta'' = \frac{\partial \eta'}{\partial t} + \frac{\partial \eta'}{\partial x}\dot{x} + \left(\frac{\partial \eta'}{\partial \dot{x}} - \frac{\partial \xi}{\partial t} - \frac{\partial \xi}{\partial x}\dot{x}\right)\ddot{x}. \tag{4b}$$

Cohen,[12] whose treatment of the solution of differential equations by Lie groups is followed most closely here, has pointed out that the solution of the second-order ordinary differential equation

$$\frac{d^2x}{dt^2} - \mathcal{F}(t,x,\dot{x}) = 0 \tag{5}$$

is equivalent to the set of first-order differential equations

$$\frac{dt}{1} = \frac{dx}{\dot{x}} = \frac{d\dot{x}}{\mathcal{F}(t,x,\dot{x})}, \tag{6}$$

which are in turn equivalent to the solution of the linear partial differential equation

$$\frac{\partial f}{\partial t} + \dot{x}\frac{\partial f}{\partial x} + \mathcal{F}(t,x,\dot{x})\frac{\partial f}{\partial \dot{x}} = 0. \tag{7}$$

The differential equations in (6) are not in the usual modern form but are expressed in a convenient, compact form where one can take any pair and write them in standard form. The characteristic equations (6) of Eq. (7) have two solutions. If $\dot{x} = v$, then Eq. (7) represents the Vlasov equation with a velocity-dependent force $\mathcal{F}(t,x,v)$. For our case the Lorentz force contains only an electric field that is velocity independent; Eq. (7) reduces then to Eq. (1) and Eq. (5) reduces to Eq. (2). The approach outlined here can be used for velocity-dependent forces.

The invariance under a one-parameter Lie (transformation) group of an nth-order nonlinear ordinary differential equation enables us to do several things. First, we can reduce the order of an equation by 1. Thus a first-order differential equation can be integrated, a second-order differential equation can be reduced to a first-order differential equation, etc. Second, a set of canonical coordinates can be defined such that in the new coordinates the differential equation is invariant under translations in one of the new variables. From the latter result with the equation of motion of the particle invariant under a Lie group we can find a new differential equation with an electric field that is independent of time in the canonical coordinates.

As an example let us take the Lewis–Leach[4] transformation between the laboratory variables (t,x) and the BGK variables $(\bar{t},\bar{x})$ where the latter variables are those for which the Vlasov equation has the BGK form. The transformation is

$$\bar{x} = \frac{x-\alpha}{\rho}, \quad \bar{t} = \int \frac{dt}{\rho^2}, \tag{8}$$

where the translation coordinate α and the time-stretching factor ρ obey the subsidiary equations

$$m\ddot{\rho} + q\Omega^2(t)\rho = qk/\rho^3, \tag{9a}$$

$$m\ddot{\alpha} + q\Omega^2(t)\alpha = qF(t). \tag{9b}$$

The overdots denote differentiation with respect to time, $\Omega^2(t)$ and $F(t)$ are arbitrary functions until the Maxwell equations are imposed, and k is a constant. For a differential equation invariant under a group Ug the new coordinate functions are $\bar{\xi}(\bar{t},\bar{x}) = 1, \bar{\eta}(\bar{t},\bar{x}) = 0$ for a differential equation invariant under translations in the new time $\bar{t}$. Hence, in the canonical coordinates the electric field is independent of time or we have transformed to a BGK reference frame. Then the following relations can be shown to hold[12]:

$$U\bar{t} = \xi(t,x)\frac{\partial \bar{t}}{\partial t} + \eta(t,x)\frac{\partial \bar{t}}{\partial x} = \bar{\xi}(\bar{t},\bar{x}) = 1, \tag{10a}$$

$$U\bar{x} = \xi(t,x)\frac{\partial \bar{x}}{\partial t} + \eta(t,x)\frac{\partial \bar{x}}{\partial x} = \bar{\eta}(\bar{t},\bar{x}) = 0. \tag{10b}$$

Equations (10a) and (10b) can be solved together with Eq. (8) to give

$$\xi(t,x)=\rho^2, \quad \eta(t,x)=\rho\dot{\rho}x+\rho^2\dot{\alpha}-\rho\dot{\rho}\alpha. \tag{11}$$

We thus have the infinitesimal transformation of a Lie group[12] that we call the Lewis–Leach group where we assume that the coordinate functions must be determined as functions of x and t. The group generator in the laboratory variables is

$$Ug=\rho^2\frac{\partial g}{\partial t}+(\rho\dot{\rho}x+\rho^2\dot{\alpha}-\rho\dot{\rho}\alpha)\frac{\partial g}{\partial x}, \tag{12}$$

and in BGK variables is

$$Ug=\frac{\partial g}{\partial \bar{t}},$$

where the latter group is in the canonical form and $(\bar{t},\bar{x})$ are the canonical variables.

We next search for the most general infinitesimal transformation that leaves the differential equation (2) for the moton of a particle invariant. The twice-extended infinitesimal transformation of Eq. (2) represented by

$$U''\left(\frac{d^2x}{dt^2}-\frac{q}{m}E(t,x)\right)=0 \tag{13}$$

gives

$$-\xi(t,x)\frac{q}{m}\frac{\partial E(t,x)}{\partial t}-\eta(t,x)\frac{q}{m}\frac{\partial E(t,x)}{\partial x}+\eta''(t,x,\dot{x}\ddot{x})=0, \tag{14}$$

where the velocity derivation of E vanishes. Upon substitution of Eq. (4b) into Eq. (14) we find

$$\left(\frac{\partial\eta}{\partial x}-2\frac{\partial\xi}{\partial t}\right)\frac{q}{m}E-\xi\frac{q}{m}\frac{\partial E}{\partial t}-\eta\frac{q}{m}\frac{\partial E}{\partial x}+\frac{\partial^2\eta}{\partial t^2}+\left(2\frac{\partial^2\eta}{\partial t\,\partial x}-\frac{\partial^2\xi}{\partial t^2}-3\frac{\partial\xi}{\partial x}\frac{q}{m}E\right)\dot{x}+\left(\frac{\partial^2\eta}{\partial x^2}-2\frac{\partial^2\xi}{\partial t\,\partial x}\right)\dot{x}^2-\frac{\partial^2\xi}{\partial x^2}\dot{x}^3=0. \tag{15}$$

The velocity dependence is explicitly given in the powers of $\dot{x}=v$. With an invariance under a group the coordinates $(t,x,\dot{x})$ vary independently. One may actually find solutions of Eq. (15) for which the first time derivative of $x,\dot{x}$, satisfies the cubic equation and is some function of (t,x). If this $\dot{x}$ differentiated results in Eq. (2), one has obtained a solution of the original differential equation. These special solutions do not help us in the solution of the Vlasov equation because $v=\dot{x}$ is an independent coordinate. Consequently the coefficients of each power of $\dot{x}$ in Eq. (15) vanish separately. These relations are

$$\frac{\partial^2\xi}{\partial x^2}=0, \tag{16a}$$

$$\frac{\partial^2\eta}{\partial x^2}-2\frac{\partial^2\xi}{\partial t\,\partial x}=0, \tag{16b}$$

$$2\frac{\partial^2\eta}{\partial t\,\partial x}-\frac{\partial^2\xi}{\partial t^2}-3\frac{\partial\xi}{\partial x}\frac{qE}{m}=0, \tag{16c}$$

$$\left(\frac{\partial\eta}{\partial x}-2\frac{\partial\xi}{\partial t}\right)\frac{q}{m}E-\xi\frac{q}{m}\frac{\partial E}{\partial t}-\eta\frac{q}{m}\frac{\partial E}{\partial x}+\frac{\partial^2\eta}{\partial t^2}=0. \tag{16d}$$

The above set of equations can be solved. After two integrations of Eq. (16a) we find that

$$\xi(t,x)=ax+b, \tag{17}$$

for a and b functions of time. Next integrate Eq. (16b) twice to give

$$\eta=\frac{da}{dt}x^2+\left(2\frac{db}{dt}+c\right)x+d, \tag{18}$$

for c and d functions of time. Then we substitute (ξ,η) into Eq. (16c). The result is

$$\frac{qE}{m}=\frac{1}{a}\left(\frac{d^2a}{dt^2}x+\frac{2}{3}\frac{dc}{dt}+\frac{d^2b}{dt^2}\right). \tag{19}$$

Since Eq. (16d) must be obeyed, we substitute ξ, η, and E into Eq. (16d). As the resultant equation is quadratic in x, we find three relations that must be satisfied but one is an identity. The resultant two differential equations are insufficient to determine a, b, c, and d. We do not develop this case further for several reasons. This case has an electric field which has at most a linear variation x or a potential V, $E=-\partial V/\partial x$, quadratic in x. Also, the complete symmetry group of the one-dimensional harmonic oscillator has already been worked out.[2] Neverltheless, we have found the general infinitesimal transformation of invariance under a Lie group of Eq. (2) for potentials quadratic in x, where

$$Ug=(ax+b)\frac{\partial g}{\partial t}+\left[\frac{da}{dt}x^2+\left(2\frac{db}{dt}+c\right)x+d\right]\frac{\partial g}{\partial x}, \tag{20}$$

and a, b, c, and d are not determined here.

If we wish a more general x dependence of the potential $V(t,x)$ or the electric field $E(t,x)$, we set $a=0$. This condition follows from Eq. (16c) where we see that with $a=0$, E is no longer constrained to be linear in x, although it may be. Henceforth, we set $a=0$, which also means that ξ depends only on time t. As a result Eq. (16a) is automatically satisfied. The next equation (16b) simplifies to

$$\frac{\partial^2\eta}{\partial x^2}=0, \tag{21}$$

from which we deduce that η is a linear function of x. Equation (16c) integrates once to give

$$2\frac{\partial\eta}{\partial x}-\frac{\partial\xi}{\partial t}=N, \tag{22}$$

where N is a constant since η is at most linear in x and ξ depends only on t. Integrating once more with respect to x we find

$$\eta=\frac{1}{2}\left(\frac{\partial\xi}{\partial t}+N\right)x+d, \tag{23}$$

for d a function of time. The relation (23) for η is substituted into Eq. (16d). We obtain

$$\left(-\frac{3}{2}\frac{\partial\xi}{\partial t}+\frac{N}{2}\right)\frac{q}{m}E-\xi\frac{q}{m}\frac{\partial E}{\partial t}-\left(\frac{\partial\xi}{\partial t}+N\right)\frac{x}{2}\frac{q}{m}\frac{\partial E}{\partial x}-\frac{dq}{m}\frac{\partial E}{\partial x}+\frac{1}{2}\frac{\partial^3\xi x}{\partial t^3}+\frac{\partial^2 d}{\partial t^2}=0. \tag{24}$$

At this point we introduce an ansatz for the electric field by

$$qE/m=qF(t)/m+G(t)x+W(t,x). \tag{25}$$

This decomposition separates out the x dependence that is explicit in Eq. (24). The form was suggested by the similarity of η found above in Eq. (23) to that for the Lewis–Leach transformation Eq. (8). Relation (25) substituted into Eq. (24) can be separated into terms of zero order in x, first order in x, and the W terms which are set equal to zero separately. W does not have terms of zero or first order in x. Three equations result in the aforementioned order:

$$\left(\frac{N}{2}-\frac{3}{2}\frac{\partial\xi}{\partial t}\right)\frac{q}{m}F-\xi\frac{q}{m}\frac{\partial F}{\partial t}-dG+\frac{\partial^2 d}{\partial t^2}=0, \tag{26a}$$

$$-\frac{3}{2}\frac{\partial\xi}{\partial t}G-\xi\frac{\partial G}{\partial t}-\frac{1}{2}\frac{\partial\xi}{\partial t}G+\frac{1}{2}\frac{\partial^3\xi}{\partial t^3}=0, \tag{26b}$$

$$\left(\frac{N}{2}-\frac{3}{2}\frac{\partial\xi}{\partial t}\right)W-\frac{\xi\partial W}{\partial t}-\left(\frac{\partial\xi}{\partial t}+N\right)\frac{x}{2}\frac{\partial W}{\partial x}-d\frac{\partial W}{\partial x}=0. \tag{26c}$$

We first solve Eq. (26b). If one sets $N=0$, one recovers the Lewis–Leach group. As Eq. (26b) does not even contain N, we let $\xi=\rho^2$ by comparison with the calculations in (4) and (8). Then Eq. (26b) becomes after some manipulation

$$\frac{\partial}{\partial t}\left(\rho^3\frac{\partial^2\rho}{\partial t^2}\right)-\frac{\partial}{\partial t}(\rho^4 G)=0. \tag{27}$$

Integrating with respect to time, we find

$$\frac{\partial^2\rho}{\partial t^2}+\frac{q}{m}\Omega^2(t)\rho=\frac{qk}{m\rho^3}, \tag{28}$$

for k an integration constant and $G=-(q/m)\Omega^2(t)$ by comparison with the results in (4) and (8). Then Eq. (28) is the same differential equation found by Lewis and Symon,[8] Eq. (9a) for ρ.

The equation for W can be rewritten as

$$\frac{\partial W'}{\partial x}\left[\frac{x}{2}\left(\frac{\partial\xi}{\partial t}+N\right)+d\right]+\xi\frac{\partial W'}{\partial t}=0, \tag{29}$$

for

$$W'=W\exp\left[-\int\frac{dt}{\xi}\left(\frac{N}{2}-\frac{3}{2}\frac{\partial\xi}{\partial t}\right)\right].$$

The characteristic equation for Eq. (29) is

$$\frac{dx}{dt}=\frac{x}{2\xi}\left(\frac{\partial\xi}{\partial t}+N\right)+\frac{d}{\xi}, \tag{30}$$

which is a linear equation in x and can be integrated. Then we call the solution $\bar{x}$,

$$\bar{x}=\frac{x}{\rho}e^{-(N/2)\bar{t}}-\int dt\frac{d}{\rho^3}e^{-(N/2)\bar{t}}=C_1, \tag{31}$$

where

$$W=[e^{(N/2)\bar{t}}/\rho^3]\,W'(\bar{x}),$$

with $\bar{t}$ defined as in Eq. (8). Note $\bar{x}$ reduces to the value in Eq. (8) for $N=0$, and the Lewis–Leach transformation results for $N=0$ if we define

$$\frac{d}{\rho^3}=\frac{\partial}{\partial t}\left(\frac{\alpha}{\rho}\right). \tag{32}$$

From Eq. (26a) we find the differential equation for α to be

$$\frac{d^2\alpha}{dt^2}+\frac{q}{m}\Omega^2(t)\alpha=\frac{q}{m}F-\frac{q}{m}\frac{N}{2\rho^3}\int dt\,\rho F. \tag{33}$$

The coordinate functions of the group generator are

$$\xi=\rho^2,\quad \eta=(\rho\dot\rho+N/2)x+\rho^2\dot\alpha-\rho\dot\rho\alpha,$$
$$\eta'=(\ddot\rho\rho+\dot\rho^2)x+(N/2-\rho\dot\rho)\dot x+\rho\dot\rho\dot\alpha+\rho^2\ddot\alpha-\rho\ddot\rho\alpha-\dot\rho^2\alpha,$$
$$\eta''=(\rho\dddot\rho+3\dot\rho\ddot\rho)(x-\alpha)+3\rho\dot\rho\ddot\alpha+\rho^2\dddot\alpha+(N/2-3\rho\dot\rho)\ddot x, \tag{34}$$

where the group generator Ug is

$$Ug=\rho^2\frac{\partial g}{\partial t}+\left[\left(\rho\dot\rho+\frac{N}{2}\right)x+\rho^2\dot\alpha-\rho\dot\rho\alpha\right]\frac{\partial g}{\partial x}.$$

In summary we have specified the group generator of the infinitesimal transformation for the Lie group with ξ a function of time only under which the one-dimensional Vlasov equation with a time-dependent electric field is invariant. The functions ρ and α satisfy the subsidiary equations (28) and (33), respectively, that are generalizations of the corresponding equations (9a) and (9b) for the Lewis–Leach transformation. Additional constraints on ρ and α may occur if Maxwell's equations are added but these are not discussed here.[9] This generator has been given for the special case of an anharmonic oscillator with cubic anharmonicity.[2]

III. GENERALIZED BGK VLASOV EQUATION

In this section we find the Vlasov equation in the generalized BGK form. First, we note the canonical coordinates $(\bar{t},\bar{x})$:

$$\bar{t}=\int\frac{dt}{\rho^2},\quad \bar{x}=\left(\frac{x-\alpha}{\rho}\right)e^{-(N/2)\bar{t}}-\frac{N}{2}\int\frac{dt\,\alpha}{\rho^3}e^{-(N/2)\bar{t}}. \tag{35}$$

The verification that these are possible canonical coordinates follows from Eqs. (10a), (10b), and (34). A transformation of Eq. (2) to these coordinates should produce a new force term independent of time in the new coordinates; we call this new force a generalized BGK force and the new reference frame, the generalized BGK frame. The time-dependent electric field from Eqs. (25), (28), and (31) is

$$E=F(t)-\Omega^2(t)x-\frac{e^{(N/2)\bar{t}}}{\rho^3}\frac{dU_e(\bar{x})}{d\bar{x}}, \tag{36a}$$

for the potential

$$V=-F(t)x+\Omega^2(t)x^2/2+(e^{N\bar{t}}/\rho^2)U_e(\bar{x}), \tag{36b}$$

where $W'(x)=-(q/m)\,(dU_e(\bar{x})/d\bar{x})$ and $U_e(\bar{x})$ should not be confused with the Lie group generator operator U or U''.

To find the Vlasov equation in the generalized BGK form or in the stationary reference frame we assume that the one-particle distribution function $f(t,x,v)$ satisfies not only the Vlasov equation but also is invariant under the group just given in Sec. II.[12] There we found the group under which the equation of motion of a particle in an electric field $E(t,x)$ is invariant but the Vlasov equation which has $E(t,x)$ in the Lorentz force is also invariant under the group.

This invariance is expressed by the following relation:

$$[U',V_a]f=-\frac{\partial\xi}{\partial t}V_a f=0, \tag{37}$$

where U' is the operator for the once-extended infinitesimal tranformation

$$U' = \xi \frac{\partial}{\partial t} + \eta \frac{\partial}{\partial x} + \eta' \frac{\partial}{\partial v}, \tag{38}$$

for $\dot{x} = v$, $\eta'(t,x,v)$ here and ξ, η, and η' are given by Eq. (34). The operator V_a is just the Vlasov operator not to be confused with the potential V,

$$V_a = \frac{\partial}{\partial t} + v \frac{\partial}{\partial x} + \frac{q}{m} E(t,x) \frac{\partial}{\partial v}, \tag{39}$$

and the commutator (alternator in Cohen) is

$$[U', V_a] f = U'(V_a f) - V_a(U'f).$$

We seek a solution that is common to both $U'f = 0$ and $V_a f = 0$. The common solution is found from the complete solution that in general is of the form

$$[U', V_a] f = r_1(t,x,v) U'f + r_2(t,x,v) V_a f,$$

that here reduces to Eq. (37).

We use two solutions of $U'f = 0$ called $\mathscr{V}(t,x,v)$ and $\mathscr{Y}(t,x,v)$ to reduce the Vlasov equation to the generalized BGK form. Let $f(t,x,v) = \bar{f}(\mathscr{Y}, \mathscr{V})$. Then

$$V_a \bar{f}(\mathscr{Y}, \mathscr{V}) = V_a \mathscr{Y} \frac{\partial \bar{f}}{\partial \mathscr{Y}} + V_a \mathscr{V} \frac{\partial \bar{f}}{\partial \mathscr{V}} = 0 \tag{40}$$

is the Vlasov equation in the stationary or generalized BGK form. If we divide by $V_a \mathscr{Y}$ we see that our equation becomes

$$\frac{\partial \bar{f}}{\partial \mathscr{Y}} + \frac{V_a \mathscr{V}}{V_a \mathscr{Y}} \frac{\partial \bar{f}}{\partial \mathscr{V}} = 0. \tag{41}$$

The function $V_a \mathscr{V} / V_a \mathscr{Y}$ must be a function of $\mathscr{Y}$ and $\mathscr{V}$ only since $\partial \bar{f} / \partial \mathscr{Y}$ and $\partial \bar{f} / \partial \mathscr{V}$ are functions of those variables even though the numerator or denominator of the fraction may not be if we do not have a Jacobian complete solution. Hence, we find in the ($\mathscr{Y}$, $\mathscr{V}$) variables a BGK-type equation which is stationary in a third coordinate that plays the role of time in these coordinates.

The next question is how do we find the variables $\mathscr{Y}$ and $\mathscr{V}$ as functions of the laboratory coordinates (t,x,v)? We go back to Eq. (13) and consider Eq. (2) as $\tilde{F}(t,x,\dot{x},\ddot{x})$:

$$U''\tilde{F} = \xi \frac{\partial \tilde{F}}{\partial t} + \eta \frac{\partial \tilde{F}}{\partial x} + \eta' \frac{\partial \tilde{F}}{\partial \dot{x}} + \eta'' \frac{\partial \tilde{F}}{\partial \ddot{x}} = 0, \tag{42}$$

where $\dot{x} = v$ and $\ddot{x} = (q/m)E(t,x)$. This equation is equivalent to the set of ordinary differential equations

$$\frac{dt}{\xi(t)} = \frac{dx}{\eta(t,x)} = \frac{d\dot{x}}{\eta'(t,x,\dot{x})} = \frac{d\ddot{x}}{\eta''(t,x,\dot{x},\ddot{x})}. \tag{43}$$

The first and second terms give

$$\frac{dx}{dt} = \frac{\eta(t,x)}{\xi(t)}, \tag{30'}$$

but that is Eq. (30) which has already been solved to give $\bar{x}$. Conventionally the solution of Eq. (30) is called $\mathscr{Y}(t,x)$ so that here we let $\mathscr{Y}(t,x) = \bar{x} = \mathscr{Y}(t,x,\dot{x})$ where there is no $\dot{x}$ dependence. The first and third terms give

$$\frac{d\dot{x}}{dt} = \frac{\eta'(t,x,\dot{x})}{\xi(t)}. \tag{44}$$

The solution of this equation is $\mathscr{V}(t,x,\dot{x})$ and is

$$\mathscr{V}(t,x,\dot{x}) = e^{-(N/2)\bar{t}} \left[\rho(\dot{x} - \dot{\alpha}) - \dot{\rho}(x - \alpha) - \frac{N}{2} \frac{\alpha}{\rho} - \frac{N^2}{4} e^{(N/2)\bar{t}} \int \frac{dt\,\alpha}{\rho^3} e^{-(N/2)\bar{t}} \right] = C_2. \tag{45}$$

The solution is found by substituting for $x(t,\bar{x})$ in $\eta'(t,x,x)$ and noting that as η' is linear in $\dot{x}$, one has a linear ordinary differential equation in $\dot{x}$. Then $\bar{x} = \mathscr{Y}(t,x)$ and $\mathscr{V}(t,x,\dot{x})$ are the new variables that appear in Eq. (41). Before we investigate possible solutions of Eq. (40) or Eq. (41) we integrate the differential equation

$$\frac{d\ddot{x}}{dt} = \frac{\eta''(t,x,\dot{x},\ddot{x})}{\xi(t)}. \tag{46}$$

Again we substitute for $x(t,\bar{x})$ and also $\dot{x}(t,x(t,\bar{x}),\mathscr{V})$ in η'' and integrate the linear differential equation in $\ddot{x}$. We find

$$\ddot{x} = \frac{q}{m} F(t) - \frac{q}{m} \Omega^2(t) x + \frac{q}{m} \frac{k\bar{x}}{\rho^3} e^{(N/2)\bar{t}} + \frac{C_3(\bar{x})}{\rho^3} e^{(N/2)\bar{t}} + \frac{N}{2} \left\{ -\frac{q}{m\rho^3} \int dt\, \rho F + \frac{e^{(N/2)\bar{t}}}{\rho^3} \int dt\, (\alpha\ddot{\rho} - \rho\ddot{\alpha}) e^{-(N/2)\bar{t}} \right\}. \tag{47}$$

This should agree with the expression for the electric field found in Eq. (36a). That agreement holds only if

$$\frac{q}{m} k\bar{x} + C_3(\bar{x}) = -\frac{q}{m} \frac{d}{d\bar{x}} U_e(\bar{x}),$$

where C_3 arises in the integration and if the fifth term on the right-hand side of Eq. (47) vanishes. The fifth term vanishes if $N = 0$ or if

$$\frac{q}{m} \int dt\, \rho F = e^{(N/2)\bar{t}} \int dt\, (\alpha\ddot{\rho} - \rho\ddot{\alpha}) e^{-(N/2)\bar{t}}. \tag{48}$$

Equation (48) can be differentiated with respect to time t to find F. The result for F and $\int dt\, \rho F$ substituted into Eq. (33) for α gives an identity which is consistent.

We now consider Eq. (40). If the Vlasov operator acts on $\mathscr{Y}$ and $\mathscr{V}$, we find by a straightforward calculation that

$$V_a \mathscr{Y} = V_a \bar{x} = \frac{\mathscr{V}}{\rho^2} - \frac{N}{2} \frac{\bar{x}}{\rho^2}, \tag{49a}$$

$$V_a \mathscr{V} = -\frac{N}{2\rho^2} \mathscr{V} - \frac{q}{\rho^2 m} \frac{d}{d\bar{x}} \tilde{U}_e(\bar{x}),$$

$$\tilde{U}_e(\bar{x}) = U_e(\bar{x}) + \frac{k\bar{x}^2}{2}. \tag{49b}$$

The stationary Vlasov equation becomes

$$\left(\mathscr{V} - \frac{N}{2} \bar{x} \right) \frac{\partial \bar{f}}{\partial \bar{x}} - \left(\frac{N}{2} \mathscr{V} + \frac{q}{m} \frac{d}{d\bar{x}} \tilde{U}_e(\bar{x}) \right) \frac{\partial \bar{f}}{\partial \mathscr{V}} = 0, \tag{50}$$

with Eq. (40) multiplied by ρ^2. If one lets $\mathscr{V}' = \mathscr{V} - (N/2)\bar{x}$, then this equation can be put in the standard BGK form but the velocity derivative coefficient is now velocity-dependent in the generalized BGK variables. Only if $N = 0$, which is the condition for the Lewis–Leach group, do we find the velocity-independent force for the stationary Vlasov equation.

The distribution function $\bar{f} = f(t,x,v)$ can be found from Eq. (50) by integrating the characteristic equation. That equation is

$$\frac{d\mathscr{V}}{d\bar{x}} = -\frac{((N/2)\mathscr{V} + (q/m)(d/d\bar{x})\tilde{U}_e(\bar{x}))}{\mathscr{V} - (N/2)\bar{x}} \tag{51}$$

Thus, the solution of the one-dimensional Vlasov equation with a time-dependent electric field for ξ a function of t only

reduces to the solution of the nonlinear, first-order differential equation (51) together with the subsidiary conditions (28) and (33). Equation (51) was also found for the anharmonic oscillator with cubic anharmonicity.[2]

IV. GENERALIZED BGK DISTRIBUTION FUNCTION

We discuss in this section the solution of the stationary Vlasov equation (50). That entails the solution of the first-order, nonlinear ordinary equation (51). This equation can be viewed as an equation for the phase plane orbits as discussed in nonlinear mechanics.[22] The equation appears simple but that simplicity is misleading and no general analytic solution has been found. The equation can be put into the form of the Emden equation, the Thomas–Fermi equation in special cases, but these have been solved numerically under the conditions that apply here or give solutions found below by simpler means.

Two cases are solvable. For $N=0$ we find the Lewis–Leach transformation as has already been pointed out. Then

$$(m/2)\mathscr{V}^2 + q\tilde{U}_e(\bar{x}) = I,$$

where $\tilde{U}_e(x)$ is now the BGK potential and the invariant I is a constant. The distribution function is a functional of the invariant I

$$f(t,x,v) = \bar{f}(\bar{x},\mathscr{V}) = f_s(m\mathscr{V}^2/2 + q\tilde{U}_e(\bar{x})). \tag{52}$$

If $N \neq 0$, we can solve Eq. (51) for $\tilde{U}_e$ quadratic in x. Since quadratic terms in x of V were removed from $U_e(\bar{x})$, this means $U_e = 0$. Also we recall that a more general form exists for this potential because ξ may depend on x as well as t. Equation (51) reduces to

$$\frac{d\mathscr{V}}{d\bar{x}} = -\frac{((N/2)\mathscr{V} + (q/m)k\bar{x})}{\mathscr{V} - (N/2)\bar{x}}. \tag{53}$$

As the numerator and denominator in Eq. (53) are homogenous functions of degree 1, the equation can be solved by the substitution $\mathscr{V} = \bar{x}Y$ (see Ref. 22) and is also invariant under the similitudinous group.[12]

The solutions of Eq. (53) are

$$\mathscr{V} + (N/2)\bar{x} = K_1, \quad qk/m = -N^2/4, \tag{54a}$$

$$\left(\mathscr{V}^2 + \frac{qk}{m}\bar{x}^2\right)^{1/2} \exp\left[-\frac{N}{2}\sqrt{\frac{m}{qk}}\tan^{-1}\left(\frac{\mathscr{V}}{\bar{x}}\sqrt{\frac{m}{qk}}\right)\right] = K_2, \quad kq > 0 \tag{54b}$$

$$\left(\mathscr{V}^2 + \frac{qk}{m}\bar{x}^2\right)^{1/2}\left(\frac{\mathscr{V} + \bar{x}\sqrt{-qk/m}}{\mathscr{V} - \bar{x}\sqrt{-qk/m}}\right)^{(N/4)(-m/qk)^{1/2}} = K_3, \quad kq < 0, \tag{54c}$$

where the invariants are given above and the distribution function is a functional of the invariant.

The first invariant is linear in v or the momentum p that is hidden in $\mathscr{V}$ and is related to a solution given by Lewis and Leach.[4] The other two invariants are not quadratic in the momentum. A special case of the invariant in Eq. (54c) squared with the appropriate value of N could be an invariant of the resonance form. Actually the invariants of Eq. (52) and Eq. (54c) can be put into the resonance form by taking the inverse.

We now relate the invariant in Eq. (54a) to the one discussed by Lewis and Leach. The distribution function $f_s(I)$ is a functional of the invariant I that satisfies the Liouville equation

$$\frac{\partial I}{\partial t} + [I, H] = 0, \tag{55}$$

where the single-particle Hamiltonian is

$$H = p^2/2m + (q/2)\Omega^2(t)x^2,$$

and the Liouville equation is identical in form to the Vlasov equation here. For the $\alpha = 0$ case considered explicitly by Lewis and Leach the invariant becomes

$$I = m(\rho e^{-(N/2)\bar{t}})\dot{x} - m\frac{d}{dt}(\rho e^{-(N/2)\bar{t}})x. \tag{56}$$

The invariant in (4) has the same form as that in Eq. (56) if a is substituted for $\rho \exp(-(N/2)\bar{t})$ but their $a = \rho\cos\bar{t}$. Actually the invariant (56) with negative N also obeys Eq. (55) for the same Hamiltonian H. To see that, we note that $\rho \exp(\pm(N/2)\bar{t})$ satisfies the following differential equation:

$$\frac{d^2}{dt^2}(\rho e^{\pm(N/2)\bar{t}}) + \frac{q}{m}\Omega^2(t)\rho e^{\pm(N/2)\bar{t}} = \left(\ddot{\rho} + \frac{N^2}{4\rho^3} + \frac{q}{m}\Omega^2(t)\rho\right)e^{-(N/2)\bar{t}} = \left(\frac{qk}{m\rho^3} + \frac{N^2}{4\rho^3}\right)e^{\pm(N/2)\bar{t}} = 0, \tag{57}$$

from Eq. (28) and Eq. (54a). Consequently, both $\pm(N/2)$ are valid solutions of Eq. (55) and (57), since for the same function $\Omega^2(t)$ two values of N hold. A linear combination of invariants is then possible. If we choose $N/2 = \pm j$, then two invariants are

$$I_1 = m\dot{x}\rho\cos\bar{t} - mx\frac{d}{dt}(\rho\sin\bar{t}),$$

$$I_2 = m\dot{x}\rho\sin\bar{t} - mx\frac{d}{dt}(\rho\cos\bar{t}), \tag{58}$$

which correspond to the Lewis–Leach solutions. Other choices are possible, of course, depending upon the choice of N.

The question arises as to the existence of other solutions for the Liouville invariant I or the Vlasov one-particle distribution function $\bar{f}(\bar{x},\mathscr{V})$. We can derive Eq. (50) by a coordinate transformation from (t,x,v) to $(\bar{t},\bar{x},\mathscr{V}')$, where $\mathscr{V}' = d\bar{x}/d\bar{t}$. We find

$$\frac{\partial\bar{f}}{\partial\bar{t}} + \mathscr{V}'\frac{\partial\bar{f}}{\partial x} - \left(N\mathscr{V}' + \frac{q}{m}\frac{dU_e'}{d\bar{x}}\right)\frac{\partial\bar{f}}{\partial\mathscr{V}'} = 0, \tag{59}$$

where $\mathscr{V}' = \mathscr{V} - (N/2)\bar{x}$, $U_e'(\bar{x}) = \tilde{U}_e(\bar{x}) + (m/q)(N^2/2)(\bar{x}^2/8)$. If $\bar{f}$ is stationary in this reference frame, Eq. (59) is equivalent to Eq. (50) upon change of variables and becomes the generalized BGK Vlasov equation. Only if $N=0$, do we find the electrostatic BGK solutions in these variables for $U_e \neq 0$. Is some clever change of variables possible that reduces Eq. (59) to the BGK form for $N \neq 0$ and $U_e \neq 0$? To discuss that question we observe that $\bar{x}(t,x)$, $\mathscr{V}(t,x,v)$ are two independent solutions of the partial differential equation $U'f = 0$. Any other solutions of $U'f = 0$ are functions of these two variables. We could introduce $\phi_1(\bar{x},\mathscr{V})$ and $\phi_2(\bar{x},\mathscr{V})$ as the solutions of $U'f = 0$ and then rewrite Eq. (50) in these new variables which might be in the electrostatic

BGK form. This procedure is, however, equivalent to a change of variables in Eq. (51). Therefore, we should look for canonical variables or an integrating factor for Eq. (51). Investigation of Eq. (51) has not revealed any other analytical solutions than those listed. Standard methods for integrating nonlinear, ordinary differential equations,[22] the invariance of the differential equation under the known Lie groups,[12] and the table of differential equations have been checked.[23]

V. DISCUSSION OF RESULTS

The solution of an exact, nonlinear, one-dimensional Vlasov equation for an electric field that depends on one spatial coordinate and time has been reduced to the solution of a nonlinear first-order, ordinary differential equation for the characteristic equation. This reduction holds for all electric fields nonlinear in the spatial coordinate and for a subclass of those linear in the spatial coordinate. The Lie method for the solution of differential equations invariant under a transformation group has started from the group generator for the point transformation. For the coordinate function ξ a function of time only, the group generator contains two functions of time that obey subsidiary differential equations that contain certain arbitrary functions. For ξ linear in the spatial coordinate only two differential equations are given for four functions of time. These undetermined functions in both cases are needed partially, at least, to satisfy additional constraints imposed by Maxwell's equations.[8,9,18]

The functional dependence of the one-particle distribution function that satisfies the exact, nonlinear, one-dimensional Vlasov equation has been given analytically for several cases. The Lewis–Leach invariant which is quadratic in the momentum has been found. For the generalized BGK Vlasov equation with an electric field linear in the spatial coordinate invariants for several ranges of integration constants have been found. One is related to the invariant linear in the momentum. Several invariants in special cases are of the resonance form.

The Lie group method of determining the functional dependence of the on-particle distribution function of the Vlasov equation has advantages and disadvantages over other approaches. The advantages are discussed first.

The general infinitesimal transformation of the Lie group has been found for the Vlasov equation where the indeterminateness of the functions of time in the two cases considered is the same as found in other methods and is partially needed to satisfy the additional constraints imposed by Maxwell's equations. Since the Lie group method includes a wide class of solutions, the class of analytical Liouville invariants is restricted, thereby. Defining the possible class of analytical Liouville invariants is much more difficult by the direct method in which the particular momentum dependence of an invariant is assumed.

Second, solution of the time-dependent Vlasov equation has been reduced for the electric field nonlinear in the spatial coordiate to a generalized BGK Vlasov equation or to a characteristic equation that is a nonlinear, first-order ordinary differential equation (51). The latter equation is in the form in which the possibility of an analytical solution is most easily appreciated. For example, in the direct method in which the momentum dependence is assumed or in the use of velocity-dependent coordinate transformations, nonlinear partial differential equations result that are so complicated that one has difficulty ascertaining whether a solution exists.

Third, the generalized BGK Vlasov equation or the characteristic equation for it is a natural starting point for approximations. One can investigate by perturbation theory distribution functions that are close to the analytical ones. For instance, if one has a potential that contains a dominant term quadratic in x and a small term cubic in x, a perturbation expansion of the distribution function about the result for the potential in x would be reasonable. On the other hand, if the integration constant N is small, an expansion of the distribution function about the Lewis–Leach result would be appropriate where the Liouville eigenfunctions could be used.

Fourth, the analysis of phase orbits for the characteristic equation as is done extensively in nonlinear mechanics would give qualitative information about the orbits. Of course, numerical integration of the orbits could be made.

The chief disadvantage of the Lie group method of point transformation for the one-dimensional Vlasov equation is that one does not choose the momentum dependence. However, for analytical invariants the ability to choose invariants may be a bit illusory if one looks at the restricted class of analytical solutions found here. The Lie group method may not be as easy to apply to systems with more variables. Lewis has generalized the invariant to a three-dimensional plasma in rectangular cartesian coordinates with an electromagnetic field and we have found the invariant in unpublished calculations in right circular cylindrical geometry for a generalization of a rigid rotator distribution function for a θ pinch. Extending the Lie group method for these cases seems more difficult than using the direct approach. However, since an invariant exists, some Lie group under which the Vlasov equation is invariant exists which could serve as a guide to finding the form of the most general one. The solutions found here by the Lie groups for point transformations are not the most general since contact transformations may also occur.

The Lie group method presented here can also be compared with other approaches that use the invariance of differential equations under Lie point translations. The first alternative approach finds the group for the invariance of the complete set of Vlasov–Maxwell equations under Lie point transformations where the method in Bluman and Cole[15] for sets of partial differential equations is extended to include integrals. Roberts[20] gives a general exposition of this method applied to the one-dimensional Vlasov–Maxwell equations. Earlier treatments included the indirect determination of group generators by Baranov[18] for the single-species plasma in a constant density, immobile background and a determination of group generators for a multispecies plasma by Axford[19] in lecture notes. The second alternative approach was suggested by a referee where the one-dimensional Vlasov equation is used with the electric field given in terms of a Green's function found from Poisson's equation. The constraint of the longitudinal current density must also be added and the purely time-dependent part of the electric field put in

explicitly. For the one-dimensional, multispecies plasma all approaches appear to give the same group when the constraints imposed by Maxwell's equation are included and a time-dependent electric field added to the field found from a Green's function. The alternative methods are more efficient than the method presented here. Nevertheless two reasons exist for presenting this method. First, the method is closest to the traditional approach used in solving the Vlasov–Maxwell equations and therefore most immediately accessible to plasma physicists. The other reason is that the alternative methods may omit possible solutions of the Vlasov–Maxwell equations. Such an example has been found. The example is a single-species plasma in a neutralizing background with a longitudinal electric field that varies with (x,t) perpendicular to a uniform magnetic field. For this plasma the Lie group solution for the Vlasov equation alone or for the Vlasov equation with the electric field in terms of a Green's function gives a more general result than for the solution of the Vlasov–Maxwell set that is invariant under a Lie point transformation. The time dependence of the electric field on the upper-hybrid frequency occurs for the first two cases but not for the last one.

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ERRATUM

Erratum: Remarks on canonical transformations in phase-space path integrals [J. Math. Phys. 24, 874 (1983)]

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Equation (1.8) should read

$$\Delta V(\bar{Q}_j) = (\hbar^2/8m)\{[f''(\bar{Q}_j)]^2/[f'(\bar{Q}_j)]^4\}.$$

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