Generating functions for IR multiplicities

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(Received 25 February 1982; accepted for publication 28 May 1982)

The construction of generating functions for multiplicities of irreducible representations from generating functions for compound characters is examined. Weyl reflection symmetry is used to simplify the procedure. Two examples involving the enumeration of SU(3) irreducible representations are discussed.

PACS numbers: 02.20. + b, 02.30. + g

1. INTRODUCTION

In the last few years, generating functions have emerged as a useful tool for the solution of a number of problems in group representation theory.[1] A single generating function (GF) enumerates, in a closed form, all irreducible representations (IR's) of finite dimension contained in some infinite set of reducible representations. This infinite set may be, for example, the set of all direct products of two IR's or the set of all IR's of some larger group. In the former case we obtain a generating function for the Clebsch–Gordan series while in the latter we obtain a GF for subgroup branching rules.

Generating functions are rational expressions whose numerators and denominators are polynomials in auxiliary variables with integer coefficients. When expanded in power series, they contain only terms with positive integer coefficients. These coefficients represent the multiplicities of the IR labeled by the corresponding powers in the auxiliary variables. In a special form, with only positive coefficients in the numerators and with denominators which are products of terms $(1 - X)$, where X is a product of powers of the auxiliary variables, the GF's provide information about the corresponding integrity basis.

Generating functions can be obtained in several ways. Simpler GF's can be guessed directly from the lower terms in the power series expansion, the result then being tested. A GF can be constructed from others by a process of "substitution."[2] Finally, generating functions can be constructed from the characters of the IR's in a manner described below. It is the last method which will concern us here.

The construction of generating functions can be a tedious procedure. During intermediate stages, before simplification, the function can "balloon" into an almost impossibly complicated form. In general, the larger the number of $(1 - X)$ denominator factors, the more complicated the GF becomes during the intermediate stages. If some of these factors can be effectively eliminated the construction can be simplified. Such an elimination has made it possible to construct several generating functions enumerating SU(2) irreducible representations.[3,4] In this paper we shall generalize the technique to IR's of any semisimple Lie group.

In Sec. 2 we review the construction of generating functions from IR characters. In Sec. 3 we derive the basic formulae of the elimination method. Some examples involving multiplicities of SU(3) IR's are presented in Sec. 4. Section 5 contains some concluding remarks.

2. CONSTRUCTION OF GF's FROM IR CHARACTERS

The character of an irreducible representation λ of a Lie group can be written

$$\chi_\lambda(\eta) = \sum_{j=1}^{d} \prod_{i=1}^{l} \eta_i^{m_{ij}}, \tag{1}$$

where d is the dimension of the IR, l is the rank of the group, m_{ij} is the ith component of the jth weight and the η_i are class labels. These characters can be determined from the relation[5]

$$\chi_\lambda(\eta) = \xi_\lambda(\eta)/\xi_0(\eta). \tag{2}$$

$\xi_\lambda(\eta)$ is the Weyl characteristic for the IR $\lambda = (\lambda_1,...,\lambda_l)$

$$\xi_\lambda(\eta) = \sum \det(S) \prod_{i,j,k=1}^{l} \eta_i^{\gamma_{ij} S_{jk}(\lambda_k + 1)}, \tag{3}$$

where the sum is over Weyl reflections, γ_{ij} is the ith component of the highest weight of the jth fundamental IR and S_{jk} are the matrices which transform the γ_{ij} under the Weyl group. The S_{jk} consist of the matrices

$$S^n_{jk} = \delta_{jk} - A_{jk}\delta_{kn} \quad (n = 1,...,l), \tag{4}$$

and all distinct products of these. A_{jk} is the Cartan matrix of the group.

Equation (3) can be used to obtain a generating function for Weyl characteristics:

$$\Xi(A,\eta) = \sum \det(S) \prod_{k=1}^{l} \left[\prod_{i,j=1}^{l} \eta_i^{\gamma_{ij} S_{jk}} \right] \times \left[1 - A_k \prod_{i,j=1}^{l} \eta_i^{\gamma_{ij} S_{jk}} \right]^{-1}. \tag{5}$$

The coefficent of $A_1^{\lambda_1}\cdots A_l^{\lambda_l}$ in the expansion of (5) is the characteristic $\xi_\lambda(\eta)$. With (2) and (5) we obtain a formal expression for the IR character generator:

$$X(A,\eta) = \Xi(A,\eta)/\Xi(0,\eta). \tag{6}$$

Again the exponents of the auxiliary variables A label the irreducible representations while the coefficients provide the corresponding character $\chi_\lambda(\eta)$. If the η are treated as auxiliary variables, then (6) becomes a weight generator. If the η are set equal to 1, then (6) becomes a generator for IR dimen-

 0022-2488/82/122217-04$02.50

sions. The character generator is a useful starting point for the construction of other generating functions.

The characteristic can be used to construct the function

$$\psi_\mu(\eta) = \xi_0(\eta) \prod_{i,j=1}^{l} \eta_i^{-\gamma_{ij}(\mu_j+1)}, \tag{7}$$

which has the property

$$[\psi_\mu(\eta)\chi_\lambda(\eta)]_{\mathrm{EX}(\eta)=0} = \delta_{\mu\lambda}, \tag{8}$$

where the instruction $\mathrm{EX}(\eta)=0$ indicates that we are to keep only terms in the expansion which are independent of the η_i. Acting on a compound character, the function $\psi_\mu(\eta)$ under the operation $\mathrm{EX}(\eta)=0$ projects out the multiplicity of the $\mathrm{IR}(\mu)$. We can therefore construct the generating function

$$\Psi(A,\eta) = \xi_0(\eta) \prod_{j=1}^{l}\left[\prod_{i=1}^{l} \eta_i^{-\gamma_{ij}}\right] \times\left[\left(1 - A_j \prod_{i=1}^{l} \eta_i^{-\gamma_{ij}}\right)\right]^{-1}. \tag{9}$$

If $\chi(\eta)$ is the character of a reducible representation which contains the irreducible representation (λ) with a multiplicity N_λ then

$$G(A) = [\Psi(A,\eta)\chi(\eta)]_{\mathrm{EX}(\eta)=0} = \sum_\lambda N_\lambda \prod_{i=1}^{l} A_i^{\lambda_i}, \tag{10}$$

is a generating function for IR multiplicities.

A particularly useful basis in which to work is one in which $\gamma_{ij} = \delta_{ij}$. In this "$\delta$-basis" we have

$$\xi_0(\eta) = \Xi(0,\eta) = \sum \det(S) \prod_{i,k=1}^{l} \eta_i^{S_{ik}}, \tag{11}$$

and

$$G(A) = \left[\chi(\eta)\xi_0(\eta) \prod_{i=1}^{l} \eta_i^{-1}(1 - A_i/\eta_i)^{-1}\right]_{\mathrm{EX}(\eta)=0}. \tag{12}$$

Equation (12) can be shown to be equivalent to

$$G(A) = \left[\chi(A)\xi_0(A) \prod_{i=1}^{l} A_i^{-1}\right]_{\mathrm{EX}(A)\geqslant 0}, \tag{13}$$

where the $\mathrm{EX}(A)\geqslant_0$ instructs us to keep only the part whose expansion contains nonnegative powers of A_i.

3. ELIMINATION OF DENOMINATOR FACTORS

Suppose the operation described in Eq. (13) is applied to a generating function $\chi(\eta,B)$ whose expansion in terms of the auxiliary variables B yields a set of compound characters. Then the resulting function $G(A,B)$ will be a generating function enumerating the irreducible representations (labeled by A) contained in reducible representations (labeled by B). The function $\chi(A,B)$ will be a sum of rational expressions whose denominators are products of factors $(1-X)$ where X is a product of powers of the variables A and B. The products X will contain only nonnegative powers of the B but some A_i in the products may have negative exponents. A systematic procedure exists for the implementation of the $\mathrm{EX}(A)\geqslant 0$ instruction. If a term has a denominator which contains the factor $(1 - PA^p)(1 - QA^{-q})$ where A is one of the variables A and P and Q are products of powers of the other variables, then the term can be replaced by a sum of two terms whose denominators contain the factors $(1 - Q^pP^q)(1 - PA^p)$ and $(1 - Q^pP^q)(1 - QA^{-q})$:

$$\frac{1}{(1-PA^p)(1-QA^{-q})} = \left(\sum_{m=0}^{p-1} \frac{Q^mA^{-mq}}{(1-PA^p)} + Q^pA^{-pq}\sum_{m=0}^{q-1} \frac{P^mA^{mp}}{(1-QA^{-q})}\right)\Big/(1-Q^pP^q). \tag{14}$$

In this way a term can be reduced, step by step, to a part with only nonnegative powers of A in its expansion and one with only negative powers, which is discarded. The other A variables are handled similarly. This procedure, and all other reduction procedures, become more difficult as the number of $(1-X)$ denominator factors increases. In this section we shall exploit the Weyl reflection symmetry of the characters to effectively reduce the number of these factors.

The function $G(A)$ defined in (13) (we will suppress the variable B) must also satisfy

$$G(A) = \chi(A)\xi_0(A) \prod_{i=1}^{l} A_i^{-1} - \sum_{S\neq I} \det(S) G(A^S) \prod_{i=1}^{l} (A_i^S/A_i), \tag{15}$$

by virtue of the Weyl reflection properties of the first term on the right-hand side. Here the reflection of the variable A_i is

$$A_i^S = \prod_{j=1}^{l} A_j^{S_{ji}}, \tag{16}$$

and the sum is over all reflections except the identity. It is easily verified that the operation $\mathrm{EX}(A)\geqslant 0$ applied to Eq. (15) gives Eq. (13) since the last term vanishes under this operation.

Suppose that we can identify a portion $D(A)$ of the denominator of $\chi(A)$ as a portion of the common denominator of $G(A)$. In other words, we can write

$$G(A) = R(A)/D(A), \tag{17}$$

and

$$\chi(A)\xi_0(A) = \phi(A)/D(A). \tag{18}$$

Then if we multiply (15) by $D(A)$ and perform the $\mathrm{EX}(A)\geqslant 0$ operation we find

$$R(A) = H(A) - \left[\sum_{S\neq I} \frac{\det(S)R(A^S)D(A)}{D(A^S)} \prod_{i=1}^{l} (A_i^S/A_i)\right]_{\mathrm{EX}(A)>0}, \tag{19}$$

where

$$H(A) = \left[\phi(A) \prod_{i=1}^{l} A_i^{-1}\right]_{\mathrm{EX}(A)>0}. \tag{20}$$

The second term on the right-hand side of Eq. (19) is nonzero for only a few terms in the expansion of $R(A^S)$ so that this equation can be solved relatively easily for $R(A)$ once $H(A)$ is known. The determination of $H(A)$ from Eq. (20) is simpler than the determination of $G(A)$ from Eq. (13) due to the reduced number of denominator factors.

4. MULTIPLICITIES OF SU(3) IR's

In this section we shall demonstrate the procedure discussed above with two examples involving the enumeration of SU(3) irreducible representations. In order to limit the number of subscripts, we shall use A,B instead of A_1, A_2 as the variables whose exponents label the IR's. The Cartan matrix for SU(3) is

$$\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

from which the S_{ij} are found to be

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} -1 & -1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ -1 & -1 \end{bmatrix} \text{ and } \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix}.$$

Corresponding to these we have the reflections

n	$\det(S)$	A^s	B^s
0	1	A	B
1	−1	$A^{-1}B$	B
2	1	$A^{-1}B$	A^{-1}
3	−1	B^{-1}	A^{-1}
4	1	B^{-1}	AB^{-1}
5	−1	A	AB^{-1}

where $n=0$ is the identity $S=I$. The function ξ_0 is

$$\begin{aligned}\xi_0(A,B) &= AB - A^{-1}B^2 + A^{-2}B \\ &\quad - A^{-1}B^{-1} + AB^{-2} - A^2B^{-1} \\ &= AB(1-A^{-2}B)(1-A^{-1}B^{-1})(1-AB^{-2}). \end{aligned} \tag{21}$$

A. SU(3) Clebsch–Gordan series

This well-known generating function provides a useful first test of our methods. The function χ in (13) and (15) is the product of two SU(3) character generators

$$\chi(A_1,B_1,A_2,B_2,A,B) = X(A_1,B_1,A,B)X(A_2,B_2,A,B), \tag{22}$$

where the exponents of A_1,B_1 and A_2,B_2 label the SU(3) IR's whose product is to be decomposed into a sum of SU(3) IR's. The final result is expected to have a common denominator factor

$$D = (1-A_1A)(1-A_2A)(1-B_1B)(1-B_2B), \tag{23}$$

and with this substitution Eq. (19) becomes, suppressing the variables A_1,B_1,A_2,B_2 for the moment,

$$\begin{aligned} R(A,B) &= H(A,B) + A_1A_2BR(0,B) + B_1B_2AR(A,0) \\ &\quad + A_1A_2B_1B_2R(0,0). \end{aligned} \tag{24}$$

With some manipulation, the characteristic generator (5) can be written, in the δ-basis,

$$\Xi(A_i,B_i,A,B) = AB\tilde{\Xi}(A_i,B_i,A,B)/((1-A_iA)(1-B_iB)), \tag{25}$$

where

$$\begin{aligned}&\tilde{\Xi}(A_i,B_i,A,B) \\ &= \sum \det(S)(1-A^s/A)(1-B^s/B)/((1-A_iA^s)(1-B_iB^s)).\end{aligned} \tag{26}$$

Using (6) to turn this into a character generator and with (18), (21), and (22) we find

$$\begin{aligned}&A^{-1}B^{-1}\phi(A,B) \\ &\quad = \frac{\tilde{\Xi}(A_1,B_1,A,B)\tilde{\Xi}(A_2,B_2,A,B)}{(1-A^{-2}B)(1-A^{-1}B^{-1})(1-AB^{-2})}. \end{aligned} \tag{27}$$

The $\mathrm{EX}(A,B)\geqslant 0$ part of this is

$$H(A,B) = A_1B_2/(1-A_1B_2) + 1/(1-A_2B_1). \tag{28}$$

After solving (24) for $R(A,B)$ and dividing by (23) we find

$$G(A_1,B_1,A_2,B_2,A,B) = \frac{(1/(1-A_1A_2B) + B_1B_2A/(1-B_1B_2A))}{(1-A_1A)(1-B_1B)(1-A_2A)(1-B_2B)(1-A_1B_2)(1-A_2B_1)} \tag{29}$$

which is the desired result.[1]

B. Polynomials in the (3,0) representation of SU(3)

We now construct the generating function $G(U,A,B)$ in which the coefficient of $U^uA^aB^b$ enumerates the (a,b) representations of SU(3) contained in the symmetric part of the direct product of u (3,0) representations. We start with the δ-basis character generator

$$\begin{aligned}\chi(U,A,B) &= [(1-UA^3)(1-UAB)(1-U)(1-UA^{-3}B^3)(1-UB^{-3})(1-UA^{-1}B^{-1}) \\ &\quad (1-UAB^{-2})(1-UA^{-1}B^2)(1-UA^2B^{-1})(1-UA^{-2}B)]^{-1}, \end{aligned} \tag{30}$$

where the coefficient of U^u in the expansion is the character of the product of u (3,0) representations of SU(3). The form of (30) suggests that we attempt to remove a common denominator factor $D=(1-UA^3)(1-UAB)$.

The function $H(U,A,B) = [D\chi\xi_0/AB]_{\mathrm{EX}(A,B)\geqslant 0}$ is found to be

$$\begin{aligned}H(U,A,B) &= (1+U^3)(1+U^2AB+U^4A^2B^2)/((1-U^2)(1-U^4)(1-U^6)(1-U^3A^3)(1-U^3B^3)) \\ &\quad - U(1+U)(1+U^3AB+U^6A^2B^2)/((1-U^2)(1-U^4)(1-U^6)(1-U^4A^3)(1-U^5B^3)). \end{aligned} \tag{31}$$

Equation (19) becomes

$$\begin{aligned}R(U,A,B) &= H(U,A,B) + R_0(B)(U^2A^2B^2 + U^3AB^4U^4B^6 - UAB - U^2B^3) + R_1(B)(U^2AB^3 + U^3B^5 - UB^2) \\ &\quad + R_2(B)(U^2B^4) + (U - U^2AB)R_{00} - U^2B^2R_{10} - U^2BR_{01}, \end{aligned} \tag{32}$$

where we use the notation

$$R(U,A,B) = \sum_i R_i(B) A^i = \sum_{ij} R_{ij} A^i B^j. \tag{33}$$

Equation (32) is easily solved by equating coefficients of appropriate powers of A and B. The required generating function is found to be

$$\begin{aligned} G(U,A,B) &= R(U,A,B)/((1-UA^3)(1-UAB)) \\ &= [(1+U^{12}B^9+U^5AB^4+U^7AB^4+U^7AB^7+U^9AB^7+U^6A^2B^5+U^8A^2B^5+U^8A^2B^8+U^{10}A^2B^8 \\ &\quad +U^3A^3B^3+U^{15}A^3B^{12})/((1-U^5B^3)(1-U^4B^6))+(U^8AB^4+U^4A^2B^2+U^6A^2B^2 \\ &\quad +U^{10}A^2B^5+U^7A^3B^3+U^8A^3B^3+U^9A^3B^3+U^{11}A^3B^6+U^7A^4B+U^9A^4B^4+U^{10}A^4B^4+U^{11}A^4B^4 \\ &\quad +U^8A^5B^2+U^9A^5B^2+U^{10}A^5B^2+U^{12}A^5B^5+U^8A^6+U^{10}A^6B^3+U^{11}A^6B^3+U^{12}A^6B^3 \\ &\quad +U^9A^7B+U^{13}A^7B^4+U^{15}A^7B^4+U^{11}A^8B^2)/((1-U^5B^3)(1-U^8A^6))+(U^3A^3+U^5A^3B^3 \\ &\quad +U^4A^4B+U^5A^4B+U^6A^5B^2+U^7A^5B^2+U^{10}A^7B+U^{11}A^7B+U^{12}A^8B^2+U^{13}A^8B^2+U^{12}A^9 \\ &\quad +U^{14}A^9B^3)/((1-U^3A^3)(1-U^8A^6))]/((1-U^4)(1-U^6)(1-UA^3)(1-U^2A^2B^2)(1-U^3B^3)). \end{aligned} \tag{34}$$

Notice that we have had to multiply numerator and denominator by $(1+UAB)$ and, for the last two terms, $(1+U^4A^3)$ in order to obtain positive coefficients in the numerators. The denominator factor $(1-U^4B^6)$ appears in the solution of Eq. (32).

5. CONCLUDING REMARKS

The technique outlined here promises to be useful in the construction of generating functions when common denominator factors are known or can be guessed. As is particularly evident in the second example, the method splits a difficult procedure into two much simpler ones. In fact, it is always possible to split the function $H(A)$ into a piece which forms a part of $R(A)$ directly and one which enters into Eq. (19) for the rest of $R(A)$. It can be seen from Eq. (32), for example, that the $\mathrm{EX}(A) > 2$ parts of $H(U,A,B)$ and $R(U,A,B)$ must be the same.

This method is quite useful in the construction of generating functions for the Clebsch–Gordan series, both because many common denominator factors are known and because Eq. (19) takes a particularly simple form. Work has recently been completed on the Clebsch–Gordan generator for G_2.[6]

As was mentioned in Sec. 1, there are several ways in which generating functions can be constructed. Regardless of the method of construction, Eq. (15) provides us with a way of testing the resulting generating function. It can be rewritten to give the δ-basis character generator in terms of the IR generator:

$$\chi(A) = \xi_0^{-1}(A) \sum_S \det(S) G(A^s) \prod_{i=1}^{l} A_i^{s}. \tag{35}$$

Both sides of Eq. (35) can be calculated on a computer for a large number of random values of the parameters. If the equation is satisfied, we can be confident that the GF has been constructed correctly. This method was used to verify Eq. (34).

ACKNOWLEDGMENT

We would like to thank R. T. Sharp for helpful discussions.

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Implementation of automorphism groups in certain representations of the canonical commutation relations

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(Received 18 May 1982; accepted for publication 25 June 1982)

Necessary and sufficient conditions are given for the unitary implementability of one-parameter unitary groups of one-particle automorphisms of the CCR algebra in representations symplectically related to the Fock representation. The criteria become particularly simple when the one-particle generator of the unitary group is positive and bounded away from zero; in this case the automorphism group is unitarily implementable only in the representations unitarily equivalent to the Fock representation. If the spectrum of the generator includes zero, however, the situation is more complicated; there then exist representations inequivalent to the Fock representation which admit unitary implementation of the automorphism group. It is also shown that whenever implementation of the automorphism group is possible, the implementing operators can be chosen to be a strongly continuous unitary group, guaranteeing the existence of a "second-quantized" self-adjoint generator.

PACS numbers: 02.20. + b, 03.65.Fd

I. INTRODUCTION

Criteria for the unitary implementability of particular automorphism groups of an abstract algebra are of great interest for the selection of physically meaningful representations of the algebra. Here necessary and sufficient conditions are found for the unitary implementability of a class of dynamical automorphisms of the algebra of the canonical commutation relations in representations symplectically related to the standard (Fock) representation. More specifically, the following situation is analyzed.

Let $\mathscr{H}$ be a separable complex Hilbert space, also regarded as a real symplectic space with sympletic form equal to the imaginary part of the inner product. Let $\mathscr{F}$ be the boson Fock space over the complex space $\mathscr{H}$, that is,

$$\mathscr{F} \equiv \mathscr{H}_0 \oplus \mathscr{H}_1 \oplus \mathscr{H}_2 \oplus \cdots,$$

where $\mathscr{H}_0 \equiv \{c\Omega \,|\, c \in \mathbb{C}\}$ is one-dimensional, $\mathscr{H}_1$ is isomorphic to $\mathscr{H}$, and $\mathscr{H}_n$ is the n-fold symmetrized tensor product of $\mathscr{H}_1$ with itself.

The Fock space $\mathscr{F}$ carries the standard irreducible representation (by unitary operators) of the Weyl group $W: \mathscr{H} \to B(\mathscr{F})$ over $\mathscr{H}$ in which

$$W(f)W(g) = e^{-iB(f,g)/2} W(f+g),$$

where B is the symplectic form, and in which $\{W(f)\Omega \,|\, f \in \mathscr{H}\}$ is total in $\mathscr{F}$. The abstract Weyl C^*-algebra $\mathscr{W}$ generated by the Weyl group (Segal[1]) 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 $\mathscr{H}$ which preserve the symplectic form B are of interest because they leave invariant the Weyl group structure, i.e., the canonical commutation relations. A *symplectic transformation* $S: \mathscr{H} \to \mathscr{H}$ is a bounded real-linear transformation with bounded inverse such that $B(Sf, Sg) = B(f, g)$ for all f and g in $\mathscr{H}$. A symplectic transformation S induces an automorphism σ on the Weyl algebra given by $\sigma(W(f)) \equiv W(Sf)$. Such an automorphism σ (or, loosely speaking, the symplectic transformation S) is *unitarily implementable* in a representation π of the Weyl algebra if there exists a unitary operator U on the carrier space of the representation such that

$$\pi(\sigma(W(f))) \equiv \pi(W(Sf)) = U\pi(W(f))U^*, \quad \text{for all } f \text{ in } \mathscr{H}.$$

The representation π_T of $\mathscr{W}$ induced via the Gel'fand–Naimark–Segal construction by the state E_T on $\mathscr{W}$ given by

$$E_T(W(f)) \equiv E_I(W(f)),$$

where T is symplectic and $E_I(A) \equiv \langle \Omega \,|\, A\Omega \rangle$ 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_T may be identified with the Fock space $\mathscr{F}$. Then with the convention that the representation symbols are dropped for the Fock representation, $\pi_T(W(f)) \equiv W(Tf)$.

This paper treats the following issue. Consider a continuous one-parameter group of unitary transformations $V_t: \mathscr{H} \to \mathscr{H}$ generated by a nonnegative-definite self-adjoint operator H; $V_t \equiv e^{itH}$. Such a group induces an automorphism group ν_t on $\mathscr{W}$ given by $\nu_t(W(f)) \equiv W(V_t f)$. The main question is, in which representations π_T of $\mathscr{W}$ symplectically related to the Fock representation can ν_t be implemented by a one-parameter unitary family on $\mathscr{F}$?

The answer depends on the spectrum of H. Theorem 1 below shows that if H is bounded away from zero, ν_t is unitarily implementable only in the representations unitarily equivalent to the Fock representation. If the spectrum of H includes zero, however, there exist representations π_T inequivalent to the Fock representation which admit implementation of the automorphism group ν_t. Explicit general criteria, in terms of H and T, for the unitarily implementability of ν_t in π_T are given in Theorem 1, and a generic example of a representation inequivalent to the Fock representation in which a one-parameter group V_t is unitarily implementable is given in Sec. VIII.

It is also shown that whenever implementation of the

[a)] Supported by National Science Foundation Grant No. PHY-79-23251. This work is based in part on results presented in a thesis to be submitted by the author in partial fulfillment of the requirements for the degree of Doctor of Philosophy at the University of California, Berkeley.

 0022-2488/82/122221-08$02.50

automorphism group ν_t is possible, the implementing unitaries can be chosen to be a strongly continuous unitary group. Thus there always exists a "second-quantized" self-adjoint generator in representations where the dynamical automorphism is unitarily implemented.

II. THE MAIN RESULT

To remove the temptation to commute it with real-linear operators, denote by Λ the operation of multiplication by the complex number i on the Hilbert space $\mathscr{H}$.

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_T be the representation of $\mathscr{W}$ induced by the symplectic transformation $T:\mathscr{H}\to\mathscr{H}$.

Let H be a nonnegative, self-adjoint, complex-linear transformation with domain $D(H)$ dense in $\mathscr{H}$, 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 unitary group generated by H, and let $\nu_t:\mathscr{W}\to\mathscr{W}$ be the automorphism induced by V_t:

$$\nu_t(W(f)) = W(V_t f) \quad \text{for all } f\in\mathscr{H}.$$

Then the automorphism ν_t is unitarily implementable in the representation π_T of $\mathscr{W}$ for all $t\in\mathbb{R}$ if and only if for some $m>0$, both $P_m(|T|^2 - I)$ and $[|T|^2, \Lambda(I-P_m)H]$ are Hilbert-Schmidt operators. In particular, if H is bounded away from zero then ν_t is unitarily implementable in π_T for all real t if and only if π_T is unitarily equivalent to the Fock representation.

Furthermore, if ν_t is unitarily implementable in π_T 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 $|T|^2 \equiv T^*T$, with T^* the real adjoint of T, and the trace in the definition of the Hilbert–Schmidt norm is defined in terms of the real inner product on $\mathscr{H}$.

These results are applicable to the specific case in which ν_t is regarded as a dynamical automorphism induced by the one-particle time development V_t, with H the one-particle Hamiltonian. In this case, H being bounded away from zero corresponds to strictly positive energy. With this physical interpretation, Theorem 1 implies that only in theories with massless excitations can the interesting situation occur that there exist representations symplectically related but inequivalent to the Fock representation which admit unitary implementation of the time development. Although this physical interpretation plays no role in the mathematics, the terms "Hamiltonian" and "energy" are used in place of "self-adjoint operator" and "spectral value" in what follows.

The proof of Theorem 1 is divided into two pieces. Sections III, IV, and V establish the necessary and sufficient conditions for the implementability of ν_t in π_T, while Secs. VI and VII prove the continuity of the implementation.

III. CONDITIONS FOR IMPLEMENTABILITY

Let ν_t be the automorphism group induced by $V_t \equiv e^{itH}$ as above, and let $T:\mathscr{H}\to\mathscr{H}$ be symplectic. The necessary and sufficient conditions stated in Theorem 1 for the implementability of ν_t in the representation π_T follow directly from Theorem 2 below, which contains the crux of the issue. The following considerations demonstrate that the unitary implementability of ν_t in π_T is equivalent to the condition (I) of Theorem 2 that $[|T|^2, V_t]$ be a Hilbert–Schmidt operator for all t.

First, note that implementability in π_T of ν_t is equivalent to the implementability in the Fock representation of the automorphism induced by the one-parameter symplectic group TV_tT^{-1}, because

$$U_t\pi_T(W(f))U_t^* = \pi_T(\nu_t(W(f))), \quad \text{for all } f\in\mathscr{H},$$

$$\text{iff } U_t\pi_T(W(f))U_t^* = \pi_T(W(V_t f)), \quad \text{for all } f\in\mathscr{H},$$

$$\text{iff } U_t W(Tf)U_t^* = W(TV_t f), \quad \text{for all } f\in\mathscr{H},$$

$$\text{iff } U_t W(f)U_t^* = W(TV_tT^{-1}f), \quad \text{for all } f\in\mathscr{H}.$$

Second, the question of implementability of a symplectic transformation S can be reduced to consideration only of the properties of S as an operator on $\mathscr{H}$. The following criterion for the unitary implementability in the Fock representation of the Weyl algebra of a given symplectic transformation S was found by Shale[2]:

There exists a unitary operator $U:\mathscr{F}\to\mathscr{F}$ such that $UW(f)U^* = W(Sf)$ for all f in $\mathscr{H}$ if and only if $(|S| - I)$ is a Hilbert–Schmidt operator.

Here again $|S| \equiv (S^*S)^{1/2}$, with S^* the real adjoint of S, and the trace in the definition of the Hilbert-Schmidt norm is taken over a real basis for $\mathscr{H}$.

So V_t is implementable in π_T if and only if TV_tT^{-1} is implementable in the Fock representation, which is the case if and only if $(|TV_tT^{-1}| - I)$ is of Hilbert–Schmidt type for all times t. Now, note that for a bounded real-linear transformation Y, $(|Y| - I)$ is a Hilbert–Schmidt operator if and only if $(Y^*Y - I)$ is a Hilbert–Schmidt operator, because the set $\mathbf{B}_{2r}$ of real-linear operators of Hilbert–Schmidt type is a *-ideal, the operator $(|Y| + I)$ has a bounded inverse, and $(Y^*Y - I) = (|Y| + I)(|Y| - I)$. Note furthermore that $(|TV_tT^{-1}|^2 - I)$ being a Hilbert–Schmidt operator is equivalent to the commutator $[|T|^2, V_t]$ being a Hilbert–Schmidt operator, because

$$(|TV_tT^{-1}|^2 - I) = T^{*-1}V_t^*(|T|^2V_t - V_t|T|^2)T^{-1},$$

and both T and V_t have bounded inverses.

Thus V_t is implementable in π_T iff $[|T|^2, V_t]$ is a Hilbert–Schmidt operator for all times t.

Now, it is clear that if T satisfies Shale's criterion, then V_t is implementable in π_T. But is it necessary that T be of Shale type for TV_tT^{-1} to be? The answer is no; if the spectrum of the Hamiltonian H which generates V_t includes zero, then other symplectic transformations T in addition to those of Shale type yield a one-parameter symplectic group TV_tT^{-1} which is of Shale type for all t. An example of such a T is given in Sec. VIII.

The properties of $|T|^2$ which embody the fact that $[|T|^2, V_t] \in \mathbf{B}_{2r}$ for all t obviously depend on the relationship between $|T|^2$ and the Hamiltonian H; Theorem 2 states these properties in terms of the spectral projection P_m for H onto energies larger than $m>0$.

Theorem 2. Let H be a nonnegative, self-adjoint, complex-linear transformation with domain $D(H)$ dense in the separable Hilbert space $\mathscr{H}$. Let $V:\mathbb{R}\to\mathbf{B}(\mathscr{H})$ be the (strongly continuous) unitary group generated by H, $V_t = e^{t\Lambda H}$, and consider an open interval $\tau\subseteq\mathbb{R}$ with $0\in\tau$. Let P_m be the spectral projection for H onto spectral values larger than m.

Let S be a symplectic transformation on $\mathscr{H}$ 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. 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 Secs. IV and V.

The statement (II) is thus the necessary and sufficient condition on $S\equiv|T|^2$ for V_t to be unitarily implementable in π_T. Note that if H is bounded away from zero, i.e., there exists an $h>0$ such that $\langle f|Hf\rangle\geqslant h\|f\|^2$ for all $f\in D(H)$, then choosing m with $0<m<h$ gives $P_m = I$, and then as a result $[|T|^2,V_t]\in\mathbf{B}_2$, for all t if and only if $(|T|^2-I)$ is a Hilbert–Schmidt operator. This implies that for such Hamiltonians H, $V_t = e^{t\Lambda H}$ is unitarily implementable in π_T only if T is unitarily implementable in the Fock representation, that is, V_t is unitarily implementable only in the representations equivalent to the Fock representation.

The example in Sec. VIII shows that the class of representations which admit implementation of V_t is actually larger than this when the spectrum of H reaches zero.

IV. PRELIMINARY LEMMAS

The proof of Theorem 2 depends on the four results which are collected here with sketches of their proofs. Repeated use is made of the facts that the class of Hilbert–Schmidt operators $\mathbf{B}_2$ on a Hilbert space $\mathscr{H}$ forms a Banach space with the norm $\|C\|_2\equiv(\mathrm{tr}\{|C|^2\})^{1/2}$, and that $\mathbf{B}_2$ is a *-ideal in the algebra $\mathbf{B}(\mathscr{H})$ of bounded operators on $\mathscr{H}$.

Lemma 1: Let A and B be bounded operators, and let $\tau\subseteq\mathbb{R}$ be an open interval containing the origin. Then $[B,e^{tA}]$ is a Hilbert–Schmidt operator for all $t\in\tau$ if and only if $[B,A]$ is a Hilbert–Schmidt operator.

Proof. If $[B,A]$ is a Hilbert–Schmidt operator, it is easily established that the power series for $[B,e^{tA}]$ converges in Hilbert–Schmidt norm. For the converse, note that if $[B,e^{tA}]$ is of Hilbert–Schmidt type, then so is

$$X(t)\equiv e^{tA}Be^{-tA}-B=(e^{t\,\mathrm{Ad}(A)}-I)B.$$

Formally,

$$t[A,B]=t\,\mathrm{Ad}(A)B=t\,\mathrm{Ad}(A)(e^{t\,\mathrm{Ad}(A)}-I)^{-1}X(t);$$

using the facts that $g(z)\equiv z(e^z-1)^{-1}$ is analytic near zero and

$$\|(\mathrm{Ad}(A))^nX\|_2\leqslant 2^n(\|A\|)^n\|X\|_2 \text{ for } n\geqslant 1,$$

it is easy to show that the formal series for $t[A,B]$ $= g(t\,\mathrm{Ad}(A))X(t)$ converges for small enough t in Hilbert–Schmidt norm. □

Lemma 2: Let H be a self-adjoint operator on (a dense domain in) a separable Hilbert space. For any $\epsilon>0$, there exists a self-adjoint (bounded) Hilbert–Schmidt-class operator K with $\|K\|_2<\epsilon$ such that $(H+K)$ has pure point spectrum.

The original proof is due to von Neumann[3]; see also Kato.[4]

Lemma 3: Let H_1 and H_2 be self-adjoint operators with a common dense domain in a separable Hilbert space, such that H_1-H_2 is (bounded and) of Hilbert–Schmidt type. Suppose $f:\mathbb{R}\to\mathbb{C}$ is a bounded measurable function such that $|f(x)-f(y)|\leqslant c|x-y|$ for some constant $c>0$. Then $f(H_1)-f(H_2)$ is of Hilbert–Schmidt type, and $\|f(H_1)-f(H_2)\|_2\leqslant c\|H_1-H_2\|_2$.

Proof: Lemma 2 is used to approximate H_j by $E_j = H_j + K_j$, where E_j has pure point spectrum and $\|K_j\|_2$ is small. Writing

$$\begin{aligned}\|f(H_1)-f(H_2)\|_2&\leqslant\|f(H_1)-f(E_1)\|_2+\|f(H_2-f(E_2)\|_2\\&\quad+\|f(E_1)-f(E_2)\|_2,\end{aligned}$$

evaluating traces in the orthonormal bases of eigenvectors of the E_j, and using the inequality for f shows

$$\begin{aligned}\|f(H_1)-f(H_2)\|_2&\leqslant c\|K_1\|_2+c\|K_2\|_2+c\|E_1-E_2\|_2\\&\leqslant 2c\|K_1\|_2+2c\|K_2\|_2+c\|H_1-H_2\|_2\end{aligned}$$

Since $\|K_j\|_2$ is arbitrarily small, the assertion follows. □

Lemma 4: Let $\{p_k|k=1,\ldots,\infty\}$ be a set of nonnegative constants, and let $\{f_k|k=1,\ldots,\infty\}$ be a sequence of positive numbers bounded away from zero, i.e., there exists an $m>0$ such that $f_k>m$ for all k. If $\Sigma_{k=1}^{\infty}p_k\sin^2(f_kt)$ converges for each t in an open interval τ containing zero, then $\Sigma_{k=1}^{\infty}p_k<\infty$.

Proof: Let $\xi(t)\equiv\Sigma_{k=1}^{\infty}p_k\sin^2(f_kt)$; $\xi(t)$ is absolutely convergent for each $t\in\tau$, and is the point-wise limit of the continuous partial sums $\xi_N(t)\equiv\Sigma_{k=1}^{\infty}p_k\sin^2(f_kt)$, so ξ is measurable. There thus exists a set $\sigma\subseteq\tau$ of finite positive measure on which ξ is bounded, say $\xi(t)\leqslant M$ for $t\in\sigma$. So $\int_\sigma dt\,\xi(t)$ exists and in fact $\int_\sigma dt\,\xi(t)\leqslant\int_\sigma dt\,M=M\mu(\sigma)>0$. Since

$$\begin{aligned}\sum_{k=1}^{N}\int_\sigma dt\,p_k\sin^2(f_kt)&=\int_\sigma dt\,\xi_N(t)\\&\leqslant\int_\sigma dt\,\xi(t)\leqslant M\mu(\sigma)\end{aligned}$$

for all N, with the right side independent of N,

$$\lim_{N\to\infty}\sum_{k=1}^{N}\int_\sigma dt\,p_k\sin^2(f_kt)\leqslant M\mu(\sigma)<\infty,$$

that is,

$$\infty>\sum_{k=1}^{\infty}p_k\int_\sigma dt\sin^2(f_kt).$$

Since $\sin^2\theta=(1-\cos(2\theta))/2$,

$$\int_\sigma dt\sin^2(f_kt)=\frac{1}{2}\mu(\sigma)-\frac{1}{2}\int_\sigma dt\cos(2f_kt).$$

The latter integral is the Fourier cosine transform of the

characteristic function of the set σ; by the Riemann–Lebesgue lemma, it vanishes as $f_k \to \infty$. Choose $L > 0$ such that $|\int_\sigma dt \cos(2ft)| < \mu(\sigma)/2$ for all $f \geqslant L$; then $\int_\sigma dt \sin^2(ft) > \mu(\sigma)/4$ for all $f \geqslant L$.

Because the sum $\Sigma_{k=1}^{\infty} p_k \int_\sigma dt \sin^2(f_k t)$ is absolutely convergent, the order of summation can be rearranged. Let $\mathscr{S} \equiv \{k \mid f_k < L\}$ and $\mathscr{B} \equiv \{k \mid f_k \geqslant L\}$. Then

$$\infty > \sum_{k\in\mathscr{S}} p_k \int_\sigma dt \sin^2(f_k t) + \sum_{k\in\mathscr{B}} p_k \int_\sigma dt \sin^2(f_k t),$$

and since each sum is positive, each is finite.

Since $\int_\sigma dt \sin^2(f_k t) > \mu(\sigma)/4$ for all $k \in \mathscr{B}$, it follows that

$$\infty > \sum_{k\in\mathscr{B}} p_k \int_\sigma dt \sin^2(f_k t) > \frac{1}{4}\mu(\sigma) \sum_{k\in\mathscr{B}} p_k,$$

and since σ has nonzero measure $\Sigma_{k\in\mathscr{B}} p_k < \infty$.

For the sum over $\mathscr{S}$, pick $r \in \tau$ such that $0 < r < \pi/L$. Then for all $k \in \mathscr{S}$, $mr < f_k r < \pi$, so that $\sin^2(f_k r)$ is bounded away from zero, that is, there exists $\delta > 0$ such that $\sin^2(f_k r) > \delta$ for all $k \in \mathscr{S}$. Thus

$$\infty > \xi(r) \geqslant \sum_{k\in\mathscr{S}} p_k \sin^2(f_k r) > \delta \sum_{k\in\mathscr{S}} p_k,$$

that is, $\Sigma_{k\in\mathscr{S}} p_k < \infty$.

Adding the two (absolutely convergent) series concludes the proof. □

V. PROOF OF THEOREM 2

Because the proof involves both the complex and real structures for the Hilbert space $\mathscr{H}$, it is useful to adopt the following notation. Let $\mathbf{B}_{2r}$ be the ideal of bounded real-linear transformations on $\mathscr{H}$ which are real-Hilbert–Schmidt operators:

$$A \in (\mathbf{B}_{2r}) \text{ if } \infty > (\|A\|_{2r})^2 \equiv \mathrm{tr}_r(A^*A) \equiv \sum_j \mathrm{Re}\langle A\rho_j | A\rho_j\rangle,$$

where $\{\rho_j\}$ is a real-orthonormal basis for the real Hilbert space $(\mathscr{H}, \mathrm{Re}\langle|\rangle)$. Let $\mathbf{B}_{2c}$ be the ideal of bounded complex-linear transformations on $\mathscr{H}$ which are complex-Hilbert–Schmidt operators:

$$A \in \mathbf{B}_{2c} \text{ if } \infty > (\|A\|_{2c})^2 \equiv \mathrm{tr}_c(A^*A) \equiv \sum_k \langle A\gamma_k | A\gamma_k\rangle,$$

where $\{\gamma_k\}$ is a complex-orthonormal basis for the complex Hilbert space $(\mathscr{H}, \langle|\rangle)$. Since $\{\gamma_k, i\gamma_k \mid k = 1,\ldots,\infty\}$ is a real-orthonormal basis for $(\mathscr{H}, \mathrm{Re}\langle|\rangle)$ whenever $\{\gamma_k \mid k = 1,\ldots,\infty\}$ is a complex-orthonormal basis for $\mathscr{H}$, if $A \in \mathbf{B}_{2c}$ then $A \in \mathbf{B}_{2r}$ and $\mathrm{tr}_r(A^*A) = 2\,\mathrm{tr}_c(A^*A)$. Every real-linear transformation $Q: \mathscr{H} \to \mathscr{H}$ is uniquely decomposed into complex-linear and complex-antilinear parts Q_l and Q_a by

$$\begin{cases} Q_l \equiv (Q + \Lambda^* Q \Lambda)/2, \\ Q_a \equiv (Q - \Lambda^* Q \Lambda)/2, \end{cases}$$

so that $Q_l \Lambda = \Lambda Q_l$ and $Q_a \Lambda = -\Lambda Q_a$. Because the trace of a complex-antilinear operator vanishes, a real-linear transformation Q is in $\mathbf{B}_{2r}$ if and only if $Q_l \in \mathbf{B}_{2r}$ and $Q_a \in \mathbf{B}_{2r}$; furthermore,

$$(\|Q\|_{2r})^2 = (\|Q_l\|_{2r})^2 + (\|Q_a\|_{2r})^2.$$

The proof of Theorem 2 proceeds as follows.

(1) Obviously (III) implies (II).

(2) To show (II) implies (I), assume that for some $m > 0$, (A) and (B) hold. Since S is self-adjoint and $\mathbf{B}_{2r}$ is a *-ideal, $P_m(S - I) \in \mathbf{B}_{2r}$ iff $(S - I)P_m \in \mathbf{B}_{2r}$.

(a) Since $(e^{t\Lambda P_m H} - I) = P_m(e^{t\Lambda P_m H} - I)$
$= (e^{t\Lambda P_m H} - I)P_m$,

$$\begin{aligned}[S, e^{t\Lambda P_m H}] &= [(S - I), (e^{t\Lambda P_m H} - I)] \\ &= (S - I)P_m(e^{t\Lambda P_m H} - I) \\ &\quad - (e^{t\Lambda P_m H} - I)P_m(S - I).\end{aligned}$$

Thus $P_m(S - I) \in \mathbf{B}_{2r}$ implies $[S, e^{t\Lambda P_m H}] \in \mathbf{B}_{2r}$ for all t.

(b) Because $(I - P_m)H$ is a bounded operator, by Lemma 1

$$[S, \Lambda(I - P_m)H] \in \mathbf{B}_{2r} \text{ iff } [S, e^{t\Lambda(I - P_m)H}] \in \mathbf{B}_{2r} \text{ for all } t \in \tau.$$

(c) Since $e^{t\Lambda H} = e^{t\Lambda P_m H + t\Lambda(I - P_m)H} = e^{t\Lambda P_m H} e^{t\Lambda(I - P_m)H}$,

$$\begin{aligned}[S, e^{t\Lambda H}] &= [S, e^{t\Lambda P_m H}] e^{t\Lambda(I - P_m)H} \\ &\quad + e^{t\Lambda P_m H}[S, e^{t\Lambda(I - P_m)H}].\end{aligned}$$

As shown above, the first term is of Hilbert–Schmidt type by the hypothesis (A), and the second term is of Hilbert–Schmidt type by hypothesis (B). So $[S, e^{t\Lambda H}] \in \mathbf{B}_{2r}$ for all t, as required.

(3) To show (I) implies (III), fix an arbitrary $m > 0$.

(a) The most involved part of the proof is to show that $[S, V_t] \in \mathbf{B}_{2r}$ for all $t \in \tau$ implies condition (A), that is, $P_m(S - I) \in \mathbf{B}_{2r}$.

(i) Choose $0 < m_1 < m_2 < m$. Let $p: \mathbb{R} \to \mathbb{R}$ be the following function:

$$p(x) \equiv \begin{cases} 0, & \text{if } x < m_1, \\ \dfrac{x - m_1}{m_2 - m_1}, & \text{if } m_1 \leqslant x \leqslant m_2, \\ 1, & \text{if } m_2 < x. \end{cases}$$

Note that $p(H) \geqslant P_m$. Since $[p(H), V_t] = 0$, $[S, V_t] \in \mathbf{B}_{2r}$ implies that $[p(H)S, V_t] \in \mathbf{B}_{2r}$.

(ii) Using Lemma 2 with the complex structure on $\mathscr{H}$, approximate H by $E \equiv H + K$, where $\|K\|_{2c} < \epsilon$ and E has a pure point spectrum. Note that with ϵ small enough, every eigenvalue ω of E is larger than $-m_0$, where $0 < m_0 < m_1$: Let $\psi \in D(E) = D(H)$ be such that $E\psi = \omega\psi$. Because H is nonnegative,

$$\begin{aligned}\omega\|\psi\|^2 &= \langle\psi|E\psi\rangle = \langle\psi|(H + K)\psi\rangle \\ &\geqslant \langle\psi|H\psi\rangle - |\langle\psi|K\psi\rangle| \\ &\geqslant -|\langle\psi|K\psi\rangle|.\end{aligned}$$

Since $|\langle\psi|K\psi\rangle| \leqslant \|\psi\|^2\|K\| \leqslant \|\psi\|^2\|K\|_{2c} < \|\psi\|^2\epsilon$, choosing $\epsilon < m_0$ gives $\omega\|\psi\|^2 > -m_0\|\psi\|^2$.

(iii) Observe that $p(x)$ satisfies the hypotheses of Lemma 3, so $p(E) - p(H) \in \mathbf{B}_{2c} \subset \mathbf{B}_{2r}$, hence $[p(H)S, V_t] \in \mathbf{B}_{2r}$ if and only if $[p(E)S, V_t] \in \mathbf{B}_{2r}$.

Observe that the function $e^{it(\cdot)}$ also satisfies the hypotheses of Lemma 3, so that $(e^{itH} - e^{itE}) \in \mathbf{B}_{2c}$, and hence $[p(H)S, e^{t\Lambda H}] \in \mathbf{B}_{2r}$ iff $[p(E)S, e^{t\Lambda E}] \in \mathbf{B}_{2r}$. Since E is complex-linear and since $Q \in \mathbf{B}_{2r}$ iff $Q_a \in \mathbf{B}_{2r}$ and $Q_l \in \mathbf{B}_{2r}$, it follows that

$[S,V_t] \in \mathbf{B}_{2r}$ implies $[p(E)S_a, e^{t\Lambda E}] \in \mathbf{B}_{2r}$.

(iv) If $A \in \mathbf{B}_{2r}$ is either purely linear or purely antilinear, then $(\|A\|_{2r})^2 = 2\Sigma_{j,k} |\langle \gamma_k | A\gamma_j \rangle|^2$ with $\{\gamma_j\}$ a basis for the complex Hilbert space. Let $\{\gamma_n\}$ be an orthonormal basis for $\mathscr{H}$ consisting of eigenvectors of E: $E\gamma_n = \omega_n \gamma_n$. Apply the trace formula to the antilinear operator $[p(E)S_a, e^{t\Lambda E}]$ to get $\|[p(E)S_a, e^{t\Lambda H}]\|_{2r}^2$

$$= 2\sum_{k,n} |\langle \gamma_n | (p(E)S_a e^{t\Lambda E} - e^{t\Lambda E} p(E)S_a)\gamma_k \rangle|^2$$

$$= 2\sum_{k,n} |(e^{-it\omega_k} - e^{it\omega_n})\langle \gamma_n | p(E)S_a \gamma_k \rangle|^2$$

$$= 8\sum_{k,n} \sin^2((\omega_k + \omega_n)t/2) |\langle p(E)\gamma_n | S_a \gamma_k \rangle|^2.$$

(v) Since $p(x)$ was chosen so that $p(E)\gamma_n = 0$ whenever $\omega_n < m_1$, it must be the case that whenever $\langle p(E)\gamma_n | S_a \gamma_k \rangle$ is nonzero,

$$(\omega_k + \omega_n) \geqslant (\omega_k + m_1) \geqslant -m_0 + m_1 > 0.$$

Imagine explicitly dropping from the absolutely convergent trace sum all terms in which the matrix element $\langle \gamma_n | p(E)S_a \gamma_k \rangle$ vanishes; the resultant collections of nonnegative constants $\{|\langle \gamma_n | p(E)S_a \gamma_k \rangle|^2\}$ and positive numbers $\{(\omega_k + \omega_n)\}$ bounded away from zero satisfy the hypotheses of Lemma 4. As a consequence, the sum

$$(\|p(E)S_a\|_{2r})^2 = \sum_{k,n} |\langle \gamma_n | p(E)S_a \gamma_k \rangle|^2$$

converges, that is, $p(E)S_a \in \mathbf{B}_{2r}$.

(vi) From $p(E)S_a \in \mathbf{B}_{2r}$ and $p(E) - p(H) \in \mathbf{B}_{2c}$ it follows that $p(H)S_a \in \mathbf{B}_{2r}$. Thus because $(p(H))^2 \geqslant (P_m)^2$,

$$\infty > \mathrm{tr}_r\{|p(H)S_a|^2\} = 2\sum_j \|p(H)S_a\gamma_j\|^2$$

$$\geqslant 2\sum_j \|P_m S_a \gamma_j\|^2 = \mathrm{tr}_r\{|P_m S_a|^2\},$$

so $P_m S_a \in \mathbf{B}_{2r}$. Now, it is easy to show that the condition for a bounded real-linear transformation Q with bounded inverse to be symplectic is that $\Lambda^* Q \Lambda = Q^{*-1}$. So S, being self-adjoint and symplectic, thus has the property that

$$S_a \equiv (S - \Lambda^* S \Lambda)/2 = (S - S^{-1})/2$$
$$= (S - I)(I + S^{-1})/2.$$

Therefore $P_m S_a = P_m (S - I)(I + S^{-1})/2$, and since $(I + S^{-1})$ is invertible,

$$P_m S_a \in \mathbf{B}_{2r} \text{ if and only if } P_m (S - I) \in \mathbf{B}_{2r}.$$

Thus $P_m (S - I) \in \mathbf{B}_{2r}$, which establishes condition (A).

(b) It remains to prove that $[S,V_t] \in \mathbf{B}_{2r}$ for all $t \in \tau$ implies condition (B), that is, $[S, \Lambda(I - P_m)H] \in \mathbf{B}_{2r}$.

Under the hypothesis, the above argument showed that $P_m(S - I) \in \mathbf{B}_{2r}$; taking the adjoint gives $(S - I)P_m \in \mathbf{B}_{2r}$, and as in paragraph (2a) above, these imply that $[S, e^{t\Lambda P_m H}] \in \mathbf{B}_{2r}$ for all t. As in paragraph (2c) above, $[S, e^{t\Lambda(I - P_m)H}]$

$$= e^{-t\Lambda P_m H}\{[S,V_t] - [S, e^{t\Lambda P_m H}] e^{t\Lambda(I - P_m)H}\},$$

and since the two terms on the right are Hilbert–Schmidt operators, $[S, e^{t\Lambda(I - P_m)H}] \in \mathbf{B}_{2r}$ for all real t. Since $(I - P_m)H$ is bounded, Lemma 1 then implies that $[S, \Lambda(I - P_m)H] \in \mathbf{B}_{2r}$, as desired.

This concludes the proof of Theorem 2. □

VI. CONTINUITY OF THE IMPLEMENTATION

Suppose that the one-parameter group of transformations $V_t = e^{t\Lambda H}$ is in fact unitarily implementable in π_T. The assertion of Theorem 1 which remains to be proved 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 ν_t is unitarily implemented. As the following considerations show, the validity of this assertion follows directly from (the somewhat technical) Theorem 3 below.

Shale[5] showed that if θ_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 θ_t in the Fock representation. Specifically, let $rSp(\mathscr{H})$ be the group of symplectic transformations satisfying Shale's criterion; the topology on $rSp(\mathscr{H})$ is defined as follows. Polar decomposition (with respect to the real adjoint) of a transformation $T \in rSp(\mathscr{H})$ gives $T = Z|T|$, where Z is complex-unitary (because it is a symplectic real isometry) and $|T|$ is a (real-) positive symplectic transformation. The topology on $rSp(\mathscr{H})$ is the product topology obtained when $rSp(\mathscr{H})$ is regarded as the Cartesian product of the space of unitary operators under the weak operator topology, with the space of positive symplectic operators under the topology induced by the Hilbert–Schmidt norm [well-defined because $(|T| - I) \in \mathbf{B}_{2r}$ for $T \in rSp(\mathscr{H})$].

Shale furthermore showed that group multiplication is continuous in this topology, so that if θ_t is a one-parameter group of implementable symplectics, continuity of θ_t at $t = 0$ implies continuity everywhere. Thus to show the existence of a continuous unitary implementation of θ_t in the Fock representation, it is sufficient to show that $\theta: \mathbb{R} \to rSp(\mathscr{H})$ is continuous at the origin.

To apply this criterion to the implementation of V_t in π_T, note that, as earlier, continuous implementation of V_t in π_T is equivalent to continuous implementation of $\theta_t \equiv TV_t T^{-1}$ in the Fock representation.

Theorem 3: Let H be a nonnegative self-adjoint complex-linear transformation with domain $D(H)$ dense in the separable Hilbert space $\mathscr{H}$. Set $V_t \equiv e^{t\Lambda H}$.

Let T be a symplectic transformation on $\mathscr{H}$ 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. Set $\theta_t \equiv TV_t T^{-1}$.

If $(|\theta_t| - I)$ is a Hilbert–Schmidt operator for all real t, then $\theta: \mathbb{R} \to rSp(\mathscr{H})$ is continuous at the origin in Shale's topology.

The proof of this theorem is in Sec. VII.

As an immediate corollary, θ_t is then continuous everywhere, and hence θ has a continuous unitary implementation in the Fock representation. Since the hypothesis here that $(|\theta_t| - I)$ be in the Hilbert–Schmidt class is equivalent

to the unitary implementability of θ_t, if follows that if V_t is unitarily implementable in π_T then the implementing unitary family can always be chosen to be a strongly continuous unitary group.

VII. PROOF OF THEOREM 3

The unitary group V_t is of course not uniformly continuous. The proof of Theorem 3 rests instead on the following result.

Lemma 5: Let $B \in \mathbf{B}_{2r}$. Let F_t be a strongly continuous one-parameter unitary group. Then $G:\mathbb{R}\to\mathbf{B}_{2r}$ given by $G(t) \equiv F_t B$ is continuous in the Hilbert–Schmidt norm.

Proof of lemma: Because $B \in \mathbf{B}_{2r}$, it is the Hilbert–Schmidt-norm limit of finite-rank operators B_j: $\lim_{j\to\infty} \|B - B_j\|_{2r} = 0$. Given $\epsilon \geqslant 0$, choose j so large that $\|B - B_j\|_{2r} < \epsilon/4$. Then

$$\begin{aligned}
&\|G(s) - G(t)\|_{2r} \\
&\quad \leqslant \|(F_s - F_t)B_j\|_{2r} + \|(F_s - F_t)(B - B_j)\|_{2r} \\
&\quad \leqslant \|(F_s - F_t)B_j\|_{2r} \\
&\qquad + \|(F_s - F_t)\|\|B - B_j\|_{2r} \\
&\quad < \|(F_s - F_t)B_j\|_{2r} + \epsilon/2.
\end{aligned}$$

Now, because B_j has finite rank, the remaining Hilbert–Schmidt norm involves a finite sum:

$$(\|(F_s - F_t)B_j\|_{2r})^2 = \sum_{k=1}^{\text{rank } B_j} \|(F_s - F_t)B_j\psi_k\|^2$$

for a suitably chosen orthonormal set $\{\psi_k\}$. Since F_t is strongly continuous, there exists $\delta > 0$ such that

$$(\|(F_s - F_t)B_j\|_{2r})^2 < \epsilon^2/4 \quad \text{whenever } |s - t| < \delta.$$

Thus $\|G(s) - G(t)\|_{2r} < \epsilon$ for $|s - t| < \delta$, which proves the lemma. □

Remark: Because $\|X^*\|_{2r} = \|X\|_{2r}$, BF_t is also continuous in the Hilbert–Schmidt norm.

To prove Theorem 3 itself, it is necessary to show that:

(i) $\lim_{t\to 0} \||\theta_t| - I\|_{2r} = 0$ and

(ii) $\lim_{t\to 0} \langle f|(Z_t - I)g\rangle = 0$ for all f and g in $\mathscr{H}$,

where Z_t is the unitary operator occurring in the real polar decomposition $\theta_t = Z_t|\theta_t|$.

(1) To prove assertion (i), first note that the hypothesis of the theorem that $(|\theta_t| - I)$ is a Hilbert–Schmidt operator for all real t implies, as in Sec. III, that for all t,

$$(|\theta_t|^2 - I) = T^{*-1}V_t^*(T^*TV_t - V_tT^*T)T^{-1} \in \mathbf{B}_{2r},$$

and hence that $[|T|^2, V_t] \in \mathbf{B}_{2r}$, for all real t. So Theorem 2 with $S \equiv |T|^2$ implies that for all $m > 0$

$$P_m(S - I) \in \mathbf{B}_{2r} \quad \text{and} \quad [S, \Lambda(I - P_m)H] \in \mathbf{B}_{2r}$$

where P_m is the spectral projection for H onto spectral values larger than m.

Since $(|\theta_t| + I)$ is a bounded invertible operator,

$$\begin{aligned}
\|(|\theta_t| - I)\|_{2r} &= \|(|\theta_t| + I)^{-1}(|\theta_t|^2 - I)\|_{2r} \\
&\leqslant \|(|\theta_t| + I)^{-1}\|\|(|\theta_t|^2 - I)\|_{2r} \\
&\leqslant \|(|\theta_t|^2 - I)\|_{2r} \\
&= \|T^{*-1}V_t^*[|T|^2, V_t]T^{-1}\|_{2r} \\
&\leqslant \|T\|\|T^{-1}\|\|[S, V_t]\|_{2r}
\end{aligned}$$

with $S \equiv |T|^2$.

Now fix $m > 0$. As in the proof of Theorem 2,

$$[S, V_t] = e^{t\Lambda P_m H}[S, e^{t\Lambda(I - P_m)H}] + [S, e^{t\Lambda P_m H}]e^{t\Lambda(I - P_m)H},$$

and since $e^{t\Lambda P_m H}$ and $e^{t\Lambda(I - P_m)H}$ are unitary,

$$\|[S, V_t]\|_{2r} \leqslant \|[S, e^{t\Lambda(I - P_m)H}]\|_{2r} + \|[S, e^{t\Lambda P_m H}]\|_{2r}.$$

In fact, each of the two commutators on the right-hand side is Hilbert–Schmidt continuous at $t = 0$, which can be seen as follows.

(a) For the first term, the fact that $\Lambda(I - P_m)H$ is a bounded operator implies that the series

$$[S, e^{t\Lambda(I - P_m)H}] = \sum_{n=1}^{\infty} \frac{t^n}{n!}[S, (\Lambda(I - P_m)H)^n]$$

is operator-norm convergent. Because $[S, \Lambda(I - P_m)H] \in \mathbf{B}_{2r}$, it is also Hilbert–Schmidt-norm convergent:

$$\begin{aligned}
&\|[S, e^{t\Lambda(I - P_m)H}]\|_{2r} \\
&\leqslant \sum_{n=1}^{\infty} \frac{|t|^n}{n!}\|[S, (\Lambda(I - P_m)H)^n]\|_{2r} \\
&\leqslant \sum_{n=1}^{\infty} \frac{|t|^n}{n!} n(\|\Lambda(I - P_m)H\|)^{n-1}\|[S, \Lambda(I - P_m)H]\|_{2r} \\
&= |t|\|[S, \Lambda(I - P_m)H]\|_{2r} \exp\{\|t\Lambda(I - P_m)H\|\}.
\end{aligned}$$

In particular,

$$\lim_{t\to 0} \|[S, e^{t\Lambda(I - P_m)H}]\|_{2r} = 0.$$

(b) For the second term, write, as in the proof of Theorem 2,

$$\begin{aligned}
&\|[S, e^{t\Lambda P_m H}]\|_{2r} \\
&\quad = \|(S - I)P_m(e^{t\Lambda P_m H} - I) \\
&\qquad - (e^{t\Lambda P_m H} - I)P_m(S - I)\|_{2r} \\
&\quad \leqslant \|(e^{t\Lambda P_m H} - I)P_m(S - I)\|_{2r} \\
&\qquad + \|(S - I)P_m(e^{t\Lambda P_m H} - I)\|_{2r}.
\end{aligned}$$

Now apply Lemma 5 twice, with $F_t \equiv e^{t\Lambda P_m H}$ and $B \equiv P_m(S - I)$ [or $B \equiv (S - I)P_m$] to conclude that

$$\lim_{t\to 0} \|[S, e^{t\Lambda P_m H}]\|_{2r} = 0,$$

as desired.

Combining these two results shows that $\lim_{t\to 0} \|[S, V_t]\|_{2r} = 0$, which establishes assertion (i).

(2) To prove assertion (ii), it is sufficient to show that

$$\lim_{t\to 0} \mathrm{Re}\langle f|(Z_t - I)g\rangle = 0 \text{ for all } f, g \in \mathscr{H}$$

because $\mathrm{Im}\langle h_1|h_2\rangle = \mathrm{Re}\langle \Lambda h_1|h_2\rangle$. Since $\theta_t = Z_t|\theta_t|$,

$$|\mathrm{Re}\langle f|(Z_t - I)g\rangle| = |\mathrm{Re}\langle f|(\theta_t - |\theta_t|)|\theta_t|^{-1}g\rangle|$$
$$= |\mathrm{Re}\langle(\theta_t^* - |\theta_t|)f|\ |\theta_t|^{-1}g\rangle|$$
$$\leqslant |\langle(\theta_t^* - |\theta_t|)f|\ |\theta_t|^{-1}g\rangle|$$
$$\leqslant \|(\theta_t^* - |\theta_t|)f\|\ \||\theta_t|^{-1}g\|.$$

(a) Now,

$$\||\theta_t|^{-1}g\|^2 = \langle|\theta_t|^{-1}g|\ |\theta_t|^{-1}g\rangle$$
$$= \mathrm{Re}\langle g|\ |\theta_t|^{-2}g\rangle$$
$$= \mathrm{Re}\langle g|\theta_t^{-1}\theta_t^{*-1}g\rangle$$
$$= \|\theta_t^{*-1}g\|^2$$
$$= \|T^{*-1}V_tT^*g\|^2$$
$$\leqslant \|T\|^2\|T^{-1}\|^2\|g\|^2 \equiv L^2,$$

with L independent of t, so that

$$|\mathrm{Re}\langle f|(Z_t - I)g\rangle| \leqslant L\ \|(\theta_t^* - |\theta_t|)f\|.$$

(b) Thus

$$|\mathrm{Re}\langle f|(Z_t - I)g\rangle| \leqslant L\ \|\{(\theta_t^* - I) - (|\theta_t| - I)\}f\|$$
$$\leqslant L\ \{\|(|\theta_t| - I)f\| + \|(\theta_t^* - I)f\|\}.$$

Since

$$\|(|\theta_t| - I)f\| \leqslant \||\theta_t| - I\|\ \|f\|$$
$$\leqslant \||\theta_t| - I\|_{2r}\|f\|,$$

and since by assertion (i), $\lim_{t\to 0}\ \||\theta_t| - I\|_{2r} = 0$, it follows that $\lim_{t\to 0}\ \|(|\theta_t| - I)f\| = 0$ for all f in $\mathscr{H}$. As for the other term, note that

$$\|(\theta_t^* - I)f\| = \|T^{*-1}(V_{-t} - I)T^*f\|,$$

so that the strong continuity of V_t implies that

$$\lim_{t\to 0}\|(\theta_t^* - I)f\| = 0 \text{ for all } f\in\mathscr{H}.$$

Thus

$$\lim_{t\to 0}|\mathrm{Re}\langle f|(Z_t - I)g\rangle| = 0 \text{ for all } f, g\in\mathscr{H},$$

which establishes assertion (ii).

(3) Since assertions (i) and (ii) are equivalent to the continuity at the origin of θ_t in Shale's topology, Theorem 3 is proved. □

VIII. AN EXAMPLE

Because the symplectic transformations satisfying Shale's criterion form a group $rSp(\mathscr{H})$ under multiplication, the set of symplectic transformations T for which TV_tT^{-1} satisfies Shale's criterion includes $rSp(\mathscr{H})$. That the inclusion is proper, and hence that conditions (A) and (B) of Theorem 2 are not merely equivalent to T being an element of $rSp(\mathscr{H})$, is shown by the following construction of a symplectic transformation T *not* in $rSp(\mathscr{H})$, but for which TV_tT^{-1} *is* in $rSp(\mathscr{H})$ for all real t.

Let the self-adjoint generator H of V_t have spectrum extending to zero. The idea is to construct from H a bounded positive linear operator A which is almost in the Hilbert–Schmidt class, in the sense that the "low-energy" eigenvalues of A are not square-summable, while those of AH are. Then it is easy to form a symplectic transformation T whose square $|T|^2$ has an antiliner part consisting precisely of A multiplied by a suitable conjugation; this T is not of Shale type but has the property that $(|TV_tT^{-1}|^2 - I)$ is a Hilbert–Schmidt operator for all t. This construction is of course motivated by the criteria (A) and (B) of Theorem 2, but the assertions of Theorem 2 are not used here.

For a concrete example, let $\mathscr{H}$ be the complex Hilbert space $L_2(\mathbb{R}^3)$ with the usual inner product $\langle f|g\rangle \equiv \int d^3p\, f^*(\mathbf{p})g(\mathbf{p})$. Again denote by A multiplication by i, and let C be the conjugation given by $(Cf)(\mathbf{p}) \equiv f^*(-\mathbf{p})$. The antilinear operator C is self-real-adjoint because

$$\mathrm{Re}\langle f|Cg\rangle = \tfrac{1}{2}(\langle f|Cg\rangle + \langle Cg|f\rangle)$$
$$= \tfrac{1}{2}(\langle g|Cf\rangle + \langle Cf|g\rangle) = \mathrm{Re}\langle Cf|g\rangle.$$

Let H be multiplication by $|\mathbf{p}|$ on its domain of self-adjointness. Such a framework is familiar from the theory of free massless scalar fields.

(1) First approximate H by an operator E with discrete eigenvalues by applying von Neumann's Lemma 2 to H: Given $\epsilon > 0$ there exists a self-adjoint operator $K\in\mathbf{B}_{2c}$ with $\|K\|_{2c} < \epsilon$ such that $E \equiv H + K$ has pure point spectrum. The eigenvectors $\{\gamma_n\}$ of E span $\mathscr{H}$, and the eigenvalues $\{\omega_n\}$ of E are dense in $(0,\infty)$ because $(0,\infty)$ is in the spectrum of H (Kato[6]). There is thus a sequence $\{\gamma_n'\}$ of eigenvectors such that the corresponding eigenvalues $\{\omega_n'\}$ form a monotonically decreasing sequence with

$$1/(n+1) < \omega_n' < 1/n.$$

(2) Now construct a positive bounded (complex-linear) operator B by specifying its action on the basis $\{\gamma_n\}$: Define say $B\gamma_n' \equiv (n^{-1/4})\gamma_n'$, and set $B\gamma_k \equiv 0$ for all γ_k not in the set $\{\gamma_n'\}$. The complex-linear operator so defined is self-adjoint and such that

$$B^4\in\mathbf{B}_{2c} \text{ but } B^2\notin\mathbf{B}_{2c}.$$

Since B is complex-linear, also $B^2\notin\mathbf{B}_{2r}$.

(3) Now set $A \equiv (B^2 + CB^2C)$. Because BC is antilinear, $CB^2C = |BC|^2$ is complex-positive. Thus A is a positive complex-linear operator which commutes with C. Because $B^2\notin\mathbf{B}_{2r}$ and C is invertible, $CB^2C\notin\mathbf{B}_{2r}$; since both terms are positive, taking the trace of A^2 in the basis $\{\gamma_n\}$ shows that $A\notin\mathbf{B}_{2r}$.

(4) This operator A has the property

$$(AC)e^{itH} - e^{itH}(AC)\in\mathbf{B}_{2r} \text{ for all real } t,$$

which can be seen as follows.

(a) Note first that because $Ce^{itH}C = e^{-itH}$, the above property is equivalent to $Ae^{itH} - e^{-itH}A\in\mathbf{B}_{2r}$ for all t.

(b) As in the proof of Theorem 2, Lemma 3 implies that $e^{itE} - e^{itH}\in\mathbf{B}_{2r}$ for all real t. It follows that

$$Ce^{itE}C - e^{-itE}$$
$$= C(e^{itE} - e^{itH})C - (e^{-itE} - e^{-itH})\in\mathbf{B}_{2r}.$$

(c) Since B^2 commutes with E on $D(E)$, B^2 commutes with $e^{\pm itE}$.

Thus

$$\mathrm{tr}_r(|B^2e^{itE} - e^{-itE}B^2|^2) = 2\,\mathrm{tr}_c(|2(\sin tE)B^2|^2)$$
$$= 8\sum_n \|(\sin tE)B^2\gamma_n'\|^2$$
$$= 8\sum_n \|(\sin t\omega_n')(1/\sqrt{n})\,\gamma_n'\|^2$$
$$= 8\sum_n \frac{1}{n}\sin^2(t\omega_n').$$

Since $\sin^2\theta \leqslant \theta^2$ for all real θ,

$$\mathrm{tr}_r(|B^2e^{itE} - e^{-itE}B^2|^2) \leqslant 8t^2\sum_n \frac{(\omega_n')^2}{n}$$
$$< 8t^2\sum_n \frac{1}{n^3} < \infty.$$

Thus $(B^2e^{itE} - e^{-itE}B^2) \in \mathbf{B}_{2r}$.

(d) Because $C^2 = I$,

$$CB^2Ce^{itE} - e^{-itE}CB^2C$$
$$= C\{(B^2e^{-itE} - e^{itE}B^2) + B^2(Ce^{itE}C - e^{-itE})$$
$$- (Ce^{-itE}C - e^{itE})B^2\}C,$$

and since each of the parenthetical expressions has been shown to be of Hilbert–Schmidt type, $(CB^2Ce^{itE} - e^{-itE}CB^2C) \in \mathbf{B}_{2r}$ also.

(e) Add the results of (c) and (d) to show that $(Ae^{itE} - e^{-itE}A) \in \mathbf{B}_{2r}$; then the fact that $(e^{itH} - e^{itE}) \in \mathbf{B}_{2r}$ for all t implies $(Ae^{itH} - e^{-itH}A) \in \mathbf{B}_{2r}$, or equivalently

$$(AC)e^{itH} - e^{itH}(AC) \in \mathbf{B}_{2r} \text{ for all } t,$$

as claimed.

(5) The final step in the construction is to define a symplectic operator T with $(T^*T)_a = AC$ so that T is not of Shale type, but TV_tT^{-1} is of Shale type.

(a) Since A is positive, the operator $R \equiv (I + A^2)^{1/2}$ is well-defined, and furthermore $R \geqslant I$ and $[R,C] = 0$. Set

$$T \equiv \frac{1}{\sqrt{2}}(R + I)^{1/2} + \frac{1}{\sqrt{2}}(R - I)^{1/2}C.$$

This T is self-real-adjoint, and

$$T^*T = R + (R^2 - I)^{1/2}C = R + AC.$$

To check that T is symplectic, note that

$$\Lambda^*T^*\Lambda = \frac{1}{\sqrt{2}}[(R + I)^{1/2} - (R - I)^{1/2}C],$$

so that

$$T(\Lambda^*T^*\Lambda) = (\Lambda^*T^*\Lambda)T = \tfrac{1}{2}[R + I - (R - I)] = I.$$

(b) To see that T is not of Shale type, note that

$$|T^*T - I|^2 = (R - I)^2 + A^2 + 2A(R - I)C,$$

and since $2A(R - I)C$ is antilinear,

$$\mathrm{tr}_r\{|T^*T - I|^2\} = \mathrm{tr}_r\{A^2 + (R - I)^2\},$$

which is not finite because $A \notin \mathbf{B}_{2r}$.

(6) The following result is useful in demonstrating that TV_tT^{-1} is in fact of Shale type.

Lemma 6: Let P be a bounded positive linear transformation, bounded away from zero, and let X be a bounded linear transformation such that $PX + XP \in \mathbf{B}_{2c}$. Then $X \in \mathbf{B}_{2c}$.

Proof: Assume, without loss of generality, that $\|P\| \leqslant 1$. Let $Q \equiv PX + XP \in \mathbf{B}_{2c}$. Then $[X,P^2] = [Q,P]$.

The crux of the proof is to show that $[X,P] \in \mathbf{B}_{2c}$. Since P is positive and $\|P\| \leqslant 1$, the series

$$P = \sqrt{P^2} = I + c_1(I - P^2) + c_2(I - P^2)^2 + c_3(I - P^2)^3 + \cdots$$

converges in norm. Thus, the series

$$[X,P] = c_1[X,(I - P^2)] + c_2[X,(I - P^2)^2]$$
$$+ c_3[X,(I - P^2)^3] + \cdots$$

also converges in norm. That this series furthermore converges in Hilbert–Schmidt norm can be seen from the fact that

$$\|[X,(I - P^2)^k]\|_{2c} \leqslant k\,\|(I - P^2)\|^{k-1}\,\|[X,(I - P^2)]\|_{2c}$$
$$= k\,\|(I - P^2)\|^{k-1}\,\|[Q,P]\|_{2c}.$$

Since P is bounded away from zero, $\lambda \equiv \|(I - P^2)\|$ is less than 1. Thus

$$\|[X,P]\|_{2c} = \left\|\sum_{k=1}^{\infty} c_k\,[X,(I - P^2)^k]\right\|_{2c}$$
$$\leqslant \sum_{k=1}^{\infty} |c_k|k\,\|(I - P^2)\|^{k-1}\,\|[Q,P]\|_{2c}$$
$$= \|[Q,P]\|_{2c}\sum_{k=1}^{\infty} |c_k|k\,\lambda^{k-1}.$$

Since this last series converges for $0 \leqslant \lambda < 1$, $XP - PX \in \mathbf{B}_{2c}$, as desired.

To finish the proof of the lemma, note that by hypothesis $XP + PX \in \mathbf{B}_{2c}$, so that both XP and PX are in $\mathbf{B}_{2c}$. Now, since P is bounded away from zero, P^{-1} is bounded, so that $X = (XP)P^{-1} \in \mathbf{B}_{2c}$.

This concludes the proof of the lemma. □

(7) To demonstrate that TV_tT^{-1} satisfies Shale's criterion although T does not, write

$$|TV_tT^{-1}|^2 - I = T^{*-1}V_t^*(|T|^2V_t - V_t|T|^2)T^{-1}$$
$$= T^{*-1}V_t^*((R + AC)V_t - V_t(R + AC))T^{-1}$$
$$= T^{*-1}V_t^*\{[AC,e^{itH}] + [R,e^{itH}]\}T^{-1}.$$

Paragraph (4) above shows that $[AC,e^{itH}] \in \mathbf{B}_{2r}$. To show that the remaining term $[R,e^{itH}]$ is also in $\mathbf{B}_{2r}$, note that

$$[R^2,e^{itH}] = [A^2,e^{itH}]$$
$$= A(Ae^{itH} - e^{-itH}A) - (e^{itH}A - Ae^{-itH})A,$$

so that, again by the results of paragraph (4), $[R^2,e^{itH}] \in \mathbf{B}_{2r}$. That is, $XR + RX \in \mathbf{B}_{2r}$, where $X \equiv [R,e^{itH}]$. Since all of these operators are complex-linear, it is even true that $XR + RX \in \mathbf{B}_{2c}$, so Lemma 6 above with $P \equiv R$ implies that $X \in \mathbf{B}_{2c}$, i.e., $[R,e^{itH}] \in \mathbf{B}_{2c} \subset \mathbf{B}_{2r}$. Thus $(|TV_tT^{-1}|^2 - I) \in \mathbf{B}_{2r}$, as was to be shown.

ACKNOWLEDGMENT

I thank Professor E. H. Wichmann for useful, stimulating discussions.

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Decomposition of the finite-dimensional fermion algebra into irreducible spaces

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(Received 15 April 1982; accepted for publication 21 May 1982)

The 2^{2n}-dimensional operator algebra constructed on n single-fermion states is decomposed into irreducible tensor operator spaces with respect to three Lie subalgebras of physical interest: (i) the Lie subalgebra associated with the group SU(n) used in Hartree–Fock theory, (ii) the Lie subalgebra associated with the group SO($2n$) used in Hartree–Bogoliubov theory, and (iii) the Lie subalgebra associated with the group SO($2n + 1$) introduced by Wybourne in atomic applications.

PACS numbers: 02.20. + b, 05.30.Fk

I. INTRODUCTION

In this paper we study the algebra generated by a finite number of creation and annihilation fermion operators. This case occurs in nuclear and atomic shell-model applications when the infinite number of single-particle states is cut off to a finite number for practical calculations. The finite-dimensional algebra generated by n creation and n annihilation fermion operators was investigated by Heise[1] in view of physical applications. Heise, however, studied this algebra especially in relation with its unitary, particle-number-conserving subalgebra. We shall consider also two other subalgebras of physical interest. These are: (i) the subalgebra corresponding to the orthogonal group SO($2n$) which mixes the n particles with the n-hole states[2] and is used in Hartree–Bogoliubov calculations[3] and (ii) a subalgebra corresponding to the orthogonal group SO($2n + 1$) introduced by Wybourne[4] and which found some interest in atomic applications.

The purpose of this paper is to decompose the finite-dimensional fermion algebra into generalized irreducible tensor operator spaces with respect to the three Lie subalgebras: the unitary SU(n), the orthogonal SO($2n$), and the orthogonal SO($2n + 1$). The irreducible tensor operator spaces (ITOS's) are irreducible representation spaces for the subalgebras with respect to the operation of commutation.

In Sec. II we review various useful properties of the fermion algebra and of its three Lie subalgebras. In particular, we specify simple basis for the three Lie subalgebras that we shall use in Sec. III for the decomposition into ITOS's. In Sec. III we decompose the fermion algebra into irreducible tensor operator spaces with respect to the three subalgebras corresponding to the groups SU(n), SO($2n$), and SO($2n + 1$). We characterize each ITOS by the highest weight (hw) of the representation, by the operator corresponding to this highest weight (hwo), and by the dimension of the irreducible representation.

II. BASIC PROPERTIES OF THE FERMION ALGEBRA AND OF ITS THREE SUBALGEBRAS

A. The algebra C

We consider n creation and n annihilation operators

$$a_1^+, \ldots, a_n^+, a_1, \ldots, a_n, \tag{1}$$

obeying the fermion anticommutation relations

$$[a_i^+, a_j]_+ = \delta_{ij}, \quad [a_i^+, a_j^+]_+ = [a_i, a_j]_+ = 0. \tag{2}$$

From the operators (1) we can construct 2^{2n} linearly independent products

$$a_{i_1}^+ a_{i_2}^+ \cdots a_{i_p}^+ a_{j_s} \cdots a_{j_2} a_{j_1} \tag{3}$$

for which we may adopt the normal ordering, i.e., creation operators first and $i_1 < i_2 \cdots < i_p, j_1 < j_2 \cdots < j_s$. These 2^{2n} products span the finite-dimensional fermion algebra. This algebra was studied in the mathematical literature, for instance by Chevalley,[5] as a Clifford algebra and we shall denote it by C.

The subspace of C spanned by products (3) containing p creation and s annihilation operators will be noted $C_{(p,s)}$. The subspace of C spanned by normal products of order k, i.e., such that $p + s = k$, will be called $C_{(k)}$. Clearly

$$\dim C_{(p,s)} = \binom{n}{p}\binom{n}{s}, \quad \dim C_{(k)} = \binom{2n}{k}. \tag{4}$$

It is useful also to consider the even and odd parts of C: The subspace of C containing the $C_{(k)}$'s with k even will be noted C_e and the subspace of C containing the $C_{(k)}$'s with k odd will be noted C_o. We have

$$\dim C_e = \dim C_o = 2^{2n-1}. \tag{5}$$

It is easy to see that C_e is an algebra while C_o is not. C_e is in fact the direct sum of two simple algebras.

To decompose C_e in simple parts, we note that the center of C_e is spanned by two elements[5]: the identity and the operator

$$e = \prod_{i=1}^{n} (2a_i^+ a_i - 1) \tag{6}$$

which satisfies the relation $e^2 = 1$. We therefore construct the two projectors

$$p_\pm = \tfrac{1}{2}(1 \pm e), \tag{7}$$

which satisfy

$$p_\pm^2 = p_\pm, \quad p_+ p_- = p_- p_+ = 0, \quad p_+ + p_- = 1. \tag{8}$$

Then C_e can be split into two simple algebras

$$C_e^+ = C_e p_+, \quad C_e^- = C_e p_- \tag{9}$$

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each of dimension 2^{2n-2} and such that $C_e^+ C_e^- = C_e^- C_e^+ = 0$.

The algebra C itself can be decomposed into a direct sum with the aid of the projectors p_+ and p_-. To see this, define $C^+ = Cp_+$ and $C^- = Cp_-$, and note that C^+ and C^- are disjoint. For, if $cp_+ = c'p_-$ $(c, c' \in C)$, multiplying by p_+ at the right on both sides, we obtain, using (8), $cp_+ = c'p_- = 0$. Moreover, any element $c \in C$ can be decomposed in a unique way as a sum $c = c_+ + c_-$ with $c_+ = cp_+$ and $c_- = cp_-$.

We have reviewed above the main properties of the finite-dimensional fermion algebra C. For other properties and especially the relation of C to the space of wavefunctions (or the space of spinors) we refer to the works 2 and 5.

B. The subalgebra L_1

In what follows we shall use mainly commutators and not the associative product, so we shall refer to Lie algebras and subalgebras instead of (associative) algebras. We shall consider first the Lie algebra associated with the realization of the unitary group U(n) which mixes creation operators (or annihilation operators) among themselves. This Lie algebra and the corresponding group are important in Hartree–Fock theory.

This unitary Lie subalgebra is spanned by the n^2 operators

$$a_i^+ a_j, \quad i,j = 1, \ldots, n. \tag{10}$$

It is not a simple algebra but it becomes simple if we take off its center which is the number operator $N = \sum_{i=1}^n a_i^+ a_i$. We call the resulting (n^2-1)-dimensional Lie subalgebra L_1. L_1 is of type A_{n-1}. It has $n-1$ simple roots $\{\alpha_i, i = 1,\ldots, n-1\}$, which satisfy the relations

$$(\alpha_i, \alpha_i) = 2, \quad (\alpha_i, \alpha_j) = k_{ij}, \tag{11}$$

where $(\ ,\ )$ is the scalar product in the root space and $k_{ij} = -1$ if α_i and α_j are adjacent and connected in the Dynkin diagram of A_{n-1} and $k_{ij} = 0$ if α_i and α_j are not directly connected. To each simple root α_i corresponds a triplet $\{H_{\alpha_i}, E_{\pm\alpha_i}\} \equiv \{H_i, E_{\pm i}\}$ of simple operators, satisfying the commutation relations

$$[H_i, E_{\pm i}]_- = \pm(\alpha_i, \alpha_i) E_{\pm i}, \quad [E_i, E_{-i}]_- = H_i,$$
$$[H_i, E_j]_- = (\alpha_i, \alpha_j) E_j, \quad [E_i, E_j]_- = q E_{\alpha_i + \alpha_j}, \tag{12}$$

where $q = \pm 1$ if α_i and α_j are directly connected and $q = 0$ if not. The $3(n-1)$ operators $\{H_i, E_{\pm i}, i = 1,\ldots,n\}$ form a simple basis of L_1 from which all other operators of L_1 can be obtained by commutation. The H_i are Cartan–Hermitian operators $(H_i^+ = H_i)$ and E_i and E_{-i} are respectively raising and lowering operators $(E_{-i} = E_i^+)$. A realization of this simple basis in terms of creation and annihilation operators is given by

$$E_i = a_i^+ a_{i+1}, \quad E_{-i} = a_{i+1}^+ a_i,$$
$$H_i = a_i^+ a_i - a_{i+1}^+ a_{i+1}, \quad i = 1,\ldots,n-1. \tag{13}$$

C. The subalgebra L_2

The Lie subalgebra L_2 of C is associated with the orthogonal group O($2n$). This group is the basic group in the Hartree–Bogoliubov theory where it mixes creation and annihilation operators to form quasiparticle operators. L_2 is spanned by the $n(2n-1)$ bilinear products

$$a_i^+ a_j^+, \quad a_i a_j, \quad a_i^+ a_j \tag{14}$$

and is of type D_n. The simple roots of L_2 satisfy relations (11) where the scalar products are determined by the Dynkin diagram of D_n. It is easily checked that a basis of $3n$ simple operators is given by

$$E_i = a_i^+ a_{i+1}, \quad E_{-i} = a_{i+1}^+ a_i,$$
$$H_i = a_i^+ a_i - a_{i+1}^+ a_{i+1}, \quad i = 1,\ldots,n-1,$$
$$E_n = a_{n-1}^+ a_n^+, \quad E_{-n} = a_n^+ a_{n-1}^+, \tag{15}$$
$$H_n = a_{n-1}^+ a_{n-1} + a_n^+ a_n - 1.$$

All other operators (14) can be obtained from the operators (15) by commutation.

D. The subalgebra L_3

The realization of the group O($2n+1$) in terms of fermion operators was considered by Wybourne.[4] Its Lie algebra L_3 contains bilinear as well as single operators

$$a_i^+ a_j^+, \quad a_i a_j, \quad a_i^+ a_j, \quad a_i^+, \quad a_i \tag{16}$$

for a total of $n(2n+1)$ operators. L_3 is of type B_n. Its simple roots satisfy

$$(\alpha_i, \alpha_i) = 2, \ i = 1,\ldots,n-1, \quad (\alpha_n, \alpha_n) = 1, \quad (\alpha_i, \alpha_j) = k_{ij}, \tag{17}$$

where $k_{ij} = -1$ if α_i and α_j are connected by a line in the Dynkin diagram and $k_{ij} = 0$ if they are not connected. A simple basis of operators for L_3 satisfying the relations (12) is given by

$$E_i = a_i^+ a_{i+1}, \quad E_{-i} = a_{i+1}^+ a_i,$$
$$H_i = a_i^+ a_i - a_{i+1}^+ a_{i+1}, \quad i = 1,\ldots,n-1,$$
$$E_n = (1/\sqrt{2}) a_n^+, \quad E_{-n} = (1/\sqrt{2}) a_n, \tag{18}$$
$$H_n = a_n^+ a_n - \tfrac{1}{2}.$$

III. DECOMPOSITION OF C INTO IRREDUCIBLE TENSOR OPERATOR SPACES

It is a matter of interest to decompose the algebra C into ITOS's with respect to the three subalgebras L_1, L_2, and L_3. Before beginning the specific decomposition, it is important to note the difference between a usual representation space for a Lie algebra L and an irreducible tensor operator space for L. For a usual representation space V of L, L acts on V by the so-called module multiplication $LV \subset V$. On the other hand, for an ITOS T of L we have $[L,T]_- \subset T$, where the commutator replaces the module multiplication.

A. Decomposition of C with respect to L_1

L_1 is spanned by the operators $\{a_i^+ a_j\}$. We remark that both C_e and C_o are stable with respect to commutation with these operators and are therefore tensor operator spaces for L_1. The same remains true when we commute the operators

$a_i^+ a_j$ with the subspaces $C_{(p,s)}$, which are thus tensor operator spaces for L_1. However, it can be seen (by taking for example a particular case) that the spaces $C_{(p,s)}$ are in general reducible.

Let us note that $C_{(p,0)}$ and $C_{(0,s)}$ are ITOS's for L_1. In fact, $C_{(p,0)}$ is the pth antisymmetrized tensor product of $C_{(1,0)}$, which is spanned by the creation operators $(a_i^+$, $i = 1,...,n)$. $C_{(1,0)}$ has hw (1,0,...,0) and its hwo is a_1^+ (corresponding to the simple basis specified in Sec. IIB). $C_{(p,0)}$ has an hw with 0's everywhere except a 1 in the pth position from the left and its hwo is $a_1^+ a_2^+ \cdots a_p^+$. We shall use the notation (1_p) for an hw with a 1 in position p from the left and 0's everywhere else. The ITOS's $C_{(0,s)}$ are adjoints to $C_{(s,0)}$. As such $C_{(0,s)}$ is the sth antisymmetrized power of $C_{(0,1)}$ which is spanned by the annihilation operators $(a_i,\ 1 = 1,...,n)$. $C_{(0,1)}$ has hw (1_{n-1}) and hwo a_n and $C_{(0,s)}$ has hw (1_{n-s}) and hwo $a_n a_{n-1} \cdots a_{n-s+1}$.

Now $C_{(p,s)}$ is the tensor product of $C_{(p,0)}$ with $C_{(0,s)}$. We use the obvious notation $(1_k 1_l)$ for an hw with 1's in the k and l positions from the left and 0's everywhere else. Dynkin[6] has shown that a tensor product like $C_{(p,s)}$ decomposes into irreducible spaces with highest weights

$$(1_p 1_{n-s}),\ (1_{p-1} 1_{n-s+1}),\ (1_{p-2} 1_{n-s+2}),\cdots, \tag{19}$$

the enumeration terminating either with an hw (0,...,0) or an hw with a single 1. Dynkin has also proved that each of the irreducible representations corresponding to the above hw's has multiplicity 1. To determine the hwo's corresponding to the hw's (19), we note first that $a_1^+ a_2^+ \cdots a_p^+ a_n \cdots a_{n-s+1}$ is the hwo corresponding to $(1_p 1_{n-s})$. The verification is done by checking that the commutators of $a_1^+ \cdots a_p^+ a_n \cdots a_{n-s+1}$ with the raising operators E_i of L_1 give zero. Then one can verify quite easily that the hwo's corresponding to the other hw's are obtained by replacing the farthest creation operator from the left and the nearest annihilation operator from the right by the number operator N. Thus the hwo corresponding to $(1_{p-1} 1_{n-s+1})$ is $a_1^+ \cdots a_{p-1}^+ N a_n \cdots a_{n-s+2}$, the hwo corresponding to $(1_{p-2} 1_{n-s+2})$ is $a_1^+ \cdots a_{p-2}^+ N^2 a_n \cdots a_{n-s+3}$, etc.

Let us take, for better illustration, a specific example. We assume $n = 4$ and want to decompose $C_{(2,2)}$ in ITOS's. The hw's occurring in the decomposition will be $(1_2,1_2) \equiv (020)$, $(1_1,1_3) \equiv (101)$ and (000). The corresponding hwo's, as easily verified, are $a_1^+ a_2^+ a_4 a_3$, $a_1^+ N a_4$, and N^2. We check in the Appendix the correctness of the decomposition of C with respect to L_1 by using dimensions.

B. Decomposition of C with respect to L_2

We take the simple basis (15) of L_2 and look for hw's and hwo's of ITOS's in C. We find that $1, a_1^+, a_1^+ a_2^+, ..., a_1^+ a_2^+ \cdots a_p^+, ..., a_1^+ a_2^+ \cdots a_n^+$ are such hwo's. This can be seen by commuting the raising operators E_i from (15) with the above operators and noting that this gives 0. The corresponding hw's (apply the Cartan operators H_i to the hwo's) are

$$(0), (1_1), (1_2), ..., (1_{n-1}), (2_n). \tag{20}$$

The dimension of the representation (1_p) of D_n is $\binom{2n}{p}$ and that of (2_n) is $\frac{1}{2}\binom{2n}{n}$. If $1, a_1^+, a_1^+ a_2^+, ..., a_1^+ a_2^+ \cdots a_n^+$ form a complete decomposition of C in ITOS's we must have the equality of dimensions: $\dim C = 1 + \binom{2n}{1} + \binom{2n}{2} + \cdots \binom{2n}{n-1} + \frac{1}{2}\binom{2n}{n} \equiv 2^{2n-1}$. But the dimension of C is 2^{2n}, the double of 2^{2n-1}.

Let us remember, however, that C is the direct sum of C^+ and C^-. Thus, we can in fact construct twice as many ITOS's in C by using the projectors $p_\pm$, viz.,

$$p_\pm, a_1^+ p_\pm, a_1^+ a_2^+ p_\pm, ..., a_1^+ a_2^+ \cdots a_n^+ p_\pm. \tag{21}$$

It is easily verified that these $(n+1)$ pairs are hwo's with the corresponding hw's (20) and that the dimension check is now correct:

$$\dim C \equiv 2^{2n} = 2\cdot 1 + 2\cdot\binom{2n}{1} + \cdots + 2\binom{2n}{n-1} + 2\left[\frac{1}{2}\binom{2n}{n}\right]. \tag{22}$$

C. Decomposition of C with respect to L_3

In the case of L_3 we shall see that pairs of adjacent ITOS's in the decomposition (22) of C with respect to L_2 mix to form an ITOS with respect to L_3. This is related to the binomial coefficient identity

$$\binom{2n}{i} + \binom{2n}{i+1} = \binom{2n+1}{i+1}. \tag{23}$$

According to Eq. (23), one can see how the dimensions of ITOS's of L_2 in Eq. (22) mix. We have now

$$\begin{aligned}\dim C \equiv 2^{2n} &= 1 + \left[\binom{2n}{0} + \binom{2n}{1}\right] + \left[\binom{2n}{1} + \binom{2n}{2}\right] + \cdots \\ &\quad + \left[\binom{2n}{n-2} + \binom{2n}{n-1}\right] \\ &\quad + \left[\binom{2n}{n-1} + \frac{1}{2}\binom{2n}{n} + \frac{1}{2}\binom{2n}{n}\right] \\ &\equiv 1 + \binom{2n+1}{1} + \binom{2n+1}{2} + \cdots \\ &\quad + \binom{2n+1}{n-1} + \binom{2n+1}{n},\end{aligned} \tag{24}$$

and we see that two ITOS's of L_2 mix to form an ITOS of L_3 for all representations of L_2 but the first and the last. The first ITOS of L_2 does not mix and the three last ITOS's of L_2 form an ITOS of L_3.

This dimension decomposition must be checked by determining the hwo's and the corresponding hw's. We assert that the following operators,

$$1, a_1^+ e, a_1^+ a_2^+, ..., a_1^+ a_2^+ \cdots a_{2k}^+, a_1^+ a_2^+ \cdots a_{2k+1}^+ e, \cdots \tag{25}$$

are hwo's for ITOS's of L_3. Note that in Eq. (25) an hwo consisting of a product of an odd number of creation operators has attached an operator e. To prove that the operators (25) are hwo's, one applies the raising operators E_i in (18). The hw's corresponding to the hwo's (25) are

$(0), (1_1), (1_2), \cdots$.

IV. CONCLUSIONS

We make now the following comments on what has been done and on possible generalizations.

First, our method can be extended to the case of an infinite number of single-particle states. Then, one has to consider infinite-dimensional algebras and subalgebras but the decomposition into ITOS's keeps probably the same structure as for the finite-dimensional case.

Secondly, it is important to note that the specific form of the hwo's depends on the realizations of the simple basis for L_1, L_2, and L_3 in terms of creation and annihilation operators. The decomposition according to hw's and the dimensions of the ITOS's remain, however, invariant and are therefore characteristic of the problem. The specification of the hwo's for the ITOS's is nevertheless useful because one can obtain from them, by using lowering operators, all the operators of the ITOS's corresponding to a specific basis of L_1, L_2, or L_3. In general, the problem of the decomposition is unique up to an automorphism of the whole algebra C.

Let us elaborate also on the usefulness of our decomposition for physical applications. As noted by Heise,[1] the study of the algebra constructed on a finite set of fermion operators is useful for the analysis and understanding of various model Hamiltonians and operators occuring in atomic and nuclear physics. These Hamiltonians and operators belong to the algebra C and therefore themselves and their eigenspaces can be studied by using our general decomposition. Our decomposition can be extended also to other symmetry subalgebras such as the symplectic or quasispin subalgebras which are used for the classification of atomic and nuclear states.

ACKNOWLEDGMENT

This work was supported in part (A. B.) by a grant from the National Sciences and Engineering Research Council of Canada and (A. N.) by a special grant from F. I. R., Université du Quebec.

APPENDIX

In this appendix a closed formula for the dimension of an irreducible representation (IR) of type (0···010···010···0) of SU($n+1$) is derived and a check for the decomposition (19) of the space $C_{(p,s)}$ with respect to L_1 is made by using dimensions.

Dynkin[6] rewrote Weyl's dimension formula in a combinatorial form and thus made it suitable for computations. We[7] unified Dynkin's formulas for all simple Lie algebras by the use of Killing–Cartan system of roots and coded the algorithm for programmable calculators. Here we use this formulation except that we have replaced the parameters $\{t_i\}$ by their values $\{n+1-i\}$.

The vector $[\Lambda_1,\Lambda_2,\ldots\Lambda_n]$ denotes the highest weight vector characterizing an IR. For A_n [i.e., SU($n+1$)] the dimension formula is given by

$$N_\Lambda = f(1)f(2_-), \tag{A1}$$

where

$$f(1) = \prod_{1\le i<n}\left[1+\frac{k_i}{n+1-i}\right],$$

$$f(2_-) = \prod_{1\le i<j<n}\left[1+\frac{k_i-k_j}{j-i}\right],$$

the k_j's satisfying the recursion relation

$$k_n = \Lambda_n,$$

$$k_{n-p} = k_{n-p+1} + \Lambda_{n-p} \quad (1\le p\le n-1). \tag{A2}$$

We consider an IR of the type defined by

$$\Lambda_p = \Lambda_q = 1, \quad \Lambda_i = 0, \quad i\neq p, q.$$

Then (A2) gives

$$k_i = \begin{cases} 0, & q+1\le i\le n,\\ 1, & p+1\le i\le q,\\ 2, & 1\le i\le p.\end{cases}$$

Consequently,

$$f(1) = \prod_{1\le i<p}\left[1+\frac{2}{n+1-i}\right]\prod_{p<i<q}\left[1+\frac{1}{n+1-i}\right]$$

which, after some algebra, reduces to

$$f(1) = \frac{(n+1)(n+2)}{(n+1-q)(n+2-p)}.$$

The other factor of N_Λ is

$$f(2_-) = \prod_{1\le i<p}\left\{\prod_{p<j<q}\left[1+\frac{1}{j-i}\right]\prod_{q<j<n}\left[1+\frac{2}{j-i}\right]\right\} \times \prod_{p<i<q}\left\{\prod_{q<j<n}\left[1+\frac{1}{j-i}\right]\right\},$$

which, after some manipulations, becomes

$$f(2_-) = \frac{q+1-p}{n+1-p}\binom{n}{p}\binom{n+1}{q+1}.$$

Finally,

$$N_\Lambda = \frac{(q+1-p)(n+1)!(n+2)!}{(q+1)!(n+1-q)!p!(n+2-p)!}, \tag{A3}$$

which can be written also for A_{n-1} [SU(n)]

$$N_\Lambda = \frac{q-p+1}{q+1}\binom{n+1}{p}\binom{n}{q}. \tag{A4}$$

We[8] know that for A_{n-1} the reflection about the midpoint is an automorphism of the Dynkin diagram. Consequently, the dimension formula must verify the relation

$$N_\Lambda(p,q) = N_\Lambda(n-q, n-p).$$

We see that our formula satisfies this test.

It is easy now to prove by induction the decomposition (19) of Sec. IIIA. We note that the equality of dimensions holds for $C_{(0,0)}$, $C_{(1,0)}$, and $C_{(0,1)}$ in (19). Now suppose that the equality of dimensions holds for $C_{(p,s)}$. To complete the induction proof, it remains to show that the equality holds also for $C_{(p+1,s+1)}$. But $\dim C_{(p+1,s+1)} \equiv \binom{n}{p+1}\binom{n}{s+1}$, and we shall prove that it equals $\dim(1_{p+1}, 1_{n-s-1}) + \dim C_{(p,s)}$. In fact this last sum can be written:

$$\frac{n-s-p-1}{n-s}\binom{n+1}{p+1}\binom{n}{n-s-1} + \binom{n}{p}\binom{n}{s} \equiv \frac{(n!)^2}{(p+1)!(n-p-1)!(s+1)!(n-s-1)!}.$$

$[(n+1)(n-s-p-1)/(n-p)(n-s) + (p+1)(s+1)/(n-p)(n-s)]$ and the expression in square brackets equals 1, which finishes the proof.

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The lifting of an İnönü–Wigner contraction at the level of universal coverings

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(Received 20 April 1982; accepted for publication 1 July 1982)

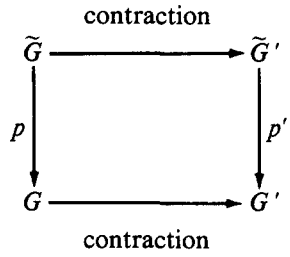
It is shown that, when the Borel cohomology of a connected Lie group G is such that all projective representations can be lifted to unitary representations of the universal covering group, then any contraction of G corresponds to a contraction of its universal covering. Three theorems are stated and proved. The results apply also to the İnönü–Wigner contraction of the Poincaré group into the Galilei group.

PACS numbers: 02.20.Qs

INTRODUCTION

After the pioneering works of Wigner and Bargman[1,2] the relationship between the classification of the PUR (projective unitary representations) of a connected Lie group and the classification of the PUR of its contraction in the İnönü–Wigner sense has become an important problem.[3] In this paper we shall study the special case of a complex connected Lie group G contracted to a "motion type" group $K(G)\circledS\mathcal{L}K(G)$ ($\circledS\equiv$semidirect product). [To fix notation, $\mathcal{L}(G)$ will denote the Lie algebra of G, $K(G)$ a maximal compact subgroup of G, $H_0^2(G,U(1))$ the second cohomology group (Borel cohomology) corresponding to trivial action of G on U(1), and $\widehat{G}$ the set of classes of projective unitary representations of G indexed by $H_0^2(G,\mathrm{U}(1))$.]

That kind of contraction can, in special cases of physical interest, be lifted at the level of universal converings.



The classical contraction $P\to g$ ($P=$ Poincaré group, $g=$ Galilean group) does not "preserve the compact part," that is $K(P)\neq K(g)$ and, in fact there are classes of PUR of g that do not appear in P. But even this contraction can be lifted in a sense described below.

Theorem I: Let G' be a contraction of G, G any connected Lie group such that $K(G)=K(G')$. Then $\widehat{G}=\widehat{G}'$.

Proof: The following isomorphism holds for every connected G:

$$H_0^2(G,\mathrm{U}(1))\cong H_0^2(K(G),\mathrm{U}(1)).$$

Then,

$$H_0^2(G',\mathrm{U}(1))\cong H_0^2(G,\mathrm{U}(1)).$$

This is because G and $K(G)$ have the same topology. Note that the isomorphism holds in spite of the fact that we include a further condition on the measurable 2-cocycles: $\sigma(a,bc)\sigma(b,c)=\sigma(a,b)\sigma(ab,c)(a,b,c\in G)$. A contraction $G\to K(G)\circledS\mathcal{L}(K(G))$ can be actually lifted to an extension of $\tilde{G}$ (the universal covering of G) which we denote by $\mathring{G}$, such that, if $p:\mathring{G}\to G$ is a continuous covering epimorphism, then applying the contravariant functor $\mathrm{Ext}_0^1(-,\mathrm{U}(1))$ we get the trivial homomorphism $\mathrm{Ext}_0^1(p,\mathrm{U}(1))\equiv 0[\mathrm{Ext}_0^1(p,\mathrm{U}(1)):\mathrm{Ext}_0^1(G,\mathrm{U}(1))\to\mathrm{Ext}_0^1(\mathring{G},\mathrm{U}(1))$.] We have the general result:

Theorem II: Let $\mathring{G}$ be a connected Lie group, G its universal covering; then $\mathring{G}\cong\mathring{G}$ (as groups).

Proof: $\mathcal{L}(\tilde{G})=\mathcal{L}(G)$ and so, also $H_0^2(\mathcal{L}(\tilde{G}),\mathbb{R})=H_0^2(\mathcal{L}(G),\mathbb{R})$. Then by a result due to Hochschild[4] we can state $\mathring{G}=\mathring{G}$.

We shall work in the special context: (1) $H_0^2(\mathcal{L}K(G),R)=0[H_0^2(\widetilde{K(G)},\mathrm{U}(1),)=0]$ [which holds in many cases of physical interest, for example, when $K(G)$ is the three-dimensional rotation group, for $K(P)$, etc. (2) G is of the form $G_1/$center of G_1, where G_1 is a connected and simply connected complex Lie group.

We shall actually see that $\mathring{G}=\tilde{G}$ and $K(G)\mathring{\circledS}\mathcal{L}(K(G))=\widetilde{K(G)\circledS\mathcal{L}(K(G))}$. [The group $\mathring{G}$ can be detected in the Levy-Leblond paper[5] dealing with the computation of all PUR of g which can be lifted to the unitary line as representations of $\mathring{g}$ (the "extended Galilean group"). Actually it is possible to "lift" at the level of the coverings the contraction $P\to g$, but in this particular case, $\mathring{P}\simeq\tilde{P}$ because $\mathrm{Ext}_0(\tilde{P},\mathrm{U}(1))=0$, so $\mathring{P}$ is a 10-dimensional group, as P, but $\mathrm{Ext}_0(\tilde{g},\mathrm{U}(1))\neq 0$ and $\mathring{g}$ is 11-dimensional over the real field $\mathbb{R}$. Even here we can "contract" $\tilde{P}$ to $\mathring{g}$ by adding an extra generator to the $\mathcal{L}(P)$ and still show that a contraction holds at the level of $\mathcal{L}(P)\to\mathcal{L}(\mathring{g})$].

In our particular context, $\mathring{G}$ is the only connected simply connected Lie group associated with the Lie algebra $\mathcal{L}(G)$.

The condition $H_0^2(\widetilde{K(G)},\mathrm{U}(1))=0$ always holds if the Lie algebra $\mathcal{L}(K(G))$ is semisimple (Whitehead's second lemma).[6]

A comparison of the Lie algebra of $\mathring{G}$ and of $K(G)\mathring{\circledS}\mathcal{L}(K(G))$ will show that one is a contraction of the other: $\mathcal{L}(\mathring{G})=L\oplus K$ (semidirect sum of the Lie algebra L and K) so that the following commutator relations hold: $[L,L]\subset L,[L,K]\subset K,[K,K]\subset K,[L,K]\neq 0$; $\mathcal{L}(K(G)\mathring{\circledS}\mathcal{L}(K(G)))=L'\oplus K'$, where $[L',L']\subset L',[K',K']\subset K'$, and $[L',K']=0$. $\mathcal{L}(\mathring{G})$ is contracted to $\mathcal{L}(K(G)\mathring{\circledS}\mathcal{L}(K(G)))$.

The condition $H_0^2(\widetilde{K(G)},\mathrm{U}(1))=0$ implies $H_0^2(\mathcal{L}(K(G)\mathring{\circledS}\mathcal{L}(K(G))),\mathbb{R})=0$. Since $K(G)$ is compact, we also get $H_0^1(\mathcal{L}(K(G)),\mathcal{L}(K(G)))=0$. (Weyl, see, e.g., MacLane[6]).

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We also have that $H_0^2(\mathcal{L}(G),\mathbb{R}) = 0$. Hence $\mathring{G}$ and $K(G)\mathring{\&}\mathcal{L}(K(G))$ are the connected simply connected Lie groups of the Lie algebras of G and $K(G)\&\mathcal{L}(K(G))$, that is their respective universal coverings. Moreover, the contraction $\mathring{G}\to K(G)\mathring{\&}\mathcal{L}(K(G))$ preserves the compact part [which is nothing but the universal covering of $K(G)$]. Hence we also get the following:

Theorem III: Under these assumptions, $\hat{\mathring{G}} \cong K(G)\hat{\mathring{\&}}\mathcal{L}(K(G))$.

Corollary: In the case of our hypothesis, PUR of G and $K(G)\&\mathcal{L}(K(G))$ can be lifted to the UR of their respective universal coverings.

As an illustration, one can consider the case exposed by Mackey in his monograph $G = \mathrm{SL}(2,\mathbb{C})/Z_2, G' =$ Euclidean group.

We have the contraction $G\to G'$, and we are in the case of our hypothesis: $\mathrm{Ext}_0(\widetilde{\mathrm{SO}(3)},\mathrm{U}(1)) = \mathrm{Ext}_0(\mathrm{SL}(2,\mathbb{C}),\mathrm{U}(1)) = 0$.

Note (1) that condition (2) is not redundant; the condition $H_0^2(\mathcal{L}(K(G)),\mathbb{R}) = 0$ does not imply $H_0^2(\mathcal{L}(G),\mathbb{R}) = 0$ for any connected Lie group G. (2) In the above illustration of Mackey,[7] G has only the principal series. Up to a set of measure 0 (with the Pontrjagin measure), the dual objects of G and of $K(G)\&\mathcal{L}(K(G))$ are such that their parameter spaces are coordinable, and the same correspondence of above can be lifted at the level of dual objects of universal coverings.

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Irreducible representations of the superalgebras type II[a)]

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(Received 18 November 1981; accepted for publication 30 June 1982)

The representation of the orthosymplectic algebras and the other members of their class are built explicitly, with simple techniques.

PACS numbers: 02.20.Qs, 11.30.Pb

1. INTRODUCTION

The "classical" Lie superalgebras[1-3] are divided into two classes or types: the Class I includes the unitary superalgebras $SU(m/n)$ and $C(n)$ [$osp(2/2n-2]$; the Class II is made of the superalgebras $osp(m/n)$ and the exceptional $F(4)$ and $G(3)$.

The difference between the two classes appears in the gradation of the Lie algebra: Class I superalgebras can be decomposed into $G_{-1}+G_0+G_1$ (with $\{G_i, G_j\} \subset G_{i+j}$); Class II superalgebras can be decomposed only into G_0+G_1, with $\{G_1, G_1\} \subset G_0$.

In other words, in the Class I case, the odd generators belong to a reducible representation of G_0, namely G_1+G_{-1}. [Example $SU(m/n)$: G_1+G_{-1} corresponds to $(\bar{m}, n)+(m, \bar{n})$ of the underlying bosonic subalgebra $SU(m)\times SU(m)\times U(1)$]; in the Class II case, the odd generators in G_1 form an irreducible representation of G_0 [for $osp(m/n)$, G_0 is $O(m)\times Sp(n)$ and G_1 is (m, n); for $F(4)$, G_0 is $O(7)\times$SU(2) and G_1 is a (8, 2) and for $G(3)$, G_0 is $G_2\times SU(2)$ and G_1 is a (7, 2)].

This modifies significantly the problems raised by the representation of these superalgebras. In a related work[4] we study the irreducible representation of $SU(m/n)$, with all the group details; with the same kind of intention we address ourselves here to the representation of the Lie superalgebras of Class II.

In which sense $osp(4/2)$ and $osp(1/2n)$ are special will be made precise in Sec. 5.

The Dynkin diagrams are related to a Cartan matrix in the same way as for a classical Lie algebra.[5]

There is a basis (chevalley basis) where it is possible to decompose the algebra into a Cartan subalgebra ($h_i | [h_i, h_j] = 0, i, j = 1,...,r$ = rank of the superalgebra), and the other generators are associated with positive and negative roots. It is always possible to extract a system of r single positive and/or negative roots $\alpha_i^{\pm}$, involving only one odd root; in terms of these roots the algebra to represent is

$$[\alpha_i^+, \alpha_j^-\} = \delta_{ij} h_i$$

($[a, b\} = \{ab\}$ if both α_i and are odd, it is a commuter otherwise) and

$$[h_i, \alpha_j^{\pm}] = \pm a_{ij} \alpha_j^{\pm}.$$

a_{ij} are the elements of the "Cartan Matrix," which can be read off the Dynkin diagram; the rules are the same as for the plain Lie algebras. Two kinds of roots are added, "grey" and "black," which correspond to the odd roots. In our cases [Dynkin diagrams are not uniquely defined in general for Lie superalgebras (Ref. 1)] for these roots the rules are grey root corresponds to a 0 in the diagonal and to a -1 for all connected entries, except the first nonzero at the right of the zero is a $+1$. A black root is the same except that there is a 2 in the diagonal.

The rank of $osp(2m/2n)$ or $osp(2n+1/2n)$ is $m+n$; on their Dynkin diagram one can recognize a $SU(n)$ and a $SO(2m)$ or $SO(2m+1)$. The odd root hides an even simple root which belongs to $Sp(2n)$. This is the source of consistency conditions for the representations which do not exist in the Class I superalgebras, the details of which we give in Secs. 2, 4, and the appendices of this paper.

This paper whose aim is to be pedagogical is organized as follows:

—In Sec. 2 a specific simple, but neither trivial nor exceptional example [$B(2, 2) = osp(5/4)$], is studied in a lot of detail.

—In Sec. 3, the $osp(m/n)$ Lie superalgebras are discussed; the parts of their anatomy and physiology relevant for us are displayed.

—In Sec. 4 we study the representation of $osp(m/n)$ in general; namely we precisely define the conditions of typicality and consistency.

—In Sec. 5 we try to clarify what is special about $B(0, n)$ and $D(2, 1, \alpha)$.

Because, unavoidably, a general study like the one we do in Secs. 3 and 4 could seem a bit abstract to an hypothetical reader interested in playing with concrete representation, we have decided to show more examples than $B(2, 2)$.

With respect to what is potentially contained in Refs. 1 and 3, this paper does not include anything mathematically new; it clarifies the meaning of the consistency conditions, and concretely shows how the representation follows. This was not made before and completes a work made with the same philosophy on $SU(m/n)$.

2. $B(2, 2) = osp(5/4)$

The generators of $osp(5/4)$ can be represented as

$$\left(\begin{array}{c|c} sp(4) & (4, 5) \\ \hline (4, 5)^T & O(5) \end{array}\right),$$

i.e., in terms of the bosonic subalgebra $Sp(4)\times O(5)$, the adjoint representation of $osp(5/4)$ is $(10, 1)_{\text{even}} + (4,5)_{\text{odd}}$

[a)] Partially supported by the Swiss National Science Foundation.

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$+(1, 10)_{\text{even}}$. In the $SU(m/n)$ case (Ref. 4) it is possible to decompose the algebra into a Cartan subalgebra and positive and negative odd and even roots. The even positive/negative roots are those of $SU(m)\times SU(n)$. The odd positive/negative roots are in $(\bar{m}, n)/(m, \bar{n})$ of $SU(m)\times SU(n)$.

This construction has to be modified in the case of $osp(m/2n)$: The odd roots do not divide so naturally into positive and negative roots, since they belong to a real respresentation of $O(m)\times Sp(2n)$.

Embedded in $Sp(2n)$ there is a $U(n)$ regularly embedded such that $2n = n + \bar{n}$. The roots are ranged as positive or negative according to whether they belong to the (m, n) or $(m, \bar{n})$ of $O(m)\times U(n)$.

The system of roots of $osp(5/4)$ is made of two parts Δ_0 for the even roots and Δ_1 for the odd roots:

$$\Delta_0 = \{ \pm\epsilon_3;\ \pm\epsilon_3 \pm \epsilon_4;\ \pm\delta_1 \pm \delta_2;\ \pm 2\delta_1; 2\delta_2\},$$
$$\Delta_1 = \{ \pm\delta_1;\ \pm\delta_2;\ \pm\epsilon_3 \pm \delta_2;$$
$$\pm\epsilon_3 \pm \delta_1;\ \pm\epsilon_4 \pm \delta_2;\ \pm\epsilon_4 \pm \delta_1\}.$$

The system of roots we choose is as follows: The even roots $\delta_1 - \delta_2, \epsilon_5 - \epsilon_4, \epsilon_4$ and the roots $\delta_2 - \epsilon_3$. (The numbers we choose are not uncorrelated with the Dynkin diagram of $osp(5/4)$.

The even simple root of $Sp(4)$, $2\delta_2$, is hidden, and is not simple here since it corresponds to the linear combination of the simple roots: $2[(\delta_2 - \epsilon_3) + (\epsilon_3 - \epsilon_n) + \epsilon_n]$.

We make the distinction between positive and negative roots in terms of $SU(2)\times O(5)$, each set belonging to a (2, 5).

This leads to the new $SU(2)\times O(5)$ gradation of $osp(5/4)$:

$$G_{-2}(3, 1)_{\text{even}} + G_{-1}(2, 5)_{\text{odd}} + G_0[(3 + 1, 1) + (1, 10)]_{\text{even}} + G_1(2, 5)_{\text{odd}} + G_2(3, 1)_{\text{even}}.$$

G_{-2} and G_2 correspond to the generators of $Sp(4)/U(2)$.

To be able to build the representation we start from a highest weight, on which we will apply all the generators corresponding to the negative roots.

The "negative" odd generators necessary to build the representation will be defined the following way:

β_2^{2-} is the generator associated with the simple odd negative roots; it corresponds to the highest weight of the (2, 5) of $SU(2)\times O(5)$.

The other odd generator are defined in the following way:

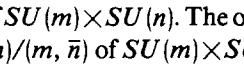
$$\beta_j^{1-} = [\beta_j^{2-}, \alpha_1^-]\ j = 2, 3, 4, \hat{4}, \hat{3}$$

and

$$\beta_3^{i-} = [\beta_2^{i-}, \alpha_3^-],\quad \beta_4^{i-} = [\beta_3^{i-}, \alpha_4^-],$$
$$\beta_{\hat{4}}^{i-} = [\beta_4^{i-}, \alpha_4^-],\quad \beta_{\hat{3}}^{i-} = [\beta_{\hat{4}}^{i-}, \alpha_3^-]; \tag{2.1}$$

their anticommuter vanishes only when it does not belong to G_{-2} or in other work is not in a (3, 1) of $SU(2)\times O(5)$.

The highest weight of an irreducible representation of $os(5/4)$ is characterized by four nonnegative integers a_1, b, a_3, a_4. (a_1, a_2, a_3, a_4) is associated with the simple roots (and corresponding to the projection of the highest weight on the corresponding simple roots).

a_1, a_3, and a_4 can be seen as characterizing a $SU(2)\times O(5)$ representation; any representations of $osp(5/4)$ can be expressed uniquely in terms of irreducible representations of $Sp(4)\times O(5)$. The highest weight corresponding to (a_1, a_2, a_3, a_4) is in the $Sp(4)\times O(5)$ representation corresponding to (), where $b = a_2 - a_3 - a_4/2$.

b is the projection on the simple roots $2\delta_2$ of $Sp(4)$ hidden by the odd simple roots. [The relation between the Cartan subalgebra of $Sp(4)\times O(5)$ and the Cartan subalgebra of $osp(5/4)$ will be given in the two next sections.]

The requirement that we are dealing with representations of $Sp(4)\times O(5)$ implies that b is a nonnegative integer (this is the first consistency condition).

In the case where $b = 0$ or 1 one requires in addition $a_2 = a_3 = a_4 = 0$ or $a_3 = a_4$, respectively.

The origin of these two additional requirements will appear more clearly when we look at explicit representations.

To get there we have still to remember that we are representing the algebra

$$[h_i, \alpha_j^{\pm}] = \pm a_{ij}\,\alpha_j^{\pm},$$
$$[\alpha_i^+, \alpha_j^-] = \delta_{ij}\,h_i, \tag{2.2}$$

where $i, j = 1, 2, 3, 4$; $\alpha_j^{\pm}$ are the generators corresponding to the simple roots and in this case the Cartan matrix reads

$$(a_{ij}) = \begin{pmatrix} 2 & -1 & & \\ -1 & 0 & +1 & \\ & -1 & 2 & -1 \\ & & -2 & 2 \end{pmatrix}. \tag{2.3}$$

It is useful to know that

$$\{\beta_j^{i+}, \beta_j^{i-}\} = N_{ij}\left(\sum_{t=i}^{2} h_t - n_3 h_3 - n_4 h_4/2\right). \tag{2.4}$$

n_3, n_4 are the number of times $\alpha_3^{\pm}$, $\alpha_4^{\pm}$ enter into the definition of $\beta_j^{i\pm}$ [cf. Eq. (2.1)], $i = 1, 2, j = 2, 3, 4$. $N_{i,j}$ is an overall factor depending on ij, which is in general easy to figure out and irrelevant for us.

An irreducible representation of $osp(5/4)$ is obtained by repeated application of the odd roots β_j^{i-} on the highest weight Λ characterized by (a_1, a_2, a_3, a_4).

The representation will be a sum of $O(5)\times Sp(4)$ representations; this is not trivial since the β_j^{i-} are in a (2, 5) of $SU(2)\times O(5)$ and not in a representation of $Sp(4)\times O(5)$.

Λ can be seen as a reducible representation of $SU(2)\times O(5)$ (characterized by a_1, a_3, a_4), all its irreducible components merging together to build up a $Sp(4)$ representation.

$\beta_j^{i-}\Lambda$ will be a reducible $SU(2)\times O(5)$ representation which will not merge in general into $Sp(4)$ representations; but this "floor" will get contributions from $\beta_{j_1}^{i_1-}\beta_{j_2}^{i_2-}\beta_{j_3}^{i_3-}\Lambda$. In effect the symmetric combinations of odd negative generators build up generators of $Sp(4)/U(2)$ belonging to the bosonic subalgebra. The antisymmetric combinations contribute to the third "floor" of the irreducible representation.

By this mechanism each floor of the representation gets an additional contribution from the product of more odd roots in the forms of additional $SU(2)\times O(5)$ representations. These new ones together with the other ones merge into $Sp(4)$ representation.

There is now the possibility that higher floors are decoupled as we will see; then the representation is called atypical.

In the case where the representation is called typical it is easy to figure out its dimensionality: it is $2^{10}\times$ multiplicity of the $Sp(4)\times O(5)$ representation of which $\tilde{\Lambda}$ is the highest weight.

$$\tilde{\Lambda} = (a_2; a_2 - \tfrac{5}{2}; a_3; a_4).$$

This comes from the fact that the representation is a sum of floors which are obtained from the lowest one by applying completely antisymmetric combinations of odd roots; the corresponding multiplicity is $\Sigma_{k=0}^{10}\binom{10}{k} = 2^{10}$.

Atypical representation: At each floor, there are well defined highest weights of a $O(5)\times SU(2)$; for example in the first floor it is $\beta_2^{2-}\Lambda$, in the second floor they are $\beta_3^{2-}\beta_2^{2-}\Lambda$ and $\beta_2^{1-}\beta_2^{2-}\Lambda$, etc. (One can verify that α_i^+ applied on these weights gives 0.)

If $\beta_2^{2+}\beta_2^{2-}\Lambda = h_2\Lambda = 0, \beta_2^{2-}\Lambda$ is disconnected from the total representation, and the $Sp(4)\times O(5)$ representation it belongs to is decoupled and the representation is "atypical." In the same way $\beta_3^{2-}\beta_2^{2-}\Lambda$ can be decoupled, $\beta_2^{2-}\Lambda$ being coupled, etc. The conditions of decoupling are easily worked out (cf. Sec. 4).

In this case they are

$$a_2 = 0,$$

$$a_2 = -(a_1 + 1),$$

which could never be fulfilled,

$$a_2 = (a_3 + 1),$$

$$a_2 = (a_3 + 1) - (a_1 + 1) = a_3 - a_1.$$

To know for which $Sp(4)\times O(5)$ representation all these weights are highest weights it is useful to notice that from (2.1), (2.2), and (2.3) one gets if,

$$\Lambda = (a_1, a_2, a_3, a_4; b = a_2 - a_3 - a_4/2),$$

then

$$\beta_2^{2-}\Lambda = (a_1 + 1, a_2, a_3 + 1, a_4; b - 1),$$

$$\beta_2^{1-}\Lambda = (a_1 - 1, a_2 + 1, a_3 + 1, a_4; b),$$

$$\beta_3^{2-}\Lambda = (a_1 + 1, a_2 - 1, a_3 - 1, a_4 + 2; b - 1),$$

$$\beta_3^{1-}\Lambda = (a_1 - 1, a_2, a_3 - 1, a_4 + 2; b),$$

$$\beta_4^{2-}\Lambda = (a_1 + 1, a_2 - 1, a_3, a_4; b - 1),$$

$$\beta_4^{1-}\Lambda = (a_1 - 1, a_2, a_3, a_4; b),$$

$$\beta_4^{2-}\Lambda = (a_1 + 1, a_2 - 1, a_3 + 1, a_4 - 2; b - 1),$$

$$\beta_4^{1}\Lambda = (a_1 - 1, a_2, a_3 + 1, a_4 - 2; b),$$

$$\beta_3^{2-}\Lambda = (a_1 + 1, a_2 - 2, a_3 - 1, a_4; b - 1),$$

$$\beta_3^{1-}\Lambda = (a_1 - 1, a_2 - 1, a_3 - 1, a_4; b).$$

The construction proceeds in the following way: Let $\Lambda = (a_1, a_2, a_3, a_4; b)$ be the highest weight of the $osp(5/4)$ representation.

$\beta_2^{2-}\Lambda = (a_1 + 1, a_2, a_3 + 1, a_4; b - 1)$ is the next $Sp(4)\times O(5)$ highest weight; it is coupled if $\beta_2^{2+}\beta_2^{2-}\Lambda = h_2\Lambda = a_2\Lambda \neq 0$ which corresponds to a condition of typicality.

$\beta_2^{2-}\Lambda$ can be part of the $osp(5/4)$ representation only if $b \geqslant 1$; if $b = 0, \beta_2^{2-}\Lambda$ had to decouple, so a_2 should be 0, which implies $a_3 = a_4 = 0$. So we get the first consistency condition.

At the next floor the two highest weights are

$$\beta_2^{1-}\beta_2^{2-}\Lambda = (a_1, a_2 + 1, a_3 + 2, a_4; b - 1)$$

[the typicality conditions associated with this weight are $a_2 \neq 0$, $a_2 \neq -a_1 - 1$ (the second is always fulfilled)] and

$$\beta_3^{2-}\beta_2^{2-}\Lambda = (a_1 + 2, a_2 - 1, a_3, a_4 + 2; b - 2)$$

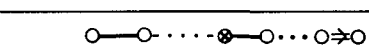
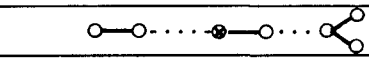
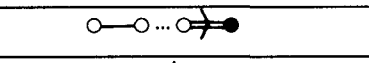
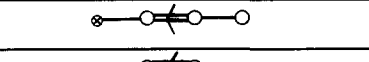
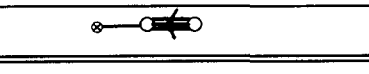
(the corresponding typicality conditions are $a_2 \neq 0$, $a_2 \neq a_3 + 1$).

If $b < 2$ this weight has to be decoupled. If that means $b = 0$, we know that implies $a_4 = a_3 = a_2 = 0$; if $b = 1$ that implies $a_2 = a_3 + 1$ and with $b = a_2 - a_3 - a_4/2$ that implies $a_4 = 0$. These are the next consistency conditions.

By applying progressively all the odd generators β_j^{i-}, that way, one can see what the whole representations can be made of.

Not belonging to the representation are all the $Sp(4)\times O(5)$ muliplets where a_1, a_3, a_4, and b are not element of Z^+. Let us look at a specific example. Let us take

TABLE I. The Class II superalgebras together with their Dynkin diagrams.

Superalgebras	Bosonic subalgebra	Odd generators	Dynkin diagram
$B(m, n) = osp(2m + 1/2n)$	$O(2m + 1)\times Sp(2n)$	$(2m + 1, 2n)$	
$D(m, n) = osp(2m/2n)$	$O(2m)\times Sp(2n)$	$(2m, 2n)$	
$D(2, 1, \alpha) = osp(4/2)_\alpha$	$SU(2)\times SU(2)\times SU(2)$	(2, 2, 2)	
$B(0, n) = osp(1/2n)$	$Sp(2n)$	$2n$	
$F(4)$	$SU(2)\times O(7)$	(2, 8)	
$G(3)$	$G_2\times SU(2)$	(7, 2)	

$\Lambda = (2, 0, 0, 0; 0)$; it is the highest weight of a (10, 1) of $Sp(4)\times O(5)$.

First floor: $\beta_2^{2-}\Lambda$ is decoupled because $a_2 = 0$. $\beta_3^{2-}\Lambda = (3, -1, -1, 2; -1)$ does not define a $Sp(4)\times O(5)$ highest weight, $\beta_2^{1-}\Lambda = (1, 1, 1, 0; 0)$ describes the highest weight of a (4, 5) of $Sp(4)\times O(5)$, and $\beta_4^{1-}\Lambda = (1, 0, 0, 0; 0)$ is not a highest weight but a weight of the (4, 5).

Second floor: $\beta_3^{1-}\beta_2^{1-}\Lambda = (0, 1, 0, 2; 0)$; it is not decoupled and is the highest weight of (1, 10) of $Sp(4)\times O(5)$. It is in fact the only $Sp(4)\times O(5)$ highest weight appearing in that floor.

It is impossible to get to a higher floor, a_1 or b would be negative.

So in summary, this atypical representation has the following $Sp(4)\times O(5)$ decomposition: (10, 1) + (4, 5) + (1, 10): it is the adjoint.

3. *osp*(*N*/2*m*)

In this section and the next we study the cases $N = 2m + 1$ and $N = 2m + 2$ with $m \geqslant 1$. We consider the special cases of $D(2, 1)$ and $B(0, m)$ in Sec. 5.

The root systems of $osp(2n + 1/2m)[B(n, m)]$ and $osp(2n/2m)[D(n, m)]$, respectively are, for $B(n, m)$,

$$\Delta_0 = \{ \pm\epsilon_i \pm \epsilon_j;\ \pm\epsilon_i;\ \pm 2\delta_l; \delta_k \pm \delta_l \},$$
$$\Delta_1 = \{ \pm\delta_k;\ \pm\epsilon_i \pm \delta_k \}, \tag{3.1}$$

and for $D(n, m)$,

$$\Delta_0\{ \pm\epsilon_i \pm \epsilon_j;\ \pm 2\delta_k;\ \pm\delta_k \pm \delta_l \},$$
$$\Delta_1 = \{ \pm\epsilon_i \pm \delta_k \}, \tag{3.2}$$

where

$$i \neq j = m + 1,...,m + n,$$
$$k \neq l = 1,...,m.$$

Δ_0 and Δ_1 correspond, respectively, to the even and odd roots.

We have already noticed in the previous section that it is possible to classify the odd generators [which are in an irreducible real representation $(N, 2m)$ of $O(N)\times Sp(2m)$] into "positive" and "negative" generators, respectively, in a (N, m) and $(N, \bar{m})$ representation of $O(N)\times SU(m)$; the $SU(m)$ being regularly embedded into $Sp(2m)$: $2m = m + \bar{m}$.

This leads to the following gradation of the $osp(N/2m)$ algebra in $SU(m)\times O(N)$:

$$G_{-2}(\overline{m(m+1)}/2, 1) + G_{-1}(\bar{m}, N) + G_0[(1, N(N-1))/2) + (1 + (m^2 - 1), 1)] + G_1(m, N) + G_2(m(m+1)/2, 1). \tag{3.3}$$

We choose the following system of simple roots: for $B(n, m)$,

$$\{\delta_1 - \delta_2; \delta_2 - \delta_3; ...; \delta_m - \epsilon_{m+1};$$
$$\epsilon_{m+1} - \epsilon_{m+2}; ...; \epsilon_{m+n}\},$$

for $D(n, m)$,

$$\{\delta_1 - \delta_2; \delta_2 - \delta_3; ...; \delta_m - \epsilon_{m+1}; \epsilon_{m+1} - \epsilon_{m+2}; ...; \epsilon_{m+n-1} \pm \epsilon_{m+n}\}.$$

These systems are directly connected to the Dynkin diagram shown in the Introduction. Following the same logic as in the previous section we are lead to specify the odd generators associated with the odd negative/positive generators.

Let β_m^{m-} be the generator associated to the simple odd root [it is a highest weight of a $(N, \bar{m})$ of $O(N)\times SU(m)$]: $\beta_m^{m-} \equiv \alpha_m^-$.

The other odd generators are defined in the following way:

$$\beta_{m+k}^{(m-j)-} = [\beta_{m+k}^{(m-j+1)-}, \alpha_{m-j}^-] = [\beta_{m+k-1}^{(m-j)-}, \alpha_{m+k}^-], \tag{3.4}$$
$$j = 1,...,m-1, \quad k = 1,...,n.$$

Furthermore, in the case $B(n, m)$, one has the following additional odd roots:

$$\tilde{\beta}_{n+m}^{(m-j)-} = [\beta_{n+m}^{(m-j)-}, \alpha_{n+m}^-], \tag{3.5}$$
$$\tilde{\beta}_{m+k}^{(m-j)-} = [\tilde{\beta}_{m+k+1}^{(m-j)-}, \alpha_{m+k}^-]. \tag{3.6}$$

In the case of $D(n, m)$,

$$\beta_{m+n}^{(m-j)-} = [\beta_{m+n-2}^{(m-j)-}, \alpha_{m+n}^-], \tag{3.7}$$
$$\beta_{m+n-1}^{(m-j)-} = [\beta_{m+n-2}^{(m-j)-}, \alpha_{m+n-1}^-], \tag{3.8}$$
$$\tilde{\beta}_{m+k}^{(m-j)-} = [\tilde{\beta}_{m+k+1}^{(m-j)-}, \alpha_{m+k}^-]. \tag{3.9}$$

In terms of the simple roots the algebra to be represented is

$$[\alpha_i^+ \alpha_j^-] = \delta_{ij} h_i, \quad i = 1,..., m-1, m+1, ...,m+n. \tag{3.10}$$
$$\{\beta_m^{m+}, \beta_m^{m-}\} = h_m, \tag{3.11}$$
$$[h_i, \alpha_j^\pm] = \pm a_{ij} \alpha_j^\pm \quad \forall i, j. \tag{3.12}$$

The elements a_{ij} of the Cartan matrix can be read off the Dynkin diagram as explained in the Introduction.

From this one can deduce

$$\{\beta_{m+k}^{(m-j)+}, \beta_{m+k}^{(m-j)-}\} = N_{jk}\left(\sum_{t=0}^{j} h_{m-t} - \sum_{t=1}^{k} h_{m+t}\right)$$
$$0 \leqslant j \leqslant m-1, \quad 0 \leqslant k \leqslant n. \tag{3.13}$$

N_{jk} is a factor irrelevant for us and in the case of $B(n, m)$,

$$\{\tilde{\beta}_{m+k}^{(m-j)+}, \tilde{\beta}_{m+k}^{(m-j)-}\} = N_{\tilde{j}k}\left(\sum_{t=0}^{j} h_{m-t} - \sum_{t=1}^{k} h_{m+t} - 2\sum_{t=k+1}^{n-1} h_{m+t} - h_{m+n}\right). \tag{3.14}$$

In the case of $D(n, m)$,

$$\{\beta_{m+n-1}^{(m-j)+}, \beta_{m+n-1}^{(m-j)-}\} = N_{jn}\left(\sum_{t=0}^{j} h_{m-t} - \sum_{t=1}^{n-1} h_{m+t}\right), \tag{3.15}$$

$$\{\beta_{m+n}^{(m-j)+}, \beta_{m+n}^{(m-j)-}\} = N_{\tilde{j}n-1}\left(\sum_{t=0}^{j} h_{m-t} - \sum_{t=1}^{n-2} h_{t+m} - h_{m+n}\right), \tag{3.16}$$

$$\{\tilde{\beta}^{(m-j)+}_{m+k}, \tilde{\beta}^{(m-j)-}_{m+k}\}$$
$$= N_{jk}\Big(\sum_{t=0}^{j} h_{m-t} - \sum_{t=1}^{k} h_{m+t} - 2\sum_{t=k+1}^{n-2} h_{m+t} - h_{m+n-1} - h_{m+n}\Big). \quad (3.17)$$

It is easy to connect the element k of the Cartan subalgebra of $Sp(2m)$, hidden in the Cartan subalgebra $\{h_i\}i = 1,...,m+n$ of the Lie superalgebra, using the relation between the corresponding roots.

In the case of $B(n, m)$ one gets

$$k = h_m - h_{m+1} - \cdots - h_{m+n-1} - \tfrac{1}{2}h_{m+n}. \quad (3.18)$$

In the case of $D(n, m)$,

$$k = h_m - h_{m+1} - \cdots - h_{m+h-2} - \tfrac{1}{2}(h_{m+n-1} + h_{m+n}). \quad (3.19)$$

4. REPRESENTATIONS OF $osp(N/2m)$

A. Typical representations

For the reasons stated in Sec. 2 the dimensions of a $osp(N/2m)$ typical irreducible representation is $2^{Nm}\times$ multiplicity of the $O(N)\times Sp(2m)$ representation to which belongs the highest $\tilde{\Lambda}$ of the $osp(N/2m)$ representation.

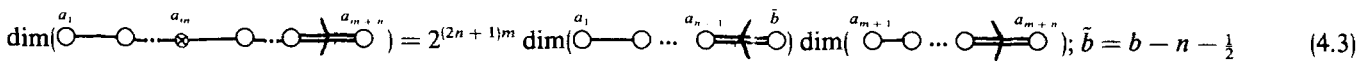
Given the nonnegative integers $(a_1,...,a_{m+n})$ characterizing the highest weight it is possible to figure out to which $Sp(2m)\times O(N)$ representation it belongs. $(a_{m+1},...,a_{m+n})$ characterizes the $O(N)$ representation; $(a_1,...,a_{m-1}, b)$ characterizes the $Sp(2m)$ representation.

b is related to a_i the same way as k is related to h_i in Eqs. (3.18) and (3.19), i.e., b is a nonnegative integer:

$$B(m, n): b = a_m - a_{m+1} - \cdots - a_{m+n-1} - \tfrac{1}{2}a_{m+n}, \quad (4.1)$$

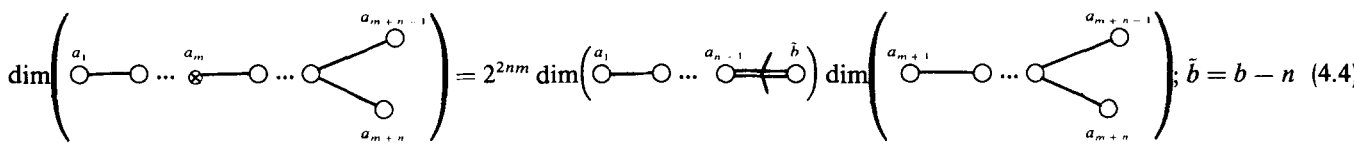
$$D(m, n): b = a_m - a_{m+1} - \cdots - a_{m+n-2} - \tfrac{1}{2}(a_{m+n-1} + a_{m+n}). \quad (4.2)$$

The dimension of a typical representation therefore corresponds to



(4.3)

for $B(n, m)$ and



(4.4)

for $D(n, m)$.

B. Atypical representations

In Sec. 2 we noticed that two kinds of mechanisms could make the dimensions of the irreducible representation smaller.

(1) Consistency requirements: All the possible $Sp(2m)\times O(N)$ highest weights which could appear, should be such highest weight, which means that the set of integers $(a_1,...,a_{m-1}, b, a_{m+1},...,a_{m+n})$ they correspond to have to be nonnegative. We have noticed in Sec. 2 that this was not always guaranteed.

This leads to consistency conditions we will come back to at the end of this section.

(2) Decouplings: We have also noticed in Sec. 2 that some $Sp(2m)\times O(N)$ highest weights appearing in higher floors could be decoupled from the $osp(N/2m)$ representation because it was impossible to get back from them to the rest of the $osp(N/2m)$ representation. This happens for some values of a_m.

In order to get the different $O(N)\times Sp(2m)$ higher-highest weights (i.e., the higher-highest weight at each floor) which make up the $osp(N/2m)$ representation, one has to apply antisymmetrically [the symmetrical combinations gives $Sp(2m)/U(m)$ generators] the odd generator β^{i-}_{j} in a certain order which can be uniquely figured out in each case by the requirement that the resulting weight is a highest weight, i.e., all the generators corresponding to positive even roots have to vanish when applied on it.

The antisymmetric product of β^{j-}_{i} is a polynomial T^{i-}_{k} of β^{j-}_{i}. The condition of decoupling are the zeros of $T^{l+}_{k}\, T^{l-}_{k}\Lambda$. In the case where

$$T^{l-}_{k} = [\, T^{(l+1)-}_{k}, \beta^{l-}_{k}\,] = [\, T^{l-}_{k-1}, \beta^{l-}_{k}\,], \quad (4.5)$$

it is possible to work the decoupling conditions in general by using exactly the same techniques as we did in Ref. 4.

The result is, for $B(n, m)$,

$$\sum_{t=0}^{j} a_{m-t} - \sum_{t=1}^{k} a_{m+t} + j - k = 0, \quad (4.6)$$

$$\sum_{t=0}^{j} a_{m-t} - \sum_{t=1}^{k} a_{m+t} - 2\sum_{t=k+1}^{n-1} a_{m+t} - a_{m+n} + k + j - 2n + 1 = 0. \quad (4.7)$$

In the case of $D(n, m)$,

$$\sum_{t=0}^{j} a_{m-t} - \sum_{t=1}^{k} a_{m+t} + j - k = 0, \quad (4.8)$$

$$\sum_{t=0}^{j} a_{m-t} - \sum_{t=1}^{n-2} a_{m+t} - a_{m+n} + j - n + 1 = 0, \quad (4.9)$$

$$\sum_{t=0}^{j} a_{m-t} - \sum_{t=1}^{k} a_{m+t} - 2\sum_{t=k+1}^{n-2} a_{m+t} - a_{m+n-1} - a_{m+n} + k + j - 2n = 0, \quad (4.10)$$

$$0 \leqslant j \leqslant m, \quad 0 \leqslant k \leqslant n-2.$$

We saw the decoupling condition at work in Sec. 2.

Since all the representations at each floor should correspond to $O(N)\times Sp(2m)$ representation, each highest weight

should correspond to a set of integers $(a_1,...,a_{m-1}, b, a_{m+1},...,a_{m+n})$, nonnegative.

Because of (4.1) and (4.2) that constrains the possible values of $a_m, a_{m+1},...,a_{m+n}$.

If $b < n$ consistency conditions appear analogous to the one we get in Sec. 2.

These conditions are

$$a_{m+b+1} = a_{m+b+2} = \cdots = a_{m+n} = 0$$

for $D(n, m)$; the case $b = n - 1$ is special [Eq. (4.10)],

$$a_{m+n-1} = a_{m+n}.$$

As we saw in Sec. 2 instead of applying blindly these results and conditions, in each specific case one should figure out explicitly the representation using the formulas of Sec. 3.

The formulas of this section give the decoupling only of the higher-highest weight at each floor; one has in addition to look at the lower-highest weights.

It is for this reason that in Appendix A we study another explicit example, $D(2, 3)$, and in Appendices B and C we study explicitly $F(4)$ and $G(3)$.

We finish this section by a somewhat cryptic remark which will become clearer in the next section when we study $B(0, n)$: an attentive reader will have noticed that there are fewer decoupling conditions in (4.6)–(4.10), than there are odd negative roots. Some odd generators do not lead to any decoupling. That is connected with the fact that the anticommutator of some odd generators build a $Sp(2m)/U(N)$ generator, i.e., contribute to the representation of the lower floor. It is essential that the corresponding decouplings do not take place to get at each floor a $Sp(2n)\times O(N)$ representation.

In Sec. 2 the odd generators which did not lead to any decoupling were β_4^{i-}.

5. SPECIAL TYPE II LIE SUPERALGEBRAS

In this section we study $B(0,n) = osp(1/2n)$ and $D(2, 1, \alpha)$.

A. $B(0/n) = osp(1/2n)$

The system of roots is

$$\Delta_0 = \{ \pm 2\delta_i;\ \pm\delta_i \pm \delta_j \},\quad i \neq j,\quad i,j = 1,...,n. \tag{5.1}$$
$$\Delta_1 = \{ \pm\delta_i \}.$$

The underlying bosonic subalgebra is $Sp(2n)$, and the odd generators are in a $2n$ of $Sp(2n)$ or a $(n + \bar{n})$ of $SU(n)$.

As simple roots we take

$$\{\delta_i - \delta_{i+1};\ \delta_n\}. \tag{5.2}$$

The Cartan matrix associated with the corresponding Dynkin diagram is the same as $O(2n + 1)$. This is probably connected to the fact that the representation of $B(0, n)$ has the same Casimirs to all orders as nonspinorial representations of $O(2n + 1)$ (Ref. 6).

The $SU(n)$ gradation of $osp(1/2n)$ is

$$G_{-2}(\bar{n}(\bar{n}+1)/2) + G_{-1}(\bar{n}) + G_0[(n^2-1)+1] + G_1(n) + G_2(n(n+1)/2). \tag{5.3}$$

By (5.1) or (5.3) one can see that no anticommutators of odd generators associated with negative (or positive) roots vanish; they all contribute to build $Sp(2n)/U(n)$ generators.

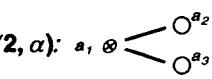
The clarification of the last remark of the last section that some readers are perhaps looking for, is a consequence of the observation we just made about the anticommutators of odd generators of $B(0, n)$.

In effect, as a result of that observation there is no decoupling conditions in $B(0, n)$ and all the representations of $B(0, n)$ are typical.

For the rest $B(0, n)$ is a simplified version of the cases we studied in the two previous sections. In particular the element k of the Cartan subalgebra of $Sp(2n)$ hidden in $osp(1/2n)$ is $k = \frac{1}{2}h_n$. So as a consistency condition one requires $b = \frac{1}{2}a_n$ to be a nonnegative integer.

The adjoint representation corresponds to $\Lambda = (a_1, a_2,...,a_n; b) = (1, 0,...; 0)$. The only other possible $Sp(2n)$ highest weight is $\beta_2^- \Lambda = (0, 1,...; 0)$.

$\Lambda + \beta_1^- \Lambda$ corresponds to $(2n)_{\text{odd}} + [n(2n+1)]_{\text{even}}$ $Sp(2n)$ irreducible representation.

B. $D(2, 1, \alpha) = osp(4/2, \alpha)$: $a_1 \otimes$ 

The root system is

$$\Delta_0 = \{ \pm 2\epsilon_i \},\quad \Delta_1 = \{ \pm\epsilon_1 \pm \epsilon_2 \pm \epsilon_3 \},\quad i = 1, 2, 3.$$

What is special about this superalgebra is that its Cartan matrix is

$$\begin{pmatrix} 0 & 1 & \alpha \\ -1 & 2 & 0 \\ -1 & 0 & 2 \end{pmatrix}. \tag{5.4}$$

This corresponds to one of the four possible systems of simple roots,

$$\{\epsilon_1 - \epsilon_2 - \epsilon_3;\ -2\epsilon_2;\ -2\epsilon_3\}.$$

The hidden even simple root is $-2\epsilon_1$. As a result the hidden element k of the Cartan subalgebra is related to h_1, h_2, h_3 by

$$k = [1/(1+\alpha)](2h_1 - h_2 - \alpha h_3), \tag{5.5}$$

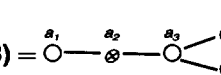
or the corresponding $SU(2)$ representation is characterized by

$$b = [1/(1+\alpha)](2a_1 - a_2 - \alpha a_3). \tag{5.6}$$

One requires b to be a nonnegative integer.

One has also to note the consistency conditions: $b = 0$ implies $a_i = 0$; $b = 1$ implies $a_3 + 1 = \pm(a_2 + 1)$. By using our techniques it is trivial to see that the representation $(a_1, a_2, a_3; b) = (1 + \alpha, 0, 0, 2)$ is the adjoint representation.

Let us finally notice that when $\alpha = 1$ this reduces to a special case of $D(n, m)$, and when $\alpha = -1$ the Cartan matrix becomes the one of $SU(2/2)$. The algebra is of Class I and [as can be seen from (5.5)] the representation is completely different; there is no more underlying $SU(2)$ and bosonic subalgebra becomes in fact $SU(2)\times SU(2)\times U(1)$.

APPENDIX A: $D(2, 3) =$  $= osp(6/4)$

The bosonic subalgebra is $Sp(4)\times O(6)$, the Cartan matrix is

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 \\ 0 & -1 & 2 & -1 & -1 \\ 0 & 0 & -1 & 2 & 0 \\ 0 & 0 & -1 & 0 & 2 \end{pmatrix},$$

and $b = a_2 - a_3 - \frac{1}{2}(a_4 + a_5)$ [Eq. (4.2)].

The generators corresponding to the odd negative roots are

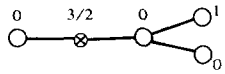
$$\beta_j^{i-}, \quad i = 1, 2, \quad j = 2, 3, 4, 5, \hat{4}, \hat{3}$$

As defined in Eqs. (3.4), (3.7), (3.8), and (3.9). They have the following effect:

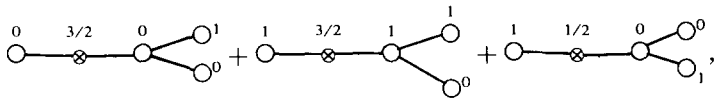
β_j^{i-} on $\Lambda = (a_1, a_2, a_3, a_4, a_5; b)$	$\{\beta_j^{i+}, \beta_j^{i-}\}$
$\beta_2^{2-}\Lambda = (a_1 + 1, a_2, a_3 + 1, a_4, a_5; b - 1)$	h_2
$\beta_3^{2-}\Lambda = (a_1 + 1, a_2 - 1, a_3 - 1, a_4 + 1, a_5 + 1, b - 1)$	$h_2 - h_3$
$\beta_4^{2-}\Lambda = (a_1 + 1, a_2 - 1, a_3, a_4 - 1, a_5 + 1, b - 1)$	$h_2 - h_3 - h_4$
$\beta_5^{2-}\Lambda = (a_1 + 1, a_2 - 1, a_3, a_4 + 1, a_5 - 1, b - 1)$	$h_2 - h_3 - h_5$
$\tilde{\beta}_4^{2-}\Lambda = (a_1 + 1, a_2 - 1, a_3 + 1, a_4 - 1, a_5 - 1, b - 1)$	$h_2 - h_3 - h_4 - h_5$
$\tilde{\beta}_3^{2-}\Lambda = (a_1 + 1, a_2 - 2, a_3 - 1, a_4, a_5, b - 1)$	$h_2 - 2h_3 - h_4 - h_5$

$$\beta_i^{1-}(a_1, a_2, a_3, a_4, a_5; b) = \beta_i^{2-}(a_1 - 2, a_2 + 1, a_3, a_4, a_5; b + 1)$$

(a) The adjoint representation corresponds to $(a_1,...,b) = (2, 0,...,0)$. Only $\beta_2^{1-}\Lambda$ and $\beta_3^{2-}\beta_2^{1-}\Lambda$ are coupled, so the $Sp(4)\times O(6)$ content of the representation is $(10, 1) + (4, 6) + (1, 15)$.

(b) The spinorial case: 

corresponds to the following representation:



i.e., in terms of $Sp(4)\times O(6)$ to $(5, 4) + (4, 20 + 4)$.

APPENDIX B: $F(4)$ = 

The adjoint is a $(21, 1) + (8, 2) + (1, 3)$ of $O(7)\times SU(2)$. The system of roots is

$$\Delta_0 = \{\pm\epsilon_i \pm \epsilon_j;\ \pm\epsilon_i;\ \pm\delta\}, \quad i, j = 2, 3, 4,$$

$$\Delta_1 = \{\tfrac{1}{2}(\pm\epsilon_2 \pm \epsilon_3 \pm \epsilon_4 \pm \delta)\}.$$

There are eight negative odd roots, the eight associated odd generators are β_1^- corresponding to the highest weights of the 8 of $O(7)$, $\beta_2^- = [\beta_1^{1-}, \alpha_2^-]$, $\beta_3^- = [\beta_2^-, \alpha_3^-]$, $\beta_4^- = [\beta_3^-, \alpha_4^-]$, $\beta_5^- = [\beta_3^-, \alpha_2^-]$, $\beta_6^- = [\beta_4^-, \alpha_2^-] = [\beta_5^-, \alpha_4^-]$, $\beta_7^- = [\beta_6^-, \alpha_3^-]$, $\beta_8^- = [\beta_7^-, \alpha_2^-]$. Modulo an irrelevant multiplicative factor the corresponding form of $\{\beta_i^+, \beta_i^-\}$ are

$$h_1;\ h_1 - h_2;\ h_1 - h_2 - 2h_3;$$

$$h_1 - h_2 - 2h_3 - 2h_4;\ h_1 - 2h_2 - 2h_3.$$

We have used the Cartan matrix

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 2 & -2 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix}.$$

The hidden element k of the Cartan algebra of $SU(2)$ is

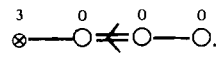
$$k = \tfrac{1}{3}(2h_1 - 3h_2 - 4h_3 - 2h_4),$$

the number b associated to k must be an integer.

The dimension of a typical representation is

$$2^8(b - 3)\dim\left(\overset{a_4}{\circ}\!\!-\!\!\overset{a_1}{\circ}\!\!\Rightarrow\!\!\overset{a_2}{\circ}\right).$$

As an example let us study the atypical representation



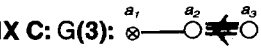
$\beta_2^-\beta_1^-\Lambda$ is a $(1, 21)$ of $SU(2)\times O(7)$. $\beta_3^-\beta_2^-\beta_1^-\Lambda$ is decoupled since

$$\beta_1^+\beta_2^+\beta_3^+\beta_3^-\beta_2^-\beta_1^-\Lambda = (h_1 - h_2 - 2h_3 - 3)(h_1 - h_2 - 1)h_1\Lambda = 0.$$

It is an atypical representation corresponding to the adjoint of $F(4)$.

Notice that the $(1, 21)$ could hide a $(1, 7)$, since we build in fact the antisymmetric product of two 8 of $O(7)$: $(8\times 8)_A = 21 + 7$.

The highest weight of the $(1, 7)$ which corresponds to $(1, 0, 0, 1; 0)$ does not appear.

APPENDIX C: G(3): 

The bosonic subgroup is $SU(2)\times G_2$; the system of roots is

$$\Delta_0 = \{\epsilon_i - \epsilon_j,\ \pm\epsilon_i,\ \pm 2\delta\}, \quad i = 1, 2, 3, \quad \epsilon_1 + \epsilon_2 + \epsilon_3 = 0.$$

$$\Delta_1 = \{\pm\epsilon_i \pm \delta,\ \pm\delta\},$$

The adjoint representation of $G(3)$ is a $(3, 1) + (2, 7) + (1, 14)$. There are seven odd negative and positive roots. The corresponding generators are taken as β_1^- corresponding to the highest weight of the $\underline{7}$ of G_2:

$$\beta_2^- = [\beta_1^-, \alpha_2^-], \quad \beta_3^- = [\beta_2^-, \alpha_3^-],$$
$$\beta_4^- = [\beta_3^-, \alpha_2^-], \quad \beta_5^- = [\beta_4^-, \alpha_2^-],$$
$$\beta_6^- = [\beta_5^-, \alpha_3^-], \quad \beta_7^- = [\beta_6^-, \alpha_2^-].$$

The corresponding forms of $\{\beta_i^+, \beta_i^-\}$ are h_1, $h_1 - h_2$, $h_1 - h_2 - 3h_3$, $h_1 - 2h_2 - 3h_3$, $h_1 - 3h_2 - 3h_3$, $h_1 - 3h_2 - 6h_3$, $h_1 - 4h_2 - 6h_3$. We have used the Cartan matrix

$$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 2 & -3 \\ 0 & -1 & 2 \end{pmatrix}.$$

The hidden element k of the Cartan subalgebra of $SU(2)$ is

$$k = \tfrac{1}{2}(h_1 - 2h_2 - 3h_3),$$

leading to the requirement that $b = \tfrac{1}{2}(a_1 - 2a_2 - 3a_3)$ be a nonnegative integer.

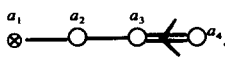
The adjoint representation corresponds to $(a_1, a_2, a_3) = (4, 0, 0) = \Lambda$. $\beta_1^-\Lambda$ is a $(2, 7)$ of $SU(2)\times G_2$, $\beta_2^-\beta_1^-\Lambda$ is a $(1, 14)$, and $\beta_3^-\beta_2^-\beta_1^-\Lambda$ is decoupled because

$$\beta_1^+\beta_2^+\beta_3^+\beta_3^-\beta_2^-\beta_1^-\Lambda = (h_1 - h_2 - 3h_3 - 4)(h_1 - h_2 - 1)h_1\Lambda = 0.$$

This is then an atypical representation. In fact no other $SU(2)\times G_2$ representation is coupled to that one.

APPENDIX D: $C(4)$

Though this corresponds to a type I superalgebra for the sake of completeness we look at this case corresponding to the following Dynkin diagram:

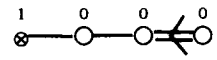


The bosonic subalgebra is $Sp(6)\times U(1)$.

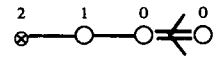
The positive and negative odd roots are in separate 6 of $Sp(6)$. There is no consistency condition and the conditions of typicality are

$$a_1 \neq 0, \quad a_1 \neq a_2 + 1, \quad a_1 \neq a_2 + a_3 + 2,$$
$$a_1 \neq a_2 + a_3 + 2a_4 + 4, \quad a_1 \neq a_2 + 2a_3 + 2a_4 + 5,$$
$$a_1 \neq 2a_2 + 2a_3 + 2a_4 + 6.$$

So, straightforwardly one gets



$= 1 + 6$ fundamental,



$= 6 + 21 + 1 + 6$ adjoint.

Note added in proof: An approach to the representation of superalgebra has been developed by Balantekin and Bars[7] using Young supertableaux. It is in close relation to the approach of Kac described here and in Ref. 4, as is shown in Ref. 8.

ACKNOWLEDGMENTS

We profited from the interest and help of the other members of our department in Geneva, in particular of Professor H. Ruegg and Professor P. Eckert.

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Reduction of tensor products with definite permutation symmetry: Embeddings of irreducible representations of Lie groups into fundamental representations of SU(*M*) and branchings

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(Received 26 March 1982; accepted for publication 30 June 1982)

We consider tensor products made out of a number of identical copies of the defining representations of Lie groups that are asymptotically free and complex. Decomposition of the tensor products into the terms with definite permutation symmetry is made by using the index sum rules and the congruence class. The results can also be used to find the branchings of SU(*M*) into a Lie group *G*, where *M* is equal to the dimension of the defining representation of *G*. Application of our results to preon dynamics is indicated in two examples.

PACS numbers: 02.20.Qs, 11.30.Pb, 11.10.Np, 11.50.Li

I. INTRODUCTION

Gauge theories are generally regarded as the theories of elementary particle interactions. In a gauge theory, whether it is a grand unified theory of "preon dynamics," one generally starts out with a certain nonabelian gauge group and writes down an invariant Lagrangian in terms of particle fields which transform as certain representations of the given gauge group. The fermion representations are usually required to satisfy additional conditions.[1] For instance, in many models the fermion representations should be complex[2] to prevent large masses for the known particles. Another requirement is that the representation should be free of triangle anomalies[3]; otherwise the theory will be unrenormalizable. The third condition often adopted is that the representations should be asymptotically free in the full gauge degree of freedom,[4] not just in the SU(3) color subgroup. Recently there have been efforts to obtain complete lists[5] of both irreducible and reducible representations that are complex, anomaly-free, and asymptotically free. We use these requirements only to get a natural limit on the representations considered in this paper.

Having chosen the representations under due conditions, one has to construct a gauge-invariant form of the Lagrangian. Here, one generally needs to know the properties of tensor products of the representations. Not only does one then need to specify how the tensor products can be computed, i.e., obtain the Clebsch–Gordan series, but also how they reduce to a direct sum of irreducible representations, each of which exhibits a definite permutation symmetry. The method of the decomposition[6] of the tensor product of n identical representations into the component with definite permutations property is called the algorithm of "plethysm."[7]

For example, consider a Yukawa coupling of the form $(f_L \otimes f_L)\phi$ in an SU(N) gauge theory, where f_L is the fermion field which belongs to the irreducible representation $\square$. We then have

$$f_L \otimes f_L = \square\!\square \oplus \begin{array}{l}\square\\\square\end{array} \oplus \square\!\!\square \,, \tag{1}$$

of which the first two terms are symmetric under interchange of f_L while the third term is antisymmetric with respect to the interchange of f_L. Hence if, for example, ϕ belongs to $\begin{array}{l}\square\!\square\\\square\end{array}$, then the corresponding Yukawa coupling must be antisymmetric under the interchange of other labels such as the family indices. The alluded permutation properties of each of the three components under the interchange of f_L can be understood as follows: Consider the fundamental representation $\square$ of SU(M), where M is equal to the dimension of the defining representation $\begin{array}{l}\square\\\square\end{array}$ in SU(N), i.e., the dimension of the fermion representation f_L. The group SU(M), in the fundamental representation, consists of all special unitary transformations of the M components of f_L; the SU(N) transformations on f_L form a subgroup, embedded in SU(M). This is referred to as nonregular embedding of SU(N) into SU(M) in this paper. The symmetric part of $(f_L \times f_L)$, i.e., the first and second terms of Eq. (1), corresponds to $\square\!\square$ in SU(M), whereas the third term of Eq. (1) corresponds to the antisymmetric representation $\begin{array}{l}\square\\\square\end{array}$ of SU(M). Such a method of decomposition with given permutation properties is what we call the algorithm of phethysm. Thus the computation of plethysm is equivalent to the direct computation of branching of SU(M)→SU(N).

In this paper, we present the computation of plethysm for the complex and asymptotically free representations of Lie groups SU(N) (type A_{N-1}), SO($4N+2$) (type D_{2N+1}), and E_6. The results of this paper have been applied to preon dynamics[8] for each of these groups with the correct Fermi statistics constraints and reported in a separate paper.[9] In particular, for SU(N) the results are given for the seven of

[a] Permanent address.

[b] Supported in part by the U. S. Department of Energy under Contract No. DE-AC02-76ER03130.A009-Task A.

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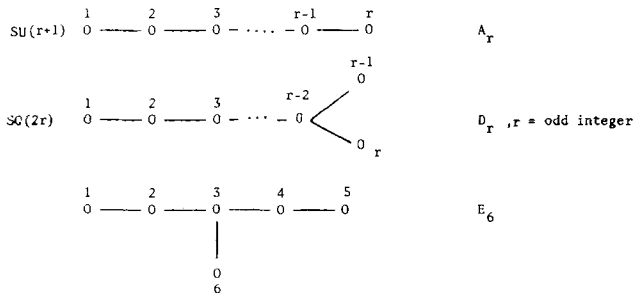

FIG. 1. Dynkin diagrams for simple Lie algebras admitting complex representations. The weight systems follow the corresponding numberings in $(a_1,a_2,\ldots,a_r)$.

nine irreducible, complex and asymptotically free representations[1]; for SO($4N+2$), the results are given for the lowest-dimensional spinor representations of D_5, D_7, and D_9 (note that D_3 is isomorphic to A_3); for E_6, we give the computation of plethysm for the fundamental representation $\underline{27}$. We have considered the direct products of at least two copies of the representation in all of these groups and in some cases the direct products up to ten copies of the representation. In fact, the recent suggestion[8] that the quarks and leptons are bound states of certain fundamental "preons" requires in general such computation of plethysm in conjunction with the requirement of Fermi statistics in the ground states.[10] Two examples showing the relevance of the results of this paper for preon dynamics will be discussed in Sec. IV. The computation of plethysm involving tensor products of several copies of the representations is also needed in tumbling gauge theories.[11]

The paper is organized as following: In Sec. II, we present the method of plethysm based on the index sum rules and congruence numbers. Section III contains the results of the decomposition of tensor products with definite permutation symmetry. The results can also be used to find the SU(M) branching into a Lie group G for the case of nonregular embedding of G into SU(M). Then we give two examples of application of our reuslts to preon dynamics in Sec. IV. Appendix A contains continuation of SU(N) indices to real N which allows us to use large values of N without the need to calculate large sums. Finally we present in Appendix B transposition rules for SU(N)-plethysm.

II. METHOD OF PLETHYSM COMPUTATION

In this section we describe the method of the decomposition of the tensor products into the components with definite permutation property. This involves two steps: The first step is to calculate the tensor products of some copies of representations, and the second step is to reduce the tensor products to a direct sum of components, each of which has definite permutation property.

There are several ways of handling these steps. For example, one may use the complete weight systems of the representation[12] to obtain the tensor products and find the highest weight terms successively. This method, however, is not only cumbersome when the dimension or rank is large but is not complete to identify the terms with definite permutation property. One may, on the other hand, use the method of the projection operators.[13] As the projection operator takes an irreducible representation of SU(M) into the representations of a group G directly, where M is the dimension of the defining representation of the fermion fields in G, the identification of the terms with given permutation properties are achieved automatically without recourse to the reduction of tensor products. But this method too becomes rapidly impractical as the dimension or rank becomes large.

The method we adopt in this paper is based on the properties of the zeroth, second, third, and fourth indices of representations as well as classification of the representations by congruence number. It is known that[14] the indices of the representations of Lie groups provide useful clues in the search of Clebsch–Gordan series as well as branching rules. In addition, the congruence number[15] reduces further the search problem by classifying the representations. Generally speaking, a representation and its complex conjugate do not have the same congruence number, thus the congruence class is useful in groups like D_{2N+1} and E_6, where the indices alone cannot distinguish a representation from its complex conjugate. Note that D_{2N+1} and E_6 are anomaly-free while in A_N the triangle anomaly, i.e., the third index, of a representation has opposite sign of that of the complex conjugate representation. It should be emphasized that the indices and congruence number satisfy certain elegant relationships that can be used easily even when the dimension of the representation or rank of the group becomes huge.

Now we proceed to introduce the indices of the representations of a semisimple Lie algebra. In general, the indices are defined differently depending on whether their order is even or odd.

The index of order $2m$ of a representation R is defined by

$$I_{2m}(R) = \sum_{M\in W(R)} (M,M)^m, \tag{2}$$

where $W(R)$ is the weight system of R and $m = 0,1,2,\ldots$. Though the indices of higher orders are known, we will use in this paper only up to the fourth index as these low-order indices can be computed simply[14] from the use of the highest weight of R. It should be obvious that $I_0(R)$ is the dimension of R as every weight contributes 1 to the sum (2). The third order index of R is defined[14] by

$$I_3(R) = a \sum_{M\in W(R)} (PM)^3, \tag{3}$$

where PM is the projection of the weight $W(R)$ on a properly chosen direction in weight space. The third order index I_3 is trivial, i.e., zero from the property of $W(R)$ for all Lie algebras except for SU(N) with $N\geqslant 3$. As noted before, I_3 for SU(N) is the triangle anomaly number. The normalization constant a of Eq. (3) can be fixed in such a way that $I_3 = 1$ for the fundamental representation of SU(N) ($N\geqslant 3$). The first index of any representation of any Lie group is zero and thus plays no useful rule. These indices can be used both to calculate tensor products and to determine branching rules.

To calculate the tensor product of the representations R and R' one has to determine the multiplicities l_i of representations R_i which appear as a direct sum:

$$R \otimes R' = \sum_{\oplus 1} l_i R_i. \tag{4}$$

The total indices of $R \otimes R'$ are related to the individual indices of R and R' in the following way[14]:

$$I_0(R \otimes R') = I_0(R) I_0(R'), \tag{5}$$

$$I_2(R \otimes R') = I_2(R) I_0(R') + I_2(R') I_0(R), \tag{6}$$

$$I_3(R \otimes R') = I_3(R) I_0(R') + I_3(R') I_0(R), \tag{7}$$

$$I_4(R \otimes R') = I_4(R) I_0(R') + I_4(R') I_0(R) + [2(r+2)/r] I_2(R) I_2(R'). \tag{8}$$

Here r is the rank of the Lie algebra. The total indices of the right-hand side of Eq. (4) are given by sums of individual indices of the representations R_i:

$$I_l(R \otimes R') = \sum_i l_i I_l(R_i) \quad (l = 0,2,3,4). \tag{9}$$

Combining Eqs. (5)–(9), one obtains four relations which will be referred to as the index sum rules for tensor products henceforth. These relations form four linear equations for the multiplicities l_i, which determine the l_i's completely if there is a unique integer solution. For sufficiently small representations (which turn out to be sufficiently large for all our purposes) there is only one source of ambiguity, the complex anomaly-free representations. Since the indices I_0, I_2, and I_4 are identical for R_i and R_i^*, they can only be distinguished by the I_3 relation, which for anomaly-free representations is identically zero. Since complex anomaly-free irreducible representations are extremely large in SU(N),[1] this problem occurs in practice only in the groups SO($4n+2$) and E_6. This ambiguity can easily be settled by means of the congruence class.[15]

The congruence class is the generalization of "N-ality" for SU(N) to any simple Lie algebra. All representations of a Lie algebra can be assigned to such a class. This class is identified by one or two numbers $C(R)$, defined modulo a certain integer n_c. For the details of this assignment we refer to Ref. 15. For our purpose, the important properties are the fact that complex conjugate representations have different congruence numbers and that each representation R_i in Eq. (4) has the same congruence number, related to the congruence classes of R and R' in the following way:

$$C(R_i) = C(R) + C(R') \pmod{n_c}. \tag{10}$$

This additional relation resolves the ambiguity.

Having determined the right-hand side of Eq. (4), we now have to identify terms with definite permutation properties. This problem is equivalent to finding the branching rules for SU(M) $\supset G$, when a representation D of G (hereafter referred to as the "defining representation") is embedded in the fundamental representation of SU(M). Of course, M must be equal to the dimension of D in G.

Irreducible representations of SU(M) can be specified by Young diagrams. On the other hand, Young diagrams also have an interpretation as representations of the permutation group. This dual interpretation is the basis of our results.

A representation R of SU(M), given by a Young diagram Y_m with m boxes, branches into a direct sum of representations of the subgroup G:

$$R \to \sum_{\oplus j} l_j R_j, \tag{11}$$

where the l_j's are integer multiplicities. The permutation group interpretation tells us that the left-hand side of Eq. (11) corresponds to those terms in the mth tensor power of D which have symmetry properties given by Y_m. To determine the multiplicities, we use the SU(M) interpretation of (11). The branching is governed by the following index sum rules[9,14]:

$$I_0(R) = \sum_j l_j I_0(R_j), \tag{12}$$

$$I_2(R) = \rho_2 \sum_j l_j I_2(R_j), \tag{13}$$

$$I_3(R) = \rho_3 \sum_j l_j I_3(R_j). \tag{14}$$

The scale factors ρ_2 and ρ_3 are only dependent on the way the subgroup is embedded in SU(M). We emphasize that they do not depend on R. Therefore, we can calculate them by choosing R equal to the fundamental representation of SU(M), which branches to the representation D of G:

$$\rho_2^{-1} = I_2(D), \tag{15}$$

$$\rho_3^{-1} = I_3(D). \tag{16}$$

Here we have used the standard normalization, $I_2 = I_3 = 1$ for the fundamental representation of SU(M). A relation similar to (13) and (14) for I_4 holds only for a few special cases and cannot be applied to SU(M) branchings.[14] Notice that relation (14) is only nontrivial for SU(N).

The tensor product is used only to limit the number of representations R_j on the right-hand side of Eq. (11). The most effective way of doing this is to use recursion in the number of boxes m of Y_m. When the results for all Young diagrams Y_{m-1} are known, one can multiply each of them with D and use relations (12)–(14) to decompose the tensor product into the terms with permutation properties defined by m-box Young diagrams. With this procedure the direct sums belonging to all m-box Young diagrams, with the exception of totally symmetric and totally antisymmetric ones, are determined several times, which can be used either as a consistency check or as additional information to rule out possible ambiguities which might arise from Eqs. (12)–(14) alone. In practice we did not encounter any persistent ambiguities.

In the special case $G = $ SU(N) the procedure can be made much more effective in the following way. The results we are calculating can be expressed entirely in terms of SU(N)-tensors, without any reference to the rank of the group. Therefore all branchings can be generalized to arbitrary N, with the understanding that Young diagrams with more than N rows should be ignored. Thus one can use the index relations with arbitrary N. For an n-box Young diagram the formula for I_0 is an nth order polynomial in N, and those for I_2 and I_3 have order $n-1$. Therefore, if n and m are the number of boxes of SU(N) and SU(M) diagrams, one gets roughly $3nm$ equations for the multiplicities from Eqs. (12)–(14), a few of which turn out to be dependent. Since the number of terms in the tensor product grows faster than the num-

ber of equations with increasing n or m, this method has its limitations. In general, even with the help of a computer, it turned out to be very hard to go beyond $nm = 12$.

In Appendix A we derive formulas for the indices which proved to be very useful for our calculations, since they are continuous in the rank of the group. This allowed us to exploit the N independence property of the index sum rules more effectively. In Appendix B we derive rules which relate the plethysms for a Young diagram Y_n of SU(N) to those for the transposed Young diagram.

III. RESULTS

Generally grand unified theories and preon dynamics require fermion representations which are anomaly-free, complex, and asymptotically free. A complete list of these representations has already been compiled. In SU(N), there is no complex irreducible representation that satisfies the requirement of both anomaly freedom and asymptotic freedom.[1] Thus one considers the reducible complex representations formed out of the anomaly-free combinations of the irreducible complex representations which are asymptotically free. It has been shown that there are nine such irreducible representations in SU(N). Of all the representations of Lie algebras, the only complex irreducible representations which are both anomaly-free and asymptotic free, are the following: the 16-, 126-, 144-dimensional representation of SO(10); the lowest dimensional spinorial representations of SO(14) and SO(18); and the 27-dimensional representation of E_6.

Now we proceed to present the results of computations of plethysm for the seven asymptotically free and complex representations $[1^4]$, $[2^2]$, $[1^3]$, $[2,1]$, $[2,1^2]$, $[2]$, and $[1^2]$ of SU(N) (see the notation for the Young diagrams below), the five irreducible representations of SO($4N + 2$) mentioned above, and the lowest dimensional representation of E_6.

A. SU(N)

Since irreducible representations for an SU(N) can be represented by simple Young diagrams, the use of the Young diagrams is convenient. We will denote a typical Young diagram that has a boxes in each of the first n rows followed by b boxes in each of the next m rows and so on by $[a^n,b^m,\cdots]$. These Young diagrams are used for both the defining representations of SU(N) and the representations of SU(M), being the dimension of the defining representation.

Table I shows the terms up to the tensor product of 12 copies with the definite permutation properties under the interchange of defining representations [2] and $[1^2]$ of SU(N). In other words, the results contained in Table I correspond to Young diagrams of SU(M) having up to ten boxes. Table II summarizes the results for the four representations $[1^4]$, $[2^2]$, $[1^3]$, and $[2,1]$ of SU(N) up to three boxes in the SU(M) Young diagrams.

B. SO($4N + 2$)

Table III gives the results for the spinorial representation of SO(10) up to five boxes in the SU(16) Young diagrams. Tables IV and V contain the results for the spinorial representations of SO(14) and SO(18) up to four and two boxes in the SU(M) Young diagram, respectively. The results for the 126- and 144-dimensional representations of SO(10) are summarized in Table VI up to three boxes.

C. E_6

Table VII summarizes the results up to six boxes. As we mentioned before, the 27-dimensional representation is the only E_6 representation which satisfies asymptotic freedom.

IV. APPLICATION OF THE RESULTS TO PREON DYNAMICS

The results of this paper can be applied to preon dynamics in which quarks and leptons are viewed as the bound states of the elementary preons. Here, we give two such examples.[9]

A. $(5 + 10^*)_L$ of SU(5) metacolor group as the preon representation

The SU(5) representation $(5 + 10^*)_L$ is anomaly-free, where L denotes the left-handed chiral state. In order for the preons to be confined, the preon representations should satisfy asymptotic freedom. The anomaly-free representation can then be repeated up to 13 times without losing asymptotic freedom. Suppose that we allow the representation $5 + 10^*$ to repeat N times, where N is an integer less than 14. Such repetition then introduces the metaflavor group $U(N)\times U(N)$, which is broken to $SU(N)\times SU(N)\times U(1)$, taking into account the instanton effects due to the metacolor group SU(5).

Let us denote the metacolor representation as

$$(5 + 10^*)_L = \alpha + \beta. \tag{17}$$

The transformation properties of α and β under metacolor group SU(5) and metaflavor group $SU(N)\times SU(N)\times U(1)$ as well as the spin group $SU_L(2)\times SU_R(2)$ are summarized as follows:

	SU(5)	SU(N)	SU(N)	U(1)	$SU_L(2)$	$SU_R(2)$	5-ality
α	$\square$	$\square$	·	Q_1	$\square$	·	1
β	$\begin{array}{l}\square\\[-4pt]\square\end{array}$	·	$\square$	Q_2	$\square$	·	3
$\bar{\alpha}$	$\bar{\square}$	$\bar{\square}$	·	$-Q_1$	·	$\square$	4
$\bar{\beta}$	$\begin{array}{l}\square\\[-4pt]\square\end{array}$	·	$\bar{\square}$	$-Q_2$	·	$\square$	2

TABLE I. The reduction of tensor products of up to six copies of [2] and $[1^2]$ of SU(N) with the symmetry of the Young diagram given in the first column. Symmetric products are given for up to eight copies of the defining representation, antisymmetric products for up to twelve copies. The table can also be used to obtain the branching of SU(M) into the representation of SU(N), when the defining representation of SU(N) is embedded in the fundamental representation of SU(M); M is the dimension of the defining representation of SU(N). For [2] and $[1^2]$, M is $N(N+1)/2$ and $N(N-1)/2$ respectively.

SU(M)	Defining Representations of SU(N)		
[1]	[2]	$[1^2]$	
[2]	[4] $[2^2]$	$[2^2]$ $[1^4]$	
$[1^2]$	[3,1]	$[2,1^2]$	
[3]	[6] [4,2] $[2^3]$	$[3^2]$ $[2^2,1^2]$ $[1^6]$	
[2,1]	[5,1] [4,2] [3,2,1]	[3,2,1] $[2^2,1^2]$ $[2,1^4]$	
$[1^3]$	$[3^2]$ $[4,1^2]$	$[3,1^3]$ $[2^3]$	
[4]	[8] [6,2] [4,4]	$[4,2^2]$ $[2^4]$	$[4^2]$ $[3^2,1^2]$ $[2^4]$ $[2^2,1^4]$ $[1^8]$
[3,1]	[7,1] [6,2] [5,3] [5,2,1]	[4,3,1] $[4,2^2]$ $[3,2^2,1]$	[4,3,1] $[3^2,1^2]$ $[3,2^2,1]$ $[3,2,1^3]$ $[2^3,1^2]$ $[2^2,1^4]$ $[2,1^6]$
$[2^2]$	[6,2] [5,2,1] $[4^2]$	$[4,2^2]$ $[3^2,1^2]$	$[4,2^2]$ $[3^2,1^2]$ $[3,2,1^3]$ $[2^4]$ $[2^2,1^4]$
$[2,1^2]$	[5,3] $[6,1^2]$ [5,2,1]	[4,3,1] $[3^2,2]$ $[4,2,1^2]$	$[4,2,1^2]$ $[3^2,2]$ $[3,2^2,1]$ $[3,2,1^3]$ $[2^3,1^2]$ $[3,1^5]$
$[1^4]$	[4,3,1] $[5,1^3]$		$[4,1^4]$ $[3,2^2,1]$
[5]	[10] [8,2] [6,4] $[6,2^2]$	$[4^2,2]$ $[4,2^3]$ $[2^5]$	$[5^2]$ $[4^2,1^2]$ $[3^2,2^2]$ $[3^2,1^4]$ $[2^4,1^2]$ $[2^2,1^6]$ $[1^{10}]$
[4,1]	[5,4,1] [5,3,2] $[5,2^2,1]$ $[4^2,2]$ [4,3,2,1] $[4,2,1^3]$ $[3^2,2^2]$	[9,1] [8,2] [7,3] [7,2,1] [6,4] [6,3,1] [6,2,2]	[5,4,1] $[4^2,1^2]$ [4,3,2,1] $[4,3,1^3]$ $[3^2,2^2]$ $[3^2,2,1^2]$ $[3^2,1^4]$ $[3,2^3,1]$ $[3,2^2,1^3]$ $[3,2,1^5]$ $[2^4,1^2]$ $[2^3,1^4]$ $[2^2,1^6]$ $[2,1^8]$
[3,2]	[8,2] [7,3] [6,4] [7,2,1] [6,3,1] 2 x [6,2²] [5,4,1]	[5,3,2] $[5,3,1^2]$ $[5,2^2,1]$ $[4^2,2]$ [4,3,2,1] $[4,2^3]$ $[3^2,2,1^2]$	$[4^2,1^2]$ [4,3,2,1] $[4,3,1^3]$ $[3^2,2^2]$ 2 x $[3^2,1^4]$ [5,3,2] $[4,2^2,1^2]$ $[3,2^3,1]$ $[3,2^2,1^3]$ $[3,2,1^5]$ $[2^4,1^2]$ $[2^3,1^4]$ $[2^2,1^6]$
$[3,1^2]$	[7,3] $[8,1^2]$ [7,2,1] 2 x [6,3,1] $[5^2]$ [5,4,1] 2 x [5,3,2] $[6,2,1^2]$	$[5,3,1^2]$ $[5,2^2,1]$ $[4,3^2]$ $[4^2,1^2]$ [4,3,2,1] $[3^2,2^2]$ $[4,2^2,1^2]$	$[5,3,1^2]$ $[4^2,2]$ [4,3,2,1] $[4,3,1^3]$ 2 x $[3^2,2,1^2]$ $[4,2^3]$ $[4,2^2,1^2]$ $[3^3,1]$ $[3,2^3,1]$ 2 x $[3^2,2^2,1^3]$ $[4,2,1^4]$ $[2^5]$ $[3,2^2,1^3]$ $[3,1^7]$
$[2^2,1]$	[6,4] [7,2,1] [6,3,1] $[6,2^2]$ [5,4,1] [5,3,2] $[6,2,1^2]$	$[5,3,1^2]$ $[5,2^2,1]$ $[4^2,2]$ [4,3,2,1] $[3^3,1]$ $[4,3,1^3]$	$[5,2^2,1]$ $[4,3^2]$ [4,3,2,1] $[4,2^2,1^2]$ $[4,3,1^3]$ $[3^2,2^2]$ $[3^2,2,1^2]$ $[3^2,1^4]$ $[4,2,1^4]$ $[3,2^3,1]$ $[3,2^2,1^3]$ $[3,2,1^5]$ $[2^4,1^2]$

SU(M)	SU(N)			
$[2,1^3]$	[6,3,1] [5,4,1] [5,3,2] [7,1³] [6,2,1²]	[5,3,1²] [4,3²] [4²,1²] [4,3,2,1] [5,2,1³]	[5,2,1³] [4,3,2,1] [4,2³] [4,2²,1²] [4,2,1⁴]	[3³,1] [3²,2,1²] [3,2³,1] [3,2²,1³] [3,1⁶]
$[1^5]$	[4²,2] [5,3,1²]	[6,1⁶]	[5,1⁵] [4,2²,1²]	[3²,2³]
[6]	[12] [10,2] [8,4] [8,2²] [6²] [6,4,2]	[6,2³] [4³] [4²,2²] [4,2⁴] [2⁶]	[6²] [5²,1²] [4²,2²] [4²,1⁴] [3⁴] [3²,2²,1²]	[5²,1⁶] [2⁶] [2⁴,1⁴] [2²,1⁸] [1¹²]
[5,1]	[11,1] [10,2] [9,3] [9,2,1] [8,4] [8,3,1] [8,2²] [7,5] [7,4,1] [7,3,2] [7,2²,1] [6,5,1]	2 x [6,4,2] [6,3,2,1] [6,2³] [5,4,3] [5,4,2,1] [5,3,2²] [5,2³,1] [4²,3,1] [4²,2²,1] [4,3,2²,1] [4,2⁴] [3,2⁴,1]	[2,1¹⁰] [2²,1⁸] [2³,1⁶] [3,2,1⁷] [2⁴,1⁴] [3,2²,1⁵] [3²,1⁶] [2⁵,1²] [3,2³,1³] [3²,2,1⁴] [4,3,1⁵] [3,2⁴,1]	2 x [3²,2²,1²] [4,3,2,1³] [4²,1⁴] [3³,2,1] [4,3,2²,1] [4²,2,1³] [5,4,1³] [4,3²,2] [4²,2²] [5,4,2,1] [5²,1²] [6,5,1]
[4,2]	[10,2] [9,3] 2 x [8,4] [9,2,1] [8,3,1] 2 x [8,2²] 2 x [7,4,1] 2 x [7,3,2] [6²] [6,5,1] 3 x [6,4,2] [7,3,1²] [7,2²,1] 2 x [6,3,2,1]	2 x [6,2³] [5,4,3] [5³,1²] 2 x [5,4,2,1] [5,3²,1] [5,3,2²] [5,3,2,1²] [5,2³,1] [4³] 2 x [4²,2²] [4,3²,1²] [4,3²,2,1] [4,2⁴] [3²,2²,1²]	[5²,1²] [5,4,2,1] [5,4,1³] 2 x [4²,2²] [4²,2,1²] 2 x [4²,1⁴] [5,3²,1] [5,3,2,1²] [4,3²,1²] 2 x [4,3,2²,1] 2 x [4,3,2,1³] [4,3,1⁵] [3³] [3³,2,1]	3 x [3²,2²,1²] 2 x [3²,2,1⁴] 2 x [3²,1⁶] [6,4,2] [4,3⁴] [4,2²,1⁴] [3,2⁴,1] 2 x [3,2³,1³] [3,2²,1⁵] [3,2,1⁷] [2⁶] 2 x [2⁴,1⁴] [2³,1⁶] [2²,1⁸]
$[4,1^2]$	[9,3] $[10,1^2]$ [9,2,1] 2 x [8,3,1] [7,5] 2 x [7,4,1] 2 x [7,3,2] [8,2,1²] [7,3,1²] [7,2²,1] [6,5,1] [6,4,2] 2 x [6,3²] 2 x [6,4,1²] 2 x [6,3,2,1]	2 x [5³,2] [5,4,3] 2 x [5,4,2,1] [5,3²,1] 2 x [5,3,2²] [6,2²,1²] [5,3,2,1²] [5,2³,1] [4²,3,1] [4,3²,2] [4²,2,1²] [4,3,2²,1] [3³,1³]	[6,4,1²] [5³,2] [5,4,2,1] [5,4,1³] 2 x [4²,2,1²] [5,3,2²] [5,3,2,1²] [4²,3,1] [4,3²,2] [4,3²,1²] 2 x [4,3,2²,1] 2 x [4,3,2,1³] [5,3,1⁴] [4,3,1⁵] [3³,2,1]	[3⁴,2²,1²] 2 x [3³,1³] 2 x [3²,2³] 2 x [3²,2,1⁴] 2 x [4,2³,1²] [3,2³,1³] [4,2²,1⁴] 2 x [3,2²,1⁵] [4,2,1⁶] [3,2,1⁷] [2⁵,1²] [2³,1⁶] [3,1⁸]
$[3^2]$	[9,3] [8,3,1] [8,2²] [7,5] [7,4,1] [7,3,2] [7,2²,1] [6,4,2] [6,3²] [6,4,1²]	[6,3,2,1] [6,2³] [5²,2] [5,4,2,1] [5,3,2²] [4²,3,1] [5,3,2,1²] [4,3,2²,1] [3³,1³]	[5,4,2,1] [4²,2,1²] [4²,1⁴] [6,3²] [5,3,2,1²] [4,3²,2] [4,3,2²,1] [4,3,2,1³] [4,3,1⁴] [3²,2²,1²]	[3³,1³] [3²,2³] [3²,2,1⁴] [3²,1⁶] [4,2³,1²] [3,2³,1³] [3,2²,1⁵] [2⁵,1²] [2³,1⁶]
[3,2,1]	[4,3,2,1³] [3³,2,1] [4,3,2²,1] [4,3²,1²] 2 x [5,3,2,1²] [5,2³,1] [4²,2²]	2 x [5,3,2²] [6,2³] [4²,2,1²] [4,3²,2] [4²,3,1] 2 x [5,3²,1] 3 x [5,4,2,1]	[6,3,2,1] [5,4,3] [5,4,2,1] [5,3²,1] 2 x [5,3,2,1²] [5,4,1³] [4²,2²]	2 x [4²,2,1²] [4²,1⁴] [5,3,2²] [4²,3,1] [4,3²,2] 2 x [4,3²,1²] 3 x [4,3,2²,1]

TABLE I. (*continued*)

SU(M)	SU(N)			
	4 x [6,3,2,1] [6,2²,1²] 2 x [7,2²,1] 2 x [5,4,3] 3 x [6,4,2] [6,3²] [5²,2] 3 x [7,3,2] [8,2²] [5,4,1³] [6,3,1³]	[5²,1²] 2 x [6,4,1²] 2 x [7,3,1²] 2 x [6,5,1] 2 x [7,4,1] 2 x [8,3,1] [8,2,1²] [9,2,1] [7,5] [8,4]	4 x [4,3,2,1³] [5,3,1⁴] 2 x [4,3,1⁵] 2 x [3³,2,1] 3 x [3²,2²,1²] [3³,1³] [3²,2³] 3 x [3²,2,1⁴] [3²,1⁶] [5,2³,1] [5,2²,1³]	[4,2⁴] 2 x [4,2³,1²] 2 x [4,2²,1⁴] 2 x [3,2⁴,1] 2 x [3,2³,1³] 2 x [3,2²,1⁵] [4,2,1⁶] [3,2,1⁷] [2⁵,1²] [2⁴,1⁴]
[3,1³]	[8,3,1] [7,4,1] [7,3,2] [9,1³] [8,2,1²] 2 x [7,3,1²] [6,5,1] [6,4,2] 2 x [6,3²] 2 x [6,4,1²] 2 x [6,3,2,1] [5²,2] [5,4,3] [5²,1²]	2 x [5,4,2,1] 2 x [5,3²,1] [5,3,2²] [7,2,1³] [6,3,1³] [6,2²,1²] [5,4,1³] [5,3,2,1²] [4²,3,1] [4,3²,2] [4²,2,1²] [4,3,2²,1] [5,2²,1³]	[6,3,1³] [5,4,2,1] [5,3,2²] [5,3,2,1²] [5,3,1⁴] [4²,3,1] [4²,2,1²] [4,3²,2] 2 x [4,3²,1²] 2 x [4,3,2²,1] 2 x [4,3,2,1³] [3³,2,1] 2 x [3³,1³] [3²,2³]	[3²,2²,1²] [3²,2,1⁴] [5,2³,1] 2 x [4,2³,1²] [5,2²,1³] [4,2⁴] 2 x [4,2²,1⁴] [3,2⁴,1] [3,2³,1³] [3,2²,1⁵] [5,2,1⁵] [4,2,1⁶] [4,1⁸]
[2³]	[4²,2²] [6,2³] [4,3²,1²] [5,3,2,1²] [5,3²,1] [5,4,2,1] [6,3,2,1] [7,2²,1] [4³]	2 x [6,4,2] [8,2²] [4²,1⁴] [6,3,1³] [3⁴] [5²,1²] [7,3,1²] [7,4,1] [6²]	[4²,2²] [4²,1⁴] [5,3²,1] [5,3,2,1²] [4,3²,1²] [4,3,2²,1] [4,3,2,1³] [4,3,1⁵] [3⁴]	2 x [3²,2²,1²] [3²,1⁶] [6,2³] [5,2²,1³] [4³] [4,2⁴] [4,2²,1⁴] [3,2³,1³] [2⁶]
[2²,1²]	[7,4,1] [6,5,1] [6,4,2] [7,3,2] [8,2,1²] [7,3,1²] [7,2²,1] [6,3²] 2 x [6,4,1²] 2 x [6,3,2,1] [5²,2] [5,4,3] 2 x [5,4,2,1]	[5,3²,1] [5,3,2²] [7,2,1³] [6,3,1³] [6,2²,1²] [5,4,1³] [5,3,2,1²] [4²,3,1] [4,3²,2] [4²,2,1²] [4,3²,1²] [5,3,1⁴]	[3,2³,1³] [3,2⁴,1] [3²,2²,1²] [3²,2,1⁴] [4,2,1⁶] [4,2²,1⁴] [4,3,1⁵] [3³,1³] 2 x [4,2³,1²] 2 x [4,3,2,1³] [3²,2³] [3³,2,1] 2 x [4,3,2²,1]	[4,3²,1²] [4²,2,1²] [5,2,1⁵] [5,2²,1³] [5,3,1⁴] [5,2³,1] [5,3,2,1²] [4,3²,2] [4²,3,1] [5,3,2²] [5,3²,1] [6,2²,1²]
[2,1⁴]	[6,4,2] [7,3,1²] [6,4,1²] [6,3,2,1] [5,4,3] [5²,1²] [5,4,2,1] [5,3²,1]	[8,1⁴] [7,2,1³] [6,3,1³] [5,4,1³] [5,3,2,1²] [4²,3,1] [4²,2²] [6,2,1⁴]	[6,2,1⁴] [5,3,2,1²] [5,2³,1] [5,2²1³] [5,2,1⁵] [4²,2²] [4,3²,2] [4,3²,1²]	[4,3,2²,1] [4,3,2,1³] [4,2³,1²] [4,2²,1⁴] [3³,2,1] [3²,2²,1²] [5,1⁷]

SU(M)	SU(N)			
[1⁶]	[4³] [5,4,2,1]	[6,3,1³] [7,1⁵]	[6,1⁶] [5,2²,1³]	[4,3,2²,1] [3⁴]
[7]	[14] [12,2] [10,4] [10,2²] [8,6] [8,4,2] [8,2³] [6²,2]	[6,4²] [6,4,2²] [6,2⁴] [4³,2] [4²,2³] [4,2⁵] [2⁷]	[7²] [6²,1²] [5²,2²] [5²,1⁴] [4²,3²] [4²,2²,1²] [4²,1⁶] [3⁴,1²]	[5²,2⁴] [5²,2²,1⁴] [3²,1⁸] [2⁶,1²] [2⁴,1⁶] [2²,1¹⁰] [1¹⁴]
[1⁷]	[5,4²,1] [5²,2²] [6,4,2,1²]	[7,3,1⁴] [8,1⁶]	[7,1⁷] [6,2²,1⁴] [5,3,2²,1²]	[4²,2³] [4,3³,1]
[8]	[2⁸] [4,2⁶] [4,2⁴] [1⁶,2⁵] [4³,2²] [6,4,2³] [8,2⁴] [4⁴] [6,4²,2] [6²,2²] [8,4,2²]	[10,2³] [6²,4] [8,4²] [8,6,2] [10,4,2] [12,2²] [8²] [10,6] [12,4] [14,2] [16]	[8²] [7²,1²] [6²,2²] [6²,1⁴] [5²,3²] [5²,2²,1²] [5²,1⁶] [4⁴] [4²,3²,1²] [4²,2⁴] [4²,2²,1⁴]	[4²,1⁸] [3⁴,2²] [3⁴,1⁴] [3²,2⁴,1²] [3²,2²,1⁶] [3²,1¹⁰] [2⁸] [2⁶,1⁴] [2⁴,1⁸] [2²,1¹²] [1¹⁶]
[1⁸]	[5²,4,2] [6,4²,1²] [6,5,2²,1]	[7,4,2,1³] [8,3,1⁵] [9,1⁷]	[8,1⁸] [7,2²,1⁵] [6,3,2²,1³]	[5,4,2³,1] [5,3³,1²] [4²,3²,2]
[1⁹]	[5³,3] [6,5,4,2,1] [7,4²,1³] [6²,2³]	[7,5,2²,1²] [8,4,2,1⁴] [9,3,1⁶] [10,1⁸]	[9,1⁹] [8,2²,1⁶] [7,3,2²,1⁴] [6,4,2³,1²]	[6,3³,1³] [5²,2⁴] [5,4,3²,2,1] [4³,3²]
[1¹⁰]	[5⁴] [6,5²,3,1] [6²,4,2²] [7,5,4,2,1²] [8,4²,1⁴]	[7,6,2³,1] [8,5,2²,1³] [9,4,2,1⁵] [10,3,1⁷] [11,1⁹]	[10,1¹⁰] [9,2²,1⁷] [8,3,2²,1⁵] [7,4,2³,1³] [7,3³,1⁴]	[6,4,3²,2,1²] [6,5,2⁴,1] [5²,3²,2²] [5,4²,3²,2,1] [4⁵,1]
[1¹¹]	[12,1¹⁰] [11,3,1⁸] [10,4,2,1⁶] [9,5,2²,1⁴] [9,4²,1⁵] [8,6,2³,1²]	[8,5,4,2,1³] [7²,2⁴] [7,6,4,2²,1] [7,5²,3,1²] [6²,5,3,2] [6,5³,1]	[11,1¹¹] [10,2²,1⁸] [9,5,2²,1⁶] [8,4,2³,1⁴] [8,3³,1³] [7,5,2⁴,1²]	[7,4,3²,2,1³] [6²,2⁵] [6,5,3²,2²,1] [6,4²,3²,1²] [5²,4,3²,2] [5,4⁴,1]
[1¹²]	[13,1¹¹] [12,5,1⁹] [11,4,2,1⁷] [10,5,2²,1⁵] [10,4²,1⁶] [9,6,2³,1³] [9,5,4,2,1⁴] [8,7,2⁴,1]	[8,6,4,2²,1²] [8,5²,3,1³] [7²,4,2³] [7,6,5,3,2,1] [7,5³,1²] [6³,3²] [6²,5²,2]	[12,1¹²] [11,2²,1⁹] [10,3,2²,1⁷] [9,4,2⁵,1⁵] [9,3³,1⁶] [8,5,2⁴,1³] [8,4,3²,2,1³] [7,6,2⁵,1]	[7,5,3²,2²,1²] [7,4²,3²,1³] [6²,3²,2³] [6,5,4,3²,2,1] [6,4⁴,1²] [5³,3³] [5²,4³,2]

TABLE II. The reduction of the tensor products of $[1^3]$ and $[1^4]$ of SU(N) up to four copies with the given symmetry property of the Young diagram in the first column. The table can also be used to obtain the branching of SU(M) into the representation of SU(N), where the defining representation of SU(N) is embedded in the fundamental representation of SU(M) such that M is the dimension of the defining representation of SU(N).

SU(M)	Defining Representations of SU(N)		
[1]	$[1^3]$	$[1^4]$	
[2]	$[2^3]$ $[2,1^4]$	$[2^4]$ $[2^2,1^4]$	$[1^8]$
$[1^2]$	$[2^2,1^2]$ $[1^6]$	$[2^3,1^2]$	$[2,1^6]$
[3]	$[3^3]$ $[3,2^2,1^2]$ $[2^3,1^3]$ $[3,1^6]$	$[3^4]$ $[3^2,2^2,1^2]$ $[3,2^3,1^3]$ $[2^4,1^4]$ $[3^2,1^6]$	$[2^6]$ $[2^3,1^6]$ $[2^2,1^8]$ $[1^{12}]$
[2,1]	$[3^2,2,1]$ $[3,2^2,1^2]$ $[2^3,1^3]$ $[3,2,1^4]$ $[2^4,1]$ $[2^2,1^5]$ $[2,1^7]$	$[3^3,2,1]$ $[3^2,2^2,1^2]$ $[3,2^3,1^3]$ 2 x $[2^4,1^4]$ $[3^2,2,1^4]$ $[3,2^4,1]$	$[3,2^2,1^5]$ $[2^5,1^2]$ $[2^3,1^6]$ $[3,2,1^7]$ $[2^2,1^8]$ $[2,1^{10}]$
$[1^3]$	$[3^2,1^3]$ $[3,2^3]$ $[2^3,1^3]$ $[2^2,1^5]$ $[1^9]$	$[3^3,1^3]$ $[3^2,2^3]$ $[3,2^3,1^3]$ $[3,2^2,1^5]$	$[2^5,1^2]$ $[2^3,1^6]$ $[3,1^9]$
[4]	$[4^3]$ $[4,3^2,1^2]$ $[3^3,1^3]$ $[4,2^4]$ $[4,2^2,1^4]$ $[3^2,2^2,1^2]$ $[3,2^3,1^3]$ $[3,2^2,1^5]$ $[2^6]$ $[4,1^8]$	$[4^4]$ $[4^2,3^2,1^2]$ $[4,3^3,1^3]$ 2 x $[3^4,1^4]$ $[4^2,2^4]$ $[4^2,2^2,1^4]$ $[4,3^2,2^2,1^2]$ $[4,3,2^3,1^3]$ $[4,3,2^2,1^5]$ $[3^4,2^2]$ $[3^3,2^3,1]$ $[3^3,2,1^5]$ 2 x $[3^2,2^4,1^2]$ $[3^2,2^3,1^4]$	2 x $[3^2,2^2,1^6]$ $[4,2^6]$ $[3,2^5,1^3]$ $[3,2^4,1^5]$ $[3,2^3,1^7]$ $[2^8]$ 2 x $[2^6,1^4]$ 2 x $[2^4,1^8]$ $[4^2,1^8]$ $[3^2,2,1^8]$ $[3^2,1^{10}]$ $[2^3,1^{10}]$ $[2^2,1^{12}]$ $[1^{16}]$
[3,1]	$[4^2,3,1]$ $[4,3^2,1^2]$ 2 x $[3^3,1^3]$ $[4,3,2^2,1]$ $[4,3,2,1^3]$ $[3^3,2,1]$ $[3^2,2^2,1^2]$ 2 x $[3^2,2,1^4]$ $[4,2^3,1^2]$ $[4,2^2,1^4]$ $[3^2,2^3]$ 2 x $[3,2^4,1]$ 2 x $[3,2^3,1^3]$ 2 x $[3,2^2,1^5]$ $[2^5,1^2]$ $[2^4,1^4]$	$[4^3,3,1]$ $[4^2,3^2,1^2]$ 2 x $[4,3^3,1^3]$ 2 x $[3^4,1^4]$ $[4^2,3,2^2,1]$ $[4^2,3,2,1^3]$ $[4^2,2^3,1^2]$ $[4^2,2^2,1^4]$ $[4,3^3,2,1]$ $[4,3^2,2^3]$ $[4,3^2,2^2,1^2]$ 2 x $[4,3^2,2,1^4]$ 2 x $[4,3,2^3,1^3]$ 2 x $[4,3,2^2,1^5]$ $[3^4,2^2]$ 2 x $[3^2,2^4,1^2]$ $[3^2,2^3,1^4]$	$[4,2^5,1^2]$ $[4,2^4,1^4]$ $[4,2^3,1^6]$ $[3^2,2^5]$ 2 x $[3,2^6,1]$ 3 x $[3,2^5,1^3]$ 3 x $[3,2^4,1^5]$ 3 x $[3,2^3,1^7]$ 2 x $[2^7,1^2]$ 2 x $[2^6,1^4]$ 3 x $[2^5,1^6]$ 2 x $[2^4,1^8]$ $[4^2,2,1^6]$ $[4,3,2,1^7]$ $[3^2,2,1^8]$ $[2^2,1^{16}]$

SU(M)	SU(N)		
	$[2^3,1^6]$ $[4,2,1^6]$ $[3,2,1^7]$ $[3,1^9]$	2 x $[3^4,2,1^2]$ 2 x $[3^3,2^3,1]$ 3 x $[3^3,2^2,1^3]$ 3 x $[3^3,2,1^5]$ 3 x $[3^2,2^4,1^2]$ 4 x $[3^2,2^3,1^4]$ 4 x $[3^2,2^2,1^6]$	$[3^2,1^{10}]$ $[3^3,1^7]$ 2 x $[3,2^2,1^9]$ 2 x $[2^3,1^{10}]$ $[3,2,1^{11}]$ $[2^2,1^{12}]$ $[2,1^{14}]$
$[2^2]$	$[4^2,2^2]$ $[4,3^2,1^2]$ $[4,3,2,1^3]$ $[3^3,2,1]$ 2 x $[3^2,2^2,1^2]$ $[3^2,2,1^4]$ $[4,2^4]$ $[4,2^2,1^4]$ $[3,2^4,1]$ $[3,2^3,1^3]$ $[3,2^2,1^5]$ $[2^6]$ 2 x $[2^4,1^4]$ $[3^2,1^6]$ $[3,2,1^7]$ $[2^2,1^8]$	$[4^3,2^2]$ $[4^2,3^2,1^2]$ $[4^2,3,2,1^3]$ $[4,3^3,2,1]$ 2 x $[4,3^2,2^2,1^2]$ $[4,3^2,2,1^4]$ $[3^4,2,1^2]$ 2 x $[3^4,1^4]$ 2 x $[3^3,2^2,1^3]$ 2 x $[3^3,2,1^5]$ $[4^2,2^4]$ $[4^2,2^2,1^4]$ $[4,3,2^4,1]$ $[4,3,2^3,1^3]$ $[4,3,2^2,1^5]$ $[3^4,2^2]$ $[3^3,2^3,1]$ 3 x $[3^2,2^4,1^2]$ 2 x $[3^2,2^3,1^4]$	3 x $[3^2,2^2,1^6]$ $[4,2^6]$ 2 x $[4,2^4,1^4]$ $[3,2^6,1]$ 2 x $[3,2^5,1^3]$ 2 x $[3,2^4,1^5]$ 2 x $[3,2^3,1^7]$ 2 x $[2^8]$ 2 x $[2^6,1^4]$ $[2^5,1^6]$ 2 x $[2^4,1^8]$ $[4,3^2,1^6]$ $[4,3,2,1^7]$ $[3^2,2,1^8]$ $[4,2^2,1^8]$ $[3,2^2,1^9]$ $[3^2,1^{10}]$ $[3,2,1^{11}]$ $[2^2,1^{12}]$
$[2,1^2]$	$[4^2,2,1^2]$ $[4,3^2,2]$ $[4,3,2^2,1]$ $[4,3,2,1^3]$ $[3^3,2,1]$ $[3^3,1^3]$ 2 x $[3^2,2^2,1^2]$ 2 x $[3^2,2,1^4]$ $[4,2^3,1^2]$ $[3^2,2^3]$ $[3,2^4,1]$ 2 x $[3,2^3,1^3]$ 2 x $[3,2^2,1^5]$ 2 x $[2^5,1^2]$ $[2^4,1^4]$ 2 x $[2^3,1^6]$ $[4,3,1^5]$ $[3^2,1^6]$ $[3,2,1^7]$ $[2^2,1^8]$ $[2,1^{10}]$	$[4^3,2,1^2]$ $[4^2,3^2,2]$ $[4^2,3,2^2,1]$ $[4^2,3,2,1^3]$ $[4,3^3,2,1]$ $[4,3^3,1^3]$ 2 x $[4,3^2,2^2,1^2]$ 2 x $[4,3^2,2,1^4]$ 2 x $[3^4,2,1^2]$ $[3^4,1^4]$ 4 x $[3^3,2^2,1^3]$ 3 x $[3^3,2,1^5]$ $[4^2,2^3,1^2]$ $[4,3^2,2^3]$ $[4,3,2^4,1]$ 2 x $[4,3,2^3,1^3]$ 2 x $[4,3,2^2,1^5]$ 2 x $[3^3,2^3,1]$ 2 x $[3^2,2^4,1^2]$ 4 x $[3^2,2^3,1^4]$ 2 x $[3^2,2^2,1^6]$ 2 x $[4,2^5,1^2]$ $[4,2^4,1^4]$	2 x $[4,2^3,1^6]$ 2 x $[3^2,2^5]$ 2 x $[3,2^6,1]$ 3 x $[3,2^5,1^3]$ 4 x $[3,2^4,1^5]$ 3 x $[3,2^3,1^7]$ 2 x $[2^7,1^2]$ $[2^6,1^4]$ 2 x $[2^5,1^6]$ $[2^4,1^8]$ $[4^2,3,1^5]$ $[4,3^2,1^6]$ $[4,3,2,1^7]$ 2 x $[3^3,1^7]$ 2 x $[3^2,2,1^8]$ $[3^5,1]$ $[4,2^2,1^8]$ 2 x $[3,2^2,1^9]$ $[2^3,1^{10}]$ $[4,2,1^{10}]$ $[3,2,1^{11}]$ $[3,1^{13}]$
$[1^4]$	$[4^2,1^4]$ $[4,3,2^2,1]$ $[3^2,2^2,1^2]$ $[3^2,2,1^4]$ $[3^2,1^6]$ $[3^4]$ $[3,2^3,1^3]$ $[2^6]$ $[2^4,1^4]$ $[2^3,1^6]$ $[2^2,1^8]$ $[1^{12}]$	$[4^3,1^4]$ $[4^2,3,2^2,1]$ $[4,3^2,2^2,1^2]$ $[4,3^2,2,1^4]$ $[4,3^2,1^6]$ $[3^3,2^3,1]$ $[3^3,2^2,1^3]$ $[3^3,2,1^5]$ $[3^3,1^7]$ $[4,3^4]$ $[4,3,2^3,1^3]$ $[3^4,2,1^2]$ $[3^2,2^3,1^4]$	$[4,2^6]$ $[4,2^4,1^4]$ $[4,2^3,1^6]$ $[3^2,2^4,1^2]$ $[3^2,2^2,1^6]$ $[3,2^6,1]$ $[3,2^5,1^3]$ $[3,2^4,1^5]$ $[3,2^3,1^7]$ $[4,2^2,1^8]$ $[3,2^2,1^9]$ $[2^6,1^4]$ $[4,1^{12}]$

TABLE III. The reduction of the tensor products of [2,1], [2,2], and [2,1²] of SU(N) up to three copies with the given symmetry property of the Young diagram in the first column. The table can also be used to obtain the branching of SU(M) into the representations of SU(N), where the defining representations [2,1], [2,2], and [2,1²] are embedded in the fundamental representation of SU(M), respectively. Here M is the dimension of the defining representation of SU(N).

SU(M)	Defining Representations of SU(N)			
[1]	[2,1]	[2,2]	[2,1²]	
[2]	[4,2] [3,2,1] [3,1³] [2⁴]	[4²] [4,2²] [3²,1²] [2⁴]	[4,2²] [4,1⁴] [3²,1²] [3,2²,1]	[3,2,1³] [2⁴] [2²,1⁴]
[1²]	[4,1²] [3²] [3,2,1] [2³,1²]	[4,3,1] [3,2²,1]	[4,2,1²] [3²,2] [3,2²,1]	[3,2,1³] [3,1⁵] [2³,1²]
[3]	[6,3] [5,3,1] [4²,1] [5,2²] [5,2,1²] [4,3,2] [4,3,1²] 2 x [4,2²,1] [3³] [3²,2,1] [4,2,1³] [3²,1³] [3,2³] [3,2²,1²] [4,1⁵]	[6²] [6,4,2] [5²,1²] [5,4,2,1] 2 x [4²,2²] [6,2³] [5,3²,1] [4³] [5,3,2,1²] [4,3²,1²] [4,3,2²,1] [4,2⁴] [3⁴] [4²,1⁴] [3²,2²,1²] [2⁶]	[6,3²] [6,2²,1²] [5,4,2,1] [5,3²,1] 2 x [5,3,2,1²] [4²,3,1] 2 x [4²,2,1²] [5,3,2²] [5,2³,1] 2 x [5,2²,1³] 2 x [4,3²,2] [4,3²,1²] 4 x [4,3,2²,1] 3 x [4,3,2,1³] 3 x [4,2³,1²] [6,1⁶] [5,3,1⁴]	[5,2,1⁵] 2 x [4,3,1⁵] [4,2²,1⁴] [4,2,1⁶] [3³,2,1] 2 x [3³,1³] [4²,1⁴] 2 x [3²,2³] 2 x [3²,2²,1²] 2 x [3²,2,1⁴] [3⁴] [3,2⁴,1] 2 x [3,2³,1³] [3²,1⁶] [3,2²,1⁵] [2⁵,1²] [2³,1⁶]
[2,1]	[6,2,1] [5,4] 2 x [5,3,1] [4²,1] [5,2²] 2 x [5,2,1²] 3 x [4,3,2] 3 x [4,3,1²] 3 x [4,2²,1] [5,1⁴] 2 x [4,2,1³] 3 x [3²,2,1] [3²,1³] [3,2³] 2 x [3,2²,1²] [3,2,1⁴] [2⁴,1]	[6,5,1] [6,4,2] [5²,1²] 2 x [5,4,2,1] 2 x [4²,2²] [6,3,2,1] [5,4,3] [5,3²,1] [5,3,2²] [4²,3,1] [4,3²,2] [5,4,1³] [5,3,2,1²] [4²,2,1²] 2 x[4,3,2²,1] [5,2³,1] [4,3²,1²] [4,2⁴] [3³,2,1] [4,3,2,1³] [3²,2²,1²] [3,2⁴,1]	[6,3,2,1] [6,2²,1²] [5,4,3] [5,4,2,1] 2 x [5,3²,1] 4 x [5,3,2,1²] 2 x [4²,3,1] 3 x [4²,2,1²] 2 x [5,3,2²] 3 x [5,2³,1] 3 x [5,2²,1³] 3 x [4,3²,2] 4 x [4,3²,1²] 6 x [4,3,2²,1] 7 x [4,3,2,1³] 5 x [4,2³,1²] [6,2,1⁴] 2 x [5,3,1⁴] 2 x [5,2,1⁵] 3 x [4,3,1⁵]	[5,1⁷] 4 x [4,2²,1⁴] 2 x [4,2,1⁶] [5,4,1³] 2 x [4²,2²] 4 x [3³,2,1] 2 x [3³,1³] [4²,1⁴] 2 x [3²,2³] 5 x [3²,2²,1²] 4 x [3²,2,1⁴] 2 x [4,2⁴] 3 x [3,2⁴,1] 3 x [3,2³,1³] [3²,1⁶] 2 x [3,2²,1⁵] [2⁵,1²] [3,2,1⁷] [2⁴,1⁴]
[1³]	[6,1³] [5,3,1] [5,2²] [5,2,1²] [4,3,2] 2 x [4,3,1²] [4,2²,1] [4,2,1³] [4²,1] [3²,2,1] [3³]	[6,3²] [6,4,1²] [5²,2] [5,4,2,1] [5,3,2²] [4²,3,1] [4,3²,2] [5,3,2,1²] [4²,2,1²] [4,3,2²,1] [3²,2³]	[6,3,1³] [6,2³] [5,4,2,1] [5,3,2²] 2 x [5,3,2,1²] [5,3,1⁴] [4²,2²] [4²,2,1²] [4²,1⁴] [5,3²,1] [5,2³,1]	2 x [4,2⁴] 2 x [4,2³,1²] 3 x [4,2²,1⁴] [4³] [4²,3,1] [3³,2,1] 2 x [3³,1³] 3 x [3²,2²,1²] [3⁴] [3²,2³] [3²,2,1⁴]
	[3²,1³] [3,2³] [3,2²,1²] [2³,1³]	[4,2³,1²] [3³,1³]	2 x [5,2²,1³] [4,3²,2] 3 x [4,3²,1²] 3 x [4,3,2²,1] 3 x [4,3,2,1³] [5,2,1⁵] [4,3,1⁵]	[3,2⁴,1] 2 x [3,2³,1³] [4,2,1⁶] [3²,1⁶] [3,2²,1⁵] [4,1⁸] [2⁶]

TABLE IV. The reduction of the tensor products of the spinor representation (0,0,0,0,1) of D_5 up to five copies with the given symmetry property of the Young diagram in the first column. The table can also be used to obtain the branching of SU(16) into the representations of D_5, where the defining representation (0,0,0,0,1) of D_5 is embedded to the fundamental representation [1] of SU(16). Square brackets are used to denote the Young diagrams of SU(16) in the first column. Representations of D_5 are given in Dynkin notation in parentheses as defined in Fig. 1.

SU(16)	Defining representation of D_5	
[1]	(0,0,0,0,1)	
[2]	(0,0,0,0,2)	(1,0,0,0,0)
[1²]	(0,0,1,0,0)	
[3]	(0,0,0,0,3)	(1,0,0,0,1)
[2,1]	(0,0,1,0,1) (1,0,0,0,1)	(0,0,0,1,0)
[1³]	(0,1,0,1,0)	
[4]	(0,0,0,0,4) (2,0,0,0,0)	(1,0,0,0,2)
[3,1]	(0,0,1,0,2) (0,1,0,0,0) (0,0,0,1,1)	(1,0,1,0,0) (1,0,0,0,2)
[2²]	(0,0,2,0,0) (0,0,0,0,0) (2,0,0,0,0)	(0,0,0,1,1) (1,0,0,0,2)
[2,1²]	(0,1,0,1,1) (0,1,0,0,0)	(0,0,0,1,1) (1,0,1,0,0)
[1⁴]	(1,0,0,2,0) (0,2,0,0,0)	
[5]	(0,0,0,0,5) (1,0,0,0,3)	(2,0,0,0,1)
[4,1]	(0,0,1,0,3) (1,0,0,0,3) (1,0,1,0,1) (0,0,0,1,2)	(1,0,0,1,0) (0,1,0,0,1) (2,0,0,0,1)
[3,2]	(0,0,2,0,1) (1,0,1,0,1) (1,0,0,0,3) (0,0,0,1,2) (0,0,1,1,0)	(2,0,0,0,1) (0,0,0,0,1) (1,0,0,1,0) (0,1,0,0,1)
[3,1²]	(1,0,0,1,0) 2 x (0,1,0,0,1) (0,0,0,1,2) (1,0,1,0,1)	(0,1,0,1,2) (1,1,0,1,0) (0,0,1,1,0) (0,0,0,0,1)
[2²,1]	(0,1,1,1,0) (1,0,1,0,1) (0,0,0,1,2) (0,0,1,1,0)	(2,0,0,0,1) (0,0,0,0,1) (1,0,0,1,0) (0,1,0,0,1)
[2,1³]	(1,0,0,2,1) (0,2,0,0,1) (1,0,0,1,0)	(0,1,0,0,1) (0,0,1,1,0) (1,1,0,1,0)
[1⁵]	(0,0,0,3,0)	(1,1,0,1,0)

Here, 5-ality is the congruence number and Q_1 and Q_2 are chosen in such a way that the $[SU(5)]^2U(1)$ anomaly vanishes. There are four candidates for the massless bound states coming from the four singlet states of metacolor SU(5):

$$\alpha^5, \quad \alpha\bar{\beta}^2, \quad \alpha^2\beta, \quad \beta^5. \tag{18}$$

The representations for the bound states are to be constructed from these candidates by imposing further Fermi statistics so as to preserve total antisymmetry under metacolor–metaflavor–spin transformation. The transformation under orbital angular momentum can be assumed to be symmetric. The metacolor singlet states constrained by Fermi statistics actually lead to the definite metaflavor wave function as we will see below.

TABLE V. The reduction of the tensor products of (0,0,0,0,2) and (1,0,0,0,1) of D_5, and (0,0,0,0,0,0,0,0,1) of D_9 up to two copies with the given symmetry property of the Young diagram in the first column. The table can also be used to obtain the branching of SU(M) into D_5 and D_9, where the defining representation (0,0,0,0,2) and (1,0,0,0,1) of D_5 and (0,0,0,0,0,0,0,0,1) of D_9 are embedded in the fundamental representation [1] of SU(M). Here M is the dimension of the defining representation. Square brackets and parentheses are used for the Young diagrams and Dynkin diagrams, respectively.

SU(M)	Defining Representations		
[1]	(0,0,0,0,2) of D_5	(1,0,0,0,1) of D_5	(0,0,0,0,0,0,0,0,1) of D_9
[2]	(0,0,0,0,4) (2,0,0,0,0) (1,0,0,0,2) (0,0,2,0,0)	(2,0,0,0,2) (0,1,1,0,0) (1,0,0,1,1) (1,1,0,0,0) (3,0,0,0,0) 2 x(0,0,0,0,2) (1,0,0,0,0)	(0,0,0,0,0,0,0,0,2) (0,0,0,0,1,0,0,0,0) (1,0,0,0,0,0,0,0,0)
$[1^2]$	(1,0,1,0,0) (0,0,1,0,2)	(2,0,1,0,0) (1,0,0,1,1) (1,1,0,0,0) 2 x(0,0,1,0,0) (0,1,0,0,2)	(0,0,0,0,0,0,1,0,0) (0,0,1,0,0,0,0,0,0)

In order to construct the ground state wavefunction consistent with Fermi statistics, it is convenient to use the antisymmetric representation of one SU(I) group, where $I = 2MN$, i.e., the product of the dimensions of the spin, metacolor, and metaflavor representations of the defining states α, β, $\bar{\alpha}$, or $\bar{\beta}$. Note $M = 5$ and 10 for $\alpha(\bar{\alpha})$ and $\beta(\bar{\beta})$, respectively.

Of the four candidates of Eq. (18), we take the state β^5 by way of explanation. Since there are five identical β's to form a fermion bound state, we take the totally antisymmetric representation $[1^5]$ of SU(I) = SU($20N$) and consider its branching to $SU_{mc}(5)\times SU_{mf}(N)\times SU_{spin}(2)$. This branching consists of three steps:

$$SU(20N) \underset{\text{step 1}}{\rightarrow} SU(10N)\times SU(2) \underset{\text{step 2}}{\rightarrow} SU(10)\times SU(N)\times SU(2) \underset{\text{step 3}}{\rightarrow} SU(5)\times SU(N)\times SU(2). \tag{19}$$

The first and second steps are special cases of the branching type SU(pq)$\supset$SU(p)$\times$SU(q), which have already been discussed extensively in the literature.[16] Our results apply to the third stage, i.e., SU(10)$\rightarrow$SU(5). This type of branching, i.e., SU(M)$\rightarrow$ the defining group particularly when M is large cannot be found in the existing literature to our knowledge.

The branching of $[1^5]$ under the first step is[16]

$$\begin{aligned}[1^5]\rightarrow&[3,1^2]\otimes[3,1^2]+[5]\otimes[1^5]+[1^5]\otimes[5]\\&+[4,1]\otimes[2,1^3]+[2,1^3]\otimes[4,1]+[3,2]\otimes[2^2,1]\\&+[2^2,1]\otimes[3,2],\end{aligned} \tag{20}$$

where the first factor in each term is the representation of SU($10N$) and the second factor is that of SU(2). Since we know that the fermion bound state β^5 must have spin $\frac{1}{2}$ and left-handed chirality, only the last term is permissible, so that the SU($10N$) representation is uniquely determined to be $[2^2,1]$. Now we proceed to observe the branching of SU($10N$) $\rightarrow$SU(10)$\times$SU(N):

$$\begin{aligned}[2^2,1]\rightarrow&[4,1]\otimes[3,2]+[3,2]\otimes[4,1]+[2,1^3]\otimes[2^2,1]\\&+[2^2,1]\otimes[2,1^3]+[4,1]\otimes[3,1^2]+[3,1^2]\otimes[4,1]\\&+[2,1^3]\otimes[3,1^2]+[3,1^2]\otimes[2,1^3]+[3,2]\otimes[3,2]\\&+[2^2,1]\otimes[2^2,1]+[3,2]\otimes[3,1^2]+[3,1^2]\otimes[3,2]\\&+[2^2,1]\otimes[3,1^2]+[3,1^2]\otimes[2^2,1]+2[3,1^2]\otimes[3,1^2]\\&+[1^5]\otimes[3,2]+[3,2]\otimes[1^5]\\&+[5]\otimes[2^2,1]+[2^2,1]\otimes[5]\\&+[4,1]\otimes[2,1^3]+[2,1^3]\otimes[4,1]+[2,1^3]\otimes[3,2]\\&+[3,2]\otimes[2,1^3]+[4,1]\otimes[2^2,1]+[2^2,1]\otimes[4,1]\\&+[3,2]\otimes[2^2,1]+[2^2,1]\otimes[3,2].\end{aligned} \tag{21}$$

Again the first factor in each term of Eq. (21) is the SU(10) representation and the second factor is the SU(N) representation.

Now we come to the most important stage of identifying the metacolor, i.e., SU(5) singlets from the branching SU(10)$\rightarrow$SU(5), for which our results of Sec. III play a crucial role. Of all representations of SU(10) in Eq. (21), we see from Table I that only the terms containing the representation $[3,1^2]$ of SU(10) can give the metacolor singlet states:

$$\begin{aligned}[3,1^2]\rightarrow&[5,3,1^2]+[4^2,2]+[4,3,2,1]+[4,3,1^3]\\&+2[3^2,2,1^2]+[4,2^3]+[4,2^2,1^2]+[3^3,1]\\&+[3,2^3,1]+2[3,2^2,1^3]+[4,2,1^4]\\&+[3,2,1^5]+[2^5]+[2^3,1^4]+[3,1^7],\end{aligned} \tag{22}$$

where $[2^5]$ is obviously the SU(5) singlet. In this way, the metaflavor representations of SU(N) are determined to be

$$2[3,1^2],\quad [2,1^3],\quad [3,2],\quad [2^2,1],\quad [4,1]. \tag{23}$$

Similarly, the metaflavor representations of α^5, $\alpha\bar{\beta}^2$, and $\alpha^2\beta$ can be obtained. These and other related subjects of preon dynamics are presented elsewhere.[9]

B. 27_L of E_6 metacolor group as the preon representation

The second example is E_6 metacolor group with preon α in the 27-dimensional (000010) representation. This representation belongs to congruence class 2 and can be repeated up to 22 times without losing asymptotic freedom. Such repetition introduces the metaflavor group SU(N) in addition.

The bound state α^3 is a singlet of E_6 and is a candidate massless bound state. The metaflavor representation of the bound state α^3 is determined by Fermi statistics in the similar way as in Subsec. A.

The branching necessary for satisfying Fermi statistics in the bound state α^3 is again through several steps:

$$SU(54N) \underset{\text{step 1}}{\rightarrow} SU(27N)\times SU(2) \underset{\text{step 2}}{\rightarrow} SU(27)\times SU(N)\times SU(2). \tag{24}$$

In the first step, the totally antisymmetric $[1^3]$ of SU($54N$) have the following SU($27N$)$\times$SU(2) branching:

$$[1^3]\rightarrow[2,1]\otimes[2,1]+[3]\otimes[1^3]+[1^3]\otimes[3]. \tag{25}$$

Only the first term can give spin $\frac{1}{2}$, and hence we find that the SU($27N$) representation is [2,1]. Under step 2 this branches

TABLE VI. The reduction of the tensor products of the spinor representation (0,0,0,0,0,0,1) of D_7 up to four copies with the given symmetry property of the Young diagram in the first column. The table can also be used to obtain the branching of SU(64) into the representation of D_7, where the defining representation (0,0,0,0,0,0,1) of D_7 is embedded in the fundamental representation [1] of SU(64). Square brackets are used to denote the Young diagrams of SU(64) in the first column. Representations of D_7 are given in Dynkin notation in parentheses as defined in Fig. 1.

SU(64)	Defining representation of D_7	
[1]	(0,0,0,0,0,0,1)	
[2]	(0,0,0,0,0,0,2)	(0,0,1,0,0,0,0)
$[1^2]$	(1,0,0,0,0,0,0)	(0,0,0,0,1,0,0)
[3]	(0,0,0,0,0,0,3)	(0,0,1,0,0,0,1)
	(1,0,0,0,0,0,1)	
[2,1]	(0,0,0,0,1,0,1)	(1,0,0,0,0,0,1)
	(0,0,1,0,0,0,1)	(0,0,0,0,0,1,0)
	(0,1,0,0,0,1,0)	
$[1^3]$	(0,0,0,0,0,1,0)	(0,0,0,1,0,1,0)
	(1,0,0,0,0,0,1)	
[4]	(0,0,0,0,0,0,4)	(2,0,0,0,0,0,0)
	(0,0,1,0,0,0,2)	(0,0,0,1,0,0,0)
	(0,0,2,0,0,0,0)	(1,0,0,0,1,0,0)
	(1,0,0,0,0,0,2)	
[3,1]	2 x (1,0,0,0,0,0,2)	(0,0,1,0,1,0,0)
	(0,0,0,0,1,0,2)	(0,0,1,0,0,0,2)
	(0,1,0,1,0,0,0)	(0,1,0,0,0,0,0)
	(1,0,0,0,1,0,0)	2 x (0,0,0,0,0,1,1)
	2 x (1,0,1,0,0,0,0)	(0,0,0,1,0,0,0)
		(0,1,0,0,0,1,1)

SU(64)	D_7	
$[2^2]$	(0,0,1,0,0,0,2)	(0,0,0,0,0,0,0)
	(0,0,0,0,2,0,0)	2 x (1,0,0,0,1,0,0)
	(0,0,2,0,0,0,0)	(0,0,0,0,0,1,1)
	(0,1,0,0,0,1,1)	(2,0,0,0,0,0,0)
	(0,2,0,0,0,0,0)	(0,0,0,1,0,0,0)
$[2,1^2]$	(0,0,0,1,0,1,1)	2 x (0,1,0,0,0,0,0)
	2 x (0,0,0,1,0,0,0)	(1,0,1,0,0,0,0)
	(0,0,1,0,1,0,0)	(1,0,0,0,1,0,0)
	2 x (0,0,0,0,0,1,1)	(0,1,0,0,0,1,1)
	2 x (1,0,0,0,0,0,2)	(0,1,0,1,0,0,0)
$[1^4]$	(0,0,1,0,0,2,0)	(0,0,0,1,0,0,0)
	(0,0,0,2,0,0,0)	(0,0,0,0,0,1,1)
	(0,0,0,0,0,0,0)	(1,0,0,0,1,0,0)
	(2,0,0,0,0,0,0)	

TABLE VII. The reduction of the tensor products of the (0,0,0,0,1,0) of E_6 up to five copies with the given symmetry property of the Young diagram in the first column. The table can also be used to obtain the branching of SU(27) into the representation of E_6, where the defining representation (0,0,0,0,1,0) of E_6 is embedded to the fundamental representation [1] of SU(27). Square brackets are used to denote the Young diagram of SU(27) and parentheses are used to denote the Dynkin diagrams of E_6 as defined in Fig. 1.

SU(27)	Defining representation of E_6	
[1]	(0,0,0,0,1,0)	
[2]	(0,0,0,0,2,0)	(1,0,0,0,0,0)
$[1^2]$	(0,0,0,1,0,0)	
[3]	(0,0,0,0,3,0)	(0,0,0,0,0,0)
	(1,0,0,0,1,0)	
[2,1]	(0,0,0,1,1,0)	(0,0,0,0,0,1)
	(1,0,0,0,1,0)	
$[1^3]$	(0,0,1,0,0,0)	
[4]	(0,0,0,0,4,0)	(0,0,0,0,1,0)
	(1,0,0,0,2,0)	(2,0,0,0,0,0)
[3,1]	(0,0,0,1,2,0)	(0,0,0,0,1,0)
	(1,0,0,0,2,0)	(0,1,0,0,0,0)
	(1,0,0,1,0,0)	(0,0,0,0,1,1)
$[2^2]$	(0,0,0,2,0,0)	(2,0,0,0,0,0)
	(1,0,0,0,2,0)	(0,0,0,0,1,1)
	(0,0,0,0,1,0)	
$[2,1^2]$	(0,1,0,0,0,0)	(0,0,1,0,1,0)
	(0,0,0,0,1,1)	(1,0,0,1,0,0)
$[1^4]$	(0,1,0,0,0,1)	
[5]	(0,0,0,0,5,0)	(0,0,0,0,2,0)
	(1,0,0,0,3,0)	(1,0,0,0,0,0)
	(2,0,0,0,1,0)	

SU(27)	E_6	
[4,1]	(0,0,0,1,3,0)	(0,1,0,0,1,0)
	(1,0,0,1,1,0)	(1,0,0,0,0,1)
	(1,0,0,0,3,0)	(1,0,0,0,0,0)
	(0,0,0,0,2,1)	(0,0,0,1,0,0)
	(2,0,0,0,1,0)	(0,0,0,0,2,0)
[3,2]	(0,0,0,0,2,0)	(2,0,0,0,1,0)
	(0,0,0,2,1,0)	(0,0,0,0,2,1)
	(1,0,0,0,3,0)	(0,0,0,0,2,0)
	(1,0,0,1,1,0)	(0,1,0,0,1,0)
	(0,0,0,1,0,1)	(1,0,0,0,0,1)
	(0,0,0,1,0,0)	(1,0,0,0,0,0)
$[3,1^2]$	(0,0,1,0,2,0)	
	(1,0,0,1,1,0)	(1,0,0,0,0,1)
	(0,1,0,0,1,0)	(0,1,0,0,1,0)
	(0,0,0,0,2,1)	(0,0,0,1,0,1)
	2 x (0,0,0,1,0,0)	(1,0,1,0,0,0)
$[2^2,1]$	(2,0,0,0,1,0)	(0,1,0,0,1,0)
	(0,0,0,1,0,0)	(0,0,0,0,2,0)
	(1,0,0,0,0,1)	(0,0,1,1,0,0)
	(1,0,0,0,0,0)	(0,0,0,1,0,1)
	(0,0,0,0,2,1)	(1,0,0,1,1,0)
$[2,1^3]$	(0,1,0,0,1,1)	(0,0,0,1,0,1)
	(1,0,0,0,0,1)	(1,0,1,0,0,0)
	(0,1,0,0,1,0)	
$[1^5]$	(1,0,0,0,0,2)	(0,2,0,0,0,0)

into $[2.1]\otimes[2.1]+[3]\otimes[2.1]+[2.1]\otimes[3]+[1^3]\otimes[2.1]+[2.1]\otimes[1^3]$. Finally, Table VII shows that the E_6 singlet (0,0,0,0,0,0) belongs to the [3] of SU(27), and the metaflavor representation of α^3 is determined as [2,1] of SU(N).

ACKNOWLEDGMENTS

We would like to thank C. Albright, W. Bardeen, E. Eichten, F. W. Lemire, W. G. McKay, J. McKay and P. Winternitz for helpful discussions. Special thanks are due to J. Patera for teaching us the plethysm method used in this paper. One of us (I.G.K.) wishes to thank members of the Fermilab Theory Group and Brown University High-Energy Theory Group for warm hospitality extended to him during the course of this work. The same author is supported in part by the Korea Traders Foundation, the Korea Science and Engineering Foundation, and the Senior Fulbright Fellowship.

APPENDIX A: CONTINUATION OF SU(N) INDICES TO REAL N

The indices of a representation, defined by Eqs. (2) and (3), can be calculated from the knowledge of the complete weight system, for any representation. For the lower indices explicit expressions for arbitrary representations have been obtained in many papers.[3,14] These formulas usually contain sums up to the rank of the group, which makes a continuation to real N impossible.

One may wonder why we are interested in such a continuation, since the groups themselves cannot be continued in the rank in a sensible way. For our purpose these formulas are advantageous in three ways. First of all they allow us to use large values of N without the need to calculate large sums. In the procedures of Sec. II large values of N are unavoidable if N is restricted to integer values. For the expressions derived in this Appendix, the computing time depends only on the structure of the Young diagram, not on N. Secondly, since the index sum rules (12)–(14) can be generalized to arbitrary integer N if $G=\mathrm{SU}(N)$, they can also be generalized to real N, when continuous functions for the indices can be found. This provides another way to avoid large values of N, since the N dependence can now be probed by small, non-integer values of N. Finally, there exists an intimate relation between a continuation of N to negative values and transposition of the Young diagram, which will be exploited in Appendix B.

Continuous formulas are already known for the dimension of an SU(N) representation and for the second- and third-order index of a few small representations.[1,3] We will present a general formula for the second and third index and indicate how the results generalize to indices of arbitrary order.

Our starting point will be the integer-N formulas for the indices. We will use the results of Perelomov and Popov.[17] The relation between the symmetrized Casimir operator J_α (in Ref. 17 denoted as I_α) and the indices defined by Eqs. (2) and (3) is

$$I_2(R)=[I_0(R)/(N^2-1)]J_2(R), \tag{A1}$$

$$I_3(R)=[2N/(N^2-1)(N^2-4)]I_0(R)J_3(R). \tag{A2}$$

The symmetrized Casimir operators can be expressed in terms of the quantities

$$S_\alpha=\sum_{i=1}^{N}(L_i^\alpha-R_i^\alpha), \tag{A3}$$

where

$$L_i=f_i-f/N+N-i, \tag{A4}$$

$$R_i=N-i, \tag{A5}$$

and f_i is the length of the ith row of the Young diagram representing R. The number of boxes of this Young diagram is f. We take from Ref. 17 the following formulas for the symmetrized Casimir operators:

$$J_2=S_2, \tag{A6}$$

$$J_3=S_3-3/2(N-1)S_2. \tag{A7}$$

The sums we want to avoid appear in (A3). Continuous expressions can be obtained by summing the parts of the summand which do not depend on f_i explicitly, and using the fact that the f_i's vanish for $i>p$, where p is the number of rows of the Young diagram. The structure of the Young diagram appears in the results in the form of the following "moments":

$$M_{nm}=\sum_{j=1}^{p}j^n[f_j]^m \quad (m\geqslant 1,\ n\geqslant 0). \tag{A8}$$

Straightforward computation yields then the following expressions:

$$J_2(R)=(1+N)M_{01}-(1/N^2)M_{01}^2+M_{02}-2M_{11}, \tag{A9}$$

$$\begin{aligned}J_3(R)=&(-1/2+3/2N+2N^2)M_{01}-(9/2+3/2N)M_{01}^2\\&+(2/N^2)M_{01}^3\\&+(M_{02}-2M_{11})(3N-3M_{01}/N)\\&+M_{03}-3M_{12}+3M_{21}-3/2(N-1)J_2(R).\end{aligned} \tag{A10}$$

The crucial point is that the moments M_{nm} depend only on the Young diagram, but not on N.

Although (A9) and (A10) have the desired properties, they can be simplified by means of the transposed moments, defined as

$$T_{nm}=\sum_{j=1}^{q}j^n[g(j)]^m, \tag{A11}$$

where q is the number of columns and $g(j)$ the length of the jth column of the Young diagram. Several relations between the moments and the transposed moments can be derived. We will only give the ones for $n+m\leqslant 3$:

$$M_{01}=T_{01}=f, \tag{A12}$$

$$T_{11}=1/2(M_{02}+M_{01}), \tag{A13}$$

$$3T_{21}-T_{11}=M_{03}+M_{02}, \tag{A14}$$

$$T_{12}+T_{11}=M_{12}+M_{11}. \tag{A15}$$

Additional relations are obtained by interchanging M and T. These relations can be proved by induction: They are trivial for the single-box Young diagram, and when a box is added to an arbitrary Young diagram the left-hand sides and right-hand sides of (A12)–(A15) change by the same amounts. We use these relations to express the indices in terms of the symmetric and antisymmetric moments:

$$S_{nm} = 1/2(M_{nm} + T_{nm}), \tag{A16}$$

$$A_{nm} = 1/2(M_{nm} - T_{nm}). \tag{A17}$$

Then we obtain the following expressions[18]:

$$J_2 = f(N - f/N) + 2A_{02}, \tag{A18}$$

$$J_3 = -\tfrac{1}{2}f(1 - N^2) - 3f^2 + 2f^3/N^2 + (3N - 6f/N)A_{02} + S_{03} - 3S_{12} + 3S_{21}. \tag{A19}$$

These formulas reveal the transformation of the indices under transposition of the Young diagram. Transposition is defined as an interchange of rows and columns, or equivalently a reflection of the Young diagram with respect to the diagonal. The moments M_{nm} and T_{nm} are interchanged by transposition, so that S_{nm} is unchanged and A_{nm} changes sign. The effect of this is equivalent to a replacement of N by $-N$, apart from an overall sign. More precisely, when $I_p(Y_m,N)$ denotes the pth-order index of the representation of SU(N) defined by the m-box Young diagram Y_m, then the following relations hold:

$$I_0(Y_m^T,N) = (-1)^m I_0(Y_m, -N), \tag{A20}$$

$$I_2(Y_m^T,N) = (-1)^{m-1} I_2(Y_m, -N), \tag{A21}$$

$$I_3(Y_m^T,N) = (-1)^{m-1} I_3(Y_m, -N), \tag{A22}$$

where T denotes transposition. Relation (A20) is a consequence of the well-known dimension formula

$$I_0 = (1/H)\prod_{i,j}(N + i - j), \tag{A23}$$

where the product is over all boxes of the Young diagram, located in the jth row and ith column; H (the product of the "hook lengths") is just a numerical factor.

The extension of our results to higher indices is straightforward, but becomes rapidly complicated.

APPENDIX B: TRANSPOSITION RULES FOR SU(N)-PLETHYSMS

In this appendix we will formulate and derive relations between tensor products with definite permutation properties of a Young diagram and its transpose.

To simplify the notation, we introduce an operation of a Young diagram Y_m on a Young diagram Y_n, denoted as $Y_m * Y_n$. This operation is defined as the mth tensor power of Y_n, symmetrized according to Y_m. The result of this operation is a direct sum of Young diagrams with nm boxes:

$$Y_m * Y_n = \sum_i l_i Y^i_{mn}, \tag{B1}$$

where i labels different Young diagrams. The multiplicities l_i can be read off from Tables I and II, for example,

$$[1^3]*[2] = [3^2] \oplus [4,1^2], \tag{B2}$$

$$[2]*[1^3] = [2^3] \oplus [2,1^4]. \tag{B3}$$

This should clarify our notation.

The transposition rules can now be formulated as follows:

(i) If n is even,

$$Y_m * Y_n^T = (Y_m * Y_n)^T, \tag{B4}$$

(ii) If n is odd,

$$Y_m^T * Y_n^T = (Y_m * Y_n)^T. \tag{B5}$$

To illustrate this, we apply these rules to (B2) and (B3):

$$[1^3]*[1^2] = [1^3]*[2]^T = ([1^3]*[2])^T = [2^3] + [3,1^3], \tag{B6}$$

$$[1^2]*[3] = [2]^T*[1^3]^T = ([2]*[1^3])^T = [3^2] + [5,1]. \tag{B7}$$

The first expression can be checked with Table I. The representation [3] is not included in the table, but one can easily check that the index sum rules (12)–(14) are satisfied. This example also illustrates the main application of the transposition rules, namely, to supplement the tables in such a way that all defining representations with not more than four boxes are included.

The validity of these rules can be demonstrated by a continuation of the rank of the group to negative values. Consider the index sum rules satisfied by (B1):

$$I_0(Y_m,M) = \sum_i l_i I_0(Y^i_{mn},N), \tag{B8}$$

$$I_p(Y_m,M)I_p(Y_n,N) = \sum_i l_i I_p(Y^i_{mn},N) \quad (p = 2,3), \tag{B9}$$

where

$$M = I_0(Y_n,N). \tag{B10}$$

These rules follow from Eqs. (12)–(16); we use the notation introduced in Appendix A for the indices of SU(N). Since the multiplicities l_i satisfy (B8)–(B10) for any value of M, we can replace N by $-N$. Then we use relations (A20)–(A22) to obtain

$$I_0(Y_m,(-1)^n I_0(Y_n^T,N)) = (-1)^{mn}\sum_i l_i I_0(Y^{iT}_{mn},N), \tag{B11}$$

$$I_p(Y_m,(-1)^n I_0(Y_n^T,N))(-1)^{n-1} I_p(Y_n^T,N) = (-1)^{mn-1}\sum_i l_i I_p(Y^{iT}_{mn},N). \tag{B12}$$

If n is even, (B11) and (B12) reduce to

$$I_0(Y_m,M^T) = \sum_i l_i I_0(Y^{iT}_{mn},N), \tag{B13}$$

$$I_p(Y_m,M^T)I_p(Y_n^T,N) = \sum_i l_i I_p(Y^{iT}_{mn},N), \tag{B14}$$

where

$$M^T = I_0(Y_n^T,N).$$

For odd n we obtain the same results, but with Y_m^T instead of Y_m.

These are exactly the equations for l_i which one would have to solve to calculate the direct sums which are equal to the left-hand sides of (B4) and (B5). We conclude that the l_i's appearing in (B1) satisfy these equations when they are associated with the transpose of Y^i_{mn}. This is exactly the content of the transposition rules (B4) and (B5). This derivation is not completely rigorous because we have not shown that the sum rules have a unique solution. In fact, although we have not found such a case, we expect that at some stage ambiguities will exist, since for large representations Y_m and Y_n the

number of equations becomes much smaller than the number of variables l_i. Such an ambiguity invalidates the derivation, but, of course, not the result.

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On a generalized Hilbert problem

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(Received 1 June 1982; accepted for publication 25 June 1982)

The problem analyzed is to find functions $f_\pm$, meromorphic in $\mathbb{C}^\pm$, respectively, with values that are linear operators on a Banach space, and such that their boundary values on $\mathbb{R}$ satisfy the equation $f_- = \omega f_+$, where the operator-valued function ω as well as the positions of the poles of $f_\pm$ and the ranges of their residues are given. Uniqueness results are obtained, under certain conditions an index is proved to exist, and the determination of $f_\pm$ is reduced to the solution of a generalization of Marchenko's fundamental equation. The results are applied to inverse scattering and inverse spectral problems.

PACS numbers: 02.30. + g

I. INTRODUCTION

A version of Hilbert's twenty first problem[1] may be stated as follows: Two functions are sought, one analytic in the upper half of the complex plane, the other in the lower half, and their boundary values on the real axis are linearly related by means of a given function. In one form or another this question has always stood at the center of the inverse scattering (inscat) problem. In its simplest version, if an eigenvalue of the S matrix for a central potential is given, its solution is the Jost function. A less trivial version arises in the case of coupled Schrödinger equations.[2] The matrix Hilbert problem that is involved there was first solved by J. Plemelj[3] by means of a linear integral equation.

The specific reason for attacking a more general form of it now is that a variant of it has been found at the core of the three-dimensional inscat problem, i.e., to determine the potential in the Schrödinger equation in $\mathbb{R}^3$ from scattering and bound-state data.[4–9] Again the solution has been reduced to that of a linear integral equation, a generalization of Marchenko's fundamental equation.[10]

The generalized form of the Hilbert problem studied in this paper deals with operator-valued functions, and its solutions are *operator-valued analytic functions*. As required for its physical applications, the data functions are assumed to differ from unity not by functions that are norm square-integrable, but by functions that are "strongly square-integrable[6,8]" on the real line.

An outline of our main results is as follows. Theorem 1 (Sec. V) establishes a one-to-one relation between the general Hilbert problem here called $H^1_\sigma(\mathcal{A},\omega)$ and a more special one here called $\hat{H}^1_\Sigma(\hat{\mathcal{A}},\Omega)$ on a larger space. Theorem 2 (Sec. VI) reduces the problem in which a solution with simple poles is sought to one whose solution is to be holomorphic. If the Hilbert problem has a solution then Theorem 3 (Sec VII) establishes the existence of an *index*, analogous to that of scalar and matrix Hilbert problems. Theorem 4 (Sec. VIII) reduces the Hilbert problem without poles to a generalization of Marchenko's fundamental linear integral equation. Theorem 5 (Sec. IX) shows that in the special case in which the underlying space is a Hilbert space and the given function differs from unity by a Hilbert–Schmidt operator with other restricted properties, the index is recognizable by means of an analog of Levinson's theorem[11] as it is in the matrix case.

Some of the analytic tools needed are provided in an appendix.

II. DEFINITIONS

We shall use the following terminology and definitions in this paper.

(1) $\mathcal{A}$ is a Banach space[12]; $\hat{\mathcal{A}} = \mathcal{A} \otimes \mathcal{A}$ is the space of two-component vectors whose components are in $\mathcal{A}$. The duals of $\mathcal{A}$ and $\hat{\mathcal{A}}$ will be denoted by $\mathcal{A}^\dagger$ and $\hat{\mathcal{A}}^\dagger$.

(2) $\mathscr{B} = \mathscr{B}(\mathcal{A})$ is the set of bounded linear operators $\mathcal{A} \to \mathcal{A}$; $\hat{\mathscr{B}} = \mathscr{B}(\hat{\mathcal{A}})$ is the set of 2×2 matrices with entries in $\mathscr{B}(\mathcal{A})$.

(3) The operators in $\mathscr{B}$ may be defined by means of their integral kernels. We define A^* as the linear operator in $\mathscr{B}$ whose kernel is the complex conjugate of that of A; $A^\dagger$ is the adjoint, i.e., the operator $\mathcal{A}^\dagger \to \mathcal{A}^\dagger$ whose kernel is the hermitian conjugate of that of A. The restriction of $A^{\dagger *}$ to $\mathcal{A}$[12] will be denoted by $\tilde{A}$. If both $A \in \mathscr{B}$ and $\tilde{A} \in \mathscr{B}$ then we shall say that $A \in \tilde{\mathscr{B}}$. We shall also use the notation $A_* = \tilde{A}^{-1}$, and ran A, nul A, dom A, and dim ran A, etc., for the range, the nullspace, the domain of definition of A, and the dimension of ran A, etc., respectively.

(4) $\mathscr{L}$ is the set of all functions [either $\mathbb{R} \to \tilde{\mathscr{B}}(\mathcal{A})$ or $\mathbb{R} \to \tilde{\hat{\mathscr{B}}}(\hat{\mathcal{A}})$, depending on the context] for which $\exists c$ such that for all $\alpha \in \mathcal{A}$

$$\int_{-\infty}^{\infty} dk\, \|\tilde{F}(k)\alpha\|^2 + \int_{-\infty}^{\infty} dk\, \|F(k)\alpha\|^2 < c\|\alpha\|.$$

(5) $\mathscr{H}^\pm$ are the sets of all functions $f \in \mathscr{L}$ that are boundary values of analytic functions holomorphic in $\mathbb{C}^+$,[13] respectively $\mathbb{C}^-$, that are such that for $\operatorname{Im} k > 0$ (or $\operatorname{Im} k < 0$) $\lim \|f(k)\| = 0$ as $|k| \to \infty$, and such that if $f \in \mathscr{H}^\pm$ then $\tilde{f} \in \mathscr{H}^\pm$. See the Appendix for some relevant remarks and Lemmas.

(6) $\mathscr{M}^\pm$ are the sets of all functions with the same properties as in $\mathscr{H}^\pm$, except that they are meromorphic in $\mathbb{C}^+$ or $\mathbb{C}^-$.

(7) If $f(k)$ is a given function then f' is the function $f'(k) = f(-k)$.

(8) A function, $\mathbb{C}^\pm \to \mathscr{B}$ (or $\mathbb{C}^\pm \to \hat{\mathscr{B}}$), is said to have a zero at k if 0 is in the point spectrum of $f(k)$. If $f \in \mathscr{H}^+$ and for

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all fixed $a\in\mathcal{h}$ and all $k\in\mathbb{C}^+$ $f(k)a\neq 0$ then f is called *zero-free*. (Similarly for $f\in\mathscr{H}^-$.)

(9) If in a neighborhood including $k=\kappa$, $f(k)$ and $[f(k)]^{-1}$ are meromorphic, at $k=\kappa$ $f(k)$ and $[f(k)]^{-1}$ both have poles, and there exists no $a\in\mathcal{h}$ such that $\lim f(k)a=0$ as $k\to\kappa$, then we will say that f has a *superpole* at κ.

III. STATEMENT OF THE HILBERT PROBLEMS

We define the following Hilbert problems.

Problem $H^1_\sigma(\mathcal{h},\omega)$: Suppose a function ω, $\mathbb{R}\to\tilde{\mathscr{B}}(\mathcal{h})$, is given, such that $(\omega-\mathbb{1})\in\mathscr{L}$ and $(\omega^{-1}-\mathbb{1})\in\mathscr{L}$. Also given is a set σ of $n=n_++n_-$ pairs, each consisting of a complex number $\kappa_m^+\in\mathbb{C}^+$ or $\kappa_m^-\in\mathbb{C}^-$, respectively, and a finite dimensional subspace $\mathscr{H}_m^+$ or $\mathscr{H}_m^-$, respectively, of $\mathcal{h}$, with $m=1,\ldots,n_\pm$. [We shall refer to the set of number κ_m^+ as τ^+, the set of κ_m^- as τ^-, the set of $-\kappa_m^-$ as $-\tau^-$, and $\tau=\tau^+\cup(-\tau^-)$. The sum of the dimensions of the spaces $\mathscr{H}_m^+$ and $\mathscr{H}_m^-$ will be denoted by λ_σ.] Find a pair of functions $f_\pm$, $\mathbb{R}\to\tilde{\mathscr{B}}(\mathcal{h})$, such that $(f_\pm-\mathbb{1})\in\mathscr{M}^\pm$, with simple poles[14] at $\kappa_m^\pm$, respectively, and residues $I_m^\pm$ there such that $\operatorname{ran} I_m^\pm=\mathscr{H}_m^\pm$, and such that $f_\pm$ satisfy the equation

$$f_-=\omega f_+. \tag{1}$$

If $\sigma=\emptyset$ we denote this problem by $H^1_0(\mathcal{h},\omega)$.

Problem $H^0_\sigma(\mathcal{h},\omega)$: ω and σ are given as in $H^1_\sigma(\mathcal{h},\omega)$. Find a pair of functions $f_\pm$, $\mathbb{R}\to\tilde{\mathscr{B}}(\mathcal{h})$, such that $f_\pm\in\mathscr{M}^\pm$, analytic in $\mathbb{C}^\pm$ except for the possibility of simple poles at $\kappa_m^\pm$, respectively, and residues $I_m^\pm$ there such that $\operatorname{ran} I_m^\pm\subset\mathscr{H}_m^\pm$, and such that $f_\pm$ satisfy (1). If $\sigma=\emptyset$ we denote this problem by $H^0_0(\mathcal{h},\omega)$.

We shall also use the notation $H^1_\sigma{}^*(\mathcal{h},\omega)=H^1_\sigma(\mathcal{h},\omega_*)$, $H^0_\sigma{}^*(\mathcal{h},\omega)=H^0_\sigma(\mathcal{h},\omega_*)$ and we shall sometimes omit the $\mathcal{h}$ or both the $\mathcal{h}$ and the ω. (In Plemelj's terminology $H^1_\sigma{}^*$ is the *accompanying* problem to H^1_σ.)

The above defined Hilbert problems will be shown to be directly related to another set of Hilbert problems that appear to be more restricted but in fact are equally general.

Problem $\hat{H}^1_\Sigma(\hat{\mathcal{h}},\Omega)$: Suppose a function Ω, $\mathbb{R}\to\tilde{\mathscr{B}}(\hat{\mathcal{h}})$, is given such that $(\Omega-\mathbb{1})\in\mathscr{L}$, and it satisfies the equation

$$\Omega'=q\Omega^{-1}q, \tag{2}$$

where

$$q=\begin{pmatrix}0 & \mathbb{1}\\ \mathbb{1} & 0\end{pmatrix}.$$

Also given is a set Σ of n pairs, each consisting of a number $\kappa_m\in\mathbb{C}^+$ and a finite-dimensional subspace $\hat{\mathscr{H}}_m$ of $\hat{\mathcal{h}}$, $m=1,\ldots,n$. (We shall refer to the set of κ_m as τ, and to the sum of the dimensions of the spaces $\hat{\mathscr{H}}_m$ as λ_Σ.) Find a function Φ, $\mathbb{R}\to\tilde{\mathscr{B}}(\hat{\mathcal{h}})$, such that $(\Phi-\mathbb{1})\in\mathscr{M}^+$ with simple poles at κ_m and residues I_m there such that $\operatorname{ran} I_m=\hat{\mathscr{H}}_m$, and Φ satisfies the equation

$$\Phi'=\Omega q\Phi q. \tag{3}$$

If $\Sigma=\emptyset$ we shall denote this problem by $\hat{H}^1_0(\hat{\mathcal{h}},\Omega)$.

Problem $\hat{H}^0_\Sigma(\hat{\mathcal{h}},\Omega)$: Ω and $\hat{\mathcal{h}}$ are given as in $\hat{H}^1_\Sigma(\hat{\mathcal{h}},\Omega)$. Find a function Φ, $\mathbb{R}\to\tilde{\mathscr{B}}(\hat{\mathcal{h}})$, such that $\Phi\in\mathscr{M}^+$, analytic in $\mathbb{R}^+$ except for the possibility of simple poles at κ_m and residues I_m there such that $\operatorname{ran} I_m\subset\hat{\mathscr{H}}_m$, and Φ satisfies (3). If $\Sigma=\emptyset$ we shall denote this problem by $\hat{H}^0_0(\hat{\mathcal{h}},\Omega)$.

We shall also use the notation $\hat{H}^1_\Sigma{}^*(\mathcal{h},\Omega)=\hat{H}^1_\Sigma(\hat{\mathcal{h}},\Omega_*)$, $\hat{H}^0_\Sigma{}^*(\hat{\mathcal{h}},\Omega)=\hat{H}^0_\Sigma(\hat{\mathcal{h}},\Omega_*)$.

It should be noted that because of (2), the problems in which the order of the operators on the right-hand side of (1) and (3) is reversed can be solved by means of solving $\hat{H}^1_\Sigma(\Omega')$.

IV. PRELIMINARY RESULTS

We start with several Lemmas concerning H^1_σ and particularly H^1_0. They will all be stated first and then proved seriatim.

Lemma 1: If $H^1_\sigma(\omega)$ has a solution then this solution is unique if and only if $H^0_\sigma(\omega)$ has only the trivial solution $f_\pm=0$.

Lemma 2: If H^1_σ has a unique solution $f_\pm$, then both f_+ and f_- are zero-free.

Lemma 3: If H^1_0 has a zero-free solution $f_\pm$ such that $(f_\pm^{-1}-\mathbb{1})\in\mathscr{M}^\pm$, then it is unique.

Lemma 4: If $H^1_0(\omega)$ has a unique solution $f_\pm$, and $f_\pm$ is such that $(f_\pm^{-1}-\mathbb{1})\in\mathscr{M}^\pm$, then $H^1_0{}^*(\omega)$ has the unique solution $g_\pm=f_{\pm *}$ and $f_\pm$, $g_\pm$, $\tilde{f}_\pm$, and $\tilde{g}_\pm$ are all zero-free.

Lemma 5: If $H^1_0(\omega)$ and $H^1_0{}^*(\omega)$ have solutions $f_\pm$ and $g_\pm$, respectively, then these solutions are unique, $f_\pm$, $g_\pm$, $\tilde{f}_\pm$, and $\tilde{g}_\pm$ are all zero-free, and $g_\pm=f_{\pm *}$.

Proof of Lemma 1: The difference between any two solutions of $H^1_\sigma(\omega)$ solves $H^0_\sigma(\omega)$. Let $g_\pm$ solve $H^0_\sigma(\omega)$; then so does $ag_\pm$ for all constants $a\in\mathbb{C}$. If $f_\pm$ solves $H^1_\sigma(\omega)$ then so does $f_\pm+ag_\pm$ for almost all a. (For a finite set of a the residues may cancel out!)□

Proof of Lemma 2: Suppose f_+ has a zero at $k=\kappa$; let P be a projection on $\operatorname{nul} f_+(\kappa)$. Then the pair of functions $g_+=f_+P(k-\kappa)^{-1}$ and $g_-=f_-P(k-\kappa)^{-1}$ solves H^0_σ. By Lemma 1, therefore, H^1_σ does not have a unique solution. Similarly if f_- has a zero.□

Proof of Lemma 3: Suppose $f_\pm$ are zero-free and $(f_\pm^{-1}-\mathbb{1})\in\mathscr{M}^\pm$. Then, in fact, $(f_\pm^{-1}-\mathbb{1})\in\mathscr{H}^\pm$. Let $g_\pm$ be another solution of H^1_0. Then $f_-^{-1}g_--\mathbb{1}=f_+^{-1}g_+-\mathbb{1}$, the left-hand side of which is in $\mathscr{H}^-$, and the right-hand side in $\mathscr{H}^+$. By Lemma A5 (see the Appendix for the Lemmas enumerated by Ax), therefore, $f_-^{-1}g_-=f_+^{-1}g_+=\mathbb{1}$. Now if f_+^{-1} or f_-^{-1} had a zero then $f_\pm-\mathbb{1}$ could not be in $\mathscr{H}^\pm$. Therefore $f_\pm^{-1}$ are zero-free, and by Lemma A1, $f_+=g_+$, $f_-=g_-$.□

Proof of Lemma 4: By Lemma 2, $f_\pm$ are zero-free and since by assumption $(f_\pm^{-1}-\mathbb{1})\in\mathscr{M}^\pm$, in fact $(f_\pm^{-1}-\mathbb{1})\in\mathscr{H}^\pm$, and hence $\tilde{f}_\pm$ are also zero-free. Since (1) implies that $f_{-*}=\omega_*f_{+*}$, $g_\pm=f_{\pm *}$ solves $H^1_0{}^*$. Since $f_\pm$ and $\tilde{f}_\pm$ are holomorphic, $g_\pm$ and $\tilde{g}_\pm$ are zero-free, and by Lemma 3, $g_\pm$ is the unique solutions of $H^1_0{}^*$.□

Proof of Lemma 5: From (1) we get $\tilde{g}_-f_--\mathbb{1}=\tilde{g}_+f_+-\mathbb{1}$. The left-hand side being in $\mathscr{H}^-$ and the right-hand side in $\mathscr{H}^+$, Lemma A5 implies that $\tilde{g}_-f_-=\tilde{g}_+f_+=\mathbb{1}$. It follows that $f_\pm$ are zero-free. Furthermore, since $f_\pm$ have bounded left inverses, they cannot have zero in their continuous spectra anywhere. Since by Lemma A3 they have inverses for sufficiently large $|k|$, by Lemma A2 they cannot have zero in their residual spectra anywhere either. Consequently $f_\pm^{-1}=\tilde{g}_\pm$,

$(f_\pm^{-1} - 1) \in \mathscr{H}^\pm$, and by Lemma 3, $f_\pm$ is unique. The rest follows by Lemma 4.□

V. CONNECTION BETWEEN H_0^1 AND $\hat{H}_0^1$

Suppose that Ω satisfies Eq. (2) and $F_\pm$ solves $H_\sigma^1(\hat{\kappa},\Omega)$. If σ is such that $\tau^+ = -\tau^-$ and $\mathscr{H}_m^+ = q\mathscr{H}_m^-$, then it follows from (1) that $\psi_\pm = qF_\mp' q$ also solves $H_\sigma^1(\hat{\kappa},\Omega)$. If the solution of $H_\sigma^1(\hat{\kappa},\Omega)$ is unique, therefore, $F_- = qF_+' q$, and thus the function $\Phi = qF_+ q$ solves $\hat{H}_\sigma^1(\hat{\kappa},\Omega)$. Therefore, for special sets σ and for Ω satisfying (2), provided that it has a unique solution, the problem $H_\sigma^1(\hat{\kappa},\Omega)$ becomes identical to the seemingly more restricted $\hat{H}_\sigma^1(\hat{\kappa},\Omega)$. In fact every $H_\sigma^1(\kappa,\omega)$ can be related to a problem $\hat{H}_\Sigma^1(\hat{\kappa},\Omega)$, as follows.

It is clear from a simple calculation that if $H_\sigma^1(\kappa,\omega)$ has a solution $f_\pm$ then

$$\Phi = \begin{pmatrix} f_+ & 0 \\ 0 & f_-' \end{pmatrix} \tag{4}$$

solves $\hat{H}_\Sigma^1(\hat{\kappa},\Omega)$, where

$$\Omega = \begin{pmatrix} \omega'^{-1} & 0 \\ 0 & \omega \end{pmatrix} \tag{5}$$

and Σ consists of the $n = n_+ + n_-$ pairs κ_m^+ and

$$\hat{\mathscr{H}}_m = \begin{pmatrix} \mathscr{H}_m^+ \\ 0 \end{pmatrix}, \quad m = 1,\ldots,n_+,$$

$-\kappa_l^-$ and

$$\hat{H}_l = \begin{pmatrix} 0 \\ \mathscr{H}_l^- \end{pmatrix}, \quad l = 1,\ldots,n_-.$$

We shall make the connection first for $H_0^1(\kappa,\omega)$, in the form of:

Theorem 1: $H_0^1(\kappa,\omega)$ has a unique solution if and only if $\hat{H}_0^1(\hat{\kappa},\Omega)$ [where Ω is related to ω by (5)] has a unique solution. The solutions of $H_0^1(\kappa,\omega)$ and $\hat{H}_0^1(\hat{\kappa},\Omega)$ are related by (4).

Proof: Suppose Ω is of the form (5) and that Φ is a solution of $\hat{\mathscr{H}}_0^1(\hat{\kappa},\Omega)$. Write it in the form

$$\Phi = \begin{pmatrix} a & b \\ c' & d' \end{pmatrix}. \tag{6}$$

Then (3) is equivalent to the two equations

$$d = \omega a, \quad c = \omega b, \tag{7}$$

and since $(\Phi - 1) \in \mathscr{H}^+$, it follows that $(a - 1) \in \mathscr{H}^+$, $(d - 1) \in \mathscr{H}^-$, $b \in \mathscr{H}^+$, $c \in \mathscr{H}^-$. Hence the pair a, d solves $H_0^1(\kappa,\omega)$, and the pair b, c solves $H_0^0(\kappa,\omega)$. The function

$$\psi = \begin{pmatrix} a + \alpha b & b \\ c' & d' + \alpha c' \end{pmatrix}$$

also solves $\hat{H}_0^1(\hat{\kappa},\Omega)$ for almost all $\alpha \in \mathbb{C}$. Therefore, if the solution of $\hat{H}_0^1(\hat{\kappa},\Omega)$ is unique, it follows by Lemma 1 that $b = c = 0$, and Φ has the form (4) where $f_\pm$ solves $H_0^1(\kappa,\omega)$. But then $f_\pm$ must be the only solution of $H_0^1(\kappa,\omega)$; if there were two, they would lead to two solutions of $\hat{H}_0^1(\hat{\kappa},\Omega)$ by (4).

Conversely, suppose that $H_0^1(\kappa,\omega)$ has a unique solution. Then that solution leads, via (4), to a solution of $\hat{H}_0^1(\hat{\kappa},\Omega)$. If $\hat{H}_0^1(\hat{\kappa},\Omega)$ has any other solution of the form (6) then the uniqueness of the solution of $H_0^1(\kappa,\omega)$ allows us to conclude from (7) by Lemma 1 that $b = c = 0$. Thus any other solution of $\hat{H}_0^1(\hat{\kappa},\Omega)$ is also of the form (4), where $f_\pm$ solves $H_0^1(\kappa,\omega)$. But these $f_\pm$ must then equal the first solution. Hence the solution of $\hat{H}_0^1(\hat{\kappa},\Omega)$ given by (4) is unique too.□

Note that if Ω has the form (5) then it satisfies Eq. (2). Conversely, if Ω has the diagonal form

$$\Omega = \begin{pmatrix} \nu & 0 \\ 0 & \omega \end{pmatrix}$$

and it satisfies (2), then $\nu = \omega'^{-1}$.

VI. REDUCTION OF H_σ^1 TO H_0^1

The Hilbert problem with poles may be reduced to one without poles. Using the set σ we construct two rational functions $\Pi_\pm^\sigma$ such that $(\Pi_\pm^\sigma - 1) \in \mathscr{M}^\pm$ with simple poles at $k = \kappa_m^\pm$, such that the ranges of their residues there equal $\mathscr{H}_m^\pm$, and $[(\Pi_\pm^\sigma)^{-1} - 1] \in \mathscr{H}^\pm$ with $\text{nul}\,(\Pi_\pm^\sigma)^{-1}(\kappa_m^\pm) = \mathscr{H}_m^\pm$, as follows.

Let $B_m^\pm = (B_m^\pm)^2 \in \tilde{\mathscr{B}}$, $m = 1,\ldots,n$, be a set of projections on $(C_m^\pm)^{-1}\mathscr{H}_m^\pm$, where

$$C_m^\pm = \left(1 + B_1^\pm \frac{2\kappa_1^\pm}{\kappa_m^\pm - \kappa_1^\pm}\right)\cdots \times \left(1 + B_{m-1}^\pm \frac{2\kappa_{m-1}^\pm}{\kappa_m^\pm - \kappa_{m-1}^\pm}\right), \tag{8}$$

then

$$\Pi_\pm^\sigma = \left(1 + B_1^\pm \frac{2\kappa_1^\pm}{k - \kappa_1^\pm}\right)\cdots\left(1 + B_n^\pm \frac{2\kappa_n^\pm}{k - \kappa_n^\pm}\right). \tag{9}$$

Clearly $\Pi_\pm^\sigma(k)$ has simple poles at $k = \kappa_m^\pm$ and nowhere else. Its residue at $\kappa_m^\pm$ is

$$R_m^\pm = 2\kappa_m^\pm C_m^\pm B_m^\pm D_m^\pm,$$

where

$$D_m^\pm = \left(1 + B_{m+1}^\pm \frac{2\kappa_{m+1}^\pm}{\kappa_m^\pm - \kappa_{m+1}^\pm}\right)\cdots \times \left(1 + B_n^\pm \frac{2\kappa_n^\pm}{\kappa_m^\pm - \kappa_n^\pm}\right).$$

Since $\text{ran}\, B_m^\pm = (C_m^\pm)^{-1}\mathscr{H}_m^\pm$, $\text{ran}\, R_m^\pm = \mathscr{H}_m^\pm$ as required. Also, since

$$(\Pi_\pm^\sigma)^{-1} = \left(1 + B_n^\pm \frac{2\kappa_n^\pm}{k + \kappa_n^\pm}\right)\cdots\left(1 + B_1^\pm \frac{2\kappa_1^\pm}{k + \kappa_n^\pm}\right),$$

$(\Pi_\pm^\sigma)^{-1}$ has all its poles in $C^\mp$, and $\Pi_\pm^\sigma$ is zero-free in $\mathbb{C}^+$. Furthermore, it is readily seen that $\text{nul}\,(\Pi_\pm^\sigma)^{-1}(\kappa_m^\pm) = \mathscr{H}_m^\pm$ and $\lim \|\Pi_\pm^\sigma\| = 1$ as $|k| \to \infty$. Thus $\Pi_\pm^\sigma$ has all the needed properties.

We remark that the projections $B_m^\pm$ are not uniquely determined by these requirements (as the kernels of the $B_m^\pm$ need not be Hermitian) and they may be chosen with other compatible properties that may be convenient.

Now define

$$f^{\sigma}_{\pm} = (\Pi^{\sigma}_{\pm})^{-1} f_{\pm}, \tag{10}$$

$$\omega^{\sigma} = (\Pi^{\sigma}_{-})^{-1} \omega \Pi^{\sigma}_{+}. \tag{11}$$

Then (1) leads to

$$f^{\sigma}_{-} = \omega^{\sigma} f^{\sigma}_{+}. \tag{1$^{\sigma}$}$$

We now pose $H^{1}_{0}(\omega^{\sigma})$. If ω is such that $(\omega - \mathbb{1}) \in \mathscr{L}$ and $(\omega^{-1} - \mathbb{1}) \in \mathscr{L}$, then ω^{σ} has the same properties, and we have

Theorem 2 (The reduction theorem): $H^{1}_{\sigma}(\omega)$ has a unique solution $f_{\pm}$, and this solution is such that $(f^{-1}_{\pm} - \mathbb{1}) \in \mathscr{M}^{\pm}$, if and only if $H^{1}_{0}(\omega^{\sigma})$ and $H^{1}_{0}{}^{*}(\omega^{\sigma})$ [where ω^{σ} is related to ω by (11)] have solutions.

Lemma 6: If $H^{1}_{0}(\omega)$ has a unique solution $f_{\pm}$, and this solution is such that $(f^{-1}_{\pm} - \mathbb{1}) \in \mathscr{M}^{\pm}$, then $(f^{-1}_{\pm} - \mathbb{1}) \in \mathscr{H}^{\pm}$.

Proof of Theorem 2: Suppose that $g_{\pm}$ solves $H^{1}_{0}(\omega^{\sigma})$, and $H^{1}_{0}{}^{*}(\omega^{\sigma})$ also has a solution. Then by Lemma 5, $g_{\pm}$ is the unique solution of $H^{1}_{0}(\omega^{\sigma})$ and it has an inverse holomorphic in $\mathbb{C}^{\pm}$. Then $f_{\pm} = \Pi^{\sigma}_{\pm} g_{\pm}$ satisfies Eq. (1), and since $g^{-1}_{\pm}$ exists, $f_{\pm}$ has the same poles in $\mathbb{C}^{\pm}$ as $\Pi^{\sigma}_{\pm}$ and its residues have the same ranges. Furthermore, $(f_{\pm} - \mathbb{1}) \in \mathscr{M}^{\pm}$ and $(f^{-1}_{\pm} - \mathbb{1}) \in \mathscr{H}^{\pm}$. If it were not unique, by Lemma 1, $H^{0}_{\sigma}(\omega)$ would have a nontrivial solution, and hence so would $H^{0}_{0}(\omega^{\sigma})$; thus $g_{\pm}$ would not be the unique solution of $H^{1}_{0}(\omega^{\sigma})$.

Conversely, suppose that $H^{1}_{\sigma}(\omega)$ has the unique solution $f_{\pm}$ and $(f^{-1}_{\pm} - \mathbb{1}) \in \mathscr{M}^{\pm}$. Then $f^{\sigma}_{\pm}$, defined by (10), satisfy Eq. (1$^{\sigma}$), and $\Pi^{\sigma}_{\pm}$ being so designed that $(\Pi^{\sigma}_{\pm})^{-1}$ annihilates the residues of $f_{\pm}$, $f^{\sigma}_{\pm}$ have no poles, and $(f^{\sigma}_{\pm} - \mathbb{1}) \in \mathscr{H}^{\pm}$. Thus it solves $H^{1}_{0}(\omega^{\sigma})$. If this solution of $H^{1}_{0}(\omega^{\sigma})$ were not unique, by Lemma 1, $H^{0}_{0}(\omega^{\sigma})$ would have a nontrivial solution, hence so would $H^{0}_{\sigma}(\omega)$ and hence, again by Lemma 1, the solution of $H^{1}_{0}(\omega)$ would not be unique. Furthermore, $(f^{\sigma}_{\pm})^{-1} = f^{-1}_{\pm} \Pi^{\sigma}_{\pm}$ so that $[(f^{\sigma}_{\pm})^{-1} - \mathbb{1}] \in \mathscr{M}^{\pm}$. Consequently by Lemma 4, $H^{1}_{0}{}^{*}(\omega^{\sigma})$ also has a unique solution.□

Proof of Lemma 6: By Theorem 2 $H^{1}_{0}(\omega^{\sigma})$ and $H^{1}_{0}{}^{*}(\omega^{\sigma})$ have solutions. The first part of the proof of Theorem 2 proves that then $(f^{-1}_{\pm} - \mathbb{1}) \in \mathscr{H}^{\pm}$.□

The use of Eqs. (10) and (11), by Theorem 2, allows us to reduce the solution of $H^{1}_{\sigma}(\omega)$ to that of $H^{1}_{0}(\omega^{\sigma})$, provided that it has a unique solution and the inverse of this solution is meromorphic. Lemma 6 implies that a unique solution of $H^{1}_{\sigma}(\omega)$ cannot have superpoles. A simple example of nonuniqueness with superpoles is provided by $\Omega = \mathbb{1}$ and $\Phi = \mathbb{1} + E(k^{2} + 1)^{-1}$, where $qEq = E$, $E^{2} = 0$.

The reduction technique may, of course, be transfered to $\hat{H}^{1}_{\Sigma}(\hat{\lambda}, \Omega)$. If Ω is defined in terms of ω as in (5) then we define

$$\Pi^{\Sigma} = \begin{pmatrix} \Pi^{\sigma}_{+} & 0 \\ 0 & \Pi^{\sigma}_{-} \end{pmatrix}, \tag{12}$$

$$\Omega^{\Sigma} = (\Pi^{\Sigma\prime})^{-1} \Omega q \Pi^{\Sigma} q, \tag{13}$$

$$\Phi^{\Sigma} = (\Pi^{\Sigma})^{-1} \Phi. \tag{14}$$

Then Ω^{Σ} is related to ω^{σ} by

$$\Omega^{\Sigma} = \begin{pmatrix} (\omega^{\sigma\prime})^{-1} & 0 \\ 0 & \omega^{\sigma} \end{pmatrix}, \tag{5$^{\sigma}$}$$

and (1$^{\sigma}$) or (3) leads to

$$\Phi^{\Sigma\prime} = \Omega^{\Sigma} q \Phi^{\Sigma} q. \tag{3$^{\Sigma}$}$$

We then have the immediate corollaries of Theorem 2 and Lemma 6:

Theorem 2′: $\hat{H}^{1}_{\Sigma}(\Omega)$ has a unique solution Φ and this solution is such that $(\Phi^{-1} - \mathbb{1}) \in \mathscr{M}^{+}$, if and only if $\hat{H}^{1}_{0}(\Omega^{\Sigma})$ and $\hat{H}^{1}_{0}{}^{*}(\Omega^{\Sigma})$ [where Ω^{Σ} is related to Ω by (13)] have solutions.

Lemma 6′: If $\hat{H}^{1}_{\Sigma}(\Omega)$ has a unique solution Φ, and this solution is such that $(\Phi^{-1} - \mathbb{1}) \in \mathscr{M}^{+}$, then $(\Phi^{-1} - \mathbb{1}) \in \mathscr{H}^{+}$.

VII. THE INDEX

The question to be answered next is whether two different Hilbert problems with the same function ω (or Ω) can both have solutions. That this is possible if the two problems differ only in the location of their poles, but not in their number, is to be expected, because that is the case in the "scalar" Hilbert problem.

Lemma 7: Let μ and σ be two sets as specified in the definition of $H^{1}_{\sigma}(\omega)$, such that[15] $\lambda_{\sigma} = \lambda_{\mu}$. If $H^{1}_{0}(\omega)$ has a unique solution $f_{\pm}$ and $(f^{-1}_{\pm} - \mathbb{1}) \in \mathscr{H}^{+}$, then $H^{1}_{\mu}(\omega)$ also has a unique solution with a holomorphic inverse.

It is clear that this Lemma has its equivalent for $\hat{H}^{1}_{\Sigma}$ but we shall not explicitly state it.

On the other hand, if the "numbers of poles," in the sense of λ_{σ} and λ_{μ}, are not equal for two sets σ and μ, then two such Hilbert problems cannot both have solutions. For this result to hold it is important that solutions with superpoles be excluded. The example given above Eq. (12) shows that if superpoles are admitted then their number may vary.

Theorem 3 (Index theorem): If $H^{1}_{\sigma}(\omega)$ and $H^{1}_{\mu}(\omega)$ have unique solutions, and the inverses of these solutions are meromorphic, then $\lambda_{\sigma} = \lambda_{\mu}$. This number will be called the *index* of ω.[16]

We shall also state its equivalent form for $\hat{H}^{1}_{\Sigma}(\Omega)$:

Theorem 3′: If $\hat{H}^{1}_{\Sigma}(\Omega)$ and $\hat{H}^{1}_{\Gamma}(\Omega)$ have unique solutions, and the inverses of these solutions are meromorphic in $\mathbb{C}^{+}$, then $\lambda_{\Sigma} = \lambda_{\Gamma}$. This number will be called the *index* of Ω.[16]

Proof of Lemma 7: Let f_{+} have a simple pole at $k = \kappa$ with residue I. Define

$$g_{+} = f_{+}\Gamma, \quad \Gamma = \mathbb{1} + C(\nu - \kappa)/(k - \nu),$$

where $C^{2} = C$. If $I(\mathbb{1} - C) = 0$ then g_{+} has no pole at $k = \kappa$, but if $\nu \in \mathbb{C}^{+}$ it has a simple pole of residue $J = f_{+}(\nu)C$ at $k = \nu$ (assuming that f_{+} has no pole or zero at ν). Thus if $\operatorname{ran}(\mathbb{1} - C) = \operatorname{nul} C = \operatorname{nul} I$ then $\dim \operatorname{ran} J = \dim \operatorname{ran} I$. We may choose an arbitrary subspace $\mathscr{H}$ with $\dim \mathscr{H} = \dim \operatorname{ran} I$ and make $\operatorname{ran} J = \mathscr{H}$ by choosing $\operatorname{ran} C = f_{+}(\nu)^{-1}\mathscr{H}$, provided only that $f_{+}(\nu)^{-1}\mathscr{H} \cap \operatorname{nul} I = \{0\}$. If we choose $\operatorname{ran}(\mathbb{1} - C) \supset \operatorname{nul} I$ with $n = \dim \operatorname{ran} C < \dim \operatorname{ran} I$ then g_{+} has a simple pole at $k = \kappa$ whose residue $I(\mathbb{1} - C)$ is such that $\dim \operatorname{ran}[I(\mathbb{1} - C)] = \dim \operatorname{ran} I - n$ and it also has a simple pole at $k = \nu$ with residue $J = f_{+}(\nu)C(\nu - \kappa)$, such that $\dim \operatorname{ran} J = n$. Thus the sum of the dimensions of the ranges of the residues at the poles at g_{+} equals that of f_{+}.

Now if $f_{\pm}$ satisfies (1) then so does $g_{\pm}$, where

$$g_- = f_- \Gamma,$$

and if $\nu \in \mathbb{C}^+$, g_- has the same poles as f_-. If $\nu \in \mathbb{C}^-$ then the dimension of the range of the residue of a pole of g_+ has been reduced by n, and a new pole of g_- has been introduced with a dimension of the range of its residue equal to n. Thus we may shift poles from g_+ to g_-. Similarly, poles may be shifted in g_- and from g_- to g_+.

Finally, if $(f_\pm^{-1} - \mathbf{1}) \in \mathscr{H}^\pm$ then $(g_\pm^{-1} - \mathbf{1}) \in \mathscr{H}^\pm$. The only pole of Γ is at κ and its residue is annihilated by $f_\pm^{-1}$.□

We shall prove the theorem in the form of Theorem 3'.

Proof of Theorem 3': By Lemma 6' the unique solutions Φ and Ψ of $\hat{H}_\Sigma^1(\Omega)$ and $\hat{H}_\Gamma^1(\Omega)$, respectively, have inverses that are holomorphic in $\mathbb{C}^+$. Define $\chi = \Psi^{-1}\Phi$. Then from (3), $\chi' = q\chi q$. Therefore χ is meromorphic in $\mathbb{C}$, and so is its inverse: $(\chi - \mathbf{1}) \in \mathscr{M}^+ \cap \mathscr{M}^-$, $(\chi^{-1} - \mathbf{1}) \in \mathscr{M}^+ \cap \mathscr{M}^-$. The poles of χ in $\mathbb{C}^+$ are those of Φ, in $\mathbb{C}^-$ those of Φ', and the poles of χ^{-1} are those of Ψ and Ψ', respectively. If any of the zeros of Ψ^{-1} (or Ψ'^{-1}) coincide with poles of Φ (or Φ') we shift them by the method used in the proof of Lemma 7.

Assume now that we have shifted the pole positions of χ, if necessary, away from zeros of Ψ^{-1} and Ψ'^{-1}. Then the dimensions of the residues of the poles of χ equals those of the corresponding ones of Φ and Φ' (and those of χ^{-1}, those of Ψ and Ψ'). We now remove the poles of χ stepwise. Without loss of generality we may assume that the sum of the dimensions of the nullspaces at the zeros of χ is not smaller than the sum of the dimensions of the ranges of the residues at its poles. Let λ be a zero of χ, and κ a simple pole with residue R. Let $B = B^2$ be the projection on a one-dimensional subspace (spanned by η) of ran R such that $B\chi(\lambda) = 0$. This projection exists, provided that ran $R \not\subset$ ran $\chi(\lambda)$. If necessary we use the method given in the proof of Lemma 7 to change ran R. Define

$$\Pi_1 = \mathbf{1} + B\left(\frac{\lambda - \kappa}{k - \lambda}\right), \quad \chi_1 = \Pi_1 \chi.$$

Since $B\chi(\lambda) = 0$, χ_1 is analytic at λ. At $k = \kappa$, χ_1 has a simple pole with residue $R_1 = (\mathbf{1} - B)R$. Therefore ran $R_1 \subset$ ran R. Furthermore, if $\exists$ a such that $\eta = R_1 a$ then $\eta = R_1 a = (\mathbf{1} - B)Ra$, and hence $B\eta = 0$; and if $\eta = R\alpha$ then $R_1\alpha = (\mathbf{1} - B)R\alpha = (\mathbf{1} - B)\eta = 0$. Thus η is not in ran R_1, and dim ran R_1 = dim ran $R - 1$. Since $\chi_1(\lambda) = \chi(\lambda) + (\lambda - \kappa)B\chi'(\lambda)$, where $\chi' = d\chi/dk$, and $B\chi(\lambda) = 0$, $\chi_1(\lambda)a = 0$ implies $\chi(\lambda)a = 0$ and $B\chi' a = 0$; therefore dim nul $\chi_1(\lambda)$ = dim nul $\chi(\lambda) - 1$. [nul $\chi(\lambda) \cap$ nul $\chi'(\lambda) = \{0\}$ because the poles of Ψ are simple.]

This procedure is repeated until all the poles of χ have been removed. The remaining factor χ_r must then, by Lemma A5, equal 1. In each step the dimensions of the ranges of the residues of χ and of its nullspaces have been lowered by 1; therefore the sums of these dimensions are equal.□

The class of Hilbert problems $H_\sigma^1(\omega)$ that have a well-defined index according to this theorem is, by Theorem 2, exactly the class that is reducible to $H_0^1(\omega^\sigma)$ and $H_0^{1*}(\omega^\sigma)$, and as we shall now see, that is solvable by a linear integral equation. This does not, however, mean that a direct method is available for determining if a given function ω (or Ω) has an index, and if so, what its numerical value is. We shall return to this question in a more restricted context in Sec. IX.

VIII. SOLUTION OF $\hat{H}_0^1$ BY AN INTEGRAL EQUATION

We now reduce the solution of $\hat{H}_0^1$ to the solution of a linear integral equation, which is a generalization of Marchenko's fundamental equation.

Theorem 4: Suppose that Ω has the properties assumed in $\hat{H}_0^1(\Omega)$. Define

$$G(\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[\Omega(k) - \mathbf{1}]qe^{ik\alpha}; \tag{15}$$

let $\mathscr{G}$ and $\mathscr{G}_\#$ be the operators on $L^2(\mathbb{R}_+) \otimes \hat{\lambda}$ whose kernel functions, $\mathbb{R}_+ \otimes \mathbb{R}_+ \to \tilde{\mathscr{B}}(\hat{\lambda})$, are $G(\alpha,\beta) = G(\alpha + \beta)$ and $G_\#(\alpha,\beta) = G(-\alpha - \beta)$, respectively. Suppose further that $\mathscr{G}$, $\tilde{\mathscr{G}}$, $\mathscr{G}_\#$, and $\tilde{\mathscr{G}}_\#$ are compact. Then:

(a) The four problems $\hat{H}_0^1(\Omega)$, $\hat{H}_0^{1*}(\Omega)$, $\hat{H}_0^1(\Omega')$, $\hat{H}_0^{1*}(\Omega')$ have solutions if and only if neither $\mathscr{G}^2$ nor $\mathscr{G}_\#^2$ has the eigenvalue 1.

(b) These solutions are unique and the solution of $\hat{H}_0^1(\Omega)$ is given by

$$\Phi(k) = \mathbf{1} + \int_0^\infty d\alpha\,\eta(\alpha)e^{ik\alpha}, \tag{16}$$

where η is the unique solution in $\mathscr{L}$ of the integral equation for $\alpha \geqslant 0$,

$$\eta(\alpha) = G(\alpha)q + \int_0^\infty d\beta\,G(\alpha + \beta)\eta(\beta)q. \tag{17}$$

The solutions of $\hat{H}_0^{1*}(\Omega)$, $\hat{H}_0^1(\Omega')$, and $\hat{H}_0^{1*}(\Omega')$ are analogously given in terms of $G_\#$, G', and $G'_\#$.

(c) If 1 is in one of the spectra of $\mathscr{G}^2$ and $\mathscr{G}_\#^2$ but not in both, then $\hat{H}_0^1(\Omega)$ and $\hat{H}_0^{1*}(\Omega)$ do not both have solutions, and neither do both $\hat{H}_0^1(\Omega')$ and $\hat{H}_0^{1*}(\Omega')$.

We remark that the solutions of $\hat{H}_0^1(\tilde{\Omega})$ and $\hat{H}_0(\Omega^{-1})$ are determined by (a) and (b).

Proof of Theorem 4: (a) Suppose first that $\hat{H}_0^1(\Omega)$, $\hat{H}_0^{1*}(\Omega)$, $\hat{H}_0^1(\Omega')$, and $\hat{H}_0^{1*}(\Omega')$ have solutions. By Lemma 5 they are unique. Let Φ solve $\hat{H}_0^1$ and define

$$\eta(\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[\Phi(k) - \mathbf{1}]e^{-ik\alpha}, \tag{18}$$

which exists in the $\mathscr{L}$ sense; since $(\Phi - \mathbf{1}) \in \mathscr{H}^+$, $\eta(\alpha) = 0$ for $\alpha < 0$. Now Eq. (3) may be written

$$\Phi' - \mathbf{1} = \Omega - \mathbf{1} + (\Omega - \mathbf{1})q(\Phi - \mathbf{1})q + q(\Phi - \mathbf{1})q,$$

the Fourier transform of which reads[17]

$$\eta = Gq + G * \eta' q + q\eta' q. \tag{19}$$

For $\alpha > 0$ this equation, explicitly written out, is Eq. (17), since $\eta'(\alpha) = \eta(-\alpha) = 0$ for $\alpha > 0$. In operator form we may write it on $\mathbb{R}_+$

$$\eta = Gq + \mathscr{G}\eta q, \tag{17'}$$

or once iterated,

$$\eta = Gq + \mathscr{G}G + \mathscr{G}^2\eta. \tag{17''}$$

Suppose now that 1 were in the spectrum of $\mathscr{G}^2$. It follows that ϵ, $\epsilon^2 = 1$, is in the spectrum of $\mathscr{G}$; let ν be a corresponding eigenfunction, $\mathscr{G}\nu = \epsilon\nu$, with components ν_1 and

ν_2. The function

$$\mu = \begin{pmatrix} \nu_1 & -\epsilon\nu_1 \\ \nu_2 & -\epsilon\nu_2 \end{pmatrix}$$

then satisfies $\mathcal{G}\mu q = -\mu$. Let ξ be its Fourier transform,

$$\xi(k) = \int_0^\infty d\alpha \mu(\alpha) e^{ik\alpha}.$$

The equation $\mathcal{G}\mu q = -\mu$ then implies, by Lemma A4, that

$$\xi' + \Omega q \xi q = \gamma \in \mathcal{H}^+$$

and it follows from (2) that γ satisfies the equation

$$\gamma' = \Omega' q \gamma q.$$

Therefore γ is a solution of $\hat{H}_0^0(\Omega')$. But since by assumption $\hat{H}_0^1(\Omega')$ and $\hat{H}_0^{1*}(\Omega')$ both have solutions, by Lemma 5 the solution of $\hat{H}_0^1(\Omega')$ is unique, and by Lemma 1, the only solution of $\hat{H}_0^1(\Omega')$ is $\gamma = 0$. Consequently $\mu = 0$, and the supposition that 1 is in the spectrum of $\mathcal{G}^2$ is false. Similarly it follows that 1 is not in the spectrum of $\mathcal{G}_\#^2$.

(b) Conversely, suppose that neither $\mathcal{G}^2$ nor $\mathcal{G}_\#^2$ have the eigenvalue 1. Since $(\Omega - \mathbf{1}) \in \mathcal{L}$ implies that $G \in \mathcal{L}$, and since $\mathcal{G}$ is compact, the inhomogeneity in (17″) is in $\mathcal{L}$ and hence (17″) has a unique solution

$$\eta = (\mathbf{1} - \mathcal{G}^2)^{-1}(Gq + \mathcal{G}G);$$

thus

$$\mathcal{G}\eta q = \mathcal{G}(\mathbf{1} - \mathcal{G}^2)^{-1}G - Gq + (\mathbf{1} - \mathcal{G}^2)^{-1}Gq = \eta - Gq,$$

and the solution of (17″) solves (17′), i.e., (17). If (17) had more than one solution then its homogeneous form would have a nontrivial solution, and hence so would that of (17″). Therefore the absence of 1 in the spectrum of $\mathcal{G}^2$ guarantees the existence of a unique solution in $\mathcal{L}$ of (17); its transpose is the unique solution in $\mathcal{L}$ of the transpose of (17).

Let η be this solution; then Φ, defined by (16), by Lemma A4, is such that

$$\Phi' - \Omega q \Phi q = \Psi \in \mathcal{H}^+.$$

It follows from (2) that Ψ satisfies the equation

$$\Psi' = -\Omega' q \Psi q. \tag{20}$$

Define

$$\xi(\alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, \Psi(k) e^{-ik\alpha}.$$

Then, just as (3) leads to (17), so (20) leads to the homogeneous integral equation for $\alpha \geqslant 0$,

$$\xi(\alpha) = -\int_0^\infty d\beta\, G(-\alpha - \beta)\xi(\beta) q,$$

or in operator form, $\xi = -\mathcal{G}_\# \xi q$, or iterated, $\xi = \mathcal{G}_\#^2 \xi$. But since by assumption $\mathcal{G}_\#$ is compact and 1 is not in the spectrum of $\mathcal{G}_\#^2$, $\mathcal{G}_\#^2$ is also compact and 1 is not in its spectrum. Consequently $\xi = 0$, and hence $\Psi = 0$. Thus Φ satisfies (3), and by Lemma A4, $(\Phi - \mathbf{1}) \in \mathcal{H}^+$; therefore it solves $\hat{H}_0^1(\Omega)$. In the same manner we solve $\hat{H}_0^{1*}(\Omega)$, to which $\mathcal{G}_\#$ is related exactly as $\mathcal{G}$ is to $\hat{H}_0^1$. By Lemma 5 therefore the solution Φ of $\hat{H}_0^1$ is unique. Similarly for $\hat{H}_0^1(\Omega')$ and $\hat{H}_0^{1*}(\Omega')$.

Part (c) is proved by recognizing that if $\mathcal{G}_\#^2$ does not have the eigenvalue 1 but $\mathcal{G}^2$ does, then the homogeneous integral equation that corresponds to (20) can only have the trivial solution and hence $\Psi = 0$. As a result, the nontrivial solution of the homogeneous form of (17) leads to a nontrivial solution of $\hat{H}_0^0(\Omega)$, and hence $\hat{H}_0^1(\Omega)$ cannot have a unique solution, by Lemma 1, and so by Lemma 5, $\hat{H}_0^1(\Omega)$ and $\hat{H}_0^{1*}(\Omega)$ cannot both have solutions. Similarly if $\mathcal{G}_\#^2$ has the eigenvalue 1 but $\mathcal{G}^2$ does not, and for $\hat{H}_0^1(\Omega')$ and $\hat{H}_0^{1*}(\Omega')$.□

IX. THE CASE OF HILBERT–SCHMIDT OPERATORS

If $\mathcal{H}$ is a Hilbert space and very much stronger assumptions are made on ω then Fredholm determinants may be defined and the index (if it exists) may be determined directly from ω without solving a Hilbert problem. This is done as follows.

Lemma 8: Suppose that $\mathcal{H}$ is a Hilbert space, that Ω has all the properties assumed in Theorem 4, and in addition, $\|\Omega - \mathbf{1}\|_2 \in L^2(\mathbb{R})$ (where $\|\cdot\|_2$ denotes the Hilbert–Schmidt norm), $\mathrm{tr}\,(\Omega - \mathbf{1}) \in L^2(\mathbb{R})$ (where tr denotes the trace), and $\mathcal{G}$ is Hilbert–Schmidt. Then the solution Φ of $\hat{H}_0^1(\Omega)$ is such that $\|\Phi - \mathbf{1}\|_2 \in L^2(\mathbb{R})$, $\mathrm{tr}\,(\Phi - \mathbf{1}) \in L^2(\mathbb{R})$, and for $k \in \mathbb{C}^+$, $\|\Phi(k) - \mathbf{1}\|_2 < \infty$, $\mathrm{tr}\,[\Phi(k) - \mathbf{1}]$ is holomorphic, $\lim \|\Phi(k) - \mathbf{1}\|_2 = 0$ and $\lim \mathrm{tr}\,[\Phi(k) - \mathbf{1}] = 0$ as $|k| \to \infty$.

Proof: Since $\|\Omega - \mathbf{1}\|_2 \in L^2(\mathbb{R})$ from (15), $\|G\|_2 \in L^2(\mathbb{R}_+)$. Because furthermore by assumption $\|\mathcal{G}\|_2 < \infty$, it follows from (17) that $\|\eta\|_2 \in L^2(\mathbb{R}_+)$, and hence by (16) $\|\Phi - \mathbf{1}\|_2 \in L^2(\mathbb{R})$ as well as $\|\Phi - \mathbf{1}\|_2 < \infty$ for $k \in \mathbb{C}^+$ and $\lim \|\Phi - \mathbf{1}\| = 0$ as $|k| \to \infty$. Taking the trace of (17) we get for $\alpha > 0$

$$\mathrm{tr}\,\eta = \mathrm{tr}\,Gq + \mathrm{tr}\,\mathcal{G}\eta q.$$

We have

$$\begin{aligned} &\int_0^\infty d\alpha |\mathrm{tr}\,[(\mathcal{G}\eta q)(\alpha)]|^2 \\ &\quad = \int_0^\infty d\alpha \left| \int_0^\infty d\beta\, \mathrm{tr}\, G(\alpha + \beta)\eta(\beta) q \right|^2 \\ &\quad \leqslant \int_0^\infty d\alpha \left(\int_0^\infty d\beta \|\eta(\beta) q\|_2 \|G(\alpha + \beta)\|_2 \right)^2 \\ &\quad \leqslant \int_0^\infty d\alpha \int_0^\infty d\beta \|G(\alpha + \beta)\|_2^2 \int_0^\infty d\gamma \|\eta(\gamma)\|_2^2 \\ &\quad < \infty, \end{aligned}$$

so $\mathrm{tr}\,\mathcal{G}\eta q \in L^2(\mathbb{R}_+)$. Also $\mathrm{tr}\,Gq \in L^2(\mathbb{R}_+)$ because by assumption $\mathrm{tr}\,(\Omega - \mathbf{1}) \in L^2(\mathbb{R})$. Consequently $\mathrm{tr}\,\eta \in L^2(\mathbb{R}_+)$, and hence by (16), $\mathrm{tr}\,(\Phi - \mathbf{1}) \in L^2(\mathbb{R})$, $\mathrm{tr}\,(\Phi - \mathbf{1})$ is holomorphic in $\mathbb{C}^+$ and tends to zero as $|k| \to \infty$ there.□

Corollary. If Ω^Σ satisfies the assumptions of Lemma 8 [where Ω^Σ is defined by (13)], then $\alpha = \det \Omega$ and $\gamma = \det \Phi$ (where det denotes the Fredholm determinant) exist, $(\alpha - 1)$ and $(\gamma - 1) \in L^2(\mathbb{R})$, γ is the boundary value of an analytic function meromorphic in $\mathbb{C}^+$, and $\lim \gamma(k) = 1$ as $|k| \to \infty$. The total number of its poles in $\mathbb{C}^+$ counting an mth-order pole m times, equals λ_Σ.

This corollary follows immediately from Lemma 8 and the properties of the Fredholm determinant.

Now note that Eq. (3) implies that $\alpha = \gamma'/\gamma$. Therefore, on the one hand,

$$\int_{-\infty}^{\infty} d \log \alpha(k) = -2 \int_{-\infty}^{\infty} d \log \gamma(k),$$

and on the other hand, completing the contour in $\mathbb{C}^+$ by a large semicircle,

$$\int_{-\infty}^{\infty} d \log \gamma(k) = 2\pi i \nu,$$

where ν is the total number of zeros of $\gamma(k)$ in $\mathbb{C}^+$, minus the total number of its poles there; $\nu = \lambda_\Sigma$. Writing $\alpha = |\alpha| e^{i\beta}$, and assuming that Ω is continuous, this leads to

$$\beta(\infty) - \beta(0) = 2\pi\lambda_\Sigma,$$

or by Theorem 3', to

Theorem 5: If Ω satisfies the assumptions of Lemma 8 and is continuous then

$$\arg \det \Omega(\infty) - \arg \det \Omega(0) = 2\pi\lambda, \tag{21}$$

where λ is the index of Ω as defined by Theorem 3'. (It is assumed here that arg det Ω is defined so as to be continuous.)

This theorem has its immediate analogue for ω in $H^1_\sigma(\omega)$:

Theorem 5': If ω is continuous and such that Ω, as defined by (5), satisfies the hypotheses of Lemma 8, then

$$\arg \det \omega(\infty) - \arg \det \omega(-\infty) = 2\pi\lambda, \tag{22}$$

where λ is the index of ω as defined by Theorem 3. (It is assumed that arg det ω is defined so as to be continuous.)

These theorems are the analog of what is known in scattering theory as Levinson's theorem.[11] If the assumption that tr $(\Omega - \mathbb{1}) \in L^2(\mathbb{R})$ is dropped then one can still get analogous results for modified Fredholm determinants but they are more complicated to state and to prove.

Note that Eq. (2) implies det $\Omega' = 1/\det \Omega$. It therefore follows from Theorem 5 that Ω and Ω' cannot both have positive indices. Theorem 3' then implies that we have the

Corollary to Theorem 5: If both $\hat{H}^1_\Sigma(\Omega)$ and $\hat{H}^1_\Gamma(\Omega')$ have unique solutions and the inverses of these solutions are meromorphic in $\mathbb{C}^+$ then $\Sigma = \Gamma = \emptyset$, i.e., both indices vanish.

The following interesting question remains unanswered: Is the vanishing of the left-hand side of (21) a sufficient condition for $\hat{H}^1_0(\Omega)$ and $\hat{H}^1_0(\Omega')$ to have unique solutions?

X. APPLICATION TO THE THREE-DIMENSIONAL INVERSE SCATTERING PROBLEM

The following family of Hilbert problems arises in the inscat problem for the Schrödinger equation in three dimensions. The space $\mathcal{A} = L^p(S^2)$, $p > 4$, where S^2 is the unit sphere in $\mathbb{R}^3$, and a point on S^2 is denoted by θ. Let $Q \in \mathcal{B}(\mathcal{A})$ be defined by $(Qf)(\theta) = f(-\theta)$ for $f \in \mathcal{A}$. If S is the S matrix and $S_x = E_x S E_x^{-1}$, where E_x is the operator (on $\mathcal{A}$) of multiplication by $\exp(ik\theta\cdot x)$, $x \in \mathbb{R}^3$, then S_x is unitary and satisfies the relations $S'_x = S^*_x$, $\tilde{S}_x = QS_xQ$. The Hilbert problem of interest is $H^1_\sigma(\tilde{S}^*_x)$, and if it has a unique solution $f_\pm$ then, $f_- = Qf'_+Q$.

In the reduction of $H^1_\sigma(\omega)$, $\omega = \tilde{S}^*_x$, to $H^1_0(\omega^\sigma)$ one requires the projections B^x_m on $(C^x_m)^{-1}\mathcal{H}^x_m$, where $\mathcal{H}^x_m = E^x_m \mathcal{H}_m$, and E^x_m is the operator of multiplication by $\exp(\kappa_m \theta\cdot x)$, $-\kappa_m^2$ being an eigenvalue. As a result, B^x_m depends on x. This x dependence is much more complicated if the kernel of B^x_m is required to be Hermitian than it would be if no such requirement were imposed. In Refs. 7 and 8 the only Hilbert problem considered was the one stated above, and the kernel of ω^σ was also restricted to be unitary. This requires the kernel of B^x_m to be Hermitian.

We may now drop this restriction and construct the projections B^x_m successively as follows: Let $(\mathbb{1} - B_m)\mathcal{H}_m = 0$. Then

$$B^x_1 = E^x_1 B_1 E^{-x}_1,$$

$$C_2 = \{\mathbb{1} + B_1[2\kappa_1/(\kappa_2 - \kappa_1)]\}$$

$$B^x_2 = E^x_1 C^{-1}_2 E^{-x}_1 E^x_2 B_2 E^{-x}_2 E^x_1 C_2 E^{-x}_1, \text{ etc.}$$

The kernels of the resulting operators $\Pi^\sigma_\pm$ will not be unitary, but the problem $H^1_\sigma(\tilde{S}^*_x)$ can be transformed to $\hat{H}^1_\Sigma$ and then reduced to $\hat{H}^1_0$, with no need for Hermitian projections B^x_m.

XI. APPLICATION TO A THREE-DIMENSIONAL INVERSE SPECTRAL PROBLEM

If the Hilbert problem that leads from the S matrix to the generalized Jost function[6–8] has a solution then there exists a uniquely defined "regular" solution ϕ of the Schrödinger equation in three dimensions that is an entire analytic function of k and has the symmetry $\phi' = Q\phi$. This solution obeys a Parseval relation with the spectral weight function $d\rho$. The inverse spectral (inspec) problem consists of the construction of the potential in the Schrödinger equation from a given $d\rho$. It is solved by solving a generalization of the linear Gel'fand–Levitan (GL) equation.[6–8] An alternative method for the solution of the inscat problem consists of the construction of $d\rho$ from a given S matrix via the generalized Jost function as an intermediary, and the subsequent solution of the inspec problem by means of the GL equation.

On the other hand, an alternative procedure for the solution of the inspec problem that has not hitherto been considered is to attempt to find the generalized Jost function from the spectral function $d\rho$, to construct the S matrix, and then to use the generalized Marchenko equation to solve the inscat problem. The relatively complicated structure of the generalized GL equation makes this a method of some interest.

According to Ref. 6, Eq. (7.13), the spectral function is expressed as

$$\frac{d\rho}{dE} = \begin{cases} (2\pi)^{-3} \tfrac{1}{2} k Q M(k) Q, & E > 0, \\ \sum_m M_m \delta(E + \kappa_m^2), & E < 0, \end{cases}$$

in terms of the generalized Jost function,[18]

$$M = (\tilde{J}J^*)^{-1} \tag{23}$$

and M_m is an operator of finite rank such that its kernel is $M_m(\theta,\theta') = \Sigma_b X^b_m(\theta) X^{b*}_m(\theta')$. The function $J(k), \mathbb{R} \to \mathcal{B}(\mathcal{A})$, $\in \mathcal{H}^+$ and it has simple zeros at $k = i\kappa_m$ such that the $X^b_m, b = 1,\ldots,N_m$, span its nullspace there. The *scale* of the X^b_m is defined by Eq. (5.20) of Ref. 6.

On the other hand, the S matrix is expressed in terms of J as[6–8]

$$S = QJ^{-1}QJ',$$

and the generalized Marchenko procedure allows a unique construction of the underlying potential in the Schrödinger equation from S.

It is clear from this account that if, in general, J^{-1} were uniquely determined by (23) together with the positions of its poles and the ranges of its residues, then $d\rho$ would contain redundant information, namely, the scale of the X_m^b. This is consistent with the realization that if the Hilbert problem $H_\sigma^1(M)$ is posed then the expected solution $f_+(k) = J(k)$, $f_-(k) = [\tilde{J}^*(k^*)]^{-1}$, is such that f_+ has *zeros*, and hence by Lemma 2 it cannot be unique.

In the absence of bound states, however, there is no such obstacle. In that case, if M satisfies the requisite conditions, $H_0^1(M)$ may be reduced to the solution of a linear integral equation by the method contained in Theorems 1 and 4, and the inspec problem may be solved by the tools of the inscat problem. If there are bound states then no such procedure is known.

APPENDIX: ANALYTIC AUXILIARIES

If f is an analytic function, $\Delta \to \mathscr{B}(\mathscr{h})$, $\Delta \subset \mathbb{C}$, then $f^{\dagger *}$ is an analytic function, $\Delta \to \mathscr{B}(\mathscr{h}^\dagger)$, whose kernel is the transpose of that of f; its restriction to $\mathscr{h}$ equals $\tilde{f}$.[19] Since $\tilde{f}$ is an operator $\mathscr{h} \to \mathscr{h}^\dagger$ it will be regarded as an analytic function only if $\tilde{f} \in \mathscr{B}$.

The inverse f^{-1} (in the operator sense) of an analytic function f is an analytic function except if one of three possibilities occurs:

(a) $f(\kappa)$ has a zero. In that case $f(\kappa)^{-1}$ does not exist.

(b) Zero is in the residual spectrum of $f(\kappa)$, i.e., $f^\dagger(\kappa)$ has a zero. Then ran $f(\kappa)$ decomposes $\mathscr{h} = \mathscr{h}_0 \oplus \text{ran } f(\kappa)$, $\mathscr{h}_0 \neq \{0\}$, and the left inverse of $f(\kappa)$ either is undefined on $\mathscr{h}_0$ or it has a zero; in neither case can it be its right inverse.

(c) Zero is in the continuous spectrum of $f(\kappa)$. In that case $f(\kappa)^{-1}$ exists but is not in $\mathscr{B}$.

In all three cases $f(\kappa)^{-1}$ is not analytic at $k = \kappa$. If $\tilde{f}$ is analytic and has a zero at κ then $f^{\dagger *}$ also has a zero and hence f^{-1} is not analytic there.

If in some region Δ, f is meromorphic and has a simple pole at κ, then so does $f^{\dagger *}$, and either f^{-1} and $f^{\dagger *-1}$ have zeros at κ, or f^{-1} and $f^{\dagger *-1}$ have simple poles, or both. [That is, there may be two vectors a and $b \in \mathscr{h}$ such that $f^{-1}a$ has a pole at κ and $\lim f(k)^{-1}b = 0$ as $k \to \kappa$.]

We shall state and then prove a sequence of lemmas that are needed.

Lemma A 1: If f and g are analytic functions, $\mathbb{C} \to \mathscr{B}$, holomorphic in an open region $\Delta \subset \mathbb{C}$, such that f is zero-free in Δ and $fg = \mathbb{1}$, then $gf = \mathbb{1}$, i.e., $f = g^{-1}$ in Δ.

Lemma A 2: Suppose f and g are analytic in an open set Δ and $fg = gf = \mathbb{1}$ there. Let κ be a boundary point of Δ such that $\exists A \in \mathscr{B}$ and $Af_0 = \mathbb{1}$, where $f_0 \in \mathscr{B}$, $\lim \|f(k) - f_0\| = 0$ as $k \to \kappa$. Then $f_0 A = \mathbb{1}$ and $\lim \|g - A\| = 0$ as $k \to \kappa$.

This lemma implies that a region in $\mathbb{C}$ in which both f and f^{-1} are analytic cannot have limit points at which zero is in the residual spectrum of f.

Lemma A 3: If $(f - \mathbb{1}) \in \mathscr{H}^+$ then for sufficiently large $|k|$, $f^{-1}(k)$ exists, is analytic, and as $|k| \to \infty$ in $\mathbb{C}^+$, $\lim \|f^{-1}(k) - \mathbb{1}\| = 0$.

Lemma A 4: If $f(\alpha) \in \mathscr{L}$ then $g(k) = \int_0^\infty d\alpha\, f(\alpha) e^{ik\alpha} \in \mathscr{H}^+$.

Lemma A 5: If $f \in \mathscr{H}^+ \cap \mathscr{H}^-$ then $f = 0$. (This lemma may be regarded as a generalization of a Corollary of Liouville's theorem.)

Proof of Lemma A 1: $gf = \mathbb{1}$ would be false only if at some point $\kappa \in \Delta$ $\mathscr{h}$ nontrivially decomposes, $\mathscr{h} = \mathscr{h}_0 \oplus \text{ran } g(\kappa)$, and either $\text{nul } f(\kappa) = \mathscr{h}_0$ or $\text{dom } f(\kappa) = \text{ran } g(\kappa)$. But f being holomorphic, $\text{dom } f = \mathscr{h}$ everywhere in Δ, and $\text{nul } f = \{0\}$ by hypothesis.□

Proof of Lemma A 2: $g = A + A(f_0 - f)g$ implies

$$\|g\| \leqslant (\|A\|)/(1 - \|A\|\,\|f - f_0\|)$$

so that $\|g(k)\|$ remains bounded as $k \to \kappa$. Then $A - g = A(f - f_0)g$ and hence $\|A - g\| \leqslant \|A\|\,\|g\|\,\|f - f_0\| \to 0$. Finally, $(f - f_0)g + f_0(g - A) = \mathbb{1} - f_0 A$ implies $\|\mathbb{1} - f_0 A\| \leqslant \|g\|\,\|f - f_0\| + \|f_0\|\,\|g - A\| \to 0$, and hence $f_0 A = \mathbb{1}$.□

Proof of Lemma A 3: Since $\lim \|f - \mathbb{1}\| = 0$ as $|k| \to \infty$, for $|k|$ sufficiently large $f^{-1}(k)$ exists and is holomorphic. Then $f^{-1} - \mathbb{1} = (f^{-1} - \mathbb{1})(\mathbb{1} - f) + (\mathbb{1} - f)$ and therefore

$$\|f^{-1} - \mathbb{1}\| \leqslant (\|f - \mathbb{1}\|)/(1 - \|f - \mathbb{1}\|) \to 0.\square$$

Proof of Lemma A 4: By Parseval's theorem $g \in \mathscr{L}$. Take $k = \lambda + i\nu > 0$, and $u \in \mathscr{h}$. Then by Schwarz's inequality

$$\|g(k)u\|^2 \leqslant \left(\int_0^\infty d\alpha\, \|f(\alpha)u\| e^{-\nu\alpha} \right)^2$$

$$\leqslant \int_0^\infty d\alpha\, \|f(\alpha)u\|^2 \int_0^\infty d\beta\, e^{-2\nu\beta} \leqslant C\|u\|\nu^{-1}$$

and similarly for $\tilde{g}u$ and their derivatives. Hence $g(k)u$ and $\tilde{g}(k)u$ are analytic in $\mathbb{C}^+$, and therefore, so are $g(k)$ and $\tilde{g}(k)$. Since for all $u \in \mathscr{h}$

$$\|g(k)u\| \,/\, \|u\| \leqslant C\nu^{-1}$$

it follows that $\lim \|g(k)\| = 0$ as $\nu \to \infty$.□

Proof of Lemma A 5: $f \in \mathscr{H}^+$ implies that $g(\alpha) = \int_{-\infty}^{\infty} dk\, f(k) e^{ik\alpha}$ exists as a function in $\mathscr{L}$ and $g(\alpha) = 0$ for $\alpha > 0$. Similarly, $f \in \mathscr{H}^-$ implies that $g(\alpha) = 0$ for $\alpha < 0$. But the only L^2 function with support at one point is $g = 0$. Hence $f = 0$.□

ACKNOWLEDGMENT

This work was supported in part by the National Science Foundation under Grant No. PHY 80-20457.

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[4] See particularly, Refs. 5–9. Earlier references can be found there. The problem discussed here is more general than that solved in Ref. 8.

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[11]N. Levinson, K. Dan. Vidensk. Selsk., Mat.-Fys. Medd. **25** (9).
[12]What we have specifically in mind is an L^p space, $p \geqslant 2$, of complex-valued functions on some given compact space, e.g., the unit sphere in $\mathbf{R}^n$. Note that then $\mathcal{H}^\dagger = L^q$, $q^{-1} + p^{-1} = 1$, $\mathcal{H}^\dagger \supset \mathcal{H}$, and $\mathcal{H}$ is dense in $\mathcal{H}^\dagger$.
[13]$\mathbf{C}^\pm$ denote the open upper and lower halves of the complex plane.
[14]We shall deal with *simple* poles only, but a generalization should not be difficult.
[15]See the statement of $H^1_\sigma(\mathcal{H},\omega)$ in Sec. III for the definition of λ_σ.
[16]This definition differs by a minus sign from that customary in the matrix case.
[17]Here $*$ denotes a convolution.
[18]Note that the notation in Refs. 7 and 8 differs from that in Ref. 6, and what is called J here and in Refs. 7 and 8 corresponds to $\bar{J}$ in Ref. 6.
[19]We are using here Ref. 12.

A class of discontinuous integrals involving Bessel functions

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(Received 13 April 1981; accepted for publication 11 September 1981)

A general theorem, which appears to be newly discovered although it is of a very classical sort, gives simple evaluations for a large class of infinite integrals containing Bessel functions in product with other suitably constrained analytic functions.

PACS numbers: 02.30. + g

Consider the following two classes of infinite integrals involving Bessel functions, where b is a real positive number:

$$I_1 = \int_0^\infty dt\, t^{\mu+1} J_\mu(bt) f(t),$$

$$I_2 = \int_0^\infty dt\, t^{\mu} N_\mu(bt) f(t). \tag{1}$$

There may be constraints upon the values of μ and upon $f(t)$ in order to give convergence of the integrals at the end points; although in many instances one may add the convergence factor $e^{-\epsilon t}$ and take the limit $\epsilon \to 0+$. The following three conditions are imposed upon the otherwise arbitrary functions $f(t)$.

(i) $f(t)$ is an analytic function in the right half-plane, Re $t \geqslant 0$;
(ii) $f(t)$ is an even function along the imaginary axis,
$f(it) = f(-it)$; (2)
(iii) $f(t)$ is bounded for large $|t|$ by $e^{a|\mathrm{Im}\, t|}$ and $b > a \geqslant 0$.

In the nomenclature of Boas,[1] $f(t)$ is an even entire function of exponential type a.

Theorem: The integrals I_1 and I_2 vanish.

The proof involves writing the Bessel functions J_μ and N_μ as linear combinations of the Hankel functions $H_\mu^{(1)}$ and $H_\mu^{(2)}$ and then, by virtue of the assumed analyticity, moving the contour of the $H_\mu^{(1)}$ integral up to the positive imaginary axis and the contour of the $H_\mu^{(2)}$ integral down to the negative imaginary axis. The portions of the contour integrals along the arc at infinity vanish by condition (iii); and the portions along the two halves of the imaginary axis cancel by virtue of condition (ii) plus the identity

$$(+i)^\mu H_\mu^{(1)}(+it) = -(-i)^\mu H_\mu^{(2)}(-it). \tag{3}$$

COMMENTS

As regards the integral I_1, the theorem can be extended to include negative real values of b and the condition (which gives rise to the identification of these as "discontinuous" integrals) reads

$$|b| > a \geqslant 0. \tag{4}$$

A familiar theorem in Fourier transforms gives

$$\int_{-\infty}^{\infty} dt\, e^{ibt} F(t) = 0, \tag{5}$$

where $F(t)$ is any entire function of exponential type a and $|b| > a$. This may be seen as a special case of our theorem, by combining the integrals I_1 for the two cases $\mu = +\frac{1}{2}$ and $\mu = -\frac{1}{2}$. It is also possible to restate our theorem in the language of Hankel transforms but this does not appear to add anything new.

The most powerful application of the theorem comes from the following.

Corollary: If condition (i) is relaxed to allow some poles in the integrals I_1 and I_2, then we get the residues picked up in moving the contours as described in the above proof.

For example, assuming the complex number z lies in the first quadrant [and f subject to the conditions (2)]

$$\int_0^\infty dt\, t^{\mu+1} J_\mu(bt) f(t)/(t^2 - z^2) = \tfrac{1}{2}\pi i z^\mu H_\mu^{(1)}(bz) f(z), \tag{6a}$$

$$\int_0^\infty dt\, t^{\mu} N_\mu(bt) f(t)/(t^2 - z^2) = \tfrac{1}{2}\pi z^{\mu-1} H_\mu^{(1)}(bz) f(z). \tag{6b}$$

Alternatively, taking x on the real positive axis and using the Principal Value prescription, we find the pair of integral transforms:

$$\text{P.V.}\int_0^\infty dt\, t^{\mu+1} J_\mu(bt) f(t)/(t^2 - x^2) = -\tfrac{1}{2}\pi x^\mu N_\mu(bx) f(x), \tag{7a}$$

$$\text{P.V.}\int_0^\infty dt\, t^{\mu} N_\mu(bt) f(t)/(t^2 - x^2) = \tfrac{1}{2}\pi x^{\mu-1} J_\mu(bx) f(x). \tag{7b}$$

FURTHER COMMENTS

Other interesting relations can be gotten from (6) by differentiating with respect to z, or by taking the Fourier transform with respect to z, or by taking the limit $z \to 0$:

$$\int_0^\infty dt\, t^{\mu-1} J_\mu(bt) f(t) = \frac{2^{\mu-1}}{b^\mu}\Gamma(\mu) f(0), \tag{8}$$

Re $\mu > 0$.

Looking at the standard reference books[2,3] and tables[4–8] of known integrals with Bessel functions one will find a great many particular results that fall within the theorem and corollary given here. Examples of the sorts of functions $f(t)$ encountered are

$$t^{2N};\ J_\nu(at) t^{-\nu};\ J_\nu(a(t^2 + p^2)^{1/2})(t^2 + p^2)^{-(1/2)\nu} \tag{9}$$

and products of these. Generalized hypergeometric functions of the type

$${}_nF_{n+1}(r_1, r_2, \ldots, r_n; s_1, s_2, \ldots, s_{n+1};\ -\tfrac{1}{4}a^2(t^2 + p^2)) \tag{10}$$

also satisfy the conditions given. The possibilities are endless.

It is most surprising that I have not been able to find any prior mention of the general results reported in this paper.

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I would also guess that the theorem could be extended to consider a class of functions larger than the Bessel functions as the kernel of the integrals.

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The commutant of a multiplication operator

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(Received 18 May 1982; accepted for publication 30 July 1982)

We determine the class of all operators commuting with a multiplication operator defined by a general piecewise continuous strictly monotonic function.

PACS numbers: 02.30.Bi, 03.65. — w

1. INTRODUCTION AND NOTATIONS

Let q be a real function defined on the finite interval $[a,b]$. Every such function defines in the space $L_2(a,b)$[1] a multiplication operator Q defined by $(Qf)(x) = q(x)f(x)$. In quantum mechanics, every multiplication operator Q corresponds to a potential field with the value $q(x)$ at the point $x\in[a,b]$.[2]

In the present paper we determine the class of all bounded operators A acting in the space $L_2(a,b)$ and commuting with a given multiplication operator Q. This class of operators is called the commutant[3] of Q. We recall that the commutant of Q (precisely, the self-adjoint elements of it) consists of the operators corresponding to observables that can be simultaneously measured with a potential given by $q(x)$.[2] It is easy to see that if q is a continuous strictly monotonic function on a bounded subset J of the real line R (i.e., separating the points of J) then, each linear bounded operator A commuting with q is a multiplication operator (see Refs. 3 and 4), i.e., there exists a function $a(x)$ such that

$$(Af)(x) = a(x)f(x) \quad \forall f\in L_2(J).$$

2. COMMUTANT OF n-PIECEWISE STRICTLY MONOTONIC FUNCTIONS

Let q be a continuous function. We say that q is an n-piecewise strictly monotonic function if there exists a subdivision of the interval $[a,b]$ by the n-points

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b,$$

such that q is strictly monotonic on each subinterval $[x_{i-1},x_i]$.

We recall that the commutant of 2-piecewise strictly monotonic function is determined in Ref. 4. Here we determine the commutant of a general continuous n-piecewise strictly monotonic function for arbitrary finite n.

Arrange the set of numbers $\{q(x_0), q(x_1),...,q(x_n)\}$ in ascending order giving them the new symbols $\{y_i, i = 0,1,2,...,k\}$;

$$y_0 < y_1 < y_2 < \cdots < y_k, \quad k\leqslant n.$$

Let $i_1 < i_2 < \cdots < i_{n_j}$, $n_j \leqslant n$ be the subset of $\{1,2,...,n\}$ such that the interval

$$I_m^{(j)} = q^{-1}(y_{j-1},y_j)\cap(x_{i_m-1},x_{i_m}) \neq \varnothing,$$
$$m = 1,2,...,n_j,$$

where $\varnothing$ denotes the empty set and $q^{-1}(y_{j-1},y_j) = \{x:q(x)\in(y_{j-1},y_j)\}$ (see Fig. 1). The collection of subintervals

$$\{I_m^{(j)}, \quad j = 1,2,...,k; \quad m = 1,2,...,n_j\}$$

can be partitioned into k equivalence classes by introducing the equivalence relation R defined by

$$I_{m_1}^{(j_1)} R I_{m_2}^{(j_2)} \Leftrightarrow q(I_{m_1}^{(j_1)}) = q(I_{m_2}^{(j_2)}),$$

where

$$q(I_{m_i}^{(j_i)}) = \{y = q(x): x\in I_{m_i}^{(j_i)}\}, \quad i = 1,2.$$

It is easy to verify that this is an equivalence relation.[5] The equivalence classes are

$$\mathscr{E}_j = \{I_1^{(j)}, I_2^{(j)},...,I_{n_j}^{(j)}\}, \quad j = 1,2,...,k.$$

It is clear that $\cup_{j=1}^{k}\cup_{m=1}^{n_j} I_m^{(j)}$ coincides with the interval $[a,b]$ except for the endpoints of the subintervals $I_m^{(j)}$ which is a finite set (i.e., has a Lebesgue measure 0).

Introduce a transformation p defined almost everywhere (a.e.) on the interval $[a,b]$ (except at the set of endpoints of $I_m^{(j)}$) by the rule: for all $x\in I_m^{(j)}, px\in I_{(m+1)(\mathrm{mod}\ n_j)}^{(j)}$ such that $q(px) = q(x)$, i.e., every point x belonging to some interval $I_m^{(j)}$ goes to the point $\bar{x} = px$ in the following subinterval of the same equivalence class where the numeration is taken modulo n_j[5] (i.e., the last subinterval is mapped into the first in the same equivalence class). In this case, it is clear that

$$p^{n_j}x = x \quad \forall x\in \bigcup_{m=1}^{n_j} I_m^{(j)} \quad \text{and} \quad \forall j\in\{1,2,...,k\}.$$

Taking N equal to the least common multiple of $\{n_1,n_2,...,n_k\}$, we see that (except at the endpoints of $I_m^{(j)}$)

$$p^N x = x \quad \text{a.e} \quad \forall x\in[a,b],$$

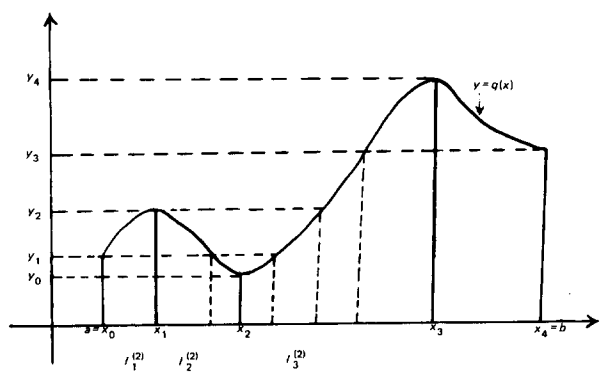

FIG. 1. An n-piecewise strictly monotonic function with $n = 4$, $k = 4$; $n_1 = 2$, $n_2 = 3$, $n_3 = 1$, $n_4 = 2$; $N = 6$.

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i.e., $p^N = e$ (a.e.), where e is the identity transformation. Consequently, $\{e, p, p^2,...,p^{N-1}\}$ forms a cyclic group of transformations of $[a,b]$ into itself.[5]

The transformation p generates an operator P acting on $L_2(a,b)$ by the formula

$$(Pf)(x) = f(px) \quad \forall f \in L_2(a,b)$$

[$f(px)$ is well defined as a function in $L_2(a,b)$, since it is defined a.e.].

The family $\{E, P, P^2,...,P^{N-1}\}$ forms a cyclic group of operators on $L_2(a,b)$, where E is the unity operator and $P^N = E$.

Lemma 1: The N roots of the unity $\{1, \omega, \omega^2,...,\omega^{N-1}\}$, $\omega = \exp\{2\pi i/N\}$ are the eigenvalues of the operator P.

Proof: Consider the eigenvalue problem $Pf = zf$. Since $P^N = E$, we have $z^N = 1$, i.e., the eigenvalues lie in the set of the N roots of the unity $\{1, \omega,...,\omega^{N-1}\}$. It remains to show that $\forall s \in \{0,1,2,...,N-1\}$, the value ω^s is an eigenvalue of P, i.e., has a corresponding nonzero eigenvector. In fact, $\forall f \in L_2(a,b)$ the function

$$f_s = \frac{1}{N} \sum_{r=0}^{N-1} \omega^{s(N-r)} P^r f, \tag{1}$$

is easily seen to be nonzero for some $f \in L_2(a,b)$ and satisfies the relation

$$\begin{aligned} Pf_s &= \frac{1}{N} \sum_{r=0}^{N-1} \omega^{s(N-r)} P^{r+1} f \\ &= \frac{1}{N} \left[\sum_{r=0}^{N-2} \omega^{s(N-r)} P^{r+1} f + \omega^s f \right] \\ &= \frac{1}{N} \left[\sum_{r=1}^{N-1} \omega^{s(N-r+1)} P^r f + \omega^s f \right] \\ &= \omega^s \frac{1}{N} \left[\sum_{r=1}^{N-1} \omega^{s(N-r)} P^r f + f \right] = \omega^s f_s. \end{aligned}$$

i.e., f_s is an eigenvector corresponding to the eigenvalue ω^s. ■

Denote by M_s the eigenspace corresponding to the eigenvalue ω^s for $s = 0,1,2,...,N-1$.

Lemma 2: The space $L_2(a,b)$ can be represented as the direct sum of the eigenspaces $\{M_s, s = 0,1,2,...,N-1\}$,

$$L_2(a,b) = M_0 \oplus M_1 \oplus \cdots \oplus M_{N-1},$$

where $\oplus$ denotes the direct sum.

Proof: Let $f \in L_2(a,b)$ be an arbitrary element. We have to prove that (see Ref. 5) f can be uniquely represented in the form

$$f = \sum_{s=0}^{N-1} f_s, \quad f_s \in M_s. \tag{2}$$

Taking f_s in the form of (1), we see that

$$\begin{aligned} \sum_{s=0}^{N-1} f_s &= \frac{1}{N} \sum_{s=0}^{N-1} \sum_{r=0}^{N-1} \omega^{s(N-r)} P^r f \\ &= \frac{1}{N} \sum_{r=0}^{N-1} P^r f \sum_{s=0}^{N-1} \omega^{s(N-r)} \\ &= \frac{1}{N} f \sum_{s=0}^{N-1} \omega^{sN} + \frac{1}{N} \sum_{r=1}^{N-1} P^r f \sum_{s=0}^{N-1} \omega^{s(N-r)} \\ &= f + \frac{1}{N} \sum_{r=1}^{N-1} P^r f \frac{1-\omega^{N(N-1)}}{1-\omega^{N-r}} = f. \end{aligned}$$

The uniqueness of the representation (2) of f is proved as follows. Let

$$f = \sum_{s=0}^{N-1} f'_s, \quad f'_s \in M_s. \tag{3}$$

Subtracting (3) from (2) and putting $f_s - f'_s = g_s$, we get

$$\sum_{s=0}^{N-1} g_s = 0, \quad g_s \in M_s.$$

Acting, successively, on the last relation by $P, P^2,...,P^{N-1}$ and noting that $P^r g_s = \omega^{r\cdot s} g_s$, we get a system of N homogeneous equations

$$\sum_{s=0}^{N-1} \omega^{r\cdot s} g_s = 0, \quad r = 0,1,2,...,N-1, \tag{4}$$

whose determinant of coefficients is

$$\begin{vmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega^{1\cdot 1} & \omega^{1\cdot 2} & \cdots & \omega^{1\cdot(N-1)} \\ 1 & \omega^{2\cdot 1} & \omega^{2\cdot 2} & \cdots & \omega^{2\cdot(N-1)} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & \omega^{(N-1)\cdot 1} & \omega^{(N-1)\cdot 2} & & \omega^{(N-1)\cdot(N-1)} \end{vmatrix}.$$

This determinant, being a special case of van der Monds determinant, is equal to the product

$$\prod_{0<r<N-1,\ 0<s<N-1,\ r<s} (\omega^r - \omega^s),$$

which is different from 0. From this, it follows that the system of Eqs. (4) has only the zero solution $g_0 = g_1 = \cdots = g_{N-1} = 0$. Hence, $f_s = f'_s$, for all $s = 0,1,2,...,N-1$. ■

Lemma 3: For every $s \in \{0,1,2,...,N-1\}$, the subspace M_s is invariant with respect to multiplication by the function q.

Proof: Let $f_s \in M_s$ be an arbitrary element. We have

$$(P(qf_s))(x) = q(px) f_s(px) = q(x)(Pf_s)(x) = \omega^s q(x) f_s(x),$$

i.e., $qf_s \in M_s$. ■

Let $\Omega = \{J : J = I^{(1)}_{m_1} \cup I^{(2)}_{m_2} \cup \cdots \cup I^{(k)}_{m_k},\ I^{(j)}_{m_j} \in \mathscr{E}_j,\ j = 1,2,...,k\}$. Denote by $L_2(J)$ the space of all square summable functions defined on J. Let $R_{sJ}: M_s \to L_2(J)$ be the restriction mappings of M_s on J for all $s \in \{0,1,2,...,N-1\}$ and all J, then we have

Lemma 4: Each restriction mapping $R_{sJ}: M_s \to L_2(J)$ is invertible for all s and all J.

Proof: It is clear that if the restriction $f_s|_{I_{m_j}}$ of a function $f_s \in M_s$ is given, then the values of f_s on the remaining components of $\mathscr{E}_j$ can be determined from the equations

$$(P^r f_s)(x) = f_s(p^r x) = \omega^{r\cdot s} f_s(x), \quad r = 1,2,...,n_j - 1.$$

Consequently, for $J = I^{(1)}_{m_1} \cup I^{(2)}_{m_2} \cup \cdots \cup I^{(k)}_{m_k}$, if the restriction $f_s|_J$ is given then, $f_s \in M_s$ can be uniquely determined (a.e.) on the whole interval $[a,b]$ by applying, successively, the relation

$$(Pf_s)(x) = \omega^s f(x).$$

This proves that R_{sJ}^{-1} exists. ■

Let A be a linear bounded operator acting in $L_2(a,b)$ and commuting with the multiplication operator defined by the

function q. According to the decomposition (2), it is sufficient to get the law of action of A on each subspace M_s. Let M_{sJ} be the restriction of M_s on J, for all $J\in\Omega$. It is clear that $M_{sJ}=L_2(J)$. Define the operator A_{sJ} on M_{sJ} by the formula

$$A_{sJ}f_{sJ}=(Af_s)|_J \quad \text{for all} \quad f_{sJ}\in M_{sJ}, \tag{5}$$

where $f_s=R_{sJ}^{-1}f_{sJ}\in M_s$.

Lemma 5: For all $J\in\Omega$, the operator A_{sJ} acts on M_{sJ} as a multiplication operator.

Proof: Let $q_J\in M_{sJ}$ be the restriction of q on $J\in\Omega$. We show now that A_{sJ} commutes with q_J. In fact, we have $q_Jf_{sJ}=(qf_s)_J$. Using (5) and the assumption that A commutes with q we get

$$\begin{aligned}A_{sJ}q_Jf_{sJ}&=A_{sJ}(qf_s)_J=(Aqf_s)|_J=(qAf_s)|_J\\&=q_J(Af_s)_J=q_JA_{sJ}f_{sJ}.\end{aligned}$$

Since q_J is separating the points of J, therefore A_{sJ} is a multiplication operator on M_{sJ}, i.e., there exists a function b_{sJ} such that

$$A_{sJ}f_{sJ}=b_{sJ}f_{sJ} \quad \text{for all} \quad f_{sJ}\in M_{sJ}.\blacksquare \tag{6}$$

Lemma 6: For every $s\in\{0,1,2,\ldots,N-1\}$, the family of functions $\{b_{sJ};J\in\Omega\}$ is compatible in the sense that if $J_1\in\Omega$, $J_2\in\Omega$, and $J_1\cap J_2=J_0$, then $b_{sJ_1}(x)=b_{sJ_2}(x)$ for all $x\in J_0$.

Proof: We have

$$\left.\begin{aligned}A_{sJ_1}f_{sJ_1}&=b_{sJ_1}f_{sJ_1} \quad \text{for all} \quad f_{sJ_1}\in M_{sJ_1},\\A_{sJ_2}f_{sJ_2}&=b_{sJ_2}f_{sJ_2} \quad \text{for all} \quad f_{sJ_2}\in M_{sJ_2}.\end{aligned}\right\} \tag{7}$$

Taking

$$\chi_{sJ_1}=\begin{cases}1 & \text{on } J_0,\\0 & \text{on } J_1\setminus J_0,\end{cases}$$

$$\chi_{sJ_2}=\begin{cases}1 & \text{on } J_0,\\0 & \text{on } J_2\setminus J_0,\end{cases}$$

It is clear that $R_{sJ_1}^{-1}\chi_{sJ_1}=R_{sJ_2}^{-1}\chi_{sJ_2}$. Denote the resulting function by χ_s. Substituting in (7) and using the definition of the operator A_{sJ}, we get

$$(A\chi_s)|_{J_1}=A_{sJ_1}\chi_{sJ_1}=b_{sJ_1}\chi_{sJ_1},$$

$$(A\chi_s)|_{J_2}=A_{sJ_2}\chi_{sJ_2}=b_{sJ_2}\chi_{sJ_2}.$$

The last two relations imply $b_{sJ_1}|_{J_0}=b_{sJ_2}|_{J_0}.\blacksquare$

The compatibility of $\{b_{sJ},J\in\Omega\}$ permits the definition of a function $b^{(s)}$ defined a.e. on the interval $[a,b]$ such that the restriction $b^{(s)}|_J$ coincides with the function b_{sJ} defined by Lemma 5. Consequently, taking (5) in mind, we see that Eq. (6) takes the form

$$Af_s=b^{(s)}f_s \quad \forall f_s\in M_s, \quad s=0,1,\ldots,N-1. \tag{8}$$

This means that the operator A acts on M_s as a multiplication operator by the function $b^{(s)}$. Using (8) and the decomposition (2) we see that

$$Af=\sum_{s=0}^{N-1}b^{(s)}f_s \quad \text{for all} \quad f\in L_2(a,b). \tag{9}$$

Substituting from (1) in (9) and putting

$$a_r=\frac{1}{N}\sum_{s=0}^{N-1}b^{(s)}\omega^{s(N-r)},$$

we get

$$\begin{aligned}Af&=\sum_{s=0}^{N-1}b^{(s)}\frac{1}{N}\sum_{r=0}^{N-1}\omega^{s(N-r)}P^rf\\&=\sum_{r=0}^{N-1}\left(\frac{1}{N}\sum_{s=0}^{N-1}b^{(s)}\omega^{s(N-r)}\right)P^rf\\&=\sum_{r=0}^{N-1}a_rP^rf \quad \text{for all} \quad f\in L_2(a,b).\end{aligned}$$

i.e., we have proved the following.

Theorem: Every continuous n-piecewise strictly monotonic function q defines a transformation p and a natural number N such that for every linear bounded operator A commuting with the multiplication operator defined by q, there exists N functions $\{a_0,a_1,\ldots,a_{N-1}\}$ such that

$$Af=\sum_{r=0}^{N-1}a_rP^rf \quad \text{for all} \quad f\in L_2(a,b),$$

where P is the operator generated by p;

$$(Pf)(x)=f(px).$$

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Carleman embedding and Lyapunov exponents

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(Received 19 March 1982; accepted for publication 10 May 1982)

We investigate the solutions of those autonomous systems with quadratic nonlinearities in a N-dimensional vector space together with the solutions of their first variational equation systems by means of the Carleman embedding. An iterative procedure based on this result is developed to evaluate the Lyapunov exponents of the considered systems. We test the method by giving some results for the Lyapunov exponents of the Lorenz model.

PACS numbers: 02.30.Hq

I. INTRODUCTION

The concepts of Carleman embedding[1] and Lyapunov exponents are related to the study of nonlinear differential equation systems and have been intensively investigated recently.[2–6] Loosely speaking the former is a method for solving the proposed system after embedding it into an infinite set of linear equations, whereas the latter reports about the asymptotic behavior of two trajectories (with respect to each other) which are close together at the initial time.

In this paper we bring these concepts together in that we use the method of Carleman to evaluate Lyapunov exponents. We consider here those autonomous systems in a N-dimensional vector space with the form

$$\frac{dy_i}{dt} = F_i(\{y_i\}) = \sum_j a_{ij} y_j + \sum_{jl} b_{ijl} y_j y_l, \quad i,j,l = 1,2,\ldots,N, \tag{1}$$

where the a_{ij} and the b_{ijl} are constant.

System (1) describes many different models in hydrodynamic and chemical reactions, etc., which display nontrivial dynamics, with the presence, e.g., of strange attractors and sequences of period-doubling bifurcations. The results we get here can be easily extended to include systems with higher polynomial nonlinearities.

The central point of our method lies on the fact that the infinite matrix M (to be defined later) resulting from the Carleman embedding of the system (1) gives rise not only to the solution of (1) itself, but also to the solution of the system of first-variational equations of (1),

$$\frac{d\delta y_i}{dt} = \sum_j a_{ij}\,\delta y_j + \sum_{jl} b_{ijl}\,(y_j(t)\delta y_l + y_l(t)\delta y_j), \tag{2}$$

whose knowledge is required for the evaluation of the Lyapunov exponents. The solution of (2) indicates how the difference δy between two trajectories evolves with time, and we have explicitly written $y_j(t)$ on the rhs of (2) to call attention to the fact that it is *not* a simple autonomous linear equation system at all.

Generally one can find approximate solutions for (1) and (2) with the help of numerical techniques. The method developed here gives a clear insight into the relation between the solutions of (1) and (2), and has simplifying advantages for the numerical computing that is required if we want to give the explicit values of the Lyapunov exponents.

This article is organized as follows: In Sec. II we introduce the concept of the Carleman embedding and use it to write down the solutions of (1) and (2). The equivalence between the Taylor series solution of (2) and the one given by the Carleman embedding is explicitly proven. In the Sec. III we define the Lyapunov exponents and discuss their meaning. Finally, a discussion of the numerical procedure, some results for the Lorenz model, and concluding remarks are presented in the Sec. IV.

II. THE CARLEMAN EMBEDDING

A. The solution of the basic system

Let us write the system (1) with the help of vector notation;

$$\frac{dx}{dt} = Ax + Bx^{[2]} \tag{3}$$

where x is the column vector of N components y_i and A is the matrix of components a_{ij}. The nonlinear terms are described by the $N \times N^2$ matrix B [$B_{ik} = b_{ijl}$, where $k = (j,l)$ and is to be labeled according to the lexicographical order], and by the vector $x^{[2]} = x \otimes x$, where $\otimes$ denotes the Kronecker product. It is convenient to introduce the Lth Kronecker power by $x^{[L]} = x^{[L-1]} \otimes x, x^{[1]} = x$, as well as the matrices

$$A_L = A \otimes I^{[L-1]} + I \otimes A_{L-1}, \quad A_1 = A,$$
$$B_L = B \otimes I^{[L-1]} + I \otimes B_{L-1}, \quad B_1 = B, \quad L = 2,3,\cdots, \tag{4}$$

with I denoting the $N \times N$ identity matrix. They will appear throughout the work with the method of Carleman.

The Carleman embedding of the system (3) amounts to first considering the components of $x^{[2]}$ as independent variables, and then to writing down their equations of motion. It can be easily shown that

$$\frac{dx^{[2]}}{dt} = A_2 x^{[2]} + B_2 x^{[3]}. \tag{5}$$

Then we consider successively the $x^{[3]}$, $x^{[4]}$,···, as independent, which leads to the infinite linear system

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$$\frac{d}{dt}\begin{pmatrix} x^{[1]} \\ x^{[2]} \\ x^{[3]} \\ \vdots \end{pmatrix} = \begin{pmatrix} A_1 & B_1 & 0 & 0 & \cdots \\ 0 & A_2 & B_2 & 0 & \cdots \\ 0 & 0 & A_3 & B_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} x^{[1]} \\ x^{[2]} \\ x^{[3]} \\ \vdots \end{pmatrix}. \tag{6}$$

We write X and M for the infinite-dimensional vector and matrix appearing in (6), and let their block components be denoted by capital indices as $X_L = x^{[L]}$ and

$$M_{L,K} = A_L \delta_{L,K} + B_L \, \delta_{L,K+1} \, .$$

The component X_1 of the solution of (6) should also furnish the solution of the system (3). Nevertheless one must proceed carefully, for the system (6) may have a broader class of solutions than that of (3); e.g., one can find C^∞ solutions for (6) whose component X_1 does not satisfy (3).[7] However, the analytical solutions of (3) and of X_1 in (6) are equal, which can be shown by comparing the terms of their Taylor series.

The formal analytical solution for X in (6) is $X(t) = e^{MT} X(0)$. If we are only interested in the component X_1, we may write

$$\begin{aligned} X_1(t) &= \sum_L (e^{MT})_{1,L} \, X_L \, (0) \\ &= \sum_L \left[I + Mt + \frac{M^2 t^2}{2!} + \cdots \right]_{1,L} X_L(0) \, . \end{aligned} \tag{7}$$

We introduce now a generalized power operation between the $N \times N$ matrix A and the $N \times N^2$ matrix B which enables the writing of both the Carleman solution and the general term of the Taylor series solution of (1) and (2) in a very compact way. So, if n, $m \in Z$ we define the matrix $\langle A^n | B^m \rangle$ by

$$\langle A^n | B^m \rangle = 0 \text{ if } n \text{ or } m < 0, \tag{8a}$$

$$\langle A^0 | B^0 \rangle = I \tag{8b}$$

$$\langle A^n | B^m \rangle = \langle A^n | B^{m-1} \rangle B_m + \langle A^{n-1} | B^m \rangle A_{m+1} \, , \tag{8c}$$

where the A_n and B_m are the matrices defined in (4).

The definitions (8c) implies that the elements of $\langle A^n | B^m \rangle$ given in terms of those of A and B contain always an n-fold product of elements of A and an m-fold product of those of B.

This justifies calling the definition (8) a kind of generalized power. In particular we have $\langle A^n | B^0 \rangle = A^n$ and $\langle A^0 | B^m \rangle = B_1 B_2 B_3 \cdots B_m$.

Now it is straightforward to verify that

$$(M^n)_{1,L} = \langle A^{n+1-L} | B^{L-1} \rangle \, , \tag{9}$$

and after inserting (9) into (7) we get

$$X_1(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \sum_{L=1}^{n+1} \langle A^{n+1-L} | B^{L-1} \rangle \, X_L(0) \, . \tag{10}$$

The expression (10), which was derived only with the help of the Carleman method, constitutes also the Taylor series solution of (1), which can be directly verified by using the definition (8) to evalutate the nth time derivative of x in (1). In the next subsection we illustrate the use of the matrices defined in (8) to verify a similar result for the case of the first variational system (2).

B. The solution of the variational equation system

Now we will show the solution of (2) may be given with the help of the Carleman embedding matrix as

$$\delta x(t; x_0, \delta x_0) = \sum_{L=1}^{\infty} (e^{Mt})_{1,L} \frac{\partial X_L(0)}{\partial x(0)} \delta x_0 \, . \tag{11}$$

In order to prove Eq. (11) it is convenient to write (2) in terms of Kronecker operations to get

$$\frac{d}{dt} \delta x = A \delta x + B (x \otimes \delta x + \delta x \otimes x) \, . \tag{12}$$

Further, we define the following $N^L \times N$ matrices Y_L, $L \geqslant 1$:

$$\begin{aligned} &Y_L = X \otimes Y_{L-1} + I \otimes X^{[L-1]}, \quad L = 2,3,\cdots, \\ &Y_1 = I \, . \end{aligned} \tag{13}$$

The Y_L are very important for our proof, since it can be shown that they satisfy the relation

$$(Y_L)_{ij} = \partial (X_L)_i / \partial y_j . \tag{14}$$

We can also use the Y_L to bring (12) into a more compact form

$$\frac{d}{dt} \delta x = (A + B Y_2) \delta x \, . \tag{15}$$

The solution of (15) written with the aid of the Taylor series is

$$\delta x(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^n}{dt^n} \delta x \Big|_{t=0} \, .$$

Using the bracket operation defined in (8) and Y_L, we will show that

$$\frac{d^n}{dt^n} \delta x \Big|_{t=0} = \sum_{L=1}^{n+1} \langle A^{n+1-L} | B^{L-1} \rangle \, Y_L(0) \delta x_0 \, . \tag{16}$$

We proceed by induction over n. For $n = 1$, (16) is evident, for it reduces to (15). If we assume (16) to be valid for $n - 1$, we get

$$\frac{d^n}{dt^n} \delta x = \sum_{L=1}^{n} \langle A^{n-L} | B^{L-1} \rangle \frac{d}{dt} (Y_L \, \delta x) \, . \tag{17}$$

In order to go further we need identity (18), which can be easily derived with some algebraic manipulations with the help of Kronecker operations and of Eq. (15),

$$\frac{d}{dt} (Y_L \, \delta x) = (A_L \, Y_L + B_L \, Y_{L+1}) \delta x \, . \tag{18}$$

After inserting (18) into (17) we arrive at

$$\begin{aligned} \frac{d^n}{dt^n} \delta x &= \sum_{L=1}^{n} \langle A^{n-L} | B^{L-1} \rangle \, [A_L \, Y_L + B_L \, Y_{L+1}] \, \delta x \, , \end{aligned} \tag{19}$$

and using the definition of the bracket operation it follows that

$$\begin{aligned} \frac{d^n}{dt^n} \delta x = \sum_{L=1}^{n} & [\langle A^{n+1-L} | B^{L-1} \rangle \\ & - \langle A^{n+1-L} | B^{L-2} \rangle B_{L-1}] \, Y_L \, \delta x \\ & + \sum_{L=1}^{n} \langle A^{n-L} | B^{L-1} \rangle B_L \, Y_{L+1} \, \delta x \, . \end{aligned} \tag{20}$$

We now observe that all the terms in the second and third series cancel each other with exception of

$$-\langle A^n|B^{-1}\rangle\, B_0\, Y_1 = 0$$

and

$$\langle A^0|B^{n-1}\rangle\, B_n\, Y_{n+1} = \langle A^0|B^n\rangle\, Y_{n+1}\,.$$

Then Eq. (16) follows immediately.

The solution of (12) given by the Taylor series is thus

$$\delta x(t;x_0,\delta x_0) = \sum_{n=0}^{\infty}\sum_{L=1}^{n+1}\frac{t^n}{n!}\langle A^{n+1-L}|B^{L-1}\rangle\, Y_L(0)\delta x_0\,, \tag{21}$$

which reduces to (11) if we use (9) and (14).

The Carleman method shows very clearly the relation between the solutions of (1) and (2). This fact has not only a formal relevance, but also for practical purposes it enables the development of a numerical procedure furnishing the solutions of both equations which are required for the evaluation of the Lyapunov exponents.

III. LYAPUNOV EXPONENTS

Let us now introduce the notation which is most used when one is concerned with the problem of defining Lyapunov exponents. Let us write the solution of (3) as

$$x(t) = T^t x_0, \quad x_0 = x(t=0)\,, \tag{22}$$

where the map T^t, which describes the evolution of any point in the phase space, is the flow induced by the vector field $F(x)$. Let $DT^t x_0$ be the matrix of partial derivatives

$$(DT^t x_0)_{ij} = \frac{\partial (T^t x_0)_i}{\partial (x_0)_j}\,. \tag{23}$$

The map $DT_t x_0$ may be so interpreted: two trajectories starting at x and $x+\delta x$, where δx is a small vector, will differ by $DT^t x_0 \delta x$ at a time t. Hence DT^t entails the same information as the solution of (2), and if knowledge of the explicit form of T^t is not possible, DT^t is formed by collecting the N column eigenvectors of (2). The rhs of (2) is time dependent through $x(t)$ and by the above quoted method one can only give an approximation for DT^t which is valid only for short time intervals. On the other hand, the Carleman method enables the evaluation of DT^t by direct differentiation of T^t [identified with the time-evolution operator in (7)] as has become clear from the last section.

The concept of Lyapunov exponents of the dynamical system (1) may be introduced in different ways.[2,3,8,9] A very illustrative one is to say that the point x_0 of the phase space has Lyapunov exponents $\lambda_1 < \lambda_2 \cdots < \lambda_N$ if there exist subspaces $E_1 \subset E_2 \subset \cdots \subset E_N$ of our vector space with the following properties:

$$E_j = \left\{ \delta x \,|\, \lim_{t\to\infty}\frac{1}{t}\ln\left[\frac{\|DT^t x_0\,\delta x\,\|}{\|\delta x\|}\right] \leqslant \lambda_j \right\}, \tag{24a}$$

$$\dim E_j = j\,, \tag{24b}$$

$$\lim_{t\to\infty}\frac{1}{t}\ln\left[\frac{\|DT^t x_0 \delta x\,\|}{\|\delta x\,\|}\right] = \lambda_j$$

$$\text{if } \delta x \in E_j \text{ but } \delta x \notin E_{j-1}\,. \tag{24c}$$

Definition (24) becomes easy to visualize if we consider a linear autonomous system with real eigenvalues. In such a case the Lyapunov exponents λ_j coincide with the eigenvalues of the system. The subspace E_j is the set of all vectors which are written as linear combinations of the eigenvectors corresponding to the j smallest eigenvalues of the system.

The largest eigenvalue λ_j of E_j is projected out by (24c). Two trajectories differing by $\delta x \in E_j$ will converge or diverge according to the negative or positive sign of λ_j. Since an arbitrary vector δx will almost always belong to E_N, the λ_N is the exponent which really decides about the diverging character of the trajectories. Moreover, it is easier to evaluate than any other λ_j.

The question concerning the existence of such exponents has been answered by Oseledec.[10] The convergence of the limits in (24) is assured for almost all x_0, provided a T^t invariant measure μ exists. The concrete evaluation of Lyapunov exponents has also been investigated, e.g., in references.[2,3] Our method presented in Sec. IV goes along the line of some of the ideas of the quoted works. We make use of the Carleman method, which besides simplifying the evaluation of the DT^t, offers the possibility of easily increasing the accuracy of the numerical work.

IV. APPROXIMATE SCHEME AND DISCUSSION

The major difficulty we are faced with while working with the Carleman embedding lies in the exact determination of the time evolution operator e^{Mt} which, as has become clear from the previous discussion, is equivalent to summing up the Taylor series for the trajectory $x(t)$. However, we can use the Carleman method as a starting point for approximative schemes which are useful in connection with computing facilities. In what follows we will take the Lorenz model[11]

$$\begin{aligned}\dot{x} &= \sigma(y-x)\,,\\ \dot{y} &= -y + rx - xz\,,\\ \dot{z} &= -bz + xy\end{aligned} \tag{25}$$

as an example and evaluate its largest Lyapunov exponent λ_3. This model belongs to the class of systems described by (1), and has been chosen as testing object because some results on its Lyapunov exponents have been published, which will be used for comparison with ours.[3] In (25), σ, r, and b are constant parameters, while x, y, and z denote the variables y_i, $i = 1,2,3$.

We consider the Carleman solution (10) for the Lorenz model. Our approximation scheme starts by cutting off M to get M_s, which contains only the first $s+1$ diagonal and the s upper-diagonal blocks. Then the approximate time-evolution operator $e^{M_s t}$ (determined, e.g., by numerical methods), applied to the cut off vector formed by the first $s+1$ block components X_L, leads to an approximate trajectory which differs from the exact one by terms of the order t^{s+1}. This fact induces us to proceed as usual in the numerical methods for differential equations: If we want to integrate Eq. (1) until a time T, we divide it in subintervals at length τ such that the error introduced in the approximate solution is sufficiently small, and integrate until T step by step. The iteration procedure for the trajectory with the help of the matrix M_s is based

TABLE I. Values for the largest Lyapunov exponent of the Lorenz model with the standard values of the parameters $\sigma = 10$, $b = 8/3$, $r = 28$. s characterizes the cutoff matrix M_s and gives also the accuracy of integration, across a step τ, of the order of τ^s. We have taken $\tau = 0.01$, and the values of λ are given after a number n of 1.4×10^5 iterations. We list the results for five arbitrary trajectories, characterized by their starting points.

Start Point \ s	4	5	6
(1.0,1.0,1.0)	0.8981	0.9009	0.9023
(-0.1,27.0,0.1)	0.9084	0.8969	0.9059
(3.0,-2.0,5.0)	0.9024	0.9045	0.9017
(-9.0,11.0,12.0)	0.9011	0.9093	0.9032
(-0.1,27.0,-0.1)	0.9153	0.9089	0.9046

on the following scheme:

$$\text{(i)}\ X_1(n\tau) = \sum_{L=1}^{s+1} (e^{M_s \tau})_{1,L}\, X_L(n\tau - \tau)\,,$$
$$\text{(ii)}\ X_L(n\tau) = X_1(n\tau)^{[L]}\,. \tag{26}$$

For the Lyapunov exponents λ_3, which we will hereafter call $\lambda(x_0,\delta x)$, we have

$$\begin{aligned}\lambda(x_0,\delta x) &= \lim_{n\to\infty} \frac{1}{n\tau} \ln\left[\frac{\| DT^{n\tau} x_0\, \delta x_0 \|}{\| \delta x \|}\right] \\ &= \lim_{n\to\infty} \frac{1}{n\tau} \\ &\quad \times \ln\left[\frac{\| DT^{\tau}(x_{n-1}) DT^{\tau}(x_{n-2}) \cdots DT^{\tau}(x_0)\delta x \|}{\| \delta x \|}\right],\end{aligned} \tag{27}$$

where we have used the properties

$$DT^{(\tau+\eta)}x = DT^{\tau}(T^{\eta}x) DT^{\tau}x$$

and

$$x_n = x(n\tau)\,. \tag{28}$$

Equation (28) follows immediately from (11) in the exact summation and is valid also within our approximation scheme if τ is small and s large. Writing $DT^{\tau}(x_{n-1})\delta x_{n-1} = \delta x_n \| DT^{\tau}(x_{n-1})\delta x_{n-1} \|$, $\delta x_0 = \delta x$, we get from (27),

$$\begin{aligned}\lambda(x_0,\delta x) &= \lim_{n\to\infty} \frac{1}{n\tau} \ln\left[\prod_{k=0}^{n-1} \frac{\| DT^{\tau}(x_k)\delta x_k \|}{\| \delta x_k \|}\right] \\ &= \lim_{n\to\infty} \frac{1}{n\tau} \sum_{k=0}^{n-1} \ln \frac{\| DT^{\tau}(x_k)\delta x_k \|}{\| \delta x_k \|}\,.\end{aligned} \tag{29}$$

$\lambda(x_0,\delta x)$ is then evaluated within our scheme with the help of the expressions (26) and (29). In each step we evaluate the $X_1(n\tau)$ and the $DT^{\tau}(x_{n-1})\delta x_{n-1}$, besides the $X_L(n\tau)$, δx_n, and $DT^{\tau}(x_n)$ which are necessary to go further with the iterative procedure.

We present some of our results for the Lorenz model obtained with the help of the above described method in Tables I and II. Those in Table II may be compared with the calculations of Shimada,[3] who has obtained the same value for λ as ours. The results in the Table I, where values of λ for different start points and increasing size of the cut off matrix M_s are presented, show a rather good convergence and support the suggestion that, for the Lorenz model, λ should not depend upon the starting point.

TABLE II. Results for the Lyapunov exponent of the Lorenz model with the Shimada values for the parameters $\sigma = 16$, $b = 4$, $r = 40$. Here we have also $\tau = 0.01$ and $n = 1.4 \times 10^5$. The starting point of the trajectory used in the evaluation of λ is (1.0, 1.0, 1.0); s has the same meaning as in the Table I.

s	4	5	6
λ	1.3704	1.3620	1.3707

We see two major practical advantages in our approximation scheme. In evaluating the Lyapunov exponents we just have to work with one time-evolution operator, which takes into account both the trajectory and its variation. This makes the separate integration of the Eqs. (1) and (2) unnecessary, requires just one basic time interval τ within the procedure, ensures equal accuracy for the evaluated time development of x and δx, and reduces the sources of possible rounding off errors.

The second interesting point refers to the possibility of easily increasing the accuracy of the procedure without any further difficult than increasing the size of the cut off matrix M_s. This remains in contrast with the normally used Runge–Kutta methods: despite their major advantage of requiring only the knowledge of the first time derivative of the variables, they become increasingly complicated if we want to get higher accuracy, and new formulae must be derived for each new case.

Concluding, we point out that the Carleman embedding has provided a useful method for evaluating Lyapunov exponents of a large class of systems. It is based on a rigorous analytic result and on an iterative numerical procedure to avoid the problem of the impossibility of determining the exact time-evolution operator. Whereas the solution of (1) by means of the Carleman embedding has already been analyzed, an investigation of the interdependency between the first variational equation and the Carleman method was needed.

Moreover, the evaluation of Lyapunov exponents enables us to test the viability of iterating the Carleman method itself, for Lyapunov exponents are quantities which may be used for comparision between our results and others. On the other hand, comparing individual trajectories of systems with sensitive dependence on the initial point, as that of Lorenz, which were obtained by two different numerical methods, makes no sense at all.

ACKNOWLEDGMENT

The author thanks Professor A. Rauh for helpful discussions and suggestions.

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Fractional approximations for linear first-order differential equations with polynomial coefficients—application to $E_1(x)$

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(Received 28 July 1981; accepted for publication 30 June 1982)

A method is described to obtain fractional approximations for linear first-order differential equations with polynomial coefficients. This approximation can give good accuracy in a large region of the complex variable plane that may include all of the real axis. The parameters of the approximation are solutions of algebraic equations obtained through the coefficients of the higher and lower powers of the variable after the substitution of the fractional approximation in the differential equation. The method is more general than the asymptotical Padé method, and it is not required to determine the power series or asymptotical expansion. A simple approximation for the exponential integral is found, which gives three exact digits for most of the real values of the variable. Approximations of higher accuracy than those of other authors are also obtained.

PACS numbers: 02.30.Hq, 02.60.Gf

I. INTRODUCTION

A main problem in physics is how to find approximations to functions defined by differential equations when no explicit solutions can be found. The usual way is to find either power series, which are usually valid for only small values of the variable, or asymptotical expansions, which are convenient for large values.[1] However in many problems in physics we have to compute the function in intermediate regions, in which either both approximations are not valid or too many terms of the power series need to be used in order to get the necessary accuracy.

For a finite interval we can find the most efficient polynomial approximation by means of orthogonal polynomials (Chebyshev or Jacobi).[2-4] The τ-method gives a procedure where the parameters of the polynomial approximation are obtained by equating like powers of the variable in the differential equation. Since the number of equations are higher than unknowns they use the parameter τ related to the Jacobi or Chebyshev polynomials in order to get a system of compatible equations. This procedure leads to fractional approximations by a transformation of the variable or by the Padé procedure. On other hand, we have published recently an extension of Padé method[5,6] where both the power series and asymptotical expansions are used to give fractional approximations. These can give the proper accuracy to the function in extensive regions of the complex plane of the variable. Those regions can include the whole real axis. As an extension of our method we show in this paper how to find fractional approximations to functions which are defined by linear first order differential equations with polynomial coefficients. In this new method we do not have to determine either the power series, or the asymptotical expansions of the function. It is well known that the solution of the above differential equations can always be obtained in a form which involves two quadratures.[1,7] However those integrals can not usually be performed and the use of rational approximations can be convenient.

In our method the unknown function is substituted in the differential equation by the quotient of two polynomial functions of unknown coefficients. In this way a set of algebraic equations for the coefficients can be found. However the number of equations is in general higher than the unknowns. If we use only the lower powers of the variable as in the power series method, the result will be equivalent to finding the Padé approximation to the exact function, which is usually convenient for small values of the variable.

As a different procedure we could use the equations derived by equating to zero the coefficients of the higher powers in about the same number as the lower powers, therefore neglecting the algebraic equations coming from intermediate powers of the variable. This is similar to using the asymptotical expansion together with the power series as in the asymptotical Padé method.[5,6] Now the rational approximation will be valid for small and large values of the variables as in the plasma dispersion function case. On the other hand, the degree of numerator and denominator polynomials can not be chosen arbitrarily as in the usual Padé method and there is a compatibility equation for the degrees of both polynomials.

In this paper we consider only the first order differential equations; further extension to higher order differential equations will be dealt with elsewhere.

In our procedure, the parameters of the fractional approximation are determined directly instead of going first through a polynomial approximation as in the τ-method. For this reason, the fractional approximation is more fitted to the differential equation and not only the coefficients, but also the degrees of the polynomials numerator and denominator are dependent on the differential equation. On the other hand, since our fractional approximation behaves as the

 0022-2488/82/122276-05$02.50

function at the infinite, this is suitable to be used instead of the function when the infinite is important, for instance, when an integration to infinity is required. Furthermore, our method leads to the parameter of the approximation in a straight way by simple algebraic equation, without requirement of intermediate step, Jacobi polynomials or computational techniques. The accuracy of the approximation increases by increasing the degree of the polynomials of the fraction.

The method has many applications: A particular case would be the function $Z(z)$.[8] An additional example considered here is the exponential integral $E_1(z)$.[9–11] In this case, we have found a very simple rational approximation which gives at least three correct digits for almost all real positive values of z, except for values near zero. The function $E_1(z)$ appears very often in physical problems where the Maxwellian distribution function is used and sometimes inside a definite integral.[12] For these cases we have also obtained an approximation with an undetermined parameter to be adjusted in order to get much better results. An approximation of higher degree is also obtained in order to compare with those found by other authors. The accuracy of our method for intermediate values is similar to that using the τ-method and computational techniques. However, the behavior at infinity is much better and outside the interval of good accuracy, the behavior is more like the function. It does not happen, as in Hasting's approximation, that for values smaller than one the approximation worsens rapidly. In relation with the fractional approximations by Bellman–Luke,[11,3] our approximation is in general much better.

In Sec. II we show the general procedure for rational approximations in first-order differential equations. The exponential integral $E_1(z)$ is treated in Sec. III. The discussion of technical aspects and conclusions are given in Sec. IV.

II. THEORETICAL TREATMENT

We consider the general first-order differential equation of the type

$$\phi(z)\frac{dw}{dz} - \Phi(z)w = \psi(z), \tag{1}$$

where $\phi(z)$, $\Phi(z)$, and $\psi(z)$ are polynomials of degree l, r, s, respectively. A solution which involves two quadratures is described in many textbooks.[1,7] However, in most cases, an explicit solution can not be found.

For instance, if $\phi(z) = 1$, $\Phi(z) = 2z$ and $\psi(z) = -2$, one solution is the plasma dispersion function $Z(z)$ which is not easily calculable.[8]

In explicit form $\phi(z)$, $\Phi(z)$, and $\psi(z)$ are defined as

$$\phi(z) = \sum_{k=0}^{l} a_k z^k, \quad \Phi(z) = \sum_{k=0}^{r} b_k z^k, \quad \psi(z) = \sum_{k=0}^{s} c_k z^k. \tag{2}$$

In order to avoid singularities at $z = 0$ we will consider $a_0 \neq 0$. If that coefficient were zero, we should consider the expansion around a new point, i.e., $z + \alpha$, where now $a_0 \neq 0$.

Let us write the solution as a rational function

$$w(z) = \frac{P_n(z)}{Q_m(z)} = \frac{\Sigma_{i=0}^{n} p_i z^i}{\Sigma_{j=0}^{m} q_j z^j}. \tag{3}$$

Substituting Eq. (3) in Eq. (1) we obtain

$$\phi(z)[P_n'(z)Q_m(z) - P_n(z)Q_m'(z)] + \Phi(z)P_n(z)Q_m(z) = \psi(z)[Q_m(z)]^2. \tag{4}$$

By grouping the powers of z, the preceding equation is written as

$$\sum_{i=0}^{m+n+l-j} z^i \left[\sum_{j=0}^{i} a_{i-j} \sum_{k=0}^{j+i} (2k-j-1)p_k q_{j-k-i}\right] + \sum_{i=0}^{m+n+r} z^i \left[\sum_{j=0}^{i} b_{i-j} \sum_{k=0}^{j} p_k q_{j-k}\right] = \sum_{i=0}^{2m+s} z^i \sum_{j=0}^{i} c_{i-j} \sum_{k=0}^{j} q_k q_{j-k}, \tag{5}$$

where conventionally we consider a_i, b_j, or c_k to be zero when $i > l, j > r$, or $k > s$, respectively. Similarly p_i or q_j are zero if $i > n$ or $j > m$, respectively.

The coefficients in both sides of Eq. (5) should be equal in order that the function $w(z)$ verifies the differential equation. However, if we do that, we find in general more equations than unknowns. Therefore a method should be given in order to delete some of the equations or as in the τ-method additional unknowns shall be included. We follow the first possibility; then we need only $(m + n)$ equations, although the number of unknowns is $(m + n + 2)$. But one of the coefficients can be chosen arbitrarily because of the proportionality factor, and the initial condition gives also an equation for the p's and q's.

One way of obtaining the correct number of equations is by equating the coefficients of the powers of z from zero to $(m + n - 1)$. Thus we obtain one of the Padé approximations to the exact function $w(z)$. This approximation will be convenient for small values of the variable z, but not for large values. However, we have shown in a previous paper, that a much better approximation is obtained if we use the asymptotical expansion together with the power series.[5] The most convenient choice was to select two more terms of the power series than of the asymptotical expansion. In a similar way we now have to use the higher powers of z together with the lower powers. To keep a complete analogy, we should choose for the actual procedure more lower powers than higher powers. For instance if $(m + n)$ is odd we can select the coefficients of the powers from zero to $(m + n - 1)/2$, and the remaining equations will be obtained from the higher powers.

We look now at the highest power in z. On the left-hand side of Eq. (5) we get a number multiplied by $p_n q_m$. Since we want an equation to define the p's and q's, the only possibility is that the highest power appears on the right-hand side too. Several cases have to be considered. To simplify, let us assume first that $r > l - 1$. Now the compatibility of the equation requires that

$$m + n + r = s + 2m, \quad m = n + r - s, \tag{6}$$

thus only n could be chosen arbitrarily.

Considering now the second case, $l - 1 > r$, we have

$$m + n + l - 1 = s + 2m, \quad m = n + l - 1 - s, \tag{7}$$

and m is also determined when n is given. However, in this

case, there is incompatibility if $l-1=s$, since $m=n$ causes the coefficient of $z^{m+n+l-1}$ to become zero. We will not consider this possibility in this paper.

From our previous discussion it is clear that we can not choose m and n arbitrarily as in the usual Padé approximation. Once n is chosen, m is determined by the Eq. (6) or (7). Since the procedure for the above two cases is very similar, for clarity we will refer hereafter only to the first case. Explicitly for $(r-s)$ odd, the p's and q's are defined by the initial condition and the coefficients of the powers

$$z^0,z^1,z^2,z^3,\ldots,z^{n+(r-s-1)/2} \text{ and } z^{n+3/2+(3r-s)/2},\ldots,z^{2n+2r-s}. \tag{8}$$

In this way we obtain from the lower powers one equation more than from the higher powers. And since the initial condition defines essentially p_0, this is equivalent to an equation of the lower power. This would be equivalent to using two terms more of the power series than of the asymptotical expansion. The case when $(r-s)$ is even can be solved similarly.

Referring now to the plasma dispersion function, the differential equation is

$$Z'(z)+2zZ(z)=-2, \tag{9}$$

with the initial condition

$$Z(0)=i\sqrt{\pi}. \tag{10}$$

For $n=1$

$$Z(z)=\frac{p_0+p_1z}{1+q_1z+q_2z^2}. \tag{11}$$

We get the proper number of equations for equating the coefficients of the power z^0, z, and z^4. The values of p and q are coincident with those obtained for $Z_{31}(s)$ in Ref. 5.

For $n=2$, the equations are obtained from the coefficients of the powers z^0, z, z^2, and z^5, z^6. The result is coincident with $Z_{42}(z)$. For $n=3$, we consider z^0, z, z^2, z^3, and z^6, z^7, and z^8, and the result is $Z_{53}(z)$. As an additional case we will consider the exponential integral function, which also shows the procedure in the case where there is a singularity at the origin.

III. APPROXIMATIONS FOR THE EXPONENTIAL INTEGRAL FUNCTION

The function

$$y(x)=e^xE_1(x), \tag{12}$$

where

$$E_1(x)=\int_x^\infty \frac{e^{-u}}{u}\,du, \tag{13}$$

is a solution of the confluent hypergeometric function for $a=b=1$.[1,9] However, for our method, we prefer to consider it as a solution of the first-order differential equation

$$\frac{dy}{dx}-y=-\frac{1}{x}. \tag{14}$$

Now for $x=0$, the coefficient a_0 is zero. If we proceed as in the plasma dispersion function case, we will find that our system of equations is incompatible. Thus we have to consider the expansions at a different point. It is preferable not to specify the point at the beginning. Thus we denote by α the expansion point and we consider the new independent variable z defined as

$$x=z+\alpha, \tag{15}$$

so that

$$y(x)=w(z). \tag{16}$$

The differential equation is now

$$(z+\alpha)\frac{dw}{dz}-(z+\alpha)w=-1, \tag{17}$$

and in relation with our previous parameters

$$l=r=1, \quad s=0, \quad m=n+1. \tag{18}$$

Considering the simplest case $n=1, m=2$, the approximated function is

$$\tilde{w}_1(z)=\underset{\text{for } n=1}{\tilde{w}(z)}=\frac{p_0+p_1z}{1+q_1z+q_2z^2} \tag{19}$$

For the highest power in z, we found

$$p_1=q_2, \tag{20}$$

and from the independent term and first-order power we get

$$\tilde{w}_1(z)=\left[\left(p_0+\frac{p(\alpha)}{D(\alpha)}z\right)\Big/\left(1+\frac{q(\alpha)}{D(\alpha)}z+\frac{p(\alpha)}{D(\alpha)}z^2\right)\right] \tag{21}$$

then

$$\tilde{y}_1(x)=\frac{p_0D(\alpha)+p(\alpha)(x-\alpha)}{D(\alpha)+q(\alpha)(x-\alpha)+p(\alpha)(x-\alpha)^2}, \tag{22}$$

where

$$\begin{aligned} p(\alpha)&=-2+(1+3\alpha)p_0-\alpha^2p_0^2,\\ q(\alpha)&=(1-\alpha)+\alpha(\alpha-2)p_0+2\alpha^2{p_0}^2,\\ D(\alpha)&=2\alpha(1-\alpha p_0-\alpha{p_0}^2). \end{aligned} \tag{23}$$

The parameter p_0 is specified by the initial conditions. The point α can be chosen arbitrarily, but p_0 is related to α. For instance if we consider $\alpha=1$, then

$$p_0=eE_1(1)=0.596347, \tag{24}$$

and

$$e^xE_1(x)\cong\frac{2-2p_0-{p_0}^2-2{p_0}^3+(-2+4p_0-{p_0}^2)x}{3p_0-5{p_0}^2+(4-9p_0+4{p_0}^2)x+(-2+4p_0-{p_0}^2)x^2}, \tag{25}$$

$$e^xE_1(x)\cong\frac{0.92465+x}{0.36598+1.86142x+x^2}. \tag{26}$$

This approximation is the simplest approximation ever found of $E_1(x)$. For $x>0.45$, the larger relative error compared with the exact function is about $3\cdot10^{-3}$ for x around 10.

In Fig. 1 we are plotting in a log–log graph the relative error versus x. As a reference we are plotting also the Bellman approximation of the same degree

$$e^xE_1(x)=[(\tfrac{1}{3}+x)/(x+x^2)] \quad \text{(Bellman)}. \tag{27}$$

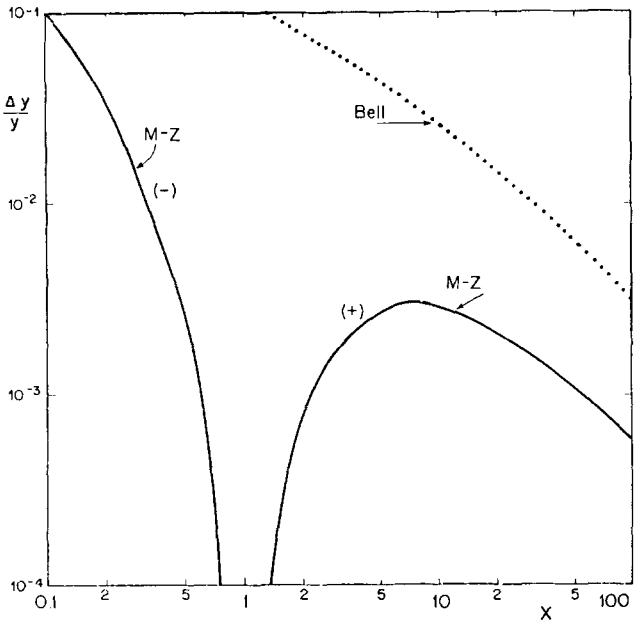

FIG. 1. Relative error of $\bar{y}_1(x) = (0.92465 + x) \times (0.36598 + 1.86142x + x^2)^{-1}$ of this work (plain line) and $\bar{y}(x) = (1/3 + x)(x + x^2)^{-1}$ of R. Bellman (pointed line) with respect to the function $e^x E_1(x)$.

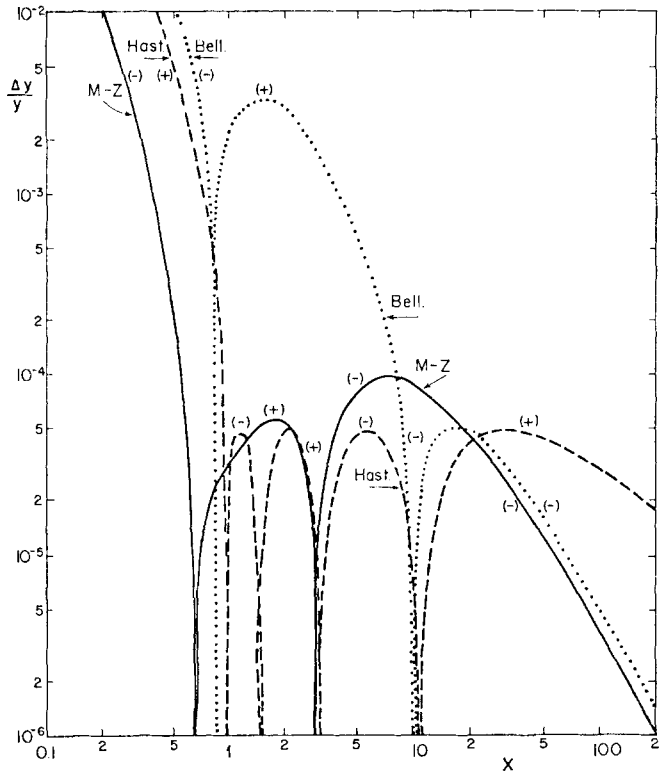

FIG. 2. Relative error of: $\bar{y}_2(x) = (1.204763 + 3.221360x + x^2) \times (0.406386 + 3.470576x + 4.221354x^2 + x^3)^{-1}$ of this work (plain line); $y(x) = (0.250621 + 2.334733x + x^2) \times (1.681534x + 3.330657x^2 + x^3)^{-1}$ of C. Hastings, Jr. (segmented line), and $y(x) = (1/16 + 2x + x^2) \times ((9/8)x + 3x^2 + x^3)^{-1}$ of R. Bellman (pointed line), with respect to the function $e^x E_1(x)$.

There are some typographical errors in the original Bellman paper that we have corrected.[13]

Considering now the approximation of the next higher degree

$$\tilde{w}_2(z) = \underset{(\text{for } n=2)}{\tilde{w}(z)} = \frac{\bar{p}_0 + \bar{p}_1 z + \bar{p}_2 z^2}{1 + \bar{q}_1 z + \bar{q}_2 z^2 + \bar{q}_3 z^3}. \tag{28}$$

From Eq. (4) or (5) we obtain the following algebraic equations:

$$\text{power } z^0\text{: } (\bar{p}_0 + \bar{p}_0\bar{q}_1 - \bar{p}_1)\alpha = 1, \tag{29a}$$

power z:

$$(\bar{p}_0 + \bar{p}_0\bar{q}_1 - \bar{p}_1) + (\bar{q}_1\bar{p}_0 + 2\bar{q}_2\bar{p}_0 - 2\bar{p}_2)\alpha = 2\bar{q}_1, \tag{29b}$$

$$\text{power } z^2\text{: } (\bar{q}_1\bar{p}_0 + \bar{p}_1 + 2\bar{q}_2\bar{p}_0 - 2\bar{p}_2) + (\bar{q}_2\bar{p}_0 + \bar{q}_1\bar{p}_1 + \bar{p}_2 + 3\bar{q}_3\bar{p}_0 + \bar{q}_2\bar{p}_1 - \bar{q}_1\bar{p}_2)\alpha = 2\bar{q}_2 + \bar{q}_1^2, \tag{29c}$$

$$\text{power } z^5\text{: } (\bar{q}_3\bar{p}_1 + \bar{q}_2\bar{p}_2 + \bar{q}_3\bar{p}_2) + (\bar{q}_3\bar{p}_2)\alpha = 2\bar{q}_2\bar{q}_3, \tag{29d}$$

$$\text{power } z^6\text{: } \bar{q}_3\bar{p}_2 = \bar{q}_3^2. \tag{29e}$$

By choosing $\alpha = 3$, we obtain

$$\begin{aligned} \bar{p}_0 &= e^3 E_1(3) = 0.2620837, \\ \bar{p}_1 &= 0.1216373, \\ \bar{p}_2 &= \bar{q}_3 = 0.1319082 \cdot 10^{-1}, \\ \bar{q}_1 &= 0.7360306, \\ \bar{q}_2 &= 0.1744005, \end{aligned} \tag{30}$$

$$e^x E_1(x) = \frac{1.204763 + 3.221360x + x^2}{0.406386 + 3.470576x + 4.221354x^2 + x^3}. \tag{31}$$

The Bellman approximation of the same degree is

$$e^x E_1(x) = \frac{\frac{1}{16} + 2x + x^2}{\frac{9}{8}x + 3x^2 + x^3}. \tag{32}$$

In Fig. 2 we plot the relative error of our approximation (M-Z Ap.) (plain line), the Hasting one (H.Ap.) of the same degree (segmented line) and the Bellman one (B.Ap.) (pointed line). For large x our approximation is better than Bellman's and much better than Hasting's. For values around one, or for intermediate values, our approximation and H.Ap. are similar (a little better H.Ap.) and both are much better than B.Ap. For values less than $x = 1$, our approximation is much better than others (except inside a narrow interval of $0.03 < x < 0.08$ in B.Ap.). The exact function $e^x E_1(x)$ becomes infinite when x goes to zero. Both H.Ap. and B.Ap. do the same and our approximation becomes finite. However H.Ap. and B.Ap. go to infinity much faster than $e^x E_1(x)$ and the error is immediately very large.

An additional advantage of our approximation in relation to H.Ap. is that all the parameters of our approximations can be obtained in a direct way without using any computer technique.

Returning to the simple general approximation given by Eq. (22), we point out that it can be useful in cases of definite integrals involving the exponential integral. The point α can be chosen now as coincident or near the lower limit of the integral. In this way the accuracy of the definite integral will be improved without using higher order polynomials.

In relation to Eq. (26) and Eq. (31), we can get an idea of the region where the approximation will fail by looking for

the poles of the denominator. The zeros of the polynomial $(0.36598 + 1.86142x + x^2)$ in Eq. (26) are on the negative real axis, therefore this approximation will be convenient on the right-hand side of the complex plane. This is in agreement with the behavior we know of $E_1(x)$, that goes logarithmically to ∞, when x goes to zero. Clearly, the approximation fails around the origin. Similarly for Eq. (31). The polynomial $(0.406386 + 3.470576x + 4.221354x^2 + x^3)$ has three real roots on the negative axis, and the approximation will be convenient on the right hand side of the complex plane.

IV. CONCLUSIONS

We have described a method of obtaining fractional approximations for the solutions of first order differential equations with polynomial coefficients. In this method the degree of the numerator polynomial $P_n(z)$ can be specified arbitrarily, but the degree of $Q_m(z)$ is determined once n is fixed. For higher values of n the accuracy of the approximation is improved.

The present method is a generalization of the asymptotical Padé method already published and the results for the plasma dispersion function are coincident. However, here we do not have to know *a priori* the power series and asymptotical expansions. In this method one of the parameters of the approximation must be determined by the initial conditions. The expansion point must be chosen to be a regular point.

We have applied the method to obtain the simplest fractional approximations for the exponential integrals, first in a general way without specifying the expansion point, and later in a particular case when $\alpha = 1$. In this case, the accuracy for most of the values is about three digits. In any case much better results can be obtained by specifying the value of the expansion point in relation to the problem to be solved. We have also obtained a second approximation one degree higher around the point $\alpha = 3$, which is much better than the approximations of the same degree published in the literature.

ACKNOWLEDGMENTS

Part of this paper was done when one of the authors (P. Martin) was on his sabbatical, first at the University of California, Los Angeles, and later at Imperial College, London, and he is greatly indebted to Professor Burton D. Fried (UCLA) and Professor Malcolm G. Haines (I.C.) for their support during this period. The authors also wish to thank Mrs. Diana Beydoun (I.C.) for typing and improving the English of the first manuscript. Research funded in part by Venezuelan Agencia CONICIT, Proj. No. 31-26-51-0606.

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[13]Corrections to Ref. 11.

Equation 1(7) (a) should read

$$Q_n(y) = 1 + \sum_{i=1}^{n} a_i y^{-i},$$

Equation 1(7) (b) should read

$$a_k = n!\,\frac{2^{-n-k}(n+1-k)}{[(n+1-k)!]^2}\prod_{l=0}^{n-k}\left(\frac{(n+1)^2-l^2}{2l+1}\right), \quad k \leqslant n.$$

$$a_k = n!, \quad k = n+1.$$

Equation 1(7) (c) should read

$$R_n(y) = P_n(y) + \sum_{i=1}^{n} a_i y^{-i} P_{n-i}(y) - a_{n+1} y^{-n-1}.$$

Equation 2(7). The denominator in the rhs should read

$$y^n |Q_n(y)|.$$

Equation 2(6). The term $-a_1 f^{(n-1)}(x)$ should read $+a_1 f^{(n-1)}(x)$.

Equation 3(4). In the lhs the denominator should read 2^{2n+i}.

Equation 3(7), 3(11), and 3(12) should read:

$$(7)\ \frac{(-1)^{n-k+1} a_{n-k+1}(k-1)!}{2^k} = \frac{n!}{2^{n+1}}\,\frac{T^{(k)}_{n+1}(-1)}{k!},$$

$$(11)\ T^{(k)}_{n+1}(-1) = (-1)^{k+n}\prod_{k=0}^{k-1}\left(\frac{(n+1)^2-k^2}{2k+1}\right), \quad k = 1,2\ldots,$$

$$= (-1)^{n+1}, \quad k = 0.$$

$$(12)\ a_k = \frac{n!2^{-n-k}(n+1-k)}{[(n+1-k)!]^2}\prod_{l=0}^{n-k}\left(\frac{(n+1)^2-l^2}{2l+1}\right), \quad k \neq n+1,$$

$$a_k = n! \quad k = n+1.$$

On the polynomial first integrals of certain second-order differential equations

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(Received 25 February 1982, accepted for publication 14 May 1982)

It is shown that *any* first integral of type $P_2(\dot{x})$—a polynomial of degree 2 in $\dot{x}$—of the differential equation $\ddot{x} = V_x$ can be obtained from a pointlike gauge symmetry of the action A_L associated to $L = \frac{1}{2}\dot{x}^2 + V(t,x)$. The same result holds for any first integral of kind $P_n(\dot{x})$ when dynamical symmetries of A_L polynomials in $\dot{x}$ are allowed. The neccessary and sufficient conditions that $V(t,x)$ must satisfy in order that $\ddot{x} = V_x$ possesses a first integral of type $P_n(\dot{x})$ have been obtained. These conditions reduce (when $n = 2$) to a condition obtained by Leach. The computational advantages and difficulties which appear in order to obtain first integrals for type $P_n(\dot{x})$ are also briefly discussed.

PACS numbers: 02.30.Jr

I. INTRODUCTION

This work has been motivated by a recent paper[1] in which Leach studied, among other things, the pointlike gauge symmetries of a Lagrangian function L of the form

$$L = \tfrac{1}{2}\dot{x}^2 + V(t,x). \tag{1}$$

The author was led to a first-order partial differential equation for $V(t,x)$ which is nothing more than the necessary and sufficient condition in order that the Lagrangian function of (1) admits a one-parameter family of pointlike gauge symmetries.

It is shown here (Sec. II) that the partial differential equation obtained in Ref. 1 is precisely the condition under which the second-order differential equation associated with (1), via the Euler–Lagrange equations, admits a first-integral quadratic in $\dot{x}$. This is important because it shows that the origin of this partial differential equation is purely algebraic, that is, the equation *arises in any method* leading to first integrals of the equation

$$\ddot{x} = V_x(t,x), \tag{2}$$

the first integrals being polynomials of degree 2 in $\dot{x}$, Now, since the method followed in Ref. 1 leads, via, the Noether theorem, to first integrals in $\dot{x}$, then $V(t,x)$ must necessarily satisfy the above mentioned condition.

It is also shown in Sec. IV that for the Lagrangians of the kind (1) any first integral of the form $P_n(\dot{x})$ (P_n being a polynomial in $\dot{x}$ of degree n) can be obtained in an infinite number of ways by considering dynamical gauge symmetries of $A_{L|_S}$ of degree n in $\dot{x}$. In order to achieve this no more restrictions on $V(t,x)$ [in addition to those required in order that Eq. (2) admits a first integral of the kind $P_n(\dot{x})$] are required. When $n = 1$ and $n = 2$ one can always achieve that the dynamical symmetries required be purely geometrical (i.e., pointlike), as those considered in Ref. 1.

The conclusion is that *only* when one is exclusively interested in obtaining the first integrals of degree 1 or 2 in $\dot{x}$, the exclusion of the dynamical symmetries [in our case the dynamical symmetires of the action integral A_L associated with (1)] is justified.

Finally, the advantages of the direct method of Sec. II over the method based on the computation of the dynamical symmetries of $A_{L|_S}$, in order to obtain first integrals of type $P_n(\dot{x})$, are discussed in Sec. V.

II. CONDITIONS IN ORDER THAT $\ddot{x} = V_x(t,x)$ ADMITS A FIRST INTEGRAL $P_n(\dot{x})$

Considering the vector field $\mathbf{X}$ given by

$$\mathbf{X} = 1\frac{\partial}{\partial t} + \dot{x}\frac{\partial}{\partial x} + V_{,x}\frac{\partial}{\partial \dot{x}},$$

associated with Eq. (2), the condition under which $P_n(\dot{x})$ be an integral of Eq. (2) can be written as

$$\mathbf{X}(P_n(\dot{x})) = 0, \tag{3}$$

and since $P_n(\dot{x})$ can be written in the form

$$P_n(\dot{x}) = \sum_{i=0}^{n} A_i(t,x)\cdot\dot{x}^i,$$

condition (3) leads to the $(n+2)$ equations

$$\begin{aligned}
&A_{0t} + A_1\cdot V_x = 0,\\
&A_{it} + A_{i-1\,x} + (i+1)A_{i+1}V_x = 0 \quad i = 1,\ldots,n-1,\\
&A_{nt} + A_{n-1\,x} = 0,\\
&A_{n\,x} = 0.
\end{aligned} \tag{4}$$

Now, from the last $(n+1)$ equations of (4) one obtains, by successive integrations with respect to the variable x, the values of $A_n(t,x),\ldots,A_0(t,x)$. Since each of these integrations introduces an arbitrary function of t, our solutions $A_n,\ldots,A_0$ depend on $(n+1)$ arbitrary functions of t. Finally, by substituting $A_0(t,x)$ and $A_1(t,x)$ in the first of equations (4) we obtain the single equation that $V(t,x)$ must satisfy in order that $P_n(\dot{x})$ be a nonbanal first integral of (2). For future reference we

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 0022-2488/82/122281-05$02.50

shall write this equation in the form

$$A_{0t} + A_1 \cdot V_{x|_S} = 0, \tag{5}$$

where the symbol $|_S$ indicates that $A_0(t,x)$ and $A_1(t,x)$ have been replaced by their values obtained via the procedure indicated above. For instance, if $n = 1$ the above procedure leads to

$$A_1 = \alpha(t) \quad A_0 = -\dot{\alpha}(t)x + \beta(t),$$

α and β being arbitrary functions of t. Therefore the condition that $V(t,x)$ must satisfy is

$$-\ddot{\alpha}x + \dot{\beta} + V_x = 0, \tag{6}$$

that is, $V(t,x)$ must have the form

$$V(t,x) = a(t)x^2 + b(t)x + c(t).$$

By the way, the generalization of this result to systems of differential equations of the form

$$\ddot{\mathbf{x}} = \nabla V(t,\mathbf{x}), \quad \mathbf{x} = (x_1,\ldots,x_m)$$

offers no difficulty, and one obtains the condition

$$-\ddot{\boldsymbol{\alpha}}(t)\cdot\mathbf{x} + \dot{\beta}(t) + \boldsymbol{\alpha}(t)\cdot\nabla V = 0,$$

while the first integral $P_1(\dot{\mathbf{x}}) = A_0(t,\mathbf{x}) + \mathbf{A}_1(t,\mathbf{x})\cdot\dot{\mathbf{x}}$, is given by

$$A_0 = -\dot{\boldsymbol{\alpha}}\cdot\mathbf{x} + \beta(t),$$

$$\mathbf{A}_1 = \boldsymbol{\alpha}(t),$$

$\boldsymbol{\alpha}(t)$ and $\boldsymbol{\beta}(t)$ being arbitrary functions of t.

When $n = 2$ one obtains from Eqs. (4),

$$A_2 = -\tfrac{1}{2}\alpha(t) \quad A_1 = \tfrac{1}{2}\dot{\alpha}x + \beta(t),$$

$$A_0 = -\tfrac{1}{4}\ddot{\alpha}x^2 - \dot{\beta}\cdot x + \alpha\cdot V - \gamma(t),$$

with α, β, and γ arbitrary functions of t. Therefore the condition to be satisfied by $V(t,x)$ is

$$\alpha\cdot V_t + (\tfrac{1}{2}\dot{\alpha}x + \beta)V_x + \dot{\alpha}V = \tfrac{1}{4}\dddot{\alpha}x^2 + \ddot{\beta}x + \dot{\gamma}. \tag{7}$$

Finally, when $n = 3$ one obtains

$$A_3 = -\lambda_3(t),$$

$$A_2 = \dot{\lambda}_3 x - \alpha/2,$$

$$A_1 = -\tfrac{1}{2}\ddot{\lambda}_3 x^2 + \tfrac{1}{2}\dot{\alpha}x + 3\lambda_3 V + \beta(t),$$

$$A_0 = \tfrac{1}{6}\dddot{\lambda}_3 x^3 - \tfrac{1}{4}\ddot{\alpha}x^2 - \dot{\beta}x + V\cdot\alpha - \int(3\dot{\lambda}_3 V + 2\dot{\lambda}_3 x V_x + 3\lambda_3 V_t)\,dx - \gamma(t), \tag{8}$$

where λ_3, α, β and γ are arbitrary functions of t. Therefore, the condition on $V(t,x)$ is given by

$$\tfrac{1}{6}\dddot{\lambda}_3\cdot x^3 - \tfrac{1}{4}\dddot{\alpha}\cdot x^2 - \ddot{\beta}x + V_t\cdot\alpha + V\dot{\alpha} - \int\left(3\frac{\partial^2}{\partial t^2}(\lambda_3 V) + \frac{\partial}{\partial t}(2\cdot\lambda_3\cdot x\cdot V_x)\right)dx - \dot{\gamma} + V_x(-\tfrac{1}{2}\ddot{\lambda}_3\cdot x^2 + \tfrac{1}{2}\dot{\alpha}x + 3\lambda_3 V + \beta) = 0,$$

that is,

$$\frac{\partial}{\partial x}\left[\dddot{\lambda}_3\frac{x^3}{6} - \frac{\ddot{\alpha}x^2}{4} - \ddot{\beta}x + V_t\cdot\alpha + V\cdot\dot{\alpha} - \dot{\gamma} + V_x\left(-\frac{\ddot{\lambda}_3}{2}x^2 + \frac{\dot{\alpha}}{2}x + 3\lambda_3 V + \beta\right)\right] = 3\frac{\partial^2}{\partial t^2}(\lambda_3\cdot V) + 2\frac{\partial}{\partial t}(x\cdot\lambda_3\cdot V_x), \tag{9}$$

which is now a nonlinear partial differential equation of second order (in V), while (7) was affine in V and its first-order derivatives. If $V(t,x)$ satisfied this equation (for convenient values of λ_3, α, β, and γ) then, $A_0,\ldots,A_3$ are immediately obtained [via (8)] by quadratures.

It is also clear that calling V_i the set formed by the functions $V(t,x)$ such that (2) admits a first integral of the type $P_i(\dot{x})$, one can obviously write $V_i \subset V_{i+1}$, even if the practical computation of all the functions $V(t,x)$ belonging to the sets V_i is quite difficult due to the complicated structure of Eq. (5) defining V_i (particularly when $i \geqslant 3$).

It would be theoretically nice to prove (or to construct a concrete counterexample disproving the proposition that follows) that any equation (2) has a first integral of type $P_n(\dot{x})$ (for certain n sufficiently high), for if this were the case the above procedure could be employed in order to obtain this first integral $P_n(\dot{x})$, possibly by quadratures. But unfortunately even if this proposition were true the practical computation of $P_n(\dot{x})$ presents difficulties due to the fact that the computation of the $(n+1)$ arbitrary functions on which $A_0,\ldots,A_n$ depends, depend in turn on the computation of solutions of differential equations which are often much more complicated than the original equation (2) we started with. This fact limits quite strongly the practical usefulness of the procedure.

Let us give an example illustrating this point. Consider the differential equation

$$\ddot{x} = t\cdot x \tag{10}$$

corresponding to the Lagrangian $L = \frac{1}{2}\dot{x}^2 + \frac{1}{2}t\cdot x^2$.

Since $V(t,x)$ has a quadratic structure in x, this differential equation certainly possesses a first integral of type $P_1(\dot{x})$. In fact $V(t,x) = \frac{1}{2}t\cdot x^2$ certainly satisfies Eq. (6) since in this case this equation reduces to

$$-\ddot{\alpha}\cdot x + \dot{\beta} + \alpha\cdot t\cdot x = 0,$$

which can certainly be satisfied by taking $\beta(t) = c$ (a constant) and $\alpha(t)$ any nontrivial solution of equation

$$-\ddot{\alpha} + \alpha t = 0. \tag{11}$$

But this last equation is of the same kind of difficulty as the original equation $\ddot{x} = t\cdot x$ we started with. Nevertheless, out of a *particular* solution of Eq. (11) one obtains (by the above procedure) a first integral of the same equation, and this is certainly an advantage.

A similar circumstance appears for Eq. (10) when we try to check out whether or not a first integral of the kind $P_2(\dot{x})$ can be found. In this case condition (7), for $V(t,x)$ given by

$$V(t,x) = \tfrac{1}{2}t\cdot x^2,$$

leads to the equation

$$\alpha\cdot x^2/2 + (\tfrac{1}{2}\dot{\alpha}\cdot x + \beta)t\cdot x + \dot{\alpha}\cdot t\cdot x^2/2 = \tfrac{1}{4}\dddot{\alpha}x^2 + \ddot{\beta}x + \dot{\gamma},$$

which can only be satisfied if α, β, and γ satisfy the system

$$\left.\begin{aligned} \tfrac{1}{2}\alpha + t\cdot\dot{\alpha} &= \tfrac{1}{4}\dddot{\alpha}, \\ \beta\cdot t &= \ddot{\beta}, \\ \dot{\gamma} &= 0. \end{aligned}\right\}$$

This system has (theoretically) infinite local solutions. The

practical computation of them is a much more serious issue. For instance if we desire a first integral of degree in $\dot{x}$ not smaller than 2, then a nontrivial solution of the equation

$$\tfrac{1}{4}\dddot{\alpha} - \dot{\alpha}t - \tfrac{1}{2}\alpha = 0$$

is necessary. Note that this equation is considerably more complicated than the original equation $\ddot{x} = tx$ under study.

These kinds of difficulties have to be taken into account and show that one cannot be too optimistic about the practical usefulness of the method.[2]

III. SYMMETRIES OF THE ACTION AND ASSOCIATED FIRST INTEGRALS

In this section we summarize the essential points leading to the Noether theorem[3] and its generalization.

Let $L(t,\mathbf{x},\dot{\mathbf{x}})$ be a nondegenerate Lagrangian (i.e., the matrix $\partial^2 L/\partial\dot{x}_i\partial\dot{x}_j$ is regular). The action integral $A_L = \int_{t_0}^{t_1} L\,dt$ is said to be gauge variant with respect to a transformation T (transforming a path $(t,x(t))$ into another path $T[t,\mathbf{x}(t)) = (t,\mathbf{x}(t))$ if a function $\Lambda_T(t,\mathbf{x},\dot{\mathbf{x}})$ can be found such that the following relation holds:

$$\int_{t_0^*}^{t_1^*} L\,dt_{|(t,\dot{\mathbf{x}}(t))} - \int_{t_0}^{t_1} L\,dt_{|(t,\mathbf{x}(t))} = \Lambda_T(P_1) - \Lambda_T(P_0),$$
$$P_0 = (t_0,\mathbf{x}(t_0),\dot{\mathbf{x}}(t_0)), \quad t_0^* = T(t_0),$$
$$P_1 = (t_1,\mathbf{x}(t_1),\dot{\mathbf{x}}(t_1)), \quad t_1^* = T(t_1), \tag{12}$$

for any path $(t,\mathbf{x}(t))$.

Consider now the one-parameter family of "dynamical transformations"[4]:

$$\tilde{t} = \mathbf{t} + \epsilon\phi(t,\mathbf{x},\dot{\mathbf{x}}),$$
$$\tilde{\mathbf{x}} = \mathbf{x} + \epsilon\psi(t,\mathbf{x},\dot{\mathbf{x}}), \tag{13}$$

where the term "dynamical" is employed because they do depend on $\dot{\mathbf{x}}$.

For this particular kind of transformation a condition to be satisfied in order that A_L be gauge variant under the family (13) is that a certain function $\Lambda_\epsilon(t,\mathbf{x},\dot{\mathbf{x}}) = \epsilon\lambda + O(\epsilon^2)$ can be found such that the following relation holds[5]

$$\frac{\partial L}{\partial t}\phi + \frac{\partial L}{\partial \mathbf{x}}\psi + \frac{\partial L}{\partial \dot{\mathbf{x}}}\theta + L\dot{\phi} = \dot{\lambda}, \tag{14}$$

where θ is defined by

$$\theta = \dot{\psi} - \dot{\phi}\cdot\dot{\mathbf{x}},$$

and the dots over ϕ, ψ, and λ indicate the total derivative with respect to t.

When condition (12) only holds for the solutions S of the Euler–Lagrange equations associated with L, condition (14) reduces to

$$\frac{\partial L}{\partial t}\phi + \frac{\partial L}{\partial \mathbf{x}}\psi + \frac{\partial L}{\partial \dot{\mathbf{x}}}\theta|_S + L\dot{\phi}\,|_S = \dot{\lambda}\,|_S, \tag{15}$$

where the symbol $|_S$ indicates that $\ddot{x}$ has to be replaced by its value obtained out of the Euler–Lagrange equations.

When (15) is satisfied we shall say that (13) is a "symmetry of $A_{L|_S}$," and under these circumstances it can be asserted that the function $I(t,\mathbf{x},\dot{\mathbf{x}})$ defined by

$$I \overset{\text{def}}{=} \frac{\partial L}{\partial \dot{\mathbf{x}}}\psi - H\cdot\phi - \lambda,$$
$$H \overset{\text{def}}{=} \frac{\partial L}{\partial \dot{\mathbf{x}}}\cdot\dot{\mathbf{x}} - L,$$

is a first integral of the Euler–Lagrange equations associated with $L(t,\mathbf{x},\dot{\mathbf{x}})$.

Moreover, assume that a certain first integral $I(t,\mathbf{x},\dot{\mathbf{x}})$ of the Euler–Lagrange equations is known. In this case the triplet

$$\left(\phi,\psi,\lambda \overset{\text{def}}{=} \frac{\partial L}{\partial \dot{\mathbf{x}}}\psi - H\phi - I\right)$$

does satisfy Eq. (15) for *any* value of $\phi(t,\mathbf{x},\dot{\mathbf{x}})$ and $\psi(t,\mathbf{x},\dot{\mathbf{x}})$.

Indeed, for the solutions of the Euler–Lagrange equations one has

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{x}}}\right) = \frac{\partial L}{\partial \mathbf{x}},$$
$$\dot{H} = -\frac{\partial L}{\partial t},$$

and on the other hand $I|_S = 0$, since I is a first integral of them; accordingly one can write

$$\begin{aligned}\dot{\lambda}\,|_S &= \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{x}}}\right)_{|_S}\cdot\psi + \frac{\partial L}{\partial \dot{\mathbf{x}}}\dot{\psi}|_S \\ &\quad - H\cdot\dot{\phi}\,|_S - \dot{H}\,|_S\cdot\phi - \dot{I}\,|_S \\ &= \frac{\partial L}{\partial \mathbf{x}}\cdot\psi + \frac{\partial L}{\partial \dot{\mathbf{x}}}\dot{\psi}|_S - H\dot{\phi}\,|_S + \frac{\partial L}{\partial t}\cdot\phi,\end{aligned}$$

and substituting the value of H we get

$$\dot{\lambda}\,|_S = \frac{\partial L}{\partial \mathbf{x}}\psi + \frac{\partial L}{\partial \dot{\mathbf{x}}}\theta|_S + L\dot{\phi}\,|_S + \frac{\partial L}{\partial t}\cdot\phi,$$

that is, Eq. (15) is automatically satisfied. Obviously the first integral associated with the triplet

$$\left(\phi,\psi,\lambda = \frac{\partial L}{\partial \dot{\mathbf{x}}}\psi - H\phi - I\right) \text{ is } I(t,\mathbf{x},\dot{\mathbf{x}}).$$

IV. APPLICATION TO THE CASE OF $L = (1/2)\dot{x}^2 + V(t,x)$

Assume now that $P_n(t,\mathbf{x},\dot{\mathbf{x}})$ is a first integral of the Euler–Lagrange equations associated with $L(t,\mathbf{x},\dot{\mathbf{x}})$, its degree (with respect to $\dot{\mathbf{x}}$) being equal to n. For instance if $L = \frac{1}{2}\dot{x}^2 + V(t,x)$ then this is certainly possible when $V(t,x)$ satisfies condition (5). In this case, and by the conclusions of Sec. III, it can be said that this first integral can be obtained as a Noether first integral provided that λ is permitted to have degree (with respect to $\dot{x}$) sufficiently high. Further, if $L(t,\mathbf{x},\dot{\mathbf{x}})$ is quadratic in $\dot{\mathbf{x}}$, $H(t,\mathbf{x},\dot{\mathbf{x}})$ will also be quadratic in $\dot{\mathbf{x}}$ and if ϕ and ψ are chosen independently of $\dot{\mathbf{x}}$ then $\lambda = (\partial L/\partial\dot{\mathbf{x}})\psi - H\phi - P_n$ has a degree equal to $\max(2,n)$. Therefore, for the case $L = \frac{1}{2}\dot{x}^2 + V(t,x)$ any first integral $P_n(\dot{x})$ can be obtained by "gauging" L with a λ of degree $\max(2,n)$. It is important to remark that this result can be achieved without any additional restrictions on $V(t,x)$. These restrictions appear only because of the requirement that Eq. (2) must possess a first integral of type $P_n(\dot{x})$.

Let us show now that for the first integral of the kind $P_2(\dot{x})$, not only ϕ and ψ but also λ can be chosen to be independent of $\dot{x}$, that is, the triplet (ϕ,ψ,λ) is purely pointlike, or

geometrical. We shall also see that this reduction is no longer possible for first integrals of the type $P_n(\dot{x})$ when $n \geqslant 3$.

Indeed, since λ and P_n are defined by

$$\lambda = \frac{\partial L}{\partial \dot{x}}\psi - H\cdot\phi - P_n,$$

$$P_n = \sum_0^n A_i(t,x)\cdot\dot{x}^i,$$

where L and H are given by:

$$L = \tfrac{1}{2}\dot{x}^2 + V(t,x),$$

$$H = \tfrac{1}{2}\dot{x}^2 - V(t,x),$$

one immediately obtains (since ϕ and ψ are free from $\dot{x}$)

$$\begin{aligned} \lambda_0 &= V\phi - A_0, \\ \lambda_1 &= \phi - A_1 \\ \lambda_2 &= -\tfrac{1}{2}\phi - A_2, \\ \lambda_k &= -A_k; \quad k \geqslant 3, \\ \lambda &\overset{\text{def}}{=} \sum_i \lambda_i(t,x)\dot{x}^i. \end{aligned} \tag{16}$$

Now, since the couple $(\phi(t,x), \psi(t,x))$ is arbitrary, it is clear that λ_1 and λ_2 can be made equal to 0, in which case the pointlike triplet is given by

$$\begin{aligned} \phi &= -2A_2(t,x), \\ \psi &= A_1(t,x), \\ \lambda &= \lambda_0 = -2A_2\cdot V - A_0. \end{aligned}$$

Therefore, any first integral of (2) quadratic in $\dot{x}$ (or affine in x) can be obtained using geometrical triplets (as those considered by Leach in Ref. 1). On the contrary, as Eqs. (16) show, for the first integrals of type $P_n(\dot{x})$, $n \geqslant 3$, the dependence of λ on $\dot{x}$ is unavoidable. Therefore, this type of first integral of (2) cannot be obtained [via the Lagrangian $\frac{1}{2}\dot{x}^2 + V(t,x)$] unless the use of triplets depending on $\dot{x}$ is allowed.

The degree in $\dot{x}$ of the triplet (ϕ,ψ,λ) can be made (when $n \geqslant 3$) less than n if ϕ and ψ are chosen of degree (with respect to $\dot{x}$) greater than 0. For example the reader can check that any first integral of type $P_3(\dot{x})$ of (2) can be obtained, via the procedure of Sec. III, [L given by (1)] out of a triplet of the kind

$$(\phi(t,x,\dot{x}),\psi(t,x,\dot{x}),\lambda(t,x,\dot{x})),$$

where ϕ, ψ, and λ are polynomials of degree 1 with respect to $\dot{x}$. In fact one can even impose that λ be identically equal to 0 (when $V \neq 0$).

The above result concerning the first integrals of Eq. (2) of type $P_n(\dot{x})$, $n < 3$, is (in general) false for the quadratic and affine integrals of the differential equations associated with $L = \frac{1}{2}\dot{\mathbf{x}}^2 + V(t,\mathbf{x})$, where $x = (x_1,\ldots,x_m)$, $m > 1$, since in this case λ is given by

$$\lambda = \frac{\partial L}{\partial \dot{\mathbf{x}}}\cdot\psi - H\cdot\phi - P_2(\dot{\mathbf{x}}),$$

and in order to achieve that λ be independent of $\dot{\mathbf{x}}$ (ϕ and ψ being functions of t and x only) $m + \frac{1}{2}m(m+1)$ conditions are to be satisfied. Since we only dispose of the $(m+1)$ undetermined functions ϕ and ψ, and $(m^2 + 3m)/2 > m + 1$, when $m > 1$, we conclude that in this case dynamical triplets are a must.

This negative result does not preclude that for a *particular* first integral of the differential equations associated with the function L,

$$L = \tfrac{1}{2}\dot{x}^2 + V(t,\mathbf{x}),$$

a pointlike triplet leading to it (via "Noether's theorem") can be found

V. FURTHER REMARKS CONCERNING THE PRACTICAL DIFFICULTIES IN THE OBTAINMENT OF A FIRST INTEGRAL OF TYPE $P_n(\dot{x})$

According to Sec. II if $V(t,x)$ satisfies condition (5), then Eq. (2) will certainly possess a first integral $P_n(\dot{x})$ of degree n with respect to $\dot{x}$. The conditions (6), (7), and (9) which V has to satisfy, when $n = 1, 2, 3$ have been obtained. Assuming that V satisfies condition (5), then, and according to Sec. IV, $P_n(\dot{x})$ can be obtained via dynamical symmetries of (when $n \geqslant 3$) and via pointlike symmetries of A_L (when $n < 3$). The question arises as to whether or not the method based on the dynamical symmetries of $A_{L|_s}$ has practical advantages over the direct method discussed in Sec. II in order to compute $P_n(\dot{x})$. Unfortunately the reply to this question is in the negative. In fact the direct method of Sec. II can only be applied once we have previously checked that $V(t,x)$ satisfies condition (5), and in order to do this a certain election of the $(n+1)$ functions appearing in Eq. (5) must be produced. Once this difficulty of selecting appropriately these functions (assuming this to be possible) has been overcome (see the examples at the end of Sec. II) then the coefficients $A_0,\ldots,A_n$ defining $P_n(\dot{x})$ are immediately obtained by quadratures. Now since condition (5) has to be always satisfied [independently of the method used in order to get the first integral $P_n(\dot{x})$ of (2)] it is clear that *any* indirect method (for instance the method based on the dynamical symmetries of $A_{L|_s}$) has disadvantages over the direct one, for in any case the first calculation to be made is to check whether or not a concrete $V(t,x)$ does or does not satisfy condition (5). But in the direct method of Sec. II it is precisely this computation (and additional quadratures) which is the *only one* necessary in order to compute $P_n(\dot{x})$, while in other indirect procedures this first step (as well as other steps, depending on the particular procedure followed) is unavoidable. For instance if the indirect procedure consists of the computation of the dynamical symmetries of $A_{L|_s}$ then it is clear from Eqs. (16) [i.e., the necessary and sufficient conditions in order that $P_n(\dot{x})$ can be obtained out of the triplet (ϕ,ψ,λ)] that this indirect procedure serves only to define the gauge function λ once the functions ϕ and ψ have been arbitrarily chosen. Therefore unless we are able to use the information contained in the function $\lambda(t,x,\dot{x})$ for other purposes this indirect procedure does not seem to offer computational advantages.

VI. SOME COMPUTATIONS CONCERNING THE DYNAMICAL SYMMETRIES OF $A_{L/s}$

As has been shown in Sec. IV any first integral of type $P_n(\dot{x})$ can be obtained out of a triplet $\phi(t,x)$, $\psi(t,x)$, $\lambda(t,x,\dot{x})$, where λ is of degree no greater than n. Assume, therefore,

that we want to compute ϕ, ψ, and λ starting from relation (15), that is, the necessary and sufficient condition in order that

$$\tilde{x} = x + \epsilon\psi(t,x),$$
$$\tilde{t} = t + \epsilon\phi(t,x)$$

be a dynamical symmetry of $A_{L|_S}$ $L = \frac{1}{2}\dot{x}^2 + V(t,x)$. In this case and for $n = 2$, ϕ, ψ, λ have to satisfy the equation

$$V_t\cdot\phi + V_x\cdot\psi + \dot{x}(\dot{\psi} - \dot{x}\dot{\phi}) + (\tfrac{1}{2}\dot{x}^2 + V)\dot{\phi} = \dot{\lambda}_0 + \dot{\lambda}_1\cdot\dot{x} + \lambda_1\cdot V_{,2} + \dot{\lambda}_2\cdot\dot{x}^2 + 2\lambda_2\cdot\dot{x}\cdot V_x, \tag{17}$$

and since ϕ and ψ are free from $\dot{x}$, (17) is equivalent to

$$V_t\cdot\phi + V_x\psi = \lambda_{0t} + \lambda_1\cdot V_x,$$
$$\psi_t + V_1\phi_x = \lambda_{0x} + \lambda_{1t} + 2V_x\cdot\lambda_2,$$
$$\psi_x - \phi_t + \tfrac{1}{2}\phi_t = \lambda_{1x} + \lambda_{2t},$$
$$-\phi_x + \tfrac{1}{2}\phi_x = \lambda_{2x}. \tag{18}$$

Solving the last three equations of this system we obtain

$$\phi = -2\lambda_2 + \alpha(t),$$
$$\psi = \lambda_1 + \tfrac{1}{2}\dot{\alpha}\cdot x + \beta(t),$$
$$\lambda_0 = \tfrac{1}{4}\ddot{\alpha}x^2 + \dot{\beta}x - 2\cdot V\cdot\lambda_2 + \gamma(t), \tag{19}$$

where $\alpha(t)$,$\beta(t)$, $\gamma(t)$, $\lambda_1(t,x)$, and $\lambda_2(t,x)$ are arbitrary functions.

Substituting (19) into (18) we get the equation

$$V_t\cdot\alpha + V_x(\tfrac{1}{2}\dot{\alpha}x + \beta) + V\cdot\dot{\alpha} = \tfrac{1}{4}\dddot{\alpha}\cdot x^2 + \ddot{\beta}\cdot x + \dot{\gamma}, \tag{20}$$

identical to Eq. (7) [that is to Eq. (17) in Ref. 1] [via the substitutions α, β, γ, $V(x)\to\rho^2$,b,c, $-V(q)$].

Now, Eq. (17) of Ref. 1 was obtained using only a pointlike function of gauge and Eq. (20) using a function λ of gauge quadratic in $\dot{x}$. It is this coincidence of the restrictions imposed on $V(t,x)$ in both cases what led us to suspect:

(i) that may first integral of type $P_2(\dot{x})$ could be obtained using exlusively pointlike triplets;

(ii) that the origin of condition (7), and in general of condition (5), was related directly to Eq. (2), and not to techniques arising by introducing pointlike or dynamical symmetries of a Lagrangian function.

The reader can check that condition (9) for V, when $n = 3$, can also be obtained by the same indirect procedure used in this section either starting from a triplet of the kind

$$(\phi(t,x),\psi(t,x),\lambda(t,x,\dot{x})),$$

where the degree in $\dot{x}$ of λ is equal to 3, or starting with a triplet of type

$$(\phi(t,x,\dot{x}),\psi(t,x,\dot{x}),\lambda(t,x,\dot{x})),$$

where ϕ, ψ, λ are polynomials in $\dot{x}$ of degree 1.

VII. FINAL REMARK

Starting from the Lagrangian (1) and considering pointlike triplets $\phi(t,x)$, $\psi(t,x)$, $\lambda(t,x)$, Noether's theorem leads to a first integral of (2) quadratic in $\dot{x}$. Therefore, $V(t,x)$ must satisfy the corresponding relation (7) of Sec. II in order that (2) can possess a first integral of this type. Conversely, as was shown in Sec. IV, if $V(t,x)$ satisfies this relation then a pointlike triplet leading to it (via Noether's theorem) can be found. Therefore, condition (7) not only guarantees than L admits a nontrival gauge-variant triplet of pointlike character but, what is more important, it guarantees that any first integral of the kind $P_2(\dot{x})$ (and not only a subset of them) can be obtained (theoretically at least, in view of the practical difficulties signaled at the end of Sec. II) in this way. The same thing can be asserted of the first integrals of the kind $P_n(\dot{x})$ when the pointlike symmetries of A_L are substituted by the dynamical symmetries of $A_{L|S}$. Therefore, pointlike symmetries of A_L are too restrictive in order to obtain first integrals of (2) of type $P_n(\dot{x})$, $n\geqslant 3$. The same thing happens with the first integrals of type $P_2(\dot{\mathbf{x}})$ of the differential equations associated with $L = \frac{1}{2}\dot{\mathbf{x}}^2 + V(t,\mathbf{x})$,$x = (x_1,\ldots,x_m)$,$m > 1$.

An interesting problem (of theoretical character) has appeared and remains unaddressed: the problem of constructing a concrete $V(t,x)$ such that Eq. (2) has no integrals of type $P_n(\dot{x})$, for every natural number n, such that $V(t,x)$ does not satisfy Eq. (5) for every value of n.

Final comment: The contents of Sec. II, and in particular the contribution by H. R. Lewis and P.G. L. Leach of Sec. III, seem to be, according to the referee not new. See *Nonlinear Problems: Present and Future*, Los Alamos National Laboratory, Conference, March 2–6, 1981 (North-Holland, Amsterdam, 1982). We have not been able to track down this reference.

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[4] See the book of Gel'fand and Fomin of Ref. 2. See also F. G. Gascón, J. Math. Phys. **18**, 1763 (1977), where some definitions and examples are given concerning transformations of symmetry not necessarily of pointlike character.

[5] See the papers by Djukiv and Vujanovic quoted in Ref. 3.

The inverse scattering problem for *LCRG* transmission lines[a)]

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(Received 25 March 1982; accepted for publication 25 June 1982)

The inverse scattering problem for one-dimensional nonuniform transmission lines with inductance $L(z)$, capacitance $C(z)$, series resistance $R(z)$ and shunt conductance $G(z)$ per unit length ($z\in\mathbb{R}$) is considered. It is reduced to the inverse scattering problem for the Zakharov–Shabat system. It is found that one can construct from the data the following functions of the travel time x:

$$\tilde{q}^{\pm}(x)=\left[\frac{1}{4}\frac{d}{dx}\left(\ln\frac{L}{C}\right)\pm\frac{1}{2}\left(\frac{R}{L}-\frac{G}{C}\right)\right]\exp\left(\mp\int_{\infty}^{x}\left(\frac{R}{L}+\frac{G}{C}\right)dy\right).$$

PACS numbers: 02.30.Jr, 02.30.Bi, 84.40.Mk

I. INTRODUCTION

In this paper we consider the inverse scattering problem (ISP) for transmission lines extending in a z direction from $z=-\infty$ to $z=\infty$, with inductance $L(z)$, capacitance $C(z)$, series resistance $R(z)$, and shunt conductance $G(z)$ per unit length. We suppose that

—$L(z)$, $C(z)$, $R(z)$, and $G(z)$ ($z\in\mathbb{R}$) are sufficiently regular real functions;

—$L(z)>0$, $C(z)>0$, $R(z)\geqslant 0$, $G(z)\geqslant 0$;

—$L(z)$ and $C(z)$ have strictly positive finite limits $L(\infty)$ and $C(\infty)$, [resp. $L(-\infty)$ and $C(-\infty)$], as $z\to\infty$ (resp. $z\to-\infty$).

$I(z,t)$ and $U(z,t)$ being, respectively, the intensity of the current and the voltage at position z and time t, we use the transmission lines equation ($z\in\mathbb{R}$):

$$\frac{\partial I}{\partial z}+C(z)\frac{\partial U}{\partial t}+G(z)U=0,$$
$$\frac{\partial U}{\partial z}+L(z)\frac{\partial I}{\partial t}+R(z)I=0. \tag{1.1}$$

For a wave of frequency k, i.e., for

$$I(z,t)=I(k,z)e^{-ikt}, \tag{1.2}$$
$$U(z,t)=U(k,z)e^{-ikt}, \tag{1.3}$$

Eq. (1.1) may be written in the form

$$\frac{dI}{dz}-ikC(z)U+G(z)U=0,$$
$$\frac{dU}{dz}-ikL(z)I+R(z)I=0. \tag{1.4}$$

In the following instead of z, we obtain the variable x defined by

$$x(z)=\int_0^z (L(u)C(u))^{1/2}\,du. \tag{1.5}$$

We also use the convention $I(k,z(x))=I(k,x)$, $L(z(x))=L(x)$, etc., justified by the one-to-one correspondence between z and x, $x(z)$ varying from $x(-\infty)=-\infty$ to $x(\infty)=\infty$. We shall see below that $x(z)$ is the travel time of waves from the origin to the position z.

The data of the ISP are the reflection coefficients to the right and to the left, $r(k)$ and $\tilde{r}(k)$, and the transmission coefficient $t(k)$, for $k>0$, and also the quantities $L(-\infty)$, $L(\infty)$, $C(-\infty)$, and $C(\infty)$. The ISP can be stated thus: what information can be obtained on L, R, C, and G from the data?, i.e., what quantities connecting L, C, R, and G can be constructed from the data?

In the lossless case, i.e., $R=G=0$, it is well known—see the survey by Kay[1]—that this ISP can be solved by reduction to the ISP for the one-dimensional Schrödinger equation

$$\text{(S)}:\quad \frac{d^2y}{dx^2}+[k^2-V(x)]y=0,\quad x\in\mathbb{R}. \tag{1.6}$$

For the solution of the ISP for (S) see Kay[2], Kay and Moses[3], and Faddeev[4]. In the lossless case, it is then found that the quantity which can be constructed from the data, is the quotient L/C as a function of the travel time x.

The lossy case with only one kind of absorption, i.e., $R=0$ or $G=0$, has been studied by Jaulent[5,6] and independently by Schmidt.[7] This ISP can be solved by reduction to the ISP for the one-dimensional Schrödinger equation with an energy-dependent potential

$$\text{(S')}:\quad \frac{d^2y}{dx^2}+[k^2-V(k,x)]y=0, \tag{1.7}$$
$$V(k,x)=V(x)+kQ(x). \tag{1.8}$$

There also exists a radial version of the ISP for the lines (i.e., $z\geqslant 0$ instead of $z\in\mathbb{R}$) which can be solved using the radial version of the ISP for (S') (i.e., $x\geqslant 0$ instead of $x\in\mathbb{R}$) (see Ref. 6). For the solution of the ISP for (S') see Jaulent and Jean,[8] Jaulent,[9,10] for the radial case ($x\geqslant 0$), and Jaulent and Jean[11] for the one-dimensional case ($x\in\mathbb{R}$). In the lossy case with $R=0$ (resp. $G=0$) it is then found that the quantities which can be constructed from the data are the quotients L/C and G/C (resp. L/C and R/L) as functions of the travel time x. In Sec. II of this paper we give some additional indications on the lossless case and the lossy case with $R=0$ or $G=0$.

In this paper we consider the general lossy case. In Sec.

a) This work has been done as part of the program "Recherche Coopérative sur Programme No. 264: Etude interdisciplinaire des problèmes inverses."

b) Physique Mathématique et Théorique, Equipe de recherche associée au C.N.R.S., No. 154.

 0022-2488/82/122286-05$02.50

III we prove that the lines equation (1.4) can be put into the form of a generalized Zakharov–Shabat system $(Z)[q^+, q^-, q_3]$:

$$\frac{dY}{dx} + ik\sigma_3 Y = \begin{pmatrix} iq_3 & q^+ \\ q^- & -iq_3 \end{pmatrix} Y, \tag{1.9}$$

with

$$Y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.10}$$

Then through $(Z)[q^+, q^-, q_3]$ we introduce the scattering data associated to the lines equation (1.4). In Sec. IV we reduce the ISP for $(Z)[q^+, q^-, q_3]$ to the well-known ISP for the Zakharov–Shabat system $(Z)[\tilde{q}^+, \tilde{q}^-, \tilde{q}_3 = 0]$. The motivation to study this ISP was first to solve nonlinear evolution equations. See Zakharov-Shabat[12], Ablowitz, Kaup, Newell, Segur,[13] and Calogero and Degasperis.[14] In Sec. V we briefly reproduce the solution of this ISP.

As a result we find that the following quantities, $\tilde{q}^+$ and $\tilde{q}^-$, can be constructed from the ISP data for the lines in the general lossy case, as functions of the travel time x:

$$\tilde{q}^{\pm}(x) = \left[\frac{1}{4} \frac{d}{dx} \left(\ln \frac{L}{C} \right) \pm \frac{1}{2} \left(\frac{R}{L} - \frac{G}{C} \right) \right] \times \exp\left(\mp \int_{\infty}^{x} \left(\frac{R}{L} + \frac{G}{C} \right) dy \right) \tag{1.11}$$

where the indices $+$ and $-$ correspond to each other. Indeed $\tilde{q}^+$ and $\tilde{q}^-$ data are equivalent to the ISP data for the lines, so that we can conclude that, although it is widely underdetermined, the ISP for the lines is theoretically solved. $\tilde{q}^+$ and $\tilde{q}^-$ represent two functional relations between $L/C, R/L$ and G/C. In order to determine the quotients $L/C, R/L$ and G/C (as functions of x) we need another relation between $L/C, R/L$ and G/C. Such is the case if we are given $R/L + G/C$ or R/L or L/C. We notice that if $R = 0$ (resp. $G = 0$) we find again the result of Ref. 6, i.e., L/C and G/C (resp. L/C and R/L) are determined from the data. Indeed these two approaches are equivalent since it has been proved by Jaulent and Miodek[15] that the ISP for the Schrödinger equation (S')$[V,Q]$ and the Zakharov–Shabat system (Z)$[\tilde{q}^+, \tilde{q}^-, \tilde{q}_3 = 0]$ are equivalent. The keystone of the proof consists in introducing the generalized Zakharov–Shabat equation (Z)$[q^+, q^-, q_3]$ and noticing that (S')$[V,Q]$ and (Z)$[\tilde{q}^+, \tilde{q}^-, \tilde{q}_3 = 0]$ are in some way "particular cases" of this equation. Furthermore, it is possible to go easily from one inversion procedure to the other.

II. THE LOSSLESS CASE AND THE CASE $R = 0$ OR $G = 0$

If $R = G = 0$ it is easy from the lines equation (1.4) to obtain

$$\frac{d}{dz}\left(\frac{1}{L(z)} \frac{dU}{dz} \right) + k^2 C(z) U = 0. \tag{2.1}$$

Using the Liouville transformation, i.e., using the variable x defined by (1.5) and setting

$$y(k,x) = \left[\frac{C(x)}{L(x)} \right]^{1/4} U(k,x), \tag{2.2}$$

we find that $y(k,x)$ satisfies the Schrödinger equation (S) with the potential

$$V(x) = \left[\frac{C(x)}{L(x)} \right]^{-1/4} \frac{d^2}{dx^2} \left[\frac{C(x)}{L(x)} \right]^{1/4}. \tag{2.3}$$

It is assumed that $V(x)$ is a sufficiently regular function going to 0 fast enough as $|x| \to \infty$. The solution of the ISP for (S) allows to construct $V(x)$ and therefore $C(x)/L(x)$.

If $R = 0$ we obtain from (1.4) the equation

$$\frac{d}{dz}\left(\frac{1}{L(z)} \frac{dU}{dz} \right) + k^2 C(z) U + ikG(z) U = 0. \tag{2.4}$$

Using the Liouville transformation defined by (1.5) and (2.2) we find that $y(k,x)$ satisfies the Schrödinger equation (S') with the potentials

$$V(x) = \left[\frac{C(x)}{L(x)} \right]^{-1/4} \frac{d^2}{dx^2} \left[\frac{C(x)}{L(x)} \right]^{1/4}, \tag{2.5}$$

$$Q(x) = -i \frac{G(x)}{C(x)}. \tag{2.6}$$

It is assumed that $V(x)$ and $Q(x)$ are sufficiently regular functions going to 0 fast enough as $|x| \to \infty$. The solution of the ISP for (S') allows one to construct $V(x)$ and $Q(x)$ and therefore $C(x)/L(x)$ and $G(x)/C(x)$. The case $G = 0$ is treated exactly in the same way by replacing $U(k,z)$ by $I(k,z)$, $L(z)$ by $C(z)$, $C(z)$ by $L(z)$, and $G(z)$ by $R(z)$.

III. REDUCTION OF THE LINES EQUATION (1.4) TO (Z) $[q^+, q^-, q_3]$ AND DEFINITION OF THE SCATTERING DATA

We use the variable x defined by (1.5) and we set

$$w_1(k,x) = \left[\frac{L(x)}{C(x)} \right]^{1/4} I(k,x), \tag{3.1}$$

$$w_2(k,x) = -\left[\frac{C(x)}{L(x)} \right]^{1/4} U(k,x), \tag{3.2}$$

$$W(k,x) = \begin{pmatrix} w_1(k,x) \\ w_2(k,x) \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{3.3}$$

Then we find that the lines equation (1.4) can be put into the form

$$\frac{dW}{dx} + ik\sigma_1 W = \begin{pmatrix} \frac{1}{4} \frac{d}{dx} \ln \frac{L}{C} & \frac{G}{C} \\ \frac{R}{L} & -\frac{1}{4} \frac{d}{dx} \ln \frac{L}{C} \end{pmatrix} W, \quad x \in \mathbb{R}. \tag{3.4}$$

One may readily put Eq. (3.4) into the form (Z) $[q^+, q^-, q_3]$ by setting

$$Y = NW, \tag{3.5}$$

$$N = N^{-1} = \frac{1}{\sqrt{2}} (\sigma_1 + \sigma_3) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{3.6}$$

$$q^{\pm}(x) = \frac{1}{4} \frac{d}{dx} \left(\ln \frac{L}{C} \right) \pm \frac{1}{2} \left(\frac{R}{L} - \frac{G}{C} \right), \tag{3.7}$$

$$iq_3(x) = \frac{1}{2} \left(\frac{R}{L} + \frac{G}{C} \right). \tag{3.8}$$

(Note that $N\sigma_3 = \sigma_1 N$).

We assume that $q^+(x)$, $q^-(x)$, and $q_3(x)$ are sufficiently regular functions going to 0 fast enough as $|x|\to\infty$. Since the trace of the matrix

$$\begin{pmatrix} iq_3 & q^+ \\ q^- & -iq_3 \end{pmatrix}$$

is 0, it is possible to introduce the scattering data for (Z) $[q^+, q^-, q_3]$ in the same way as in the well-known case $q_3 = 0$. Instead of (Z) $[q^+, q^-, q_3]$ it is technically convenient to consider both systems (Z)$^\pm[q^+, q^-, q_3]$:

$$\frac{dY^\pm}{dx} + ik\sigma_3 Y^\pm = \begin{pmatrix} \pm iq_3 & q^\pm \\ q^\mp & \mp iq_3 \end{pmatrix} Y^\pm. \tag{3.9}$$

If $Y^-(k,x)$ is a solution of (Z)$^-$ then $\sigma_1 Y^-(-k,x)$ is a solution of (Z)$^+$. This symmetry property allows one to reduce the study of two types of Jost solutions at $+\infty$ (or at $-\infty$) to only one.

The right and left Jost solutions of (Z)$^\pm$, $F^\pm(k,x)$ and $\overleftarrow{F}^\pm(k,x)$, are defined as

$$F^\pm(k,x) \underset{x\to\infty}{\sim} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ikx}, \quad \overleftarrow{F}^\pm(k,x) \underset{x\to-\infty}{\sim} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx}. \tag{3.10}$$

$\sigma_1 F^\mp(-k,x)$ and $\sigma_1 \overleftarrow{F}^\mp(-k,x)$ are also Jost solutions of (Z)$^\pm$ with

$$\sigma_1 F^\mp(-k,x) \underset{x\to\infty}{\sim} \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx}, \quad \sigma_1 \overleftarrow{F}^\mp(-k,x) \underset{x\to-\infty}{\sim} \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ikx}. \tag{3.11}$$

Using standard arguments (see Ref. 13 for example) one can prove that $F^\pm(k,x)$ and $\overleftarrow{F}^\pm(k,x)$ are analytic in k for Im $k>0$ and continuous for Im $k\geqslant 0$. $F^\pm(k,x)$ and $\sigma_1 F^\mp(-k,x)$ [resp. $\overleftarrow{F}^\pm(k,x)$ and $\sigma_1 \overleftarrow{F}^\mp(k,x)$] form a fundamental system of solutions of (Z)$^\pm$ for $k\in\mathbb{R}$. The reflection coefficients to the right and to the left, $r^\pm(k)$ and $\overleftarrow{r}^\pm(k)$, and the transmission coefficient $t^\pm(k)$ associated with (Z)$^\pm$ are defined for $k\in\mathbb{R}$ by

$$\overleftarrow{F}^\pm(k,x) = \frac{r^\pm(k)}{t^\pm(k)} F^\pm(k,x) + \frac{1}{t^\pm(k)} \sigma_1 F^\mp(-k,x), \tag{3.12}$$

$$F^\pm(k,x) = \frac{\overleftarrow{r}^\pm(k)}{t^\pm(k)} \overleftarrow{F}^\pm(k,x) + \frac{1}{t^\pm(k)} \sigma_1 \overleftarrow{F}^\mp(-k,x). \tag{3.13}$$

It follows from (3.10)–(3.13) that there exist two solutions of (Z)$^\pm$: $\overleftarrow{\Psi}^\pm(k,x)$ $[= t^\pm(k)\overleftarrow{F}^\pm(k,x)]$ and $\Psi^\pm(k,x)$ $[= t^\pm(k)F^\pm(k,x)]$ such that $(k\in\mathbb{R})$

$$\overleftarrow{\Psi}^\pm(k,x) \underset{x\to-\infty}{\sim} t^\pm(k)\begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx} \underset{x\to\infty}{\sim} r^\pm(k)\begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ikx} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx}, \tag{3.14}$$

$$\Psi^\pm(k,x) \underset{x\to-\infty}{\sim} \overleftarrow{r}^\pm(k)\begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-ikx} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ikx} \underset{x\to\infty}{\sim} t^\pm(k)\begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{ikx}. \tag{3.15}$$

The scattering matrix associated with (Z)$^\pm$ is defined by

$$S^\pm(k) = \begin{pmatrix} t^\pm(k) & r^\pm(k) \\ \overleftarrow{r}^\pm(k) & t^\pm(k) \end{pmatrix}, \quad k\in\mathbb{R}. \tag{3.16}$$

The function $1/t^\pm(k)$ is analytic for Im $k>0$ and continuous for Im $k\geqslant 0$. We assume that this function has no zero for Im $k\geqslant 0$, i.e., (Z)$^\pm$ has no bound state (square integrable solution). This point should be studied thoroughly. Indeed, in the case $R = G = 0$ one can prove a similar but weaker result for Eq. (1.7) (see Ref. 6).

We deduce from (3.5), (3.6), (3.14), and (3.15) that there exist two solutions of (3.4), $\overleftarrow{w}(k,x)$ and $W(k,x)$ such that

$$\overleftarrow{W}(k,x) \underset{x\to-\infty}{\sim} t^+(k)\begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-ikx} \underset{x\to\infty}{\sim} r^+(k)\begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{ikx} + \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-ikx}, \tag{3.17}$$

$$W(k,x) \underset{x\to-\infty}{\sim} \overleftarrow{r}^+(k)\begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-ikx} + \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{ikx} \underset{x\to\infty}{\sim} t^+(k)\begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{ikx}. \tag{3.18}$$

Therefore [use (1.5), (3.1)–(3.3)] there exist two solutions of the lines equation (1.4),

$$\begin{pmatrix} \overleftarrow{I}(k,z) \\ \overleftarrow{U}(k,z) \end{pmatrix} \text{ and } \begin{pmatrix} I(k,z) \\ U(k,z) \end{pmatrix},$$

such that

$$\overleftarrow{I}(k,z) \underset{z\to-\infty}{\sim} \left[\frac{C(-\infty)}{L(-\infty)}\right]^{1/4} t^+(k) e^{-ikx(z)} \underset{z\to\infty}{\sim} \left[\frac{C(\infty)}{L(\infty)}\right]^{1/4} \{r^+(k)e^{ikx(z)} + e^{-ikx(z)}\}, \tag{3.19}$$

$$\overleftarrow{U}(k,z) \underset{z\to-\infty}{\sim} -\left[\frac{L(-\infty)}{C(-\infty)}\right]^{1/4} t^+(k) e^{-ikx(z)} \underset{z\to\infty}{\sim} -\left[\frac{L(\infty)}{C(\infty)}\right]^{1/4} \{-r^+(k)e^{ikx(z)} + e^{-ikx(z)}\}, \tag{3.20}$$

$$I(k,z) \underset{z\to-\infty}{\sim} \left[\frac{C(-\infty)}{L(-\infty)}\right]^{1/4} \{\overleftarrow{r}^+(k)e^{-ikx(z)} + e^{ikx(z)}\} \underset{z\to\infty}{\sim} \left[\frac{C(\infty)}{L(\infty)}\right]^{1/4} t^+(k) e^{ikx(z)}, \tag{3.21}$$

$$U(k,z) \underset{z\to-\infty}{\sim} -\left[\frac{L(-\infty)}{C(-\infty)}\right]^{1/4} \{\overleftarrow{r}^+(k)e^{-ikx(z)} - e^{ikx(z)}\} \underset{z\to\infty}{\sim} \left[\frac{L(\infty)}{C(\infty)}\right]^{1/4} t^+(k) e^{ikx(z)}. \tag{3.22}$$

We see on Eqs. (3.19)–(3.22) that $r^+(k)$, $\overleftarrow{r}^+(k)$, and $t^+(k)$ represent also for the lines equation (1.4) the reflection coefficients to the right and to the left and the transmission coefficient for the frequency k $(k>0)$. Furthermore, recalling (1.2), (1.3), and (1.5), it is clear that

$$v(z) = (L(z)C(z))^{-1/2} \tag{3.23}$$

is the local wave velocity at point z and that $x(z)$ is the travel time of waves from the origin to the position z.

The ISP for the line is the construction of quantities connecting L, C, R, and G from the data of $S^+(k)$ $(k>0)$, $L(\infty)$, $L(-\infty)$, $C(-\infty)$, and $C(\infty)$. q^+, q^-, and iq_3 being real [see Eqs. (3.7) and (3.8)], one can prove that

$$\overline{S^+(k)} = S^+(-k), \quad k\in\mathbb{R}, \tag{3.24}$$

where $\overline{S^+(k)}$ is the complex conjugate matrix of $S^+(k)$. Therefore $S^+(k)$ $(k\in\mathbb{R})$ is determined by $S^+(k)$ $(k>0)$. $S^-(k)$

($k\in\mathbb{R}$) is also determined because of the general identity

$$S^{\pm}(k)^{t}S^{\mp}(-k)=I, \tag{3.25}$$

where "t" means "transposed" and I is the 2×2 identity matrix. So the data $S^{+}(k)$ ($k>0$) imply the data $r^{+}(k)$ and $r^{-}(k)$ ($k\in\mathbb{R}$). For this reason we consider in what follows the ISP associated with (Z) $[q^{+}, q^{-}, q_3]$ from the data of $r^{+}(k)$ and $r^{-}(k)$ ($k\in\mathbb{R}$).

IV. REDUCTION OF THE ISP FOR (Z) $[q^{+}, q^{-}, q_3]$ TO THE ISP FOR (Z) $[\tilde{q}^{+}, \tilde{q}^{-}, \tilde{q}_3=0]$

Let us write the generalized Zakharov–Shabat equation $(Z)^{\pm}[q^{+}, q^{-}, q_3]$ [id. Eq. (3.9)] in the form

$$\left(\frac{d}{dx}\mp iq_3\sigma_3\right)Y^{\pm}+ik\sigma_3 Y^{\pm}=\begin{pmatrix}0 & q^{\pm}\\ q^{\mp} & 0\end{pmatrix}Y^{\pm}, \tag{4.1}$$

and let us notice that

$$\frac{d}{dx}\mp iq_3\sigma_3=M^{\mp}(x)\left(\frac{d}{dx}\right)\circ M^{\pm}(x), \tag{4.2}$$

$$\sigma_3=M^{\mp}(x)\sigma_3 M^{\pm}(x), \tag{4.3}$$

where

$$M^{\pm}(x)=\exp\left(\mp i\int_{\infty}^{x}q_3(y)\sigma_3\,dy\right)=\begin{pmatrix}\exp\left(\mp i\int_{\infty}^{x}q_3(y)\,dy\right) & 0\\ 0 & \exp\left(\pm i\int_{\infty}^{x}q_3(y)\,dy\right)\end{pmatrix}. \tag{4.4}$$

It is then easy to see that $\tilde{Y}^{\pm}$ defined by

$$\tilde{Y}^{\pm}=M^{\pm}(x)Y^{\pm}, \tag{4.5}$$

is a solution of the Zakharov–Shabat system $(Z)^{\pm}[\tilde{q}^{+}, \tilde{q}^{-}, \tilde{q}_3=0]$ with

$$\tilde{q}^{\pm}=q^{\pm}\exp\left(\mp 2i\int_{\infty}^{x}q_3(y)\,dy\right). \tag{4.6}$$

The Jost solutions of $(Z)^{\pm}[q^{+}, q^{-}, q_3]$ and $(Z)^{\pm}[\tilde{q}^{+}, \tilde{q}^{-}, \tilde{q}_3=0]$ are connected by

$$\tilde{F}^{\pm}(k,x)=M^{\pm}(x)F^{\pm}(k,x), \tag{4.7}$$

$$\overleftarrow{\tilde{F}}^{\pm}(k,x)=\exp\left(\mp i\int_{-\infty}^{\infty}q_3(y)\,dy\right)M^{\pm}(x)\overleftarrow{F}^{\pm}(k,x). \tag{4.8}$$

From (3.12), (3.13), (4.7), and (4.8) it is easy to obtain the connection between the scattering data ($k\in\mathbb{R}$)

$$\tilde{r}^{\pm}(k)=r^{\pm}(k), \tag{4.9}$$

$$\overleftarrow{\tilde{r}}^{\pm}(k)=\exp\left(\pm 2i\int_{-\infty}^{\infty}q_3(y)\,dy\right)\overleftarrow{r}^{\pm}(k), \tag{4.10}$$

$$\tilde{t}^{\pm}(k)=\exp\left(\pm i\int_{-\infty}^{\infty}q_3(y)\,dy\right)t^{\pm}(k). \tag{4.11}$$

Note that this result is a particular case of a lemma used in Ref. 15. So we are led to solve the ISP for the Zakharov–Shabat system $(Z)^{\pm}[\tilde{q}^{+}, \tilde{q}^{-}, \tilde{q}_3=0]$ from the data of $\tilde{r}^{+}(k)=r^{+}(k)$ and $\tilde{r}^{-}(k)=r^{-}(k)$ for $k\in\mathbb{R}$. Because of Eqs. (4.6), (3.7), and (3.8), the potentials $\tilde{q}^{+}$ and $\tilde{q}^{-}$, solutions of this ISP, are connected to L, C, R, and G through Eq. (1.11).

We remark that it would be quite possible to introduce the ISP data for the lines [see formulas (3.19)–(3.22)] by using the Zakharov–Shabat system $(Z)[\tilde{q}^{+}, \tilde{q}^{-}, \tilde{q}_3=0]$ instead of the generalized Zakharov–Shabat system (Z) $[q^{+}, q^{-}, q_3]$ as done in Sec. III. The choice of the intermediate step $(Z)[q^{+}, q^{-}, q_3]$ may be justified by the following remarks:

—The equation $[q^{+}, q^{-}, q_3]$ is more directly connected with the lines equation (1.4) than the equation (Z) $[\tilde{q}^{+}, \tilde{q}^{-}, \tilde{q}_3=0]$ and is no more difficult to investigate;

—The potentials q^{+}, q^{-}, and iq_3 have the nice property of being real and thus lead to the nice relation (3.24).

V. SOLUTION OF THE ISP FOR (Z) $[\tilde{q}^{+}, \tilde{q}^{-}, \tilde{q}_3=0]$

The starting point is the following representation formula for the Jost solution $\tilde{F}^{\pm}(k,x)$ of $(Z)^{\pm}[\tilde{q}^{+}, \tilde{q}^{-}, \tilde{q}_3=0]$:

$$\tilde{F}^{\pm}(k,x)=\begin{pmatrix}0\\ 1\end{pmatrix}e^{ikx}+\int_{x}^{\infty}K^{\pm}(x,y)e^{iky}dy, \tag{5.1}$$

where the kernel

$$K^{\pm}(x,y)=\begin{pmatrix}K_1^{\pm}(x,y)\\ K_2^{\pm}(x,y)\end{pmatrix}$$

is such that

$$K_1^{\pm}(x,x)=-\frac{1}{2}\tilde{q}^{\pm}(x), \tag{5.2}$$

$$K_2^{\pm}(x,x)=\frac{1}{2}\int_{x}^{\infty}\tilde{q}^{+}(y)\tilde{q}^{-}(y)\,dy. \tag{5.3}$$

The insertion of (5.1) into (3.12) and the use of contour integration in the complex k plane yield the inversion equations

$$\sigma_1 K^{\pm}(x,y)=\begin{pmatrix}0\\ 1\end{pmatrix}p^{\mp}(x+y)+\int_{x}^{\infty}p^{\mp}(y+t)K^{\mp}(x,t)\,dt,\quad y\geqslant x,\quad x\in\mathbb{R}, \tag{5.4}$$

where $p^{+}(x)$ and $p^{-}(x)$ are the scalar functions connected to the data $\tilde{r}^{+}(k)$ and $\tilde{r}^{-}(k)$ ($k\in\mathbb{R}$) by

$$p^{\pm}(x)=-\frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{r}^{\pm}(k)e^{ikx}dk \tag{5.5}$$

(we recall that we have assumed that there is no bound state). Therefore the steps of the solution of this ISP are:

(a) construct p^{+} and p^{-} from $\tilde{r}^{+}(k)$ and $\tilde{r}^{-}(k)$ ($k\in\mathbb{R}$) using Eq. (5.5);

(b) find the solution (K^{+}, K^{-}) of the system of integral equations (5.4);

(c) obtain $[\tilde{q}^{+}, \tilde{q}^{-}]$ from (K^{+}, K^{-}) using Eq. (5.2).

ACKNOWLEDGMENT

This research has been sponsored by NATO (Research Grant No. 057.81).

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Two-dimensional scattered fields: A description in terms of the zeros of entire functions

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(Received 21 May 1981; accepted for publication 7 August 1981)

A general description of n-dimensional Fourier transforms is given in terms of their complex zero surfaces. The properties of these surfaces are analyzed and then applied to two-dimensional scattered electromagnetic fields in the Fraunhofer region. It is shown that the properties of two-dimensional fields differ inherently from those of one-dimensional fields and that they lead to a reduced ambiguity for object reconstruction from intensity data. A way of estimating this ambiguity is given.

PACS numbers: 02.30.Nw, 02.30.Fn, 42.30.Kq

I. INTRODUCTION

The theory of Fourier transforms, and in particular its extension in the complex domain, has been applied to a variety of problems in physics. One of these applications has been the description of one-dimensional scattered fields, where among other useful results, it gave a measure of the ambiguity of object reconstruction from intensity data.

In this paper we aim to formulate a description of n-dimensional Fourier transforms using the theory of functions of several complex variables. We will then discuss its application to the description of two-dimensional scattered fields by complex functions of two complex variables. We aim to show that the one-dimensional theory is a special case which does not generalize to the n-dimensional theory.

Consequently the one-dimensional description of scattered fields is inadequate for an analysis of the two-dimensional case and can lead to false results.

We proceed by analyzing the consequences of the above difference on the modeling of scattered fields in two dimensions. This will lead to an understanding of the different type of inherent ambiguity involved in the reconstruction of two-dimensional objects from their energy spectra.

The above questions have not, to my knowledge, been considered in their most general form. The two attempts made in this area have been limited in scope. The treatment by Bruck and Sodin[1] is based on the assumption that the object is a set of discrete points, and although most of their results hold in this special case, it is not clear that they can be generalized to continuous objects.

Such problems have also been illustrated in a paper by Huiser and van Toorn,[2] where no such assumption about the object is made. These authors, though, assume that the function describing the field has at least one polynomial factor; this assumption is not necessary. They then proceed to show that this would lead to ambiguities in the object reconstruction. In this paper we will consider the problem in its most general form, making no assumptions about either space—the object space or the Fourier space.

In the first part of this paper a short exposition of the main properties of the one-dimensional model for scattered fields will be given. Since we propose to put forward a two-dimensional description, this is useful as an introduction to this type of model and for comparison purposes in the rest of the paper.

The second part of the paper will be devoted to the properties of functions of several complex variables applicable to Fourier transforms and two-dimensional scattered fields. In this part we will discuss the uniqueness of object reconstruction in two dimensions.

In a following paper we will show explicitly how the zeros of the two-dimensional Fourier transform encode the information about the conjugate space in two particular cases: when the object is confined to a circular or a square aperture.

II. THE ONE-DIMENSIONAL MODEL

It is well known that a relationship exists between the scattered field in the Fraunhofer region and the object wave which is given by the Fourier transform

$$F(x) = \int_{-a}^{a} f(t) e^{ixt}\, dt, \tag{2.1}$$

where $F(x)$ is the scattered field and $f(t)$ the object wave. This Fourier transform relationship can be used to continue the scattered field into the complex plane $\mathbb{C}$, by use of the fact that[3]

$$F(x+iy) = \int_{-a}^{a} f(t) e^{ixt} e^{-yt}\, dt$$

or

$$F(z) = \int_{-a}^{a} f(t) e^{izt}\, dt, \tag{2.2}$$

where $z = x + iy$.

A theorem by Paley and Wiener[4] states that (2.1) is a sufficient and necessary condition for $F(z)$ to be an entire function of exponential type a, i.e., so that we can always write

$$|F(z)| \leqslant A e^{a|z|}. \tag{2.3}$$

This fact together with Hadamard's theorem[5] gives a unique description of $F(z)$ in terms of its zero locations, i.e.,

$$F(z) = C z^{p} \prod_{n=-\infty}^{\infty} (1 - z/z_n), \tag{2.4}$$

where the z_n are the zero locations for a specific $F(z)$. It follows from (2.1), (2.2), and (2.4) that all the information about

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the object wave is uniquely encoded by the positions of the zeros of $F(z)$. It can be shown[6] that the zero positions encode uniquely the frequency, phase, and amplitude of harmonics in the conjugate space.

It is interesting to note that in optics, i.e., at high frequencies, the only experimentally measurable quantity is the scattered-intensity distribution. To reconstruct the object wave from this distribution one has to take into account an ambiguity, which viewed from the point of view of analytic functions can be described as follows: The zeros of the scattered intensity are those of the scattered field and its complex conjugate

$$I(x) = |F(x)|^2 = F(x)F^*(x)$$

$$\therefore I(x) = Cx^{2p} \prod_{n=-\infty}^{\infty} (1 - x/z_n)(1 - x/z_n^*),$$

where we have written * for the complex conjugate. Given an intensity distribution with $2N$ complex zeros, there are 2^N possibilities for the zero locations of $F(z)$. The phase problem then can be reduced to the problem of locating the zeros of $F(z)$, and the ambiguity of the object reconstruction from intensity data can be described in terms of the ambiguity of zero location.

To recapitulate, in the one-dimensional model, the field is described by an infinite product of factors each of which is of the form $(1 - x/z_n)$, where z_n is the nth zero of $F(z)$. Each of these zero positions encodes uniquely information about the object.

III. THE N-DIMENSIONAL MODEL

In this section we will give the relevant properties of functions of several complex variables, used to describe Fourier transforms. Most of the time we will consider the case of n complex variables, and only in the examples we will let $n = 2$ for simplicity (but without loss of generality).

In what follows all references to n dimensions will mean n complex dimensions unless specified otherwise. We will denote by $\mathbb{C}^n$ the complex n-dimensional space, by $\mathbb{R}^n$ the real n-dimensional space. The variable in $\mathbb{C}^n$ will be denoted by $z = (z_1,...,z_n)$, where $z_i = x_i + iy_i$; $x_i, y_i \in \mathbb{R}$. The variable in the conjugate space will be denoted by $t = (t_i,...,t_n)$; $t_i \in \mathbb{R}$.

The first part, Sec. IIIA, will be devoted mostly to the global theory of functions of several complex variables, i.e., the properties of these functions which can be defined in all of $\mathbb{C}^n$. These properties will be used to formulate a general description of two-dimensional scattered fields. We will also give an estimate of the inherent ambiguity of object reconstruction from two-dimensional intensity data.

In the second part, Sec. IIIB, the local properties of functions of several complex variables will be analyzed. The local properties allow a detailed description of what is happening in the neighborhood of each point of the complex space. These properties cannot be carried directly to global ones—which we need—but are indispensable in the analysis of the zeros of functions of several complex variables. In fact it is impossible to describe their behavior in any complete way using only the global properties, as will become apparent later. We will then refine our description of two-dimensional scattered fields using these properties; we will also give a more refined estimate of the factors governing the ambiguity of object reconstruction from power spectra.

A. Global theory

In accordance with the one-dimensional model we will assume a Fourier transform relationship between the object wave and the scattered field in the Fraunhofer region. Then a well-known theorem by Plancherel and Pólya[7] states that:

Theorem 1: For a function $F(z)$ of n complex variables to be entire of exponential type, and square integrable when considered for real values of its n arguments, it is necessary and sufficient that it can be represented in the form

$$F(z_1,...,z_n) = \int_{-\infty}^{\infty} \cdots \int f(t_1,...,t_n) \exp[i(z_1t_1 + ... + z_nt_n)] \times dt_1...dt_n, \tag{3.1}$$

where $f(t)$ is a square-integrable function for all its n variables, and vanishes at every point outside a bounded domain.

This implies that $F(z)$ satisfies the inequality[7]

$$|F(z_1,...,z_n)| \leqslant A \exp[a(|z_1| + \cdots + |z_n|)], \tag{3.2}$$

where a and A are positive constants. Inequality (3.2) is valid for all complex values of the variables $z_1,...,z_n$.

It is easy to prove,[8] that functions of $n \geqslant 2$ complex variables do not have isolated zeros. Their zeros are always continuous "lines" (in this context, a "line" means an $(n-1)$-dimensional surface). It will become obvious that this is one of the most significant difference between the one- and two-dimensional descriptions. To go further in the analysis of the zero lines it is necessary to introduce some concepts from the theory of analytic sets, which describes the zeros of analytic functions. The following definition will make more precise our concept of a zero line.

Definition 1: Analytic set[9]: Let $B \subset \mathbb{C}^n$ be a region, M a subset of B, and $(a) \in B$ a point. M is called analytic at (a) if there exists an open neighborhood $U = U(a) \in B$ and functions $f_1,...,f_l$ holomorphic in U such that

$$U \cap M = \{z \in U: f_1(z) = \cdots = f_l(z) = 0\}.$$

M is called analytic in B if M is analytic at every point in B.

In particular the set $M(f) \subset B$ defined by

$$M(f) = \{z \in B: f(z) = 0\},$$

where f is holomorphic in B, is also an analytic set. $M(f)$ will be called the zero set of the function f.

Definition 2: Reducible analytic set[9]: An analytic set $M \subset B$ is called reducible if there exist analytic subsets $i = 1, 2$, such that

1. $M = M_1 \cup M_2$,
2. $M_i \neq M$, $i = 1, 2$.

If M is not reducible it is called irreducible.

We will call an entire function $F(z)$ globally reducible if it can be written as the product of two entire functions for all $z \in \mathbb{C}^n$. Otherwise it will be called globally irreducible. Notice that global irreducibility does not imply that F is irreducible everywhere. It is enough that one of the functions comprising its product is nonanalytic at one point for F to be globally irreducible.

Next we will introduce the fundamental theorem of this section, due to Osgood.[10] In Appendix A we show how a proof for this theorem can be constructed.

Theorem 2: An entire function $F(z)$ which has zeros and does not vanish identically can be uniquely decomposed in a finite or infinite product of globally irreducible factors. This product has the form

$$F(z) = \prod_{m=1}^{N} [F_m(z)e^{\gamma_m}]^{l_m} \quad (N \leqslant \infty), \tag{3.3}$$

where the $F_m(z)$ are globally irreducible entire functions and the e^{γ_m} are convergence factors, with the γ_m polynomials in z. The exponents l_m are integers.

In Appendix A it is shown, that each $F_m(z)$ in (3.3) describes an irreducible analytic set and that the union of all these sets forms the zero set of $F(z)$. Here we will just use this fact to discuss the properties of the zero lines of $F(z)$.

From the above we can see two crucial differences between (3.3) and the Hadamard product (2.4). The first is that the form of each factor in (3.3) is not known, and depends entirely on the zero set of F. The second difference is that each factor describes not necessarily one, but several zero lines, which cannot be separated.

In the case of scattered fields, the usual practice in one dimension is to try to determine the zero locations of the field from those of the scattered intensity. It is easily seen from the above, that zero location from a two-dimensional intensity recording is not enough to determine the field. To form the irreducible analytic set described by each $F_m(z)$ in (3.3) it is essential to determine the way each of the zero lines is related to the others. For example, if an attempt were made to fit polynomials to these lines, without knowing the specific relations between them, the resulting product of factors would be either unphysical, or Fourier-transform to an object wave which bears no relation whatsoever to the real one.

We can also look at this from the point of view of information encoding. In one dimension, all information about the function describing the field is encoded uniquely by the positions of the zeros, which thus constitute "units of information." In two dimensions information is encoded uniquely by irreducible combinations of zero lines, i.e., combinations which can be expressed in one and only one way. Consequently, in two dimensions, each irreducible zero set is a unit of information, and there exists an infinite variety of these. The way each of these "units" encodes information is by both the position and the specific combinations of the zero lines it describes. The uniqueness of irreducible zero sets ensures that each unit encodes a unique feature of the object. The uniqueness of the product (3.3) ensures that each object wave is uniquely encoded by the zero lines of the scattered field.

To determine the probability of occurrence of irreducible factors in the field we cannot use the argument that there are more irreducible than reducible functions, as is done by Bruck and Sodin.[1] The opposite is actually true, as can be easily seen from a simple statistical argument. Consider a finite subset of the set of all irreducible functions, with N elements. Then, combining these we can create $\Sigma_{k=1}^{N} N/(N-k)!k!$ reducible ones. Although the set of all entire functions contains an infinite number of both types of functions, using the above argument it can be deduced that it contains more reducible than irreducible ones. It may be possible to give a different estimate of the number of irreducible factors in the field, but this can only be done by imposing additional physical constraints on the mathematical model.

If the scattered intensity data contains $2N$ complex zero lines (N lines from the field and N from its complex conjugate) then we have three possibilities.

(a) The field is completely separable in terms of its two variables, i.e., we can write

$$F(z_1,z_2) = F_1(z_1)F_2(z_2). \tag{3.4}$$

Since each of the $F_i (i = 1,2)$ is now a one-dimensional function we can decompose it in a Hadamard product (2.4) and therefore the ambiguity is that of the one-dimensional case: if F_1 has M zeros and F_2 has K zeros, where $M + K = N$, then the ambiguity is $2^{M+K} = 2^N$.

(b) The field is not separable in terms of its two variables. Then we have the case described by (3.3), where each F_m describes a set of nonseparable zero lines, i.e., if the field has N zero lines the ambiguity is going to be 2^L, where L is the number of irreducible factors describing these lines, and $L \leqslant N$.

(c) Cases (a) and (b) together. For this case, Hadamard's theorem can be used to factor the separable part [case (a)] and then Theorem 2 can be applied to the rest of the function. The ambiguity can be worked out as a combination of the ambiguities of (a) and (b).

It will be seen later than any effect to separate parts of the irreducible zero set described by each F_m into its components (elements) has the effect of destroying the analytic character of the function, and consequently the finite support of the object wave is lost.

Since $F(z_1,z_2)$ is an entire function of exponential type and is also square-integrable on the real plane $\mathbb{R}^2$, it must have an infinite number of zero lines. Otherwise $F(x_1,x_2)$ would tend to infinity as $|x_1|, |x_2| \to \infty$, and consequently it would not be square-integrable. In Appendix B we will show that the asymptotic behavior of $F(z)$ is defined by the edge of the scattering aperture in the object space. Since the factors in (3.3) are entire functions this fact imposes a strong condition on their behavior *even in the finite part of* $\mathbb{C}^n$. Consequently this behavior is displayed by their zero sets everywhere. This important property of zero sets has no counterpart in the one-dimensional case, where the behavior of the zeros in the finite part of $\mathbb{C}$ is independent of the asymptotic behavior of the function.

To show how these properties can be used in practice we will consider an aperture of regular fixed shape and size with its edge preset to a specific constant value, containing some object. We assume also that the Fourier transform of the empty aperture is known. The fact that the edge has been preset to a specific constant value, implies that the asymptotic behavior of the field has been fixed to be that of the Fourier transform of the empty aperture. Thus, the product (3.3) of the field, scattered by this configuration in the object space, will contain at least the asymptotic part of the aperture func-

tion, which will, of course, still be a function of exponential type, i.e., we have

$$F(z_1,z_2) = G(z_1,z_2)\prod_{m=1}^{N}\left[F_m(z_1,z_2)e^{\gamma m}\right]^{l_m} \quad (N\leqslant\infty),$$

where $G(z_1,z_2)$ is the part of the Fourier transform of the aperture, and is a function of exponential type. Rewriting this as

$$F(z_1,z_2)/G(z_1,z_2) = \prod_{m=1}^{N}\left[F_m(z_1,z_2)e^{\gamma m}\right]^{l_m} \quad (N\leqslant\infty),$$

we can use a well-known theorem[11-13] which states that the quotient of two functions of exponential type is either a function of exponential type or a polynomial. If it is a function of exponential type then the object can be considered to be a convolution, which implies that the new function is similar to G, since the apertures of both have to be constant on their edge. This argument can be repeated until there are only polynomial factors in the field.

More specifically, choosing a square or circular aperture as the original one, it is easy to see from the above argument that the product in the Fourier space cannot contain any nonpolynomial factors. To show this we need only consider the fact that both aperture functions can be expressed as infinite products. Furthermore, the only way of getting a square or circular aperture by convolution is by convolving with another square or circular aperture, respectively. The result is now obvious.

The fact that we have preset the aperture allows us to infer even more. Since the asymptotic behavior is known *a priori*, we know that all functions in the product, polynomials or not, must have the same asymptotic behavior. Thus, for example, the asymptotic behavior of the zero surfaces of $J_1[(z_1^2+z_2^2)^{1/2}]/(z_1^2+z_2^2)^{1/2}$ which is the Fourier transform of a circular aperture of edge equal to one, is that of $z_1^2+z_2^2-a^2=0$. This can be easily deduced from the infinite product for this function.[14] Thus asymptotically we have that all the zero surfaces of an object contained in such an aperture (keeping the value on the edge equal to one) must be like $z_1 = \pm iz_2$, which is the asymptotic behavior of the circle given above.

In the next section we will analyze the zero lines in more detail showing how each of the lines defined by the F_m is related to the others, forming with them a single entity, the irreducible zero set of the function F_m. We will then show that in two dimensions, this leads to a reduced ambiguity for object reconstruction from intensity data.

B. Local theory

As we pointed out in the introduction, the local properties of analytic functions are needed for a detailed analysis of the behavior of analytic sets. In Sec. IIIA we stated that each factor F_m, in the product (3.3), is a globally irreducible entire function, but nothing was said about its zero set, except that it is irreducible. We will now proceed to analyze further these zero sets.

It is well known[9,10] that any neighborhood in $\mathbb{C}^n$ intersects only a finite number of the components of an analytic set. This fact allows us to use the Weierstrass preparation theorem, to simplify the zero set of the original function to that of a pseudopolynomial (see Definition 4)—locally, of course. When the original function is a polynomial, one can dispense with this theorem, and use Theorem 4 directly to analyze the behavior of its zero set.

To proceed further we need the local definition of reducibility.

Definition 3: Locally reducible function[8]: Let $B\subset\mathbb{C}^n$ be a domain, $(a)\in B$ a point. Let g be a function analytic in some neighborhood $U(a)\in B$ of (a) such that $g(a)=0$. Then g will be called reducible at the point (a) if there exist two functions, analytic in $U(a)$, such that:

$$g(z) = g_1(z)g_2(z) \quad z\in U(a)$$

and

$$g_1(a) = g_2(a) = 0. \tag{3.5}$$

If g is not reducible it will be called irreducible.

As was stated in Sec. III A, global irreducibility does not necessarily imply local irreducibility.

The basic theorem of this section is the Weierstrass preparation theorem. This theorem serves as a preparation for the examination of the zeros of analytic functions. For this theorem we will limit ourselves to the case $n=2$, which differs slightly from the general case. The concept of a distinguished pseudo- polynomial of order k, which will be used in this theorem, will also be introduced for $n=2$; the general case is identical.

Definition 4: Distinguished pseudopolynomial[8]: Let $(a)=(a_1,a_2)$ be a point in $\mathbb{C}^2$, $U=U(a)$ an open neighborhood of this point. A function $G(z)$ which can be represented in this neighborhood in the form

$$G(z_1,z_2) = A_0(z_1)(z_2-a_2)^k + A_1(z_1)(z_2-a_2)^{k-1} + \cdots + A_k(z_1), \tag{3.6}$$

where the $A_i (i=0,\ldots,k)$ are functions of the variable z_1 analytic in this neighborhood, is called a pseudopolynomial of order k, with center at the point a_1. A pseudopolynomial for which the coefficient A_0 is nonzero in $U(a)$ is called distinguished.

In what follows we will take $A_0=1$, since we can always divide the coefficients A_i by A_0 [$\neq 0$ in $U(a)$]. We are now ready to state the Weierstrass preparation theorem. As mentioned above we will state it in a restricted form, for functions of two complex variables.

Theorem 3: The Weierstrass preparation theorem[8]: If the function $F(z_1,z_2)$ is holomorphic at the point (a_1,a_2), while $F(a_1,a_2)=0$ and $F(z_1,z_2)\not\equiv 0$, then in some bicylinder $\{|z_1|<r,\ |z_2|<h\}$

$$F(z_1,z_2) = (z_1-a_1)^{\mu}G(z_1,z_2)\Omega(z_1,z_2), \tag{3.7}$$

where $G(z_1,z_2)$ is a distinguished pseudopolynomial of order k

$$G(z_1,z_2) = (z_2-a_2)^k + A_1(z_1)(z_2-a_2)^{k-1} + \cdots + A_k(z_1),$$

and $A_i(a)=0$, $i=0,\ldots,k$. The integers k,μ are positive or zero. The functions $\Omega(z_1,z_2)$ is holomorphic at (a_1,a_2) and $\Omega(a_1,a_2)\neq 0$. The functions A_i and Ω are uniquely defined by the conditions of the theorem.

The factor $(z_1-a_1)^{\mu}$ can be used only in the case $n=2$.

It is included in order to cover the possibility of $F(a_1,z_2)\equiv 0$, i.e., that the factorization of F has the form

$$F(z_1,z_2) = f_1(z_1)f_2(z_1,z_2), \tag{3.8}$$

where $f_1(a_1) = 0$ for all z_2. In Sec. IIIA we have referred to this case as the third possibility for the product form of the scattered field. On the other hand, if $n > 2$, one has to make a coordinate transformation to exclude the case $F(a_1,\ldots,a_{n-1},z_n)\equiv 0$ (Ref. 8).

The Weierstrass preparation theorem does not imply reducibility for $F(z_1,z_2)$, since $\Omega(a_1,a_2)\neq 0$ (cf. Definition 3). Conversely, if F is reducible at (a_1,a_2) G will also be reducible there. If F is irreducible so is G. (Ref. 15). This is to be expected if the theorem is to be used to examine the properties of the zero lines of F.

A function F, holomorphic in the neighborhood of some point (a) will have a unique decomposition (3.7) in some open bicylinder $V(a)$ about this point. The uniqueness of this decomposition, plus the fact that G has the same zero lines as F in $V(a)$ allows an examination of the zeros of G rather than F, and this is much simpler. In case the F_m are polynomials the following discussion applies directly, without the use of Theorem 3. In particular, it can be used by letting the A_i be polynomials in z_1, instead of analytic functions.

It is well known from conventional algebra[16] that whenever the discriminant $\Delta_G(z_1)$ of a pseudopolynomial $G(z_1,z_2)$ is zero at a point (a_1), then G has a multiple root there, i.e.. $k\geqslant 2$ zero lines meet at (a_1), and at that point G has a root of order k in z_2. If $\Delta_G\equiv 0$, then G has multiple factors. Without loss of generality we can assume that G has no multiple factors, since in such a case the respective componens of their zero sets are equal.

In order to analyze the structure of the zero sets of analytic functions, the structure of the zero sets of pseudopolynomials must be determined. This may be done by means of the following theorem.[9]

Theorem 4: Let $B\subset\mathbb{C}$ be a domain, $G(z_1,z_2) = z_2^k - A_1(z_1)z_2^{k-1} + \cdots + (-1)^k A_k(z_1)$ a pseudopolynomial without multiple factors. The $A_i(z_1)$ $(i = 1,\ldots,k)$ are functions analytic in B. Let

$$M_G = \{(z_1,z_2)\in B\times\mathbb{C}: G(z_1,z_2) = 0\}$$

and

$$D_G = \{z_1\in B:\Delta_G(z_1) = 0\}.$$

Thus M_G and D_G are analytic sets and

1. For $z_1^0\in B - D_G$ there exist an open neighborhood $U(z_1^0)\subset B - D_G$ and holomorphic functions $f_1,\ldots,f_k$ on U, with $f_\nu(z_1)\neq f_\mu(z_1)$ for $\nu\neq\mu$ and $z_1\in U$, such that

$$G(z_1,z_2) = (z_2 - f_1(z_1))\cdots(z_2 - f_k(z_1)) \tag{3.9}$$

for all $z_1\in U$.

2. The points of D_G are "branch points," that is, above a point $z_1\in D_G$ there always lie fewer than k points of the set M_G.

In general there are only two kinds of branch points (for any $n > 1$), as shown in the following example.

Let $G(z_1,z_2) = z_2^2 - z_1^2(z_1 - 1)$, a globally irreducible function. The discriminant of G is

$$\Delta_G(z_1) = 4z_1^2(z_1 - 1).$$

Clearly

$$D_G = \{z_1\in\mathbb{C}:\Delta_G(z_1) = 0\} = \{0\}\cup\{1\}.$$

Let us choose two domains $B_1 = \{z_1\in\mathbb{C}:|z_1| < 1\}$ and $B_2 = \{z_1\in\mathbb{C}:|z_1|\geqslant 1\}$. In B_1 we have:

$$M_G = \{(z_1,z_2)\in B_1\times\mathbb{C}: G(z_1,z_2) = 0\}.$$

For $z_1^0\in B_1 - D_G$ there is a neighborhood $U(z_1^0)\subset B_1 - D_G$ and above U we have a decomposition of the form (3.9)

$$G(z_1,z_2) = [z_2 - z_1(z_1 - 1)^{1/2}][z_2 + z_1(z_1 - 1)^{1/2}]. \tag{3.10}$$

and

$$M_G = \{(z_1,z_2)\in B_1\times\mathbb{C}: z_2 = z_1(z_1 - 1)^{1/2}\}$$
$$\cup\{(z_1,z_2)\in B_1\times\mathbb{C}: z_2 = -z_1(z_1 - 1)^{1/2}\},$$

since both functions in (3.10) are analytic in B_1. Above $D_G = \{0\}$ in B_1, the two analytic sets coincide but both remain analytic at this point. In this case one speaks of pseudobranching.

For $z_1^0\in B_2 - D_G$ and $U(z_1^0)\subset B_2 - D_G$ we have the same decomposition (3.10) but now $D_G = \{1\}$ and above it we have the branch point of the Reimann surface of $z_1(z_1 - 1)^{1/2}$. Clearly neither of the factors in (3.10) is analytic and consequently G is locally irreducible. Here $M_G = \{(z_1,z_2)\in B_2\times\mathbb{C}: G(z_1,z_2) = 0\}$ and it is irreducible since it consists of the Riemann surface of $z_1(z_1 - 1)^{1/2}$. M_G yields a two-sheeted covering above $B_2 - D_G$ and a branch point above $D_G = \{1\}$.

Therefore in $(B_1\cup B_2)\times\mathbb{C} = \mathbb{C}^2$ the zero set of G is irreducible and it consists of the two branches of $z_1(z_1 - 1)^{1/2}$, with the branch point above $z_1 = 1$ and a pseudobranch point above $z_1 = 0$.

If in the neighborhood of a branch point there are m branches of the zero set of a functions, we will call it a branch point of multiplicity m (e.g., in the above example $m = 2$). It is obvious from the above example that if the zero set of a function has a branch point of multiplicity m, then it is m-times irreducible—locally and globally. If the function is a polynomial of order m then it is completely irreducible. This is true also if it has m branch points of multiplicity two.

Returning to the original problem we are now able to analyze the zero set of each F_m in (3.3) as follows. Each F_m defines an irreducible analytic set. In the neighborhood of every point of this set we can use the Weierstrass preparation theorem to write a unique decomposition (3.7). For each pseudopolynomial defined this way we write a product (3.9) which locally describes the zero lines of F_m.

Then, if F_m is irreducible at a point, and $k\geqslant 2$ zero lines from its zero set coincide there, we have a branch point of multiplicity k. If F_m is reducible there then we have a pseudobranch point of order k; of course both cases can exist simultaneously. Since F_m must be an entire function, it is true that each branch surface must have its counterpart in F_m, so that the function does not have branch points. But it is not true that "the zero lines are described by analytic functions."[17] It is the total collection of lines for each factor F_m which forms an irreducible zero set, and not each line individually.

Here, the reason behind the fact that the removal of a

zero line may destroy the band limitation of the object wave, becomes obvious: If a branch surface is removed, the function is no longer entire and thus cannot represent a physical field. Obviously it cannot Fourier-transform back to a physical object wave with finite support. (The usual practice of "flipping" a zero line, i.e., multiplying the Fourier transform $F(z)$ by $G^*(z^*)/G(z)$, where $G(z)$ describes one or more zero lines of an irreducible zero set, has the effect of removing these lines from this set. However unless $G(z)$ describes the whole set, i.e., unless $G(z) \equiv F_m(z)$ the analyticity of the field is destroyed by this operation.)

We can easily show this by an example. It is well known that the scattered field from a circular aperture is given by $aJ_1(ar)/r$, where a is the radius of the aperture. This function can be written as a Hadamard product since it is essentially a one-dimensional function due to its circular symmetry. We have (with $r^2 = x_1^2 + x_2^2$)

$$aJ_1(ar)/r = a \prod_{n=-\infty}^{\infty} (1 - r^2/\alpha_n^2), \tag{3.11}$$

where $J_1(a\alpha_n) = 0$ for all n. It will be shown in a following paper that the removal of one or more factors from (3.11) leaves its band limitation intact. Let us write one of these factors in the form

$$\frac{1}{\alpha_n^2}(\alpha_n^2 - x_1^2 - x_2^2)$$

$$= -\frac{1}{\alpha_n^2}[x_2 - (\alpha_n^2 - x_1^2)^{1/2}][x_2 + (\alpha_n^2 - x_1^2)^{1/2}].$$

This decomposition is possible everywhere except at the points $x_1 = \pm \alpha_n$. If now one of these factors is removed, the object wave is no longer band-limited. This is because the remaining factor contains one branch of the double surface with the branch point. Thus the product no longer forms an analytic function. In Fig. 1 two different such zeros have been removed from the field; the objects shown are no longer confined in a finite domain.

We have shown why one must invert each F_m as a whole [here each factor $(1 - r^2/\alpha_n^2)$ essentially forms a double zero line] and not individual zero lines: each F_m describes a unique and interrelated set of lines, which are inseparable—in essence we have shown what global irreducibility means, and its relation with the analyticity of the field. The ambiguity of object reconstruction can be directly related to the number of branch points in the field; if there are m branch points, of multiplicity $k_1,\ldots,k_m$ the ambiguity is reduced from 2^N to $2^{N-(\Sigma_{i=1}^m k_i)}$. If $\Sigma_{i=1}^m k_i$ is comparable to N, then the determination of the correct object wave from the intensity data is facilitated to a large extent. Of course, if $\Sigma_{i=1}^m k_i = N$, there are only two reconstructions possible: the object wave and its 180° "twin image," which is not too serious an ambiguity.

Unfortunately, the existence of pseudobranching complicates the situation, since it is not apparent how one could distinguish between the two cases, i.e., given a power spectrum it is not possible to determine the number of branch points in a straightforward way, since any zero crossing could be either a branch or a pseudobranch. A further complication is introduced by the fact that branching and pseudobranching can coexist at a point, which does not allow an easy determination of the multiplicity of a branch.

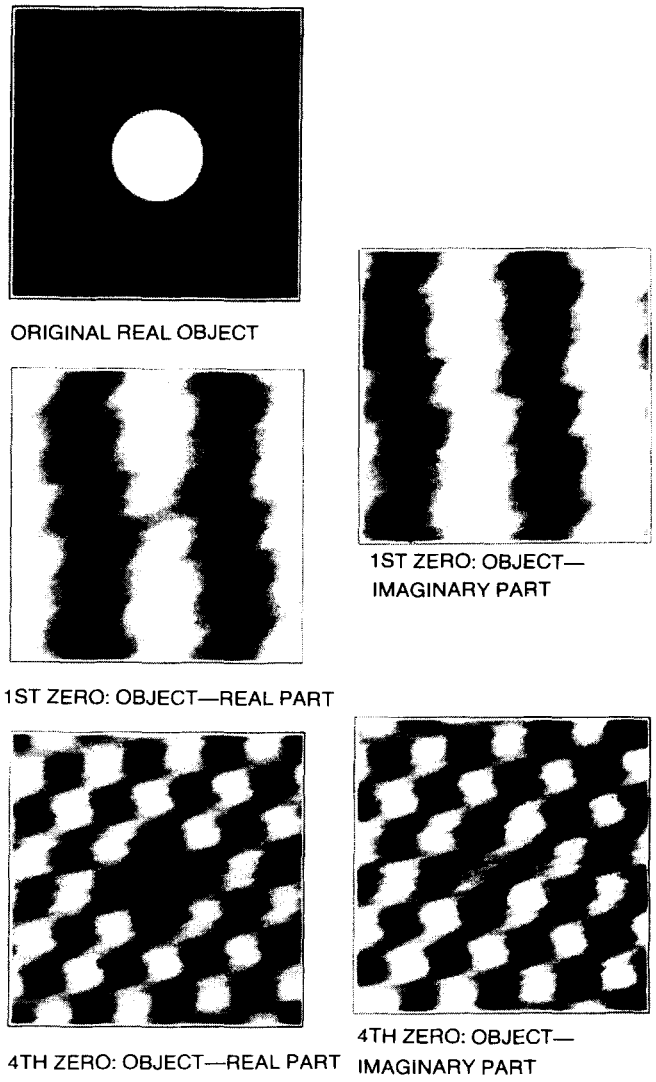

FIG. 1. Loss of finite object support resulting from the removal of one branch of the first and fourth zero circles of $aJ_1(ar)/r$, the Fourier transform of the original real object.

As we have shown in Sec. IIIA, the probability of occurrence of reducible functions in the field is higher than that of irreducible functions. This implies that the probability of occurrence of pseudobranches is higher than that of branches. It should be emphasized once again though, that the above argument was made on purely mathematical grounds. Work is being done to determine the physical significance of branching and pseudobranching, which would then allow an examination of this probability on physical grounds.

IV. CONCLUSIONS

The aim of this paper was two-fold: to formulate a general description of n-dimensional Fourier transforms in terms of the zero surfaces of functions of several complex variables and to apply this description to certain aspects of two-dimensional scattered fields.

In Sec. IIIA it was shown that n-dimensional Fourier transforms can be described by entire functions of exponential type factorable in terms of irreducible entire functions. Each of these functions was shown to define a finite or infinite number of zero lines which form irreducible analytic sets— the units of information in n dimensions.

This description was then applied to two-dimensional scattered fields, to show that for a nonseparable field the ambiguity of object reconstruction from intensity data depends on the number of irreducible factors present and not on the number of zero lines, in contrast with the one-dimensional case. Then the asymptotic behavior of functions of two complex variables was discussed. It was shown that the zero lines in the field have to comply with the asymptotic behavior determined by the aperture. Consequently, since they are of infinite extent, this must also involve a specific behavior in the finite part of $\mathbb{C}^n$, a property which has no counterpart in one-dimensional functions. These properties were used to show how it can be ensured that the product expressing the field in the Fourier space contains only polynomial factors of known asymptotic behavior. The only *a priori* conditions imposed in the object space are that the aperture must be square or circular and that the value on its edge be kept equal to a constant.

The existence of irreducible analytic sets was explained in Sec. IIIB, through the branching behavior of their defining functions. Two cases were distinguished: branching and pseudobranching. This was used to refine the measure of ambiguity for object reconstruction from two-dimensional intensity data. It was shown that this ambiguity is equal to the difference between the number of zero lines present and the number of branch points (counting their multiplicities). In other words, each irreducible zero set must be flipped as a whole; otherwise the function loses it analytic character.

On the other hand, the existence of pseudobranching does not allow a straightforward determination, either of the number of branch points or of their multiplicity, i.e., it is not possible to count the number of zero crossings and equate them with the number of branches. The same goes for the multiplicity of each branch point, since branch and pseudobranch may coincide. From purely mathematical considerations, the probability of occurrence of irreducible factors was shown to be lower than that of reducible ones.

We have also shown that the one-dimensional theory does not generalize to n dimensions, since none of the above properties could have been derived from a one-dimensional description. The difference between the two descriptions hinges on the fact that the zeros of n-dimensional functions ($n \geqslant 2$) are lines and not points. From this all the other differences follow in a natural way.

In a following paper this description will be applied to two particular cases, fields scattered from objects confined to square and circular apertures. These exhibit the characteristic behavior of two-dimensional scattered fields and can be used to show how information is encoded by their respective zero lines. In this paper exact forms will be derived for the encoding of information in each case, and through this it will be shown that information encoding is aperture-dependent.

ACKNOWLEDGMENTS

The author would like to thank Professor R. E. Burge and Mr. G. Ross for their helpful advice. He is also grateful to Dr. M. A. Fiddy, Dr. T. J. Hall, and Dr. P. van Toorn for stimulating discussions and advice.

This work was supported by a three year scholarship given to the author by Queen Elizabeth College.

APPENDIX A: OSGOOD'S PRODUCT THEOREM

Although the proof of the theorem for the factorization of functions of several complex variables is given by Osgood,[10] his formulation of the proof is rather difficult to follow from a contemporary viewpoint. Thus it seemed useful to include a sketch of a proof of his theorem. In addition, the fact that analytic sets are defined locally seems to contradict the fact that they can be described by global functions. It was felt that this point needed clarification. What folllows is by no means a proof of this theorem, but shows how a proof can be constructed.

Let $M(F)$ be the zero set of some entire function F. Now, any analytic set M can be uniquely decomposed into a locally finite, countable system of analytic subsets (M_i) such that $U_{i\in\mathbb{N}} M_i = M$ (Ref. 9). Let $M = M(f)$; M then is defined in the whole of $\mathbb{C}^n$. Using Cousin's second theorem,[8] the functions defining each M_i (now defined for all of $\mathbb{C}^n$) can be connected to form global functions F_i.

Let us now take the product of the F_i, including convergence factors e^{γ_i} which contain no finite zeros, and let G represent this product.

$$G(z) = \prod_{i=1}^{N} [F_i(z) e^{\gamma_i(z)}]^{l_i} \quad (N \leqslant \infty). \tag{A1}$$

(The l_i are introduced because several of the components M_i may be equal.)

Since $U_{i\in\mathbb{N}} M_i = M$ it is easy to see that F/G is an entire function without zeros, i.e., $F/G = e^H$, where H is an entire function. By distributing e^H over the F_m we get (A1).

APPENDIX B: THE ASYMPTOTIC BEHAVIOR OF FOURIER TRANSFORMS IN TWO VARIABLES

Here we aim to show that the edge of the scattering aperture defines the asymptotic behavior of the field. Let us take the object to be a function of r, θ. Then, using the complex form of the Fourier transform we can write

$$\int_0^{2\pi} d\theta \int_0^{r_0(\theta)} dr\, r f(r,\theta) e^{iz_1 r\cos\theta} e^{iz_2 r\sin\theta} = F(z_1,z_2), \tag{B1}$$

where $F(z_1,z_2)$ is the scattered field in the Fraunhofer region and $r_0(\theta)$ is some continuous function of θ. Taking the left-hand side of (B1) and integrating by parts twice with respect to r, we have

$$\int_0^{2\pi} d\theta \int_0^{r_0(\theta)} r\,dr f(r,\theta)\,d\left[\frac{\exp[ir(z_1\cos\theta + z_2\sin\theta)]}{i(z_1\cos\theta + z_2\sin\theta)}\right]$$

$$= \int_0^{2\pi} d\theta \frac{\exp[ir_0(\theta)(z_1\cos\theta + z_2\sin\theta)]}{(z_1\cos\theta + z_2\sin\theta)}$$

$$\times\left\{ - ir_0(\theta) f(r_0(\theta),\theta) \right.$$

$$\left. + \frac{f'(r_0(\theta),\theta)}{(z_1\cos\theta + z_2\sin\theta)} + \frac{r_0(\theta) f'(r_0(\theta),\theta)}{(z_1\cos\theta + z_2\sin\theta)}\right\}$$

$$+ \int_0^{r_0(\theta)} dr\, O\left[(z_1\cos\theta + z_2\sin\theta)^{-3}\right], \qquad \text{(B2)}$$

where the prime denotes the derivative with respect to r.

The dominant term in the above expression, as $|z_1|$, $|z_2| \to \infty$ is the first. This implies that the behavior of the zero lines of $F(z_1,z_2)$ for large values of its arguments is determined by the values $r_0(\theta) f(r_0(\theta),\theta)$, i.e., the edge of the aperture. In general the behavior of the zero lines of the field are determined by the first nonzero term of the integration by parts. It is evident from (B2) that this term is going to be some derivative of $f(r,\theta)$ (with respect to r) evaluated at $r = r_0(\theta)$.

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Global solution to a nonlinear integral evolution problem in particle transport theory

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(Received 18 May 1982; accepted for publication 30 July 1982)

Existence and uniqueness of the solution to a nonlinear integral evolution equation, arising in particle transport theory, is discussed and proved for any time interval $[0,T]$. This is pursued by a suitable application of the contracting mapping principle to the study of the nth power A^n of the relevant nonlinear inhomogeneous integral operator A.

PACS numbers: 02.30.Rz

INTRODUCTION

In a previous paper we have discussed a class of nonlinear integral evolution equations arising in particle transport theory.[1] This class of equations originated from integrating along the trajectory the nonlinear integro-differential Boltzmann equation that governs the space-independent, velocity- and time-dependent distribution function $f(\bar{v},t)$ of the particles considered in the following physical situation. In the interior of an unbounded host medium, consisting of certain field particles (f.p.), a spatially uniform source injects at the time $t=0$ a burst of certain other particles—of mass m, and to be referred to as test particles (t.p.)—with an intensity of Q_0 t.p. per unit volume and with a velocity distribution $S(\bar{v})$ such that $\int_{R_3} d\bar{v}\, S(\bar{v}) = 1$. The t.p. so emitted diffuse then in the host medium by binary collisions either between themselves and against the f.p. of the host medium itself. It is supposed that the cross sections, relevant to all the collisions considered, are of the $1/|\bar{v}|$-type, and no external forces act on the system. The objective is thus to determine the distribution function $f(\bar{v},t)$ of the t.p. that have been injected at $t=0$, and to study how it evolves for $t>0$. If the host medium is taken to be free of t.p. up to $t=0$, then the sought distribution function must be subject to the initial condition $f(\bar{v},0) = Q_0 S(\bar{v})$.

In the present paper we aim at extending the results obtained in Ref. 1 along a two-fold direction. First, we shall assume that the same system as considered in Ref. 1 is now also subject to the action of an external conservative force. Secondly, we shall show here—for a general time-dependent force—that existence and uniqueness of the solution to the new class of nonlinear integral evolution equations, that now originates, can be proved for any time interval $[0,T]$, whereas in Ref. 1 the ultimate goal has been the construction of a rigorous iterative scheme in a finite interval $[0,T_0]$, T_0 being a value of T fixed once for all.

Studies of global solutions for the space-independent nonlinear integro-differential Boltzmann equation have been reported in the literature (see, for instance, Refs. 2–6. Recent reviews, that include also studies of global and local solutions for the space-dependent case, are those of Refs. 7 and 8). We underline that the present approach differs from those proposed in Refs. 2–6 at least in the following four main respects. (i) We refer to the integral version of the nonlinear integro-differential Boltzmann equation as it is, in turn, derived in the frame of the so-called scattering kernel formulation. (ii) The relevant scattering probability distribution is taken to be quite general, and is not restricted to any special class of encounters. (iii) The effects of an external force are fully incorporated in the theory. (iv) In force of both the $1/|\bar{v}|$- approximation for the cross sections and the spatial uniformity of the problem we succeed in producing and solving the exact autonomous continuity equation for the zeroth moment of the unknown distribution function, namely the total density $n(t)$. The knowledge of $n(t)$ is, indeed, crucial for the explicit calculation of the relevant kernel associated with the nonlinear inhomogeneous integral operator, say A, to be dealt with.

The paper is organized as follows. After the outline of the problem is given, we prove, by neglecting removal effects, that A^n is, for sufficiently large n, and with respect to any interval $[0,T]$, a contraction operator mapping a certain ball B of an appropriate Banach space E into itself. A relevant fixed point theorem then applies, and consequently existence and uniqueness of the solution are proved. As an example, an exact analytical solution of the problem is at last reported according to a suitable specialization of both the scattering probability distribution and the law of dependence of the external force on time.

1. OUTLINE OF THE PROBLEM

In the frame of the scattering kernel formulation the space-independent nonlinear integro-differential Boltzmann equation, governing the distribution function $f(\bar{v},t)$ of the t.p. to be considered, reads as[1]

$$\frac{Df(\bar{v},t)}{Dt} + [\hat{\nu}_R(\bar{v}) + \nu(\bar{v},t)]f(\bar{v},t) = G(\bar{v},t),$$

$$(\bar{v}\in R_3; t\in(0,+\infty)). \tag{1}$$

In Eq. (1)

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \frac{\bar{F}(t)}{m}\cdot\bar{\nabla}_{\bar{v}}, \tag{2a}$$

is the substantial derivative of f, $\bar{\nabla}$ being the symbol of the gradient,

$$\hat{\nu}_R(\bar{v}) = |\bar{v}|N\hat{\sigma}_R(|\bar{v}|), \tag{2b}$$

where N is the assigned total density of the f.p., is the collision frequency for the removal of t.p. by the f.p.,

 0022-2488/82/122299-05$02.50

$$\nu(\bar{v},t) = \nu_S(\bar{v},t) + \nu_R(\bar{v},t)$$
$$= \int_{R_3} d\bar{v}''\sigma(|\bar{v}-\bar{v}''|)|\bar{v}-\bar{v}''|f(\bar{v}'',t)$$
$$(\sigma = \sigma_S + \sigma_R). \tag{2c}$$

is the collision frequency, scattering plus removal, of the t.p. between themselves, and

$$G(\bar{v},t) = Q(\bar{v},t) + I_S(\bar{v},t)$$
$$= Q(\bar{v},t) + \int_{R_3}\int_{R_3} d\bar{v}'d\bar{v}''f(\bar{v}',t)f(\bar{v}'',t)$$
$$\times\sigma_S(|\bar{v}'-\bar{v}''|)|\bar{v}'-\bar{v}''|\Pi(\bar{v}',\bar{v}''\to\bar{v}), \tag{2d}$$

includes all the gain terms, namely the external source $Q(\bar{v},t)$, and the scattering-in integral $I_S(\bar{v},t)$, respectively.

We recall also that the zeroth moment

$$n(t) = \int_{R_3} d\bar{v}f(\bar{v},t), \tag{3}$$

is the (unknown) total density of the t.p. considered, whereas the scattering probability distribution $\Pi(\bar{v}',\bar{v}''\to\bar{v})$—which is a nonnegative function on $R_3\otimes R_3\otimes R_3$—summable with respect to $\bar{v}$—obeys the normalization condition

$$\int_{R_3} d\bar{v}\Pi(\bar{v}',\bar{v}''\to\bar{v}) = 1, \tag{4a}$$

and the symmetry condition

$$\Pi(\bar{v}',\bar{v}''\to\bar{v}) = \Pi(\bar{v}'',\bar{v}'\to\bar{v}), \tag{4b}$$

with respect to the velocities $\bar{v}'$ and $\bar{v}''$ before collision.

For the scattering-in integral we have at last

$$\int_{R_3} d\bar{v}I_S(\bar{v},t) = \int_{R_3} d\bar{v}\nu_S(\bar{v},t)f(\bar{v},t). \tag{5}$$

We specialize now Eq. (1) according to the following hypothesis: (i) The external source is taken to be of pulsed type, namely

$$Q(\bar{v},t) = Q_0S(\bar{v})\delta(t), \tag{6}$$

where Q_0 is the intensity, $S(\bar{v})$ is a nonnegative function on R_3 such that

$$\int_{R_3} d\bar{v}S(\bar{v}) = 1, \tag{6a}$$

and $\delta(t)$ is the symbol for the delta Dirac function. (ii) All the cross sections obey the $1/|\bar{v}|$-law, that is

$$\hat{\sigma}_R(|\bar{v}|) = \hat{C}_R/|\bar{v}|, \tag{7a}$$
$$\sigma_\alpha(|\bar{v}'-\bar{v}''|) = C_\alpha/|\bar{v}'-\bar{v}''|, \tag{7b}$$

$\hat{C}_R$ and $C_\alpha(\alpha = S,R)$ being appropriate positive constants. There follows thus that

$$\hat{\nu}_R(\bar{v}) = \hat{C}_RN, \tag{8a}$$
$$\nu(\bar{v},t) = Cn(t) = (C_S + C_R)n(t), \tag{8b}$$

and

$$\int_{R_3} d\bar{v}I_S(\bar{v},t) = C_Sn^2(t). \tag{8c}$$

Equation (1) reduces then to

$$\frac{Df(\bar{v},t)}{Dt} + [\hat{C}_RN + Cn(t)]f(\bar{v},t)$$
$$= C_S\int_{R_3}\int_{R_3} d\bar{v}'d\bar{v}''f(\bar{v}',t)f(\bar{v}'',t)\Pi(\bar{v}',\bar{v}''\to\bar{v}), \tag{9}$$

to be integrated upon the initial condition

$$f(\bar{v},0) = Q_0S(\bar{v}). \tag{9a}$$

When it is allowed to integrate along the trajectory of the general t.p., we obtain for the integral version of Eq. (9) the result

$$f(\bar{v},t) = Q_0S[\bar{v}(0)]T_0(t)$$
$$+ C_S\int_0^t du\int_{R_3}\int_{R_3} d\bar{v}'d\bar{v}''K(\bar{v},\bar{v}',\bar{v}'';t,u)f(\bar{v}',u)f(\bar{v}'',u), \tag{10}$$

which represents a nonlinear integral equation for $f(\bar{v},t)$, of Volterra's type with respect to time. The kernel of Eq. (10) is given by

$$K(\bar{v},\bar{v}',\bar{v}'';t,u) = T(t,u)\Pi[\bar{v}',\bar{v}''\to\bar{v}(u)], \tag{11}$$

where

$$T(t,u) = e^{-\hat{C}_RN(t-u)}\exp\left[-C\int_u^t n(u')du'\right], \tag{12a}$$

with

$$T_0(t) = T(t,0), \tag{12b}$$

and

$$\bar{v}(u)\equiv\bar{v}(\bar{F};t;u) = \bar{v} - \int_u^t du'\frac{\bar{F}(u')}{m}, \tag{12c}$$

the latter following from integrating the Newton law of motion upon the final condition $\bar{v}(t) = \bar{v}$.

With $\bar{v}(u)$ expressed by Eq. (12c), the kernel K is not any longer "globally" separable as it is in the case without any force acting on the system. Indeed, in the limit of $\bar{F}\to 0$, we realize that K becomes the product of a function of time $T(t,u)$—which is the kernel relevant to the Volterra nature of the equation—by a function $\Pi(\bar{v}',\bar{v}''\to\bar{v})$ of the velocities alone. Thus both Eq. (9) and Eq. (10) reduce to the corresponding equations dealt with in Ref. 1. We also notice that in Eq. (10), $S(\bar{v})$, $\Pi(\bar{v}',\bar{v}''\to\bar{v})$, and $\bar{F}(t)$ are so far general functions of their respective arguments.

2. THE TOTAL DENSITY $n(t)$ AND THE FACTOR $T(t,u)$

Equations (9) and (10) become fully explicit once $n(t)$ is known. It can be indeed determined autonomously from the continuity equation, the latter being derived by integrating either Eq. (9) or Eq. (10) over the velocity domain and assuming that the exchange of the order of the relevant functional operations be permissible. The same result is obtained, namely the nonlinear Bernouilli equation

$$n'(t) + C_RNn(t) + C_Rn^2(t) = 0, \tag{13}$$

provided we take into account that in the case of Eq. (10)

$$\int_{R_3} d\bar{v}S\left(\bar{v} - \int_0^t du'\frac{\bar{F}(u')}{m}\right) = 1, \tag{14a}$$

and

$$\int_{R_3} d\bar{v}\Pi\left(\bar{v}',\bar{v}''\to\bar{v} - \int_u^t du'\frac{\bar{F}(u')}{m}\right) = 1. \tag{14b}$$

We remark that Eq. (13) holds for any S, Π and $\bar{F}$.

The general solution to Eq. (13), satisfying the initial condition

$$n(0) = Q_0, \tag{15}$$

is therefore the same as in the case $\bar{F} = 0$, namely

$$n(t) = Q_0\hat{C}_R N\left[(\hat{C}_R N + Q_0 C_R)e^{\hat{C}_R N t} - Q_0 C_R\right]^{-1}, \tag{16}$$

which for large t behaves exponentially like $e^{-\hat{C}_R N t}$, as physically expected.

The factor $T(t,u)$, appearing in the kernel of Eq. (10), can be then determined as

$$T(t,u) = H(t)H^{-1}(u), \tag{17}$$

with

$$H(t) = e^{-\hat{C}_R N t}\left[(\hat{C}_R N + Q_0 C_R) - Q_0 C_R e^{-\hat{C}_R N t}\right]^{-C/C_R}. \tag{17a}$$

3. THE CASE WITHOUT REMOVAL

When both $\hat{C}_R$ and C_R tend to zero, then

$$n(t) = \text{const} = Q_0, \tag{18a}$$

for all t, and consequently

$$T(t,u) = H(t-u) = e^{-C_S Q_0(t-u)}, \tag{18b}$$

is not only separable, but also of displacement type. We rewrite then Eq. (10) in an operational form as

$$Af = f, \tag{19}$$

where A is the nonlinear inhomogeneous operator defined by

$$\begin{aligned} Af = {} & Q_0 S[\bar{v}(0)]e^{-C_S Q_0 t} \\ & + C_S\int_0^t du\, e^{-C_S Q_0(t-u)}\int_{R_3}\int_{R_3} d\bar{v}'d\bar{v}'' \\ & \times f(\bar{v}',u)f(\bar{v}'',u)\Pi[\bar{v}',\bar{v}''\to\bar{v}(u)]. \end{aligned} \tag{20}$$

4. THE OPERATOR A AS A CONTRACTION OPERATOR. EXISTENCE AND UNIQUENESS OF THE SOLUTION TO EQUATION (19)

If T_0 is a positive constant, let us consider the four-dimensional domain $R_3 \otimes [0,T_0]$, and denote by E the Banach space of the functions $\varphi(\bar{v},t)$, defined on $R_3 \otimes [0,T_0]$, which are continuous in t for almost every $\bar{v}\in R_3$, and summable in $\bar{v}$ for any $t\in[0,T_0]$. If

$$\|\varphi\|_t = \int_{R_3} d\bar{v}|\varphi(\bar{v},t)| \tag{21a}$$

denotes the L_1-norm of $\varphi(\bar{v},t)$ with respect to $\bar{v}$, the norm in E is defined as

$$|||\varphi||| = \max_{t\in[0,T_0]}\|\varphi\|_t. \tag{21b}$$

Let then B denote the closed ball of E centered at the origin and having radius Q_0 (in other words, $|||\varphi|||\leqslant Q_0$ if $\varphi\in B$). We now verify that A maps B into itself, namely $AB\subset B$. As we may change the relevant integration order, we get in fact for $\varphi\in B$

$$\begin{aligned} |A\varphi| \leqslant {} & Q_0 S[\bar{v}(0)]e^{-C_S Q_0 t} \\ & + C_S\int_0^t du\, e^{-C_S Q_0(t-u)}\int_{R_3}\int_{R_3} d\bar{v}'d\bar{v}'' \\ & \times|\varphi(\bar{v}',u)\varphi(\bar{v}'',u)|\Pi[\bar{v}',\bar{v}''\to\bar{v}(u)], \end{aligned} \tag{22}$$

and successively, accounting for Eqs. (14),

$$\begin{aligned} \|A\varphi\|_t &\leqslant Q_0 e^{-C_S Q_0 t} + C_S\int_0^t du e^{-C_S Q_0(t-u)}\|\varphi\|_u^2 \\ &\leqslant Q_0 e^{-C_S Q_0 t} + \frac{|||\varphi|||^2}{Q_0}(1 - e^{-C_S Q_0 t}) \leqslant Q_0, \end{aligned} \tag{23a}$$

from which

$$|||A\varphi||| \leqslant Q_0, \tag{23b}$$

that is, A maps B into itself. Q. E. D.

We prove now that A is a contraction. Recalling also Eq. (4b), we have successively

$$\begin{aligned} A\varphi - A\psi = {} & C_S\int_0^t du\, e^{-C_S Q_0(t-u)}\int_{R_3}\int_{R_3} d\bar{v}'d\bar{v}''[\varphi(\bar{v}',u) + \psi(\bar{v}',u)] \\ & \times[\varphi(\bar{v}'',u) - \psi(\bar{v}'',u)]\Pi[\bar{v}',\bar{v}''\to\bar{v}(u)], \end{aligned} \tag{24a}$$

$$\begin{aligned} |A\varphi - A\psi| \leqslant {} & C_S\int_0^t du\, e^{-C_S Q_0(t-u)}\int_{R_3}\int_{R_3} d\bar{v}'d\bar{v}''|\varphi(\bar{v}',u) \\ & + \psi(\bar{v}',u)||\varphi(\bar{v}'',u) - \psi(\bar{v}'',u)|\Pi[\bar{v}'\bar{v}''\to\bar{v}(u)], \end{aligned} \tag{24b}$$

$$\begin{aligned} \|A\varphi - A\psi\|_t &\leqslant C_S\int_0^t du\, e^{-C_S Q_0(t-u)}\|\varphi+\psi\|_u\|\varphi-\psi\|_u \\ &\leqslant C_S|||\varphi+\psi|||\,|||\varphi-\psi||| \\ &\quad\times\int_0^t du\, e^{-C_S Q_0(t-u)} \\ &\leqslant 2(1 - e^{-C_S Q_0 t})|||\varphi-\psi|||, \end{aligned} \tag{24c}$$

$$|||A\varphi - A\psi||| \leqslant 2(1 - e^{-C_S Q_0 T_0})|||\varphi-\psi|||. \tag{24d}$$

If $2(1 - e^{-C_S Q_0 T_0}) < 1$, then A is a contraction. This requires thus that

$$T_0 < \frac{\ln 2}{C_S Q_0}, \tag{25}$$

which is the same result already obtained for the case $\bar{F} = 0$. We realize that this occurs because $\bar{v}(u)$ differs from $\bar{v}$ only by a displacement so that nothing changes when integrating S or Π over $\bar{v}\in R_3$.

On the basis of Eqs. (23b) and (25) we can thus conclude—as a straightforward application of the contracting mapping principle[9]—that, also for the present case of $\bar{F}\neq 0$, there is only one fixed point of the operator A in the ball B of radius Q_0 centered at the origin of the Banach space E considered. However, the proof of existence and uniqueness we have come up with so far is only local, since $[0,T_0]$ is a fixed finite interval.

We show next that, even accounting for a force $\bar{F}\neq 0$, we can extend our proof of existence and uniqueness to any time interval $[0,T]$. Let indeed T be a general positive constant and check if there exists a sufficiently large integer n so that A^n be still a contraction operator. We first prove by induction that, for $\varphi,\psi\in B$,

$$||A^n\varphi - A^n\psi||_t \leqslant \frac{2^n}{(n-1)!}\gamma(n,C_S Q_0 t)|||\varphi-\psi|||, \quad (26)$$

where $\gamma(n,x)$ denotes the incomplete gamma function defined as[10]

$$\gamma(n,x) = \int_0^x dz\, z^{n-1}e^{-z} = (n-1)!\left(1 - e^{-x}\sum_{k=0}^{n-1}\frac{x^k}{k!}\right). \quad (27)$$

Indeed, if Eq. (26) is true for $n-1$, then we have

$$\begin{aligned}
&||A^n\varphi - A^n\psi||_t \\
&\leqslant 2C_S Q_0 e^{-C_S Q_0 t}\int_0^t du\, e^{C_S Q_0 u}||A^{n-1}\varphi - A^{n-1}\psi||_u \\
&\leqslant 2^n C_S Q_0 e^{-C_S Q_0 t}|||\varphi-\psi|||\int_0^t du \\
&\quad\times\left[e^{C_S Q_0 u} - \sum_{k=0}^{n-2}\frac{(C_S Q_0 u)^k}{k!}\right] \\
&= 2^n\left[1 - e^{-C_S Q_0 t}\sum_{k=0}^{n-1}\frac{(C_S Q_0 t)^k}{k!}\right]|||\varphi-\psi|||. \quad \text{Q.E.D.}
\end{aligned} \quad (28)$$

As $\gamma(n,x)$, for a fixed $n \geqslant 1$, is a positive, monotonically increasing function of $x > 0$, then, by taking the norm with respect to t of both sides of Eq. (28), we get

$$|||A^n\varphi - A^n\psi||| \leqslant \frac{2^n}{(n-1)!}\gamma(n,C_S Q_0 T)|||\varphi-\psi|||. \quad (29)$$

For A^n to be a contraction, it is then sufficient to verify that for a fixed T

$$\frac{2^n}{(n-1)!}\gamma(n,C_S Q_0 T) \leqslant \frac{(2C_S Q_0 T)^n}{(n-1)!} < 1. \quad (30)$$

As $n \to +\infty$, $(2C_S Q_0 T)^n/(n-1)!$ tends to zero so that for any fixed T there exists a value n, say, $n_0 = n_0(T)$, such that the condition, Eq. (30), is satisfied for any $n > n_0$.

We have thus extended existence and uniqueness of the solution to Eq. (19) to any time interval $[0,T]$. In this sense we can then speak of a global solution to Eq. (19) itself.

5. AN ANALYTICAL SOLUTION TO EQ. (19)

Let us assume that the scattering probability distribution $\Pi(\bar v', \bar v'' \to \bar v)$ be given by the following model

$$\Pi(\bar v', \bar v'' \to \bar v) = \psi(\bar v), \quad (31)$$

that is, it is independent of both the velocities $\bar v'$ and $\bar v''$ before collision, and depends only on the velocity $\bar v$ after collision. This means that the scattered t.p. forget at once their previous history and are pushed towards an equilibrium distribution $\psi(\bar v)$. Then the solution to Eq. (19) is directly supplied by the equation itself and reads as

$$\begin{aligned}
f(\bar v,t) &= Q_0 S[\bar v(0)]e^{-C_S Q_0 t} \\
&\quad + C_S Q_0^2\int_0^t du\, e^{-C_S Q_0(t-u)}\psi[\bar v(u)].
\end{aligned} \quad (32)$$

A physical application of Eq. (32) is the one according to which $\psi(\bar v)$ is taken to coincide with the Maxwellian distribution

$$M(\bar v) = (\beta/\pi)^{3/2}e^{-\beta|\bar v|^2} \quad (\beta = m/2k_B T), \quad (33a)$$

and for the force $\bar F(t)$ we refer, without loss of generality, to a force parallel to the x_3-axis of the form

$$\bar F(t) = \bar k_3[F + F_0 H(t)U(t-t_0)], \quad (33b)$$

that is, at a certain time $t_0 > 0$ a time-dependent force $F_0 H(t)$ is suddenly superimposed to a constant force already acting on the system.

Accounting for Eqs. (33), Eq. (32) can be rewritten as

$$\begin{aligned}
f(\bar v,t) &= Q_0 S\left(\bar v - \bar k_3\frac{F}{m}t\right)e^{-C_S Q_0 t} \\
&\quad + C_S Q_0^2\int_0^t du\, e^{-C_S Q_0(t-u)} \\
&\quad\times M\left[\bar v - \bar k_3\frac{F}{m}(t-u)\right]
\end{aligned} \quad (34a)$$

for $t < t_0$, and

$$\begin{aligned}
f(\bar v,t) &= Q_0 S\left[\bar v - \bar k_3\frac{F}{m}t - \bar k_3\frac{F_0}{m}\int_{t_0}^t du'\, H(u')\right]e^{-C_S Q_0 t} \\
&\quad + C_S Q_0^2\int_0^{t_0} du\, e^{-C_S Q_0(t-u)} \\
&\quad\times M\left[\bar v - \bar k_3\frac{F}{m}(t-u) - \bar k_3\frac{F_0}{m}\int_{t_0}^t du'\, H(u')\right] \\
&\quad + C_S Q_0^2\int_{t_0}^t du\, e^{-C_S Q_0(t-u)} \\
&\quad\times M\left[\bar v - \bar k_3\frac{F}{m}(t-u) - \bar k_3\frac{F_0}{m}\int_u^t du'\, H(u')\right],
\end{aligned} \quad (34b)$$

for $t > t_0$, respectively.

In the simple case when $H(t) = 1$, we have then explicitly

$$\begin{aligned}
f(\bar v,t) &= Q_0 S\left[v_1, v_2, v_3 - \frac{F}{m}t - \frac{F_0}{m}(t-t_0)U(t-t_0)\right]e^{-C_S Q_0 t} \\
&\quad + \frac{\pi^{1/2}}{2}C_S Q_0 t_F \exp\left[\frac{F_0}{F}C_S Q_0(t-t_0)U(t-t_0)\right] \\
&\quad\times\exp[\tfrac{1}{2}C_S Q_0 t_F - \beta^{1/2}v_3)^2] \\
&\quad\times\left\{\operatorname{erfc}\left[\tfrac{1}{2}C_S Q_0 t_F + \frac{t-t_0}{t_{F+F_0}}U(t-t_0) - \beta^{1/2}v_3\right]\right. \\
&\quad - \operatorname{erfc}\left[\tfrac{1}{2}C_S Q_0 t_F + \frac{t}{t_F}\right. \\
&\quad \left.\left. + \frac{t-t_0}{t_{F_0}}U(t-t_0) - \beta^{1/2}v_3\right]\right\}Q_0 M(\bar v) \\
&\quad + \frac{\pi^{1/2}}{2}C_S Q_0 t_{F+F_0}U(t-t_0)\exp[(\tfrac{1}{2}C_S Q_0 t_{F+F_0} \\
&\quad - \beta^{1/2}v_3)^2]\left\{\operatorname{erfc}(\tfrac{1}{2}C_S Q_0 t_{F+F_0} - \beta^{1/2}v_3)\right. \\
&\quad \left.- \operatorname{erfc}\left(\tfrac{1}{2}C_S Q_0 t_{F+F_0} + \frac{t-t_0}{t_{F+F_0}} - \beta^{1/2}v_3\right)\right\}Q_0 M(\bar v),
\end{aligned} \quad (35)$$

where, for a given force F, t_F is the characteristic time

$$t_F = \frac{m}{F\beta^{1/2}}, \quad (35a)$$

representing the time that takes F to accelerate at t.p. at rest up to a speed $\beta^{-1/2}$.

In the case when $S(\bar{v}) = M(\bar{v})$, then the solution $f(\bar{v},t)$, Eq. (35), can be recast as the product of $Q_0 M(\bar{v})$ times a distortion factor depending on v_3 and t as well as on the parameters t_0, F, F_0, m, β, C_S and Q_0.

When $t \to +\infty$, we get

$$\lim_{t \to +\infty} f(\bar{v},t) = \frac{\pi^{1/2}}{2} C_S Q_0 t_{F+F_0} e^{(\frac{1}{2}C_S Q_0 t_{F+F_0} - \beta^{1/2} v_3)^2} \times \operatorname{erfc}(\tfrac{1}{2} C_S Q_0 t_{F+F_0} - \beta^{1/2} v_3) Q_0 M(\bar{v}), \tag{36}$$

namely, the asymptotic limit of f is, in any case, the product of $Q_0 M(\bar{v})$ times the stationary distortion factor that would be in order for the constant force $F + F_0$ in absence of external source, as physically expected. (In all the preceding equations erfc denotes the complementary error function as defined in Ref. 10).

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Nonclassical fields with singularities on a moving surface

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(Received 30 November 1981; accepted for publication 18 June 1982)

Fields with singularities on a moving surface S with boundary ∂S can be represented as distributions which have their support concentrated on S and ∂S. This paper considers such fields of the form $F = \{f\} + \lambda\delta_{\tilde{S}}$, where $\{f\}$ is the distribution determined by a field f and $\lambda\delta_{\tilde{S}}$ is a Dirac delta distribution with density λ concentrated on the tube $\tilde{S}$ swept out by the moving surface. A straightforward calculation of the distributional gradient, curl, divergence, and time derivative of such fields yields fields of the following general form: $G = \{g\} + \alpha\delta_{\tilde{S}} + \beta\delta_{\partial\tilde{S}} + \gamma\nabla_n(\cdot)\delta_{\tilde{S}}$. The density α is shown to contain all the information which is customarily presented in the jump conditions for fields with singularities at a moving interface. Examples from electromagnetic field theory are presented to show the significance of the other terms $\{g\}, \beta\delta_{\partial\tilde{S}}$, and $\gamma\nabla_n(\cdot)\delta_{\tilde{S}}$.

PACS numbers: 02.30.Sa, 03.50.De, 02.30.Jr

I. INTRODUCTION

In a recent paper[1] Costen derived the jump conditions for fields with step-function and δ-function singularities on a moving interface, and thereby extended the treatment given to this subject in many standard textbooks, notably in Jackson's well-known book.[2] Costen's methods are essentially the same as those employed by Jackson. In this paper I will show how these results of Costen follow from a direct calculation of the distributional gradient, curl, divergence, and time derivatives of nonclassical fields (distributions). These calculations also exhibit other features which are not accounted for in Costen's paper, but which are shown to be of physical significance in several examples taken from electricity and magnetism.

The theoretical advantages of the use of distribution theory, as opposed to the traditional methods of Costen and Jackson, should be widely recognized, if for no other reason than the remarkable ease with which the distributional calculus handles the field singularities which arise in many physical phenomena. A well-known example from electrostatics is the solution of the field equations $\mathrm{div}(\mathscr{E}) = 4\pi\rho$ and $\mathrm{curl}(\mathscr{E}) = 0$ when the charge distribution $\rho = \sigma\delta_S$ is concentrated on a stationary surface (interface) between two media. A solution of the form $\mathscr{E} = \{\mathbf{e}\}$ is sought, where $\mathbf{e}$ is a smooth (differentiable) field off the surface and $\{\mathbf{e}\}$ denotes the nonclassical distributional field determined by $\mathbf{e}$. The distributional calculus gives

$$\mathrm{div}(\mathscr{E}) = \{\mathrm{div}(\mathbf{e})\} + \hat{n}\cdot[\mathbf{e}]\delta_S,$$
$$\mathrm{curl}(\mathscr{E}) = \{\mathrm{curl}(\mathbf{e})\} + \hat{n}\times[\mathbf{e}]\delta_S,$$

where $[\mathbf{e}] = \mathbf{e}_+ - \mathbf{e}_-$ is the jump in $\mathbf{e}$ across the surface. Thus, to determine $\mathscr{E}$, a classical field $\mathbf{e}$ must be found which satisfies

$$\left.\begin{aligned}\mathrm{div}(\mathbf{e}) &= 0\\ \mathrm{curl}(\mathbf{e}) &= 0\end{aligned}\right\} \text{ off of } S,$$
$$\left.\begin{aligned}\hat{n}\cdot[\mathbf{e}] &= 4\pi\sigma\\ \hat{n}\times[\mathbf{e}] &= 0\end{aligned}\right\} \text{ on } S.$$

Numerous other examples from Jackson[2] or other standard textbooks can be treated in a similar manner. Schwartz's remarkably nice textbook,[3] ostensibly written to promote this unifying aspect of distribution theory[4] among the physical scientists, treats several such examples in this manner. I have written this paper to show that the method of Schwartz may be extended to the physical situation discussed in Costen's paper.

Some preliminary definitions and discussion are presented in the next section. The customary treatment of nonclassical tensor fields (distributional tensor fields) on space–time is modified to time-dependent fields on space. The reason for this is to allow the results to be presented in terms of classical vector analysis. Sections III and IV give the formulas for the distributional gradient, curl, divergence, and time derivatives of distributional fields of the forms $F = \{f\}$ and $F = \lambda\delta_{\tilde{S}}$. The derivations of the formulas are briefly indicated. In Sec. V Costen's jump conditions are shown to follow from the formulas in the previous sections. In Sec. VI two examples from electromagnetic field theory are given to illustrate the physical significance of singularities in nonclassical fields and to advocate the distributional approach.

II. PRELIMINARY DEFINITIONS AND DISCUSSION

Consider a two-dimensional surface S embedded in three-dimensional Euclidean space R^3. The surface is assumed to be smooth and to have smooth boundary ∂S (which may be empty). More general cases can be reduced to this situation. Suppose that the surface is set in motion by a smooth flow $\{\Phi_t\}$ generated by a smooth vector field $\mathbf{U}$ on R^3. Thus each $\Phi_t : R^3 \to R^3$ is a smooth map, indexed smoothly by the time t, and

$$\frac{\partial}{\partial t}\Phi_t(\mathbf{r}) = \mathbf{U}(\Phi_t(\mathbf{r})),$$
$$\Phi_0(r) = r$$

for each r and t. The positions of the surface and its boundary at time t are then given by $S_t = \Phi_t(S)$ and $\partial S_t = \Phi_t(\partial S)$. It is convenient to have each S_t also described by $S_t = \{\mathbf{r}\in R^3 | h(\mathbf{r},t) = 0\}$, where h is a scalar field with nonzero gradient at each point. Then the unit vector field on R^3 defined by $\hat{n}(\mathbf{r},t) = \nabla h(\mathbf{r},t)/|\nabla h(\mathbf{r},t)|$ is a unit normal to S_t at

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each point $\mathbf{r}$ on S_t. Additionally assume that by a similar device $\hat{l}(\mathbf{r},t)$ is a unit vector field which is tangent to ∂S_t at points $\mathbf{r}$ on ∂S_t. The speed of propagation of the surface in the direction of the normal is given by $N(\mathbf{r},t) = \hat{\mathbf{n}}(\mathbf{r},t)\cdot\mathbf{U}(\mathbf{r})$. The tube generated by the moving surface is defined as

$$\tilde{S} = \{(\mathbf{r},t) \in R^4 | h(\mathbf{r},t) = 0\}.$$

The various aspects of differential geometry and distribution theory needed here can be found in Refs. 4, 5, and 6. Because I wish to present the results of this paper in the form of classical vector analysis, it is necessary to include some remarks and definitions here on how tensor analysis on tensor fields in R^4 can be modified to fit the time-dependent R^3 point of view.

A scalar field (on R^4) is a smooth function $\psi: R^4 \to R^1$ and can be considered, in the obvious way, to be a time-dependent scalar field on R^3. A vector field (on R^4) is a smooth cross section of the tangent bundle. A time-dependent vector field on R^3 is then by definition a vector field $\mathbf{v}$ on R^4 for which $\mathbf{v}(r^4) = 0$ (here $\mathbf{v}$ is considered as a derivation and $r^4: R^4 \to R^1$ is the projection on the time coordinate). For a coordinate system x^1, x^2, x^3 on R^3 there is a natural extension x^1, x^2, x^3, r^4 to a coordinate system on R^4, and in this coordinate system each time-dependent vector field $\mathbf{v}$ on R^3 has local representation

$$\mathbf{v} = v^1\mathbf{e}_1 + v^2\mathbf{e}_2 + v^3\mathbf{e}^3 = v_1\mathbf{e}^1 + v_2\mathbf{e}^2 + v_3\mathbf{e}^3$$

in terms of the local basis and reciprocal basis for which $\mathbf{e}^i\cdot\mathbf{e}_j = \delta_{ij}$ and $\mathbf{e}^4 = \mathbf{e}_4$. Let $\mathbf{e}_i\cdot\mathbf{e}_j = g_{ij}, g = \det((g_{ij}))$, and assume the orientation is chosen so that g is positive. The use of such coordinate systems will be adhered to from now on. The various differential forms needed will be written without the exterior product symbol, e.g., $dx^1\,dx^2$ instead of $dx^1 \wedge dx^2$. The differential one-forms on R^4 are dx^1, dx^2, dx^3, and $dr^4 = dt$. The volume element is the differential three-form on R^4 defined by $dV = g^{1/2}\,dx^1\,dx^2\,dx^3$, while the four-volume element is $dV\,dt$. The area element is $dA = g^{1/2}(n^1\,dx^2\,dx^3 + n^2\,dx^3\,dx^1 + n^3\,dx^1\,dx^2)$, where $\hat{n} = n^1e_1 + n^2e_2 + n^3e_3$ is the unit normal field previously defined. The line element is $dl = g^{1/2}(l^1\,dx^1 + l^2\,dx^2 + l^3\,dx^3)$. It should be noticed that by use of a suitable parameterization of $\tilde{S}$ one can show that

$$\begin{aligned}\int_{\tilde{S}} \psi\,dV &= \int_{\tilde{S}} \psi N\,dA\,dt \\ &= \int_{\tilde{S}} \psi(U^1\,dx^2\,dx^3 \\ &\quad + U^2\,dx^3\,dx^1 + U^3\,dx^1\,dx^2)\,dt. \qquad (1)\end{aligned}$$

These generalities with coordinate systems are necessary to obtain a simpler proof of the results in Sec. IV by use of a special coordinate system. This special coordinate system is constructed by choosing x^1, x^2, and x^3 so that on a neighborhood of the tube swept out by S_t in R^3, $\mathbf{e}_1$ and $\mathbf{e}_2$ are tangent to S_t and $\mathbf{e}_3 = \hat{n}$ (this can be done first for S and then can be extended to S_t by means of the flow). In this coordinate system, $n^1 = n^2 = 0$, $n^3 = 1$, and consequently

$$dA\,dt = g^{1/2}\,dx^1\,dx^2\,dt \qquad (2)$$

holds on the tube $\tilde{S}$. The Levi–Civita connection (absolute differential) on R^4 is denoted by ∇, and the covariant derivative of the tensor field τ along a vector field $\mathbf{v}$ is $\nabla_{\mathbf{v}}(\tau) = \nabla\tau\cdot\mathbf{v}$. The divergence and curl are defined in the usual way. This completes the differential geometry needed here.

Distributional scalar and vector fields (on R^4) are, by definition, continuous linear functionals on the respective spaces of scalar and vector fields with compact support (the continuity is with respect to a standard topology). A time-dependent distributional scalar field on R^3 is defined to be a distributional scalar field f on R^4. The value of f at ψ is denoted by $\langle f|\psi\rangle$. If a distributional vector field $\mathbf{F}$ on R^4 is restricted to acting only on time-dependent vector fields v on R^3, then the resulting linear functional is called a time-dependent distributional vector field on R^3, and the value of $\mathbf{F}$ at $\mathbf{v}$ is denoted again by $\langle\mathbf{F}|\mathbf{v}\rangle$. Henceforth I will refer to time-dependent (distributional) scalar and vector fields on R^3 simply as (distributional) fields. The principal examples of distributional fields used in this paper are as follows: suppose that ψ and $\mathbf{v}$ are fields which are not necessarily smooth. The corresponding distributional fields $\{\psi\}$ and $\{\mathbf{v}\}$ are defined by

$$\langle\{\psi\}|\alpha\rangle = \int_{R^4} \psi\alpha\,dV\,dt,$$

$$\langle\{\mathbf{v}\}|\mathbf{w}\rangle = \int_{R^4} \mathbf{v}\cdot\mathbf{w}\,dV\,dt,$$

where α and $\mathbf{w}$ are fields with compact support. In addition define the distributional fields $\psi\delta_{\tilde{S}}$ and $\mathbf{v}\delta_{\tilde{S}}$ by

$$\langle\psi\delta_{\tilde{S}}|\alpha\rangle = \int_{\tilde{S}} \psi\alpha\,dA\,dt,$$

$$\langle\mathbf{v}\delta_{\tilde{S}}|\mathbf{w}\rangle = \int_{\tilde{S}} \mathbf{v}\cdot\mathbf{w}\,dA\,dt.$$

The differential operators ∇, curl, divergence, and $\partial/\partial t$ are extended to operators on distributional fields in the following way: for a distributional scalar and vector field f and $\mathbf{F}$, the distributional fields ∇f, curl($\mathbf{F}$), div($\mathbf{F}$), $\partial\mathbf{F}/\partial t$, and $\partial f/\partial t$ are defined by

$$\begin{aligned}\langle\nabla f|\mathbf{w}\rangle &= -\langle f|\mathrm{div}(\mathbf{w})\rangle, \\ \langle\mathrm{curl}(\mathbf{F})|\mathbf{w}\rangle &= +\langle\mathbf{F}|\mathrm{curl}(\mathbf{w})\rangle, \\ \langle\mathrm{div}(\mathbf{F})|\alpha\rangle &= -\langle\mathbf{F}|\nabla\alpha\rangle, \\ \langle\partial\mathbf{F}/\partial t|\mathbf{w}\rangle &= -\langle\mathbf{F}|\partial\mathbf{w}/\partial t\rangle, \\ \langle\partial f/\partial t|\alpha\rangle &= -\langle f|\partial\alpha/\partial t\rangle,\end{aligned}$$

where α and $\mathbf{w}$ are fields with compact support. If ψ and $\mathbf{v}$ are fields which are smooth everywhere except possibly on $\tilde{S}$, then $\nabla\psi$, curl($\mathbf{v}$), div($\mathbf{v}$), $\partial\mathbf{v}/\partial t$, and $\partial\psi/\partial t$ denote the fields obtained by taking the derivatives in the classical sense off of $\tilde{S}$ and assigning arbitrary values on $\tilde{S}$. One can verify that if ψ and $\mathbf{v}$ are smooth everywhere in R^4, then $\nabla(\{\psi\}) = \{\nabla\psi\}$, $\mathrm{curl}(\{\mathbf{v}\}) = \{\mathrm{curl}(\mathbf{v})\}$, $\mathrm{div}(\{\mathbf{v}\}) = \{\mathrm{div}(\mathbf{v})\}$, $\partial\{\mathbf{v}\}/\partial t = \{\partial\mathbf{v}/\partial t\}$, and $\partial\{\psi\}/\partial t = \{\partial\psi/\partial t\}$. The next two sections extend these calculations to fields with singularities.

III. GRAD, CURL, DIV, AND $\partial/\partial t$ FOR FIELDS WITH STEP-FUNCTION DISCONTINUITIES

Consider a scalar field ψ and a vector field $\mathbf{v}$ which are smooth on $R^4 \setminus \tilde{S}$. Then

$$\nabla(\{\psi\}) = \{\nabla\psi\} + [\psi]\hat{n}\delta_{\tilde{S}}, \tag{3}$$

$$\mathrm{curl}(\{\mathbf{v}\}) = \{\mathrm{curl}(\mathbf{v}\} + \hat{n}\times[\mathbf{v}]\delta_{\tilde{S}}, \tag{4}$$

$$\mathrm{div}(\{\mathbf{v}\}) = \{\mathrm{div}(\mathbf{v})\} + \hat{n}\cdot[\mathbf{v}]\delta_{\tilde{S}}, \tag{5}$$

$$\partial\{\mathbf{v}\}/\partial t = \{\partial\mathbf{v}/\partial t\} - N[\mathbf{v}]\delta_{\tilde{S}}, \tag{6}$$

$$\partial\{\psi\}/\partial t = \{\partial\psi/\partial t\} - N[\psi]\delta_{\tilde{S}}. \tag{7}$$

These results are easily derived by using integration by parts together with a limiting process. The limiting process is related to the Gaussian pillbox argument and is necessitated by the fact that ψ and $\mathbf{v}$ are not assumed to be differentiable on the moving surface. To get around this, let S_t^ϵ denote the surface which lies at distance ϵ from the surface S_t and let B_t^ϵ be the solid which has S_t^ϵ for boundary. The corresponding tube $\tilde{S}_\epsilon$ and four-volume $\tilde{B}_\epsilon$ swept out in space–time by S_t^ϵ and B_t^ϵ are defined in the natural way. Let $\hat{n}_\epsilon(x,t)$ be a unit vector field which is normal to S_t^ϵ at points x on the surface. Notice that the quantity $\psi\hat{n}_\epsilon \to -[\psi]\hat{n}$, as $\epsilon\to 0$. Similar statements hold for the other quantities involved. In the following proofs the Cartesian coordinate system will be used and d will denote the exterior derivative operator.

Proof of (3): From the definition

$$\langle\nabla\{\psi\}|\mathbf{w}\rangle = -\langle\{\psi\}|\mathrm{div}(\mathbf{w})\rangle = -\int_{R^4}\psi\,\mathrm{div}(\mathbf{w})\,dV\,dt.$$

However, off of $\tilde{S}$

$$\begin{aligned}
&-\psi\,\mathrm{div}(\mathbf{w})\,dV\,dt\\
&\quad= -\psi\left(\frac{\partial w^1}{\partial x^1}+\frac{\partial w^2}{\partial x^2}+\frac{\partial w^3}{\partial x^3}\right)dx^1\,dx^2\,dx^3\,dt\\
&\quad= \begin{cases}\left(\dfrac{\partial\psi}{\partial x^1}w^1+\dfrac{\partial\psi}{\partial x^2}w^2+\dfrac{\partial\psi}{\partial x^3}w^3\right)dx^1\,dx^2\,dx^3\,dt,\\ -d(\psi(w^1\,dx^2\,dx^3+w^2\,dx^3\,dx^1+w^3\,dx^1\,dx^2)\,dt).\end{cases}
\end{aligned}$$

Thus integration by parts over $\tilde{B}_\epsilon$ gives

$$-\int_{\tilde{B}_\epsilon}\psi\,\mathrm{div}(\mathbf{w})\,dV\,dt = \int_{\tilde{B}_\epsilon}\nabla\psi\cdot\mathbf{w}\,dV\,dt - \int_{\tilde{S}_\epsilon}\psi\hat{n}_\epsilon\cdot\mathbf{w}\,dA\,dt.$$

Taking the limit as $\epsilon\to 0$ gives the result.

Proof of (4): From the definition

$$\langle\mathrm{curl}\{\mathbf{v}\}|\mathbf{w}\rangle = \langle\{\mathbf{v}\}|\mathrm{curl}(\mathbf{w})\rangle = \int_{R^4}\mathbf{v}\cdot\mathrm{curl}(\mathbf{w})\,dV\,dt.$$

However, off of $\tilde{S}$

$$\begin{aligned}
&\mathbf{v}\cdot\mathrm{curl}(\mathbf{w})\,dV\,dt\\
&\quad= \left(v_1\left(\frac{\partial w_3}{\partial x_2}-\frac{\partial w_2}{\partial x_3}\right)+v_2\left(\frac{\partial w_1}{\partial x_3}-\frac{\partial w_3}{\partial x_1}\right)\right.\\
&\qquad\left.+v_3\left(\frac{\partial w_2}{\partial x_1}-\frac{\partial w_1}{\partial x_2}\right)\right)dx^1\,dx^2\,dx^3\,dt\\
&\quad= \left\{\left(w_1\left(\frac{\partial v_3}{\partial x_2}-\frac{\partial v_2}{\partial x_3}\right)+w_2\left(\frac{\partial v_1}{\partial x_3}-\frac{\partial v_3}{\partial x_1}\right)\right.\right.\\
&\qquad\left.\left.+w_3\left(\frac{\partial v_2}{\partial x_1}-\frac{\partial v_1}{\partial x_2}\right)\right)dx^1\,dx^2\,dx^3\,dt,\right.\\
&\qquad+d\left((w_2v_3-w_3v_2)\,dx^2\,dx^3+(w_3v_1-w_1v_3)\,dx^3\,dx^1\right.\\
&\qquad\left.+(w_1v_2-w_2v_1)\,dx^1\,dx^2\right)dt.
\end{aligned}$$

Integrating by parts over $\tilde{B}_\epsilon$ gives

$$\int_{\tilde{B}_\epsilon}\mathbf{v}\cdot\mathrm{curl}(\mathbf{w})\,dV\,dt = \int_{\tilde{B}_\epsilon}\mathrm{curl}(\mathbf{v})\cdot\mathbf{w}\,dV\,dt + \int_{\tilde{S}_\epsilon}(\mathbf{v}\times\hat{n}_\epsilon)\cdot\mathbf{w}\,dA\,dt.$$

Taking the limit as $\epsilon\to 0$ gives the result.

Proof of (5): From the definition

$$\langle\mathrm{div}\{\mathbf{v}\}|\alpha\rangle = -\langle\{\mathbf{v}\}|\nabla\alpha\rangle = -\int_{R^4}\mathbf{v}\cdot\nabla\alpha\,dV\,dt.$$

However, off of $\tilde{S}$

$$\begin{aligned}
&-\mathbf{v}\cdot\nabla\alpha\,dV\,dt\\
&\quad= -\left(v^1\frac{\partial\alpha}{\partial x^1}+v^2\frac{\partial\alpha}{\partial x^2}+v^3\frac{\partial\alpha}{\partial x^3}\right)dx^1\,dx^2\,dx^3\,dt\\
&\quad= \begin{cases}\left(\dfrac{\partial v^1}{\partial x^1}+\dfrac{\partial v^2}{\partial x^2}+\dfrac{\partial v^3}{\partial x^3}\right)\alpha\,dx^1\,dx^2\,dx^3\,dt,\\ -d(\alpha(v^1\,dx^2\,dx^3+v^2\,dx^3\,dx^1+v^3\,dx^1\,dx^2)dt).\end{cases}
\end{aligned}$$

Thus integrating by parts over $\tilde{B}_\epsilon$ gives

$$-\int_{\tilde{B}_\epsilon}\mathbf{v}\cdot\nabla\alpha\,dV\,dt = \int_{\tilde{B}_\epsilon}\mathrm{div}(\mathbf{v})\alpha\,dV\,dt - \int_{\tilde{S}_\epsilon}\mathbf{v}\cdot\hat{n}_\epsilon\alpha dA\,dt.$$

Taking the limit as $\epsilon\to 0$ gives the result.

Proof of (6): This follows from formula (7).

Proof of (7): From the definition

$$\langle\partial\{\psi\}/\partial t\,|\alpha\rangle = -\langle\{\psi\}|\partial\alpha/\partial t\rangle = -\int_{R^4}\psi\frac{\partial\alpha}{\partial t}\,dV\,dt.$$

However, off of $\tilde{S}$

$$-\psi\frac{\partial\alpha}{\partial t}\,dx^1\,dx^2\,dx^3\,dt = \frac{\partial\psi}{\partial t}\alpha\,dx^1\,dx^2\,dx^3\,dt + d(\psi\alpha\,dx^1\,dx^2\,dx^3).$$

Integrating by parts over $\tilde{B}_\epsilon$ gives

$$-\int_{\tilde{B}_\epsilon}\psi\frac{\partial\alpha}{\partial t}\,dV\,dt = \int_{\tilde{B}_\epsilon}\frac{\partial\psi}{\partial t}\alpha\,dV\,dt + \int_{\tilde{S}_\epsilon}\psi\alpha\,dV.$$

Taking the limit as $\epsilon\to 0$ results in

$$\langle\partial\{\psi\}/\partial t\,|\alpha\rangle = \langle\{\partial\psi/\partial t\}|\alpha\rangle - \int_{\tilde{S}}[\psi]\alpha\,dV.$$

The use of identity (1) now gives the result.

This completes the proofs in this section, dealing with fields having step-function singularities on a moving surface. The next section provides the corresponding results for fields with δ-function singularities on a moving surface.

IV. GRAD, CURL, DIVERGENCE, AND $\partial/\partial t$ FOR FIELDS WITH DELTA FUNCTION SINGULARITIES

Consider the distributional scalar field $\alpha\delta_{\tilde{S}}$ and vector field $\mathbf{K}\delta_{\tilde{S}}$ with smooth density fields α and $\mathbf{K}$. Then

$$\nabla(\alpha\delta_{\tilde{S}}) = \begin{cases}(\nabla\alpha - \hat{n}\nabla_{\hat{n}}\alpha + 2\Omega\alpha\hat{n})\delta_{\tilde{S}},\\ +\alpha(\hat{n}\times\hat{l})\delta_{\partial\tilde{S}} - \alpha\nabla_{\hat{n}}(\hat{n}\cdot)\delta_{\tilde{S}},\end{cases} \tag{8}$$

$$\mathrm{curl}(\mathbf{K}\delta_{\tilde{S}}) = \begin{cases}(\nabla(\mathbf{K}\cdot\hat{n})\times\hat{n} + (\hat{n}\cdot\mathrm{curl}\,\mathbf{K})\hat{n} + \nabla_{\mathbf{K}\times\hat{n}}(\hat{n}))\delta_{\tilde{S}},\\ +((\mathbf{K}\cdot\hat{n})\hat{l} - (\mathbf{K}\cdot\hat{l})\hat{n})\delta_{\partial\tilde{S}} + (\mathbf{K}\times\hat{n})\cdot\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}},\end{cases} \tag{9}$$

$$\operatorname{div}(\mathbf{K}\delta_{\tilde{S}}) = \begin{cases} (\hat{n}\cdot\operatorname{curl}(\hat{n}\times\mathbf{K}))\delta_{\tilde{S}}, \\ +(\mathbf{K}\times\hat{n})\cdot\hat{l}\delta_{\partial\tilde{S}} - \mathbf{K}\cdot\hat{n}\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}}, \end{cases} \tag{10}$$

$$\frac{\partial}{\partial t}(\alpha\delta_{\tilde{S}}) = \begin{cases} \left(\dfrac{\partial\alpha}{\partial t} + N\nabla_{\hat{n}}\alpha - 2\Omega N\alpha\right)\delta_{\tilde{S}}, \\ +\hat{l}\cdot(\hat{n}\times\mathbf{U})\alpha\delta_{\partial\tilde{S}} + N\alpha\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}}, \end{cases} \tag{11}$$

$$\frac{\partial}{\partial t}(\mathbf{K}\delta_{\tilde{S}}) = \begin{cases} \left(\dfrac{\partial\mathbf{K}}{\partial t} + N\nabla_{\hat{n}}\mathbf{K} - 2\Omega N\mathbf{K}\right)\delta_{\tilde{S}}, \\ \hat{l}\cdot(\hat{n}\times\mathbf{U})\mathbf{K}\delta_{\partial\tilde{S}} + N\mathbf{K}\cdot\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}}. \end{cases} \tag{12}$$

In these formulas $\Omega(\mathbf{x},t)$ is the mean curvature of the surface S_t at the point $\mathbf{x}$, and the distributions $\alpha\nabla_{\hat{n}}(\hat{n}\cdot)\delta_{\tilde{S}}$, $(\mathbf{K}\times\hat{n})\cdot\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}}$, etc. are defined in the natural way:

$$\langle\alpha\nabla_{\hat{n}}(\hat{n}\cdot)\delta_{\tilde{S}}|\mathbf{w}\rangle = \langle\alpha\delta_{\tilde{S}}|\nabla_{\hat{n}}(\hat{n}\cdot\mathbf{w})\rangle,$$
$$\langle(\mathbf{K}\times\hat{n})\cdot\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}}|\mathbf{w}\rangle = \langle\mathbf{K}\times\hat{n}\delta_{\tilde{S}}|\nabla_{\hat{n}}\mathbf{w}\rangle.$$

Just as in the last section these results follow from integration by parts. Here, however, there is no limiting process ($\epsilon\to 0$). In all the proofs below the special coordinate system described in the introduction is used. This is not absolutely necessary, but the special property given in Eq. (2) greatly shortens the proofs.

Proof of (8):

$$\begin{aligned}
\langle\nabla(\alpha\delta_{\tilde{S}})|\mathbf{w}\rangle &= -\int_{\tilde{S}}\alpha\,\operatorname{div}(\mathbf{w})\,dA\,dt \\
&= -\int_{\tilde{S}}\alpha\left(\frac{\partial}{\partial x^1}(g^{1/2}w^1) + \frac{\partial}{\partial x^2}(g^{1/2}w^2) + \frac{\partial}{\partial x^3}(g^{1/2}w^3)\right)dx^1\,dx^2\,dt \\
&= \begin{cases} \displaystyle\int_{\tilde{S}}\left(\frac{\partial\alpha}{\partial x^1}w^1 + \frac{\partial\alpha}{\partial x^2}w^2 - \alpha\frac{\partial}{\partial x^3}(g^{1/2})w^3\right)dx^1\,dx^2\,dt \\ \displaystyle\int_{\partial\tilde{S}}\alpha\,g^{1/2}(w^2\,dx^1 - w^1\,dx^2)\,dt - \int_{\tilde{S}}\alpha\frac{\partial w^3}{\partial x^3}\,g^{1/2}\,dx^1\,dx^2\,dt \end{cases} \\
&= \begin{cases} \displaystyle\int_{\tilde{S}}(\nabla\alpha - \hat{n}\nabla_{\hat{n}}\alpha + 2\Omega\alpha\hat{n})\cdot\mathbf{w}\,dA\,dt, \\ \displaystyle\int_{\partial\tilde{S}}\alpha(\hat{n}\times\hat{l})\cdot\mathbf{w}\,dl\,dt - \int_{\tilde{S}}\alpha\nabla_{\hat{n}}(\hat{n}\cdot\mathbf{w})\,dA\,dt. \end{cases}
\end{aligned}$$

Proof of (9):

$$\begin{aligned}
\langle\operatorname{curl}(\mathbf{K}\delta_{\tilde{S}}|\mathbf{w}\rangle &= \int_{\tilde{S}}\left(K_1\left(\frac{\partial w_3}{\partial x_2} - \frac{\partial w_2}{\partial x_3}\right) + K_2\left(\frac{\partial w_1}{\partial x_3} - \frac{\partial w_3}{\partial x_1}\right) + K_3\left(\frac{\partial w_2}{\partial x_1} - \frac{\partial w_1}{\partial x_2}\right)\right)dx^1\,dx^2\,dt \\
&= \begin{cases} \displaystyle\int_{\tilde{S}}\left(w_1\frac{\partial K_3}{\partial x_2} - w_2\frac{\partial K_3}{\partial x_1} + \left(\frac{\partial K_2}{\partial x_1} - \frac{\partial K_1}{\partial x_2}\right)w_3\right)dx^1\,dx^2\,dt \\ \displaystyle\int_{\partial\tilde{S}}K_3(w_1\,dx^1 + w_2\,dx^2)\,dt - w_3(K_1\,dx^1 + K_2\,dx^2)dt \\ \displaystyle\int_{\tilde{S}}\left(K_2\frac{\partial w_1}{\partial x_3} - K_1\frac{\partial w_2}{\partial x_3}\right)dx^1\,dx^2\,dt \end{cases} \\
&= \begin{cases} \displaystyle\int_{\tilde{S}}(\nabla(\mathbf{K}\cdot\hat{n})\times\hat{n} + (\operatorname{curl}\mathbf{K}\cdot\hat{n})\hat{n})\cdot\mathbf{w}\,dA\,dt, \\ \displaystyle\int_{\partial\tilde{S}}((\mathbf{K}\cdot\hat{n})\hat{l} - (\mathbf{K}\cdot\hat{l})\hat{n})\cdot\mathbf{w}\,dl\,dt, \\ \displaystyle\int_{\tilde{S}}(\nabla_{\mathbf{K}\times\hat{n}}(\hat{n})\cdot\mathbf{w} + (\mathbf{K}\times\hat{n})\cdot\nabla_{\hat{n}}\mathbf{w})\,dA\,dt. \end{cases}
\end{aligned}$$

In the last equality the following identity was used:

$$\nabla_{\mathbf{K}\times\hat{n}}(\hat{n})\cdot\mathbf{w} + (\mathbf{K}\times\hat{n})\cdot\nabla_{\hat{n}}\mathbf{w} = \frac{1}{g^{1/2}}\left(K_2\frac{\partial w_1}{\partial x_3} - K_1\frac{\partial w_2}{\partial x_3}\right)$$

which holds in the special coordinate system being used.

Proof of (10):

$$\begin{aligned}
\langle\operatorname{div}(\mathbf{K}\delta_{\tilde{S}})|\beta\rangle &= -\int_{\tilde{S}}\mathbf{K}\cdot\nabla\beta\,dA\,dt \\
&= -\int_{\tilde{S}}\left(K^1\frac{\partial\beta}{\partial x^1} + K^2\frac{\partial\beta}{\partial x^2} + K^3\frac{\partial\beta}{\partial x^3}\right)g^{1/2}\,dx^1\,dx^2\,dt
\end{aligned}$$

$$= \begin{cases} \int_{\tilde{S}} \left[\frac{1}{g^{1/2}} \left(\frac{\partial}{\partial x^1}(g^{1/2}K^1) + \frac{\partial}{\partial x^2}(g^{1/2}K^2) \right)\beta - K^3 \frac{\partial \beta}{\partial x^3} \right] g^{1/2}\, dx^1\, dx^2\, dt \\ \int_{\partial \tilde{S}} \beta\, g^{1/2}(K^2\, dx^1 - K^1\, dx^2)\, dt \end{cases}$$

$$= \begin{cases} \int_{\tilde{S}} (\hat{n}\cdot \mathrm{curl}(\hat{n}\times \mathbf{K})\beta - (\mathbf{K}\cdot\hat{n})\nabla_{\hat{n}}\beta)\, dA\, dt, \\ \int_{\partial \tilde{S}} \hat{l}\cdot(\mathbf{K}\times\hat{n})\beta\, dl\, dt. \end{cases}$$

Proof of (11):

$$\left\langle \frac{\partial}{\partial t}(\alpha\delta_{\tilde{S}}) | \beta \right\rangle = -\int_{\tilde{S}} \alpha \frac{\partial \beta}{\partial t} g^{1/2}\, dx^1\, dx^2\, dt$$

$$= \begin{cases} \int_{\tilde{S}} \left(\frac{\partial \alpha}{\partial t} + \alpha \frac{\partial}{\partial t}(\log g^{1/2}) \right)\beta\, g^{1/2}\, dx^1\, dx^2\, dt \\ \int_{\tilde{S}} \left(\frac{\partial \alpha}{\partial x^3}\beta\, g^{1/2} + \alpha \frac{\partial \beta}{\partial x^3} g^{1/2} + \alpha\beta \frac{\partial}{\partial x^3}(g^{1/2}) \right) dx^1\, dx^2\, dx^3 \\ - \int_{\partial \tilde{S}} \alpha\beta\, g^{1/2}\, dx^1\, dx^2 \end{cases}$$

$$= \begin{cases} \int_{\tilde{S}} \left(\frac{\partial \alpha}{\partial t} + \alpha \frac{\partial}{\partial t}(\log g^{1/2}) + N\nabla_{\hat{n}}\alpha - 2N\Omega\alpha \right)\beta\, dA\, dt, \\ \int_{\partial \tilde{S}} \hat{l}\cdot(\hat{n}\times \mathbf{U})\alpha\beta\, dl\, dt + \int_{\tilde{S}} \alpha N \nabla_{\hat{n}}\, \beta\, dA\, dt. \end{cases}$$

This last equality makes use of the property in Eq. (1) and a similar property for the line integral. The last equation above shows that in an arbitrary coordinate system

$$\frac{\partial}{\partial t}(\alpha\delta_{\tilde{S}}) = \left(\frac{\partial \alpha}{\partial t} + \alpha \frac{\partial}{\partial t}(\log g^{1/2}) + N\nabla_{\hat{n}}\alpha - 2N\Omega\alpha + N\alpha\nabla_{\hat{n}}(\cdot) \right)\delta_{\tilde{S}} + \hat{l}\cdot(\hat{n}\times \hat{U})\alpha\delta_{\partial\tilde{S}}.$$

Thus formula (11) follows since in Cartesian coordinates $g = 1$.

Proof of (12): This follows from formula (11).

V. THE JUMP CONDITIONS

In this section it will be shown that the jump conditions given in Costen's paper follow easily from Eqs. (3)–(12) given here in Secs. III and IV. By combining the results in these equations, it is seen that if the distributional gradient, curl, divergence, or time derivative is taken of a field with the form

$$F = \{ f \} + \lambda\delta_{\tilde{S}},$$

then the resulting field has the form

$$G = \{ g \} + \alpha\delta_{\tilde{S}} + \beta\delta_{\partial\tilde{S}} + \gamma\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}}.$$

This field is the sum of distributions: $G_0 = \{ g \}$, $G_S = \alpha\delta_{\tilde{S}}$, $G_{\partial S} = \beta\delta_{\partial\tilde{S}}$, and $G'_S = \gamma\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}}$ with different orders of singularities. It should be noted that if

$$\overline{G} = \{ \bar{g} \} + \bar{\alpha}\delta_{\tilde{S}} + \bar{\beta}\delta_{\partial\tilde{S}} + \bar{\gamma}\nabla_{\hat{n}}(\cdot)\delta_{\tilde{S}},$$

then $G = \overline{G}$ not only implies that $G_0 = \overline{G}_0$, $G_S = \overline{G}_S$, $G_{\partial S} = \overline{G}_{\partial S}$, $G'_S = \overline{G}'_S$, but also that for the respective densities $g = \bar{g}$ on $R^4 \setminus \tilde{S}$, $\alpha = \bar{\alpha}$ on $\tilde{S}$, $\beta = \bar{\beta}$ on $\partial\tilde{S}$, and $\gamma = \bar{\gamma}$ on $\tilde{S}$. These last equations between the densities g,α,β,γ and $\bar{g},\bar{\alpha},\bar{\beta},\bar{\gamma}$ are called the jump conditions.

The jump conditions of Costen only involve the G_S part of the above decompositions (actually just the densities). For example if

$$G = \mathrm{div}(\mathbf{F}),$$

then by my Eqs. (5) and (10)

$$G_S = (\hat{n}\cdot[\, \mathbf{f}\,] + \hat{n}\cdot\mathrm{curl}(\hat{n}\times\lambda))\delta_{\tilde{S}}.$$

Also if

$$G = \frac{\partial \mathbf{F}}{\partial t},$$

then

$$G_S = \left(-N[\mathbf{f}] + \frac{\partial \lambda}{\partial t} + N\nabla_{\hat{n}}\lambda - 2\Omega N\lambda \right)\delta_{\tilde{S}}.$$

The density in this last equation is the negative of Costen's density since I have chosen to use $dA\, dt$ and $dV\, dt$ as the tube and four-volume elements instead of $dt\, dA$ and $dt\, dV$. The rest of Costen's formulas follow in a similar manner. The examples in the next section will indicate why the densities in the other terms G_0, $G_{\partial S}$, and G'_S should not be neglected in the treatment of the jump conditions.

VI. PHYSICAL INTERPRETATIONS AND EXAMPLES

Before giving the first example it will be convenient to introduce some notation. The convolution of the distributional scalar field ρ with a scalar field α (with compact support) is the field given by $(\rho * \alpha)(\mathbf{x}) = \langle \rho | \alpha_{\mathbf{x}} \rangle$, where $\alpha_{\mathbf{x}}(\mathbf{y},t) = \alpha(\mathbf{x} - \mathbf{y},t)$. The convolution involving a distributional vector field $\mathbf{J}$ is done componentwise. In Cartesian coordinates $\langle \mathbf{e}_i \rangle$ the components of $\mathbf{J}$ are the distributional scalar fields J_i defined by $\langle J_i | \alpha \rangle = \langle \mathbf{J} | \alpha \mathbf{e}_i \rangle$. The various convolution operations are then defined by

$$\mathbf{J}*\alpha = (J_1*\alpha)\mathbf{e}^1 + (J_2*\alpha)\mathbf{e}^2 + (J_3*\alpha)\mathbf{e}^3,$$
$$\mathbf{J}*\mathbf{v} = J_1*v^1 + J_2*v^2 + J_3*v^3,$$
$$\mathbf{J}\wedge\mathbf{v} = (J_2*v_3 - J_3*v_2)\mathbf{e}_1 + (J_3*v_1 - J_1*v_3)\mathbf{e}_2 + (J_1*v_2 - J_2*v_1)\mathbf{e}_3.$$

The position vector field on R^3 is denoted by $\mathbf{x} = x^1\mathbf{e}_1 + x^2\mathbf{e}_2 + x^3\mathbf{e}_3$ and its magnitude is the scalar field denoted by $|\mathbf{x}|$.

In the first example let me show how fields of the form

$$\mathscr{P} = \{\mathbf{P}\} + \mathbf{p}\delta_S$$

and

$$\mathscr{M} = \{\mathbf{M}\} + \mathbf{m}\delta_S$$

can be interpreted as a polarization field $\mathscr{P}$ arising from an electric dipole distribution and as a magnetization field $\mathscr{M}$ arising from a magnetic dipole distribution. As is well known these fields contribute to the electric and magnetic fields indirectly through effective (virtual) charge and current distributions ρ_e and $\mathbf{J}_m$. Distribution theory explains all of this directly as follows. The usual intuitive arguments suggest that the contributions of $\mathscr{P}$ and $\mathscr{M}$ to the potential functions of the electric and magnetic fields are given by

$$\Phi_e = \mathscr{P}*\frac{\mathbf{x}}{|\mathbf{x}|^3},$$
$$\mathbf{A}_m = \mathscr{M}\wedge\frac{\mathbf{x}}{|\mathbf{x}|^3}.$$

However, the distributional calculus gives

$$\mathscr{P}*\frac{\mathbf{x}}{|\mathbf{x}|^3} = \mathscr{P}*\nabla\left(\frac{1}{|\mathbf{x}|}\right) = -\operatorname{div}(\mathscr{P})*\frac{1}{|\mathbf{x}|},$$
$$\mathscr{M}\wedge\frac{\mathbf{x}}{|\mathbf{x}|^3} = \mathscr{M}\wedge\nabla\left(\frac{1}{|\mathbf{x}|}\right) = \operatorname{curl}(\mathscr{M})*\frac{1}{|\mathbf{x}|}.$$

These identities suggest defining the effective charge and current distributions by

$$\rho_e = -\operatorname{div}(\mathscr{P}),$$
$$\mathbf{J}_m = \operatorname{curl}(\mathscr{M}),$$

which is the customary procedure. The formulas from Secs. III and IV may be used to express ρ_e and $\mathbf{J}_m$ in terms of $\mathbf{P},\mathbf{p}$ and $\mathbf{M},\mathbf{m}$. The potentials Φ_e and $\mathbf{A}_m$ are then expressible as follows (for clarity the variable y has been suppressed in several places as, for instance, $\operatorname{curl}(\mathbf{M}) = \operatorname{curl}(\mathbf{M})(\mathbf{y})$, $\hat{\mathbf{n}} = \hat{\mathbf{n}}(\mathbf{y})$, etc.):

$$\Phi_e(\mathbf{x}) = \begin{cases} -\displaystyle\int_{R^3}\frac{\operatorname{div}(\mathbf{P})}{|\mathbf{x}-\mathbf{y}|}\,dV(\mathbf{y}) + \int_S\frac{\hat{\mathbf{n}}\cdot\operatorname{curl}(\mathbf{p}\times\hat{\mathbf{n}}) - \hat{\mathbf{n}}\cdot[\mathbf{P}]}{|\mathbf{x}-\mathbf{y}|}\,dA(\mathbf{y}) \\ +\displaystyle\int_{\partial S}\frac{(\hat{\mathbf{l}}\times\hat{\mathbf{n}})\cdot\mathbf{p}}{|\mathbf{x}-\mathbf{y}|}\,dl(\mathbf{y}) + \int_S\frac{(\mathbf{p}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3}\,dA(\mathbf{y}) \end{cases}$$

$$\mathbf{A}_m(\mathbf{x}) = \begin{cases} \displaystyle\int_{R^3}\frac{\operatorname{curl}(\mathbf{M})}{|\mathbf{x}-\mathbf{y}|}\,dV(\mathbf{y}) + \int_S\frac{\hat{\mathbf{n}}\times[\mathbf{M}] + \nabla(\mathbf{m}\cdot\hat{\mathbf{n}})\times\hat{\mathbf{n}} + (\hat{\mathbf{n}}\cdot\operatorname{curl}(\mathbf{m}))\hat{\mathbf{n}}}{|\mathbf{x}-\mathbf{y}|}\,dA(\mathbf{y}), \\ +\displaystyle\int_S\frac{\nabla_{\mathbf{m}\times\hat{\mathbf{n}}}(\hat{\mathbf{n}})}{|\mathbf{x}-\mathbf{y}|}\,dA(\mathbf{y}) + \int_{\partial S}\frac{(\mathbf{m}\cdot\hat{\mathbf{n}})\hat{\mathbf{l}} - (\mathbf{m}\cdot\hat{\mathbf{l}})\hat{\mathbf{n}}}{|\mathbf{x}-\mathbf{y}|}\,dl(\mathbf{y}), \\ +\displaystyle\int_S\frac{(\mathbf{m}\times\hat{\mathbf{n}})\hat{\mathbf{n}}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3}\,dA(\mathbf{y}). \end{cases}$$

For simplicity in the above formulas, it has been assumed that the surface is stationary. One can readily see that these formulas reduce to the formulas in Jackson's book when $\mathbf{p} = 0 = \mathbf{m}$. It should be noted that the last two terms in the equations Φ_e and A_m are not accounted for in the work of Costen. All of the terms involving $\mathbf{p}$ and $\mathbf{m}$ arise naturally from the mathematics and their physical significance is explained by the following intuitive argument, which also suggests various ways of experimentally realizing these dipole distributions. It is apparent that some of the terms are zero when $\mathbf{p}$ and $\mathbf{m}$ are either tangent or normal to the surface at each point, and so the argument will proceed under one of these assumptions (the general case follows by resolving into tangential and normal components).

One imagines the electric dipole $\mathbf{p}$ to be represented by an infinitesimal arrow with a positive charge at the head, an equal negative charge at the tail, and the amount of charge times the length of the arrow equal to $|\mathbf{p}|$. These arrows are embedded in the surface S with their various orientations coinciding with the various directions of $\mathbf{p}$. Firstly, when $\mathbf{p}$ is everywhere normal to S, the two ends of each arrow protrude on opposite sides of S and all the arrow heads together form a surface with charge density $\mathbf{p}\cdot\hat{\mathbf{n}}$, while all the tails form a surface with charge density $-\mathbf{p}\cdot\hat{\mathbf{n}}$. These two surfaces, considered infinitesimally close to one another, constitute an electric dipole layer whose contribution to $\Phi_e(\mathbf{x})$ is easily seen to be (cf. Ref. 2, p. 37) $\int_S(\mathbf{p}\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}\cdot(\mathbf{x}-\mathbf{y})|\mathbf{x}-\mathbf{y}|^{-3}dA(\mathbf{y})$. Secondly, if the dipole arrows are everywhere tangent to the surface then two adjacent arrows, lined up head to tail, tend to have their respective head and tail charges combine (cancel if equal in amount), and the net charge is measured by the surface divergence of $\mathbf{p}$, which [cf. the proof of Eq. (10)] is given by $\hat{\mathbf{n}}\cdot\operatorname{curl}(\mathbf{p}\times\hat{\mathbf{n}})$. The reason for this divergence term is explained by taking a small curvilinear square with $\mathbf{p}$ everywhere tangent to two of its sides and normal to the others. The integral of the surface divergence over this square is equal to the line integral of $\mathbf{p}$ around the sides, and this latter integral is, by construction, equal to the difference in strength of $\mathbf{p}$ on the two normal sides. Thus, a net surface charge density arises. An additional contribution to the potential arises at the boundary ∂S from the dipoles which protrude through and create a net line charge density of $(\hat{\mathbf{l}}\times\hat{\mathbf{n}})\cdot\mathbf{p}$.

One imagines the magnetic dipole $\mathbf{m}$ to be represented

by an infinitesimally small current loop (in the shape of a curvilinear square) lying in a plane perpendicular to $\mathbf{m}$ with the direction of current flow determined by the direction of $\mathbf{m}$ and with the current strength times the area of the loop determined by $|\mathbf{m}|$. Firstly, when $\mathbf{m}$ is everywhere tangent to the surface S, one can conceive of each current loop as straddling the surface S, with two sides of the loop running along two adjacent normals and the other two sides of the loop connecting the normal sides and running along at equal distances on each side of S. The totality of these latter two sides forms two surfaces infinitesimally close together, one with current density $\mathbf{m}\times\hat{\mathbf{n}}$ and the other with current density $-\mathbf{m}\times\hat{\mathbf{n}}$. Such a configuration is a magnetic dipole layer and its contribution to $\mathbf{A}_m(\mathbf{x})$ is easily reasoned to be $\int_S (\mathbf{m}\times\hat{\mathbf{n}})\hat{\mathbf{n}}\cdot(\mathbf{x}-\mathbf{y})|\mathbf{x}-\mathbf{y}|^{-3}dA(y)$. There is an additional contribution from the currents $\mathbf{m}\times\hat{\mathbf{n}}$ and $-\mathbf{m}\times\hat{\mathbf{n}}$ flowing on opposite sides of each current loop. These sides, connecting the normal sides, have different lengths (except where S is flat) due to the variation in the normal $\hat{\mathbf{n}}$ along the direction of $\mathbf{m}\times\hat{\mathbf{n}}$. This variation is measured by $\nabla_{\mathbf{m}\times\hat{\mathbf{n}}}(\hat{\mathbf{n}})/|\mathbf{m}|$ and the resulting surface current density is $\nabla_{\mathbf{m}\times\hat{\mathbf{n}}}(\hat{\mathbf{n}})$. Next, the sides of the current loops which are normal to S have currents running in the normal direction which combine (perhaps cancel) along adjacent sides. The net effect is a current density $\hat{\mathbf{n}}\cdot(\mathrm{curl}(\mathbf{m}))\hat{\mathbf{n}}$ distributed over S and a current density $-(\mathbf{m}\cdot\hat{\mathbf{l}})\hat{\mathbf{n}}$ distributed along ∂S. Secondly, in the case where $\mathbf{m}$ is everywhere normal to the surface S, a vector identity gives $\hat{\mathbf{n}}\cdot\mathrm{curl}(\mathbf{m})=0$, and so one is left only with the surface current density $\nabla(\mathbf{m}\cdot\hat{\mathbf{n}})\times\hat{\mathbf{n}}$ and the line current density $(\mathbf{m}\cdot\hat{\mathbf{n}})\hat{\mathbf{l}}$. These densities are present since now all the current loops form a grid on the surface with the currents in the sides of adjacent loops combining (perhaps cancelling) all the way out to the boundary ∂S where one is left with a net current flowing around the boundary circuit.

The second example involves Maxwell's equations:

$$\mathrm{div}(\mathscr{D})=\rho,$$
$$\mathrm{curl}(\mathscr{H})-\frac{\partial\mathscr{D}}{\partial t}=\mathbf{J},$$
$$\mathrm{curl}(\mathscr{E})+\frac{\partial\mathscr{B}}{\partial t}=0,$$
$$\mathrm{div}(\mathscr{B})=0.$$

Let $\rho=\{\rho_0\}+\rho_1\delta_{\tilde{S}}+\rho_2\delta_{\partial\tilde{S}}+\rho_3\nabla(\cdot)\delta_{\tilde{S}}$ and $\mathbf{J}=\{\mathbf{J}_0\}+\mathbf{J}_1\delta_{\tilde{S}}+\mathbf{J}_2\delta_{\partial\tilde{S}}+\mathbf{J}_3\nabla(\cdot)\delta_{\tilde{S}}$ be decompositions of ρ and $\mathbf{J}$ into distributions with supports on $R^4\backslash\tilde{S}$, on $\tilde{S}$, and on $\partial\tilde{S}$, respectively. To find nonclassical solutions of Maxwell's equations, assume that the fields have the form

$$\mathscr{D}=\{\mathbf{d}\}+\mathbf{D}\delta_{\tilde{S}},$$
$$\mathscr{H}=\{\mathbf{h}\}+\mathbf{H}\delta_{\tilde{S}},$$
$$\mathscr{E}=\{\mathbf{e}\}+\mathbf{E}\delta_{\tilde{S}},$$
$$\mathscr{B}=\{\mathbf{b}\}+\mathbf{B}\delta_{\tilde{S}}.$$

Substituting these fields in the field equations and calculating the derivatives in the distributional sense gives the following sets of equations:

$$\mathrm{div}(\mathbf{d})=\rho_0,$$
$$\mathrm{curl}(\mathbf{h})-\partial\mathbf{d}/\partial t=\mathbf{J}_0,$$
$$\mathrm{curl}(\mathbf{e})+\partial\mathbf{b}/\partial t=0,$$
$$\mathrm{div}(\mathbf{b})=0. \tag{13}$$

These equations are to hold on $R^4\backslash\tilde{S}$.

$$\hat{\mathbf{n}}\cdot([\mathbf{d}]+\mathrm{curl}(\hat{\mathbf{n}}\times\mathbf{D}))=\rho_1, \tag{14}$$
$$\hat{\mathbf{n}}\cdot([\mathbf{b}]+\mathrm{curl}(\hat{\mathbf{n}}\times\mathbf{B}))=0, \tag{15}$$
$$\left\{\begin{aligned}&\hat{\mathbf{n}}\times([\mathbf{h}]-\nabla(\mathbf{H}\cdot\hat{\mathbf{n}}))+\nabla_{\mathbf{H}\times\hat{\mathbf{n}}}(\hat{\mathbf{n}})\\&+(\hat{\mathbf{n}}\cdot\mathrm{curl}\,\mathbf{H})\hat{\mathbf{n}}+N[\mathbf{d}]-\frac{\partial\mathbf{D}}{\partial t}-N\nabla_{\hat{\mathbf{n}}}\mathbf{D}+2\Omega N\mathbf{D}\end{aligned}\right\}=\mathbf{J}_1, \tag{16}$$
$$\left\{\begin{aligned}&\hat{\mathbf{n}}\times([\mathbf{e}]-\nabla(\mathbf{E}\cdot\hat{\mathbf{n}}))+\nabla_{\mathbf{E}\times\hat{\mathbf{n}}}(\hat{\mathbf{n}})\\&+(\hat{\mathbf{n}}\cdot\mathrm{curl}\,\mathbf{E})\hat{\mathbf{n}}-N[\mathbf{b}]+\frac{\partial\mathbf{B}}{\partial t}+N\nabla_{\hat{\mathbf{n}}}\mathbf{B}-2\Omega N\mathbf{B}\end{aligned}\right\}=0. \tag{17}$$

Equations (14)–(17) are to hold on $\tilde{S}$.

$$(\mathbf{D}\times\hat{\mathbf{n}})\cdot\hat{\mathbf{l}}=\rho_2, \tag{18}$$
$$(\mathbf{H}\cdot\hat{\mathbf{n}})\hat{\mathbf{l}}-(\mathbf{H}\cdot\hat{\mathbf{l}})\hat{\mathbf{n}}+\hat{\mathbf{l}}\cdot(\mathbf{U}\times\hat{\mathbf{n}})\mathbf{D}=\mathbf{J}_2, \tag{19}$$
$$(\mathbf{E}\cdot\hat{\mathbf{n}})\hat{\mathbf{l}}-(\mathbf{E}\cdot\hat{\mathbf{l}})\hat{\mathbf{n}}-\hat{\mathbf{l}}\cdot(\mathbf{U}\times\hat{\mathbf{n}})\mathbf{B}=0, \tag{20}$$
$$(\mathbf{B}\times\hat{\mathbf{n}})\cdot\hat{\mathbf{l}}=0. \tag{21}$$

Equations (18)–(21) are to hold on $\partial\tilde{S}$. Of course the interpretation of these sets of equations is that (13) constitutes the usual Maxwell equations governing the classical parts $\mathbf{d}$, $\mathbf{h}$, $\mathbf{e}$, and $\mathbf{b}$ of the fields on each side of the moving surface. Equations (14)–(17) are the jump conditions that hold on the moving surface, while Eqs. (18)–(21) are the jump conditions that hold on the boundary of the moving surface. The additional set of equations connected with ρ_3 and $\mathbf{J}_3$ has not been listed. Equations (14)–(17) are the ones given by Costen in dealing with this example, and are seen to reduce to the jump conditions given in Jackson's book (where $\mathbf{D}=\mathbf{H}=\mathbf{E}=\mathbf{B}=0$). It should be noted that the last two equations of Costen [Eqs. (16) and (17) here] have particularly simple resolutions along the normal direction: by taking the dot product with $\hat{\mathbf{n}}$ on both sides of these equations and using Eqs. (14)–(15) and some vector identities, one arrives at

$$\hat{\mathbf{n}}\cdot\left(\mathrm{curl}\,\mathbf{H}-\frac{\partial\mathbf{D}}{\partial t}-\mathbf{J}_1\right)=N(\mathrm{div}(\mathbf{D})-\rho_1),$$
$$\hat{\mathbf{n}}\cdot\left(\mathrm{curl}\,\mathbf{E}+\frac{\partial\mathbf{B}}{\partial t}\right)=0.$$

VII. CONCLUSION

The techniques employed in this paper concerning fields with singularities to the second order can, in principle, be extended to fields with singularities of higher order. Regularity theorems from distribution theory quarantee that every distributional field (with compact support) is essentially a finite sum of derivatives of continuous functions. Taking derivatives then just increases the order. Thus, calculations like those in Secs. III and IV may be carried out, but they

yield complicated results. Simplifications and unification (even of the results given here) can be obtained by extending the treatment to distributional rank-k tensor fields on space–time. These topics will be discussed in another paper.

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The inverse problem of the calculus of variations applied to continuum physics

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(Received 11 March 1982; accepted for publication 25 June 1982)

Necessary and sufficient conditions for a differential system of equations to admit a variational formulation are established by having recourse to Vainberg's theorem which provides also a systematic method for producing the sought functional. An application of the method to the Lagrangian description of fluid dynamics leads to a new variational principle which, while being fully general, reveals a hierarchy between variational approaches to fluid dynamics. Next, the method is applied in an attempt to obtain new variational formulations in various areas of research pertaining to continuum physics: water wave models, elasticity, heat conduction in solids, dynamics of anharmonic crystals, and electromagnetism. Owing to the power of the method, relevant variational formulations are found whenever the given system allows them. The paper places particular emphasis on equations which have, or are supposed to have, soliton solutions.

PACS numbers: 02.30.Wd, 03.40.Gc, 03.50.De, 03.40.Dz

1. INTRODUCTION

At first sight it could seem that the importance of variational principles is due to their being alternate approaches to direct applications of local physical laws. This look, though, is fairly unrealistic: variational formulations of the laws of continuum physics may be the only rigorous way to express such laws. This is so because the fundamental principles of continuum physics are global in character while local forms of the laws are generated from them only if the involved fields are endowed with suitable smoothness properties. However, this smoothness is very often unnatural in that it rules out point sources and discontinuities. In conclusion, there are physical phenomena which can be adequately modeled mathematically only in a variational setting.

Yet, further aspects weigh in favor of variational formulations. First, a single functional accounts for all of the intrinsic features of the problem at hand: differential equations, boundary and jump conditions. Second, variational formulations may serve to unify diverse fields and constitute natural means for approximating[1] or finding[2] the solution. Third, the variational approach allows a systematic connection between symmetries and conservation laws.[3] Fourth, sometimes a Lagrangian turns out to be more fundamental than the resulting equations of motion as it happens, for example, in Feynman's path integral formulation of quantum mechanical systems. Finally, it is an astonishing feature that the overwhelming majority of equations having soliton solutions are the local counterparts of some variational problem.[4]

These considerations are enough for justifying the importance of getting new variational formulations and, more specifically, of solving the inverse problem of the calculus of variations which consists of finding the functional whose stationary points are described by a given set of equations. Until recently, however, the search for functionals was practiced as an art merely based on trick transformations of the given equation. Physically, when a functional can be specified through a Lagrangian L, the difficulty relies on the fact that the standard presciption $L = T - V$ only works for conservative particlelike systems.

A first systematic attempt to solve the problem dates back to Darboux[5] who succeeded in the case of one unknown function only. The case of two unknown functions was solved by Douglas[6] in 1941; since then a number of papers appeared on the subject—see, e.g., Refs. 7–11. The inverse problem was definitely solved by Vainberg[12] within the framework of functional analysis; he showed that the question of existence of a variational principle (potentialness) is equivalent to determining whether or not an operator is self-adjoint. The importance of Vainberg's work was rightly emphasized by Tonti[13] who derived operational formulas to check the self-adjointness of differential operators. Subsequently, more general operational formulas were obtained and applied by Atherton and Homsy.[14] Recently, a series of papers was written by Santilli[9] in connection with a thorough investigation of Lagrangian formulations of second-order systems; as a result Santilli rediscovered the self-adjointness condition characterizing potential operators. Finally, we mention that Gurtin[15] set up a variational formulation, involving a convolution bilinear form, for linear initial value problems. Gurtin's approach was re-examined by Tonti[16] who, on appealing to Vainberg's theorem, arrived at a more direct procedure. A convolution bilinear form is involved also in the work by Kanal and Moses[17] where a variational principle for Fredholm equation, and then for the Gel'fand–Levitan equation and the Korteweg–de Vries equation, is exhibited.

In spite of the literature referred to above, we believe that further attention should be paid to Vainberg's theorem especially with the twofold purpose of bearing evidence of the power of the theorem and of finding new variational formulations in continuum physics. With this in mind, here we attempt to obtain new variational formulations in various areas of research (e.g., vectorial solitons) and to remedy deficiences of previous formulations (e.g., fluid dynamics). To this end, in Sec. 2, we restate Vainberg's theorem and then, in

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Sec. 3, we apply it to the Lagrangian description of fluid dynamics. So we are able to set up a variational principle delivering the continuity equation too as an Euler–Lagrange equation; a detailed comparison with known variational formulations is also presented (Sec. 4). Next, Sec. 5 provides a number of variational principles pertaining to various branches of continuum mechanics: water wave models, elasticity, heat conduction in solids, dynamics of anharmonic crystals. Finally, Sec. 6 yields three variational formulations for electromagnetism. The general operational formulas to check the potentialness of operators, defined by an arbitrary number of nonlinear differential equations in an arbitrary number of independent variables and of arbitrary order (developed in the Appendix), are used throughout. Besides involving an extensive application of Vainberg's theorem, this paper delivers many new Lagrangians; the systematic way of producing them witnesses the power of the theorem.

2. POTENTIALNESS OF A DIFFERENTIABLE OPERATOR

Let X, Y be Banach spaces over the field of real numbers $\mathbf{R}$ (obvious generalizations hold when the Banach spaces are over the field of complex numbers $\mathbf{C}$). For each subset U of Y we let $\mathcal{N}(U;X)$ denote the vector space over $\mathbf{R}$ of all operators from U into X. If the range of an operator belongs to $\mathbf{R}$ then the operator is called a functional. The symbol $\|\cdot\|$ denotes the norm of both X and Y while ω stands for a suitable convex subset of Y and X^* for the conjugate (dual) space of X. Letting $v\in X$ and $z\in X^*$, $\langle v,z\rangle$ represents a bilinear functional (pairing) satisfying the condition that whenever $\langle v,z\rangle = 0$ for every $v\in X$ ($z\in X^*$) then $z(v)$ is the null element of $X^*(X)$. In the instance when $X = X^*$ is a real Hilbert space of functions from a domain $\mathscr{D}\subset\mathbf{R}^n$ into an m-dimensional vector space $\mathbf{V}$, then $\langle\cdot,\cdot\rangle$ may be taken as the inner product on X

$$\langle v,z\rangle = \int_{\mathscr{D}} v(x)\cdot z(x)d\mathscr{V}, \tag{2.1}$$

where "$\cdot$" denotes the inner product on $\mathbf{V}$, or, if $\mathscr{D} = [x_1,x_2]$ in $\mathbf{R}$, as the convolution product

$$\langle v,z\rangle = \int_{x_1}^{x_2} v(x_2 - x)\cdot z(x)dx. \tag{2.2}$$

Suppose that $U\subset Y$ is an open set and $u\in U$. An operator $N\in\mathcal{N}(U;X)$ is said to have a Gâteaux variation at u if

$$VN(u|h) = \lim_{\lambda\to 0}\frac{N(u+\lambda h) - N(u)}{\lambda}, \tag{2.3}$$

namely,

$$\lim_{\lambda\to 0}\|(1/\lambda)[N(u+\lambda h) - N(u)] - VN(u|h)\| = 0,$$

exists for each direction $h\in Y$. The operator $VN(u|\cdot)\in\mathcal{N}(Y;X)$ is called the Gâteaux variation of N at u. Letting $\alpha\in\mathbf{R}$, it is immediate from the definition (2.3) that $VN(u|\alpha h) = \alpha VN(u|h)$, which makes $VN(u|h)$ a homogeneous operator in h. If, further, $VN(u|h)$ is a bounded linear operator in h from Y into X, then the operator N is said to have a Gâteaux differential at u which will be denoted by $DN(u|h)$. Also, in view of the linearity on h, we may write

$$DN(u|h) = N'(u)h, \quad h\in Y,$$

which defines the Gâteaux derivative $N'(u)$; in the case of functionals

$$Df(u|h) = f'(u)h := \langle f'(u),h\rangle.$$

If the Gâteaux variation $Vf(u|h)$ of a functional f exists at each point of $\omega\subset Y$, then for any two points u, $u+h\in\omega$ the Lagrange formula

$$f(u+h) - f(u) = Vf(u+\tau h|h), \quad \tau\in(0,1), \tag{2.4}$$

holds. The counterpart of (2.4) for operators is

$$\langle N(u+h) - N(u),z\rangle = \langle VN(u+\tau h|h),z\rangle, \tag{2.5}$$

where $\tau\in(0,1)$ depends on z.

A bilinear operator G on pairs (u_1,u_2) of elements $u_1,u_2\in Y$ is called symmetric if $G(u_1,u_2) = G(u_2,u_1)$. Now let $Y = X$ be a real Hilbert space. For any linear operator N on X we define the adjoint operator N^* of N through the relation

$$\langle v,N(u)\rangle = \langle N^*(v),u\rangle, \quad u,v\in X.$$

If $N = N^*$ then N is said to be self-adjoint. Hence, because the symmetry of $\langle\cdot,\cdot\rangle$ implies that $\langle v,N(u)\rangle = \langle N(u),v\rangle$, the bilinear functional $G(u,v) := \langle N(u),v\rangle$ is symmetric if and only if N is self-adjoint.

An operator $N\in\mathcal{N}(X;X)$ is potential on $U\subset X$ if there exists a functional f such that $f'(u) = N(u)$ for every $u\in U$. Moreover, $f'(u) = N(u)$ allows us to write

$$\frac{d}{d\lambda}f(u_0+\lambda(u-u_0)) = Df(u_0+\lambda(u-u_0)|u-u_0) = \langle N(u_0+\lambda(u-u_0)),u-u_0\rangle.$$

The obvious integration yields

$$f(u) = f(u_0) + \int_0^1\langle N(u_0+\lambda(u-u_0)),u-u_0\rangle d\lambda. \tag{2.6}$$

Whenever the pairing $\langle\cdot,\cdot\rangle$ coincides with (2.1) the functional f determines the Lagrangian (density)

$$L(u) = (u-u_0)\cdot\int_0^1 N(u_0+\lambda(u-u_0))d\lambda, \tag{2.7}$$

whereby

$$f(u) = f(u_0) + \int_{\mathscr{D}} L(u)d\mathscr{V}, \quad \mathscr{D}\subset\mathbf{R}^n.$$

These preliminaries enable us to exhibit a detailed proof of Vainberg's theorem.[12]

Theorem. Suppose that

(1) N is an operator from X into X^*,

(2) N has a linear Gâteaux differential $DN(u|h)$ at every point of the ball B: $\|u-u_0\|\leqslant r$,

(3) the bilinear functional $\langle DN(u|h),k\rangle$ on $h,k\in X$ is continous in u at every point of the ball B.

Then a necessary and sufficient condition for N to be potential in the ball B is that

$$\langle DN(u|h),k\rangle = \langle DN(u|k),h\rangle \tag{2.8}$$

for every $h,k\in X$ and every $u\in B$.

Proof: Look first at the necessity. We known that there exists a functional f such that $\langle N(u),\eta\rangle = Df(u|\eta)$, $u\in U$, $\eta\in X$. Consider now $u\in B$ and $h,k\in X$, $\|h\| = \|k\| = 1$, and choose $\alpha,\beta\in\mathbf{R}$ such that $u+\alpha h+\beta k\in B$. The expression

$$\Delta = f(u+\alpha h+\beta k) - f(u+\alpha h) - f(u+\beta k) + f(u)$$

may be given the form,

$$\Delta = \phi(u+\beta k) - \phi(u)$$

by letting $\phi(u) = f(u+\alpha h) - f(u)$. So ϕ is Gâteaux differentiable and then, in view of the Lagrange formula (2.4), we can write

$$\begin{aligned}\Delta &= D\phi(u+\tau_1\beta k \mid \beta k)\\ &= \beta\langle N(u+\alpha h+\tau_1\beta k),k\rangle\\ &\quad -\beta\langle N(u+\tau_1\beta k),k\rangle, \quad \tau_1\in(0,1).\end{aligned}$$

Accordingly, on appealing to the Lagrange formula (2.5) we obtain

$$\Delta = \alpha\beta\langle DN(u+\tau_2\alpha h+\tau_1\beta k \mid h),k\rangle, \quad \tau_2\in(0,1). \tag{2.9}$$

On the other hand, put

$$\psi(u) = f(u+\beta k) - f(u);$$

following along an analogous procedure we arrive at

$$\Delta = \alpha\beta\langle DN(u+\tau_3\alpha h+\tau_4\beta k \mid k),h\rangle, \quad \tau_3,\tau_4\in(0,1). \tag{2.10}$$

Comparison between (2.9) and (2.10) delivers

$$\begin{aligned}&\langle DN(u+\tau_2\alpha h+\tau_1\beta k \mid h),k\rangle\\ &\quad = \langle DN(u+\tau_3\alpha h+\tau_4\beta k \mid k),h\rangle.\end{aligned}$$

Taking the limit as $\alpha\to 0, \beta\to 0$ yields the desired result (2.8).

As to the sufficiency, we have to prove that, in view of (2.8), $N(u) = f'(u)$ for some functional f; it seems then natural to look at the functional (2.6). Letting $u, u+h\in B$, it follows from (2.6) that

$$\begin{aligned}&f(u+h) - f(u)\\ &\quad = \int_0^1 \langle N(u_0+\lambda(u-u_0)+\lambda h),h\rangle d\lambda\\ &\qquad + \int_0^1 \langle N(u_0+\lambda(u-u_0)+\lambda h)\\ &\qquad - N(u_0+\lambda(u-u_0)),u-u_0\rangle d\lambda.\end{aligned} \tag{2.11}$$

It is convenient to express the second integral, say I, in the form

$$\begin{aligned}I &= \int_0^1\left[\int_0^\lambda \frac{\partial}{\partial\sigma}\langle N(u_0+\lambda(u-u_0)+\sigma h),u-u_0\rangle d\sigma\right]d\lambda\\ &= \int_0^1\left[\int_0^\lambda \langle DN(u_0+\lambda(u-u_0)+\sigma h \mid h),u-u_0\rangle d\sigma\right]d\lambda.\end{aligned}$$

On using the hypothesis (2.8) and on interchanging the order of integration, we arrive at

$$\begin{aligned}I = \int_0^1 &\langle N(u_0+(u-u_0)+\sigma h)\\ &- N(u_0+\sigma(u-u_0)+\sigma h),h\rangle d\sigma.\end{aligned}$$

Then, substitution into (2.11) yields

$$f(u+h) - f(u) = \int_0^1 \langle N(u+\sigma h),h\rangle d\sigma.$$

Application of the mean value theorem to the right-hand side gives

$$f(u+h) - f(u) = \langle N(u+\tau h),h\rangle, \quad \tau\in(0,1).$$

Letting $h\to\lambda h$ we have

$$\lim_{\lambda\to 0}\frac{f(u+\lambda h)-f(u)}{\lambda} = \langle N(u),h\rangle, \quad h\in X,$$

that is

$$N(u) = f'(u). \qquad \square$$

In this paper we are concerned with the inner product (2.1) and, in order to emphasize the essence of our analysis, we disregard possible boundary terms. In other words, we are dealing with operators devoid of initial and boundary conditions (formal operators[13,14]) and then the potentialness condition (2.8) is considered up to boundary terms. Of course, whenever we have variational formulations with fixed end point conditions the boundary terms vanish identically and this makes formal potential operators be in fact potential operators.

When N is a continuous, possibly not differentiable, operator the potentialness condition is expressed through the independence of $\int_\ell \langle N(u),du\rangle$ of the path ℓ of integration. In this connection we observe that, in the case of formal operators, on changing the path of integration we obtain, in addition, boundary terms which are being disregarded.

As a last observation, we remark that sometimes the potential condition (2.8) is referred to as symmetry condition[13] or self-adjointness condition.[9]

3. VARIATIONAL FORMULATION OF FLUID DYNAMICS VIA THE LAGRANGIAN DESCRIPTION

Look at an inviscid fluid whose motion is described in terms of the time t and the Lagrangian (Cartesian) coordinates $\mathbf{X} = (X_1, X_2, \ldots, X_n)\in\mathscr{R}, \mathscr{R}$ being a suitable reference configuration; although physical reasons suggest that $n\leqslant 3$, we allow n to be arbitrary. Letting $\mathbf{x} = (x_1, x_2, \ldots, x_n)$, $\mathbf{x} = \mathbf{x}(\mathbf{X},t)$ is the position vector of the particle $\mathbf{X}$ at time t. In terms of the function $\mathbf{x} = \mathbf{x}(\mathbf{X},t)$ we may define the matrix $x_{aA} = \partial x_a/\partial X_A$ $(a, A = 1,2,\ldots,n)$, its determinant $J = \det(x_{aA})$, and its inverse $X_{Aa} = \partial X_A/\partial x_a$. Letting $\rho(\rho_0)$ be the mass density in the present (reference) configuration and p be the pressure, the equation of motion and the continuity equation in the Lagrangian description are, respectively,

$$\rho x_{a,tt} + X_{Ma}p_{,M} = 0, \tag{3.1}$$

$$J\rho - \rho_0 = 0, \tag{3.2}$$

the summation convention being in force and a comma denoting partial derivatives, namely $f_{,t} = \partial f(\mathbf{X},t)/\partial t$, $f_{,M} = \partial f(\mathbf{X},t)/\partial X_M$. To Eqs. (3.1) and (3.2) we must add the energy equation. Here we confine ourselves to adiabatic flows; accordingly the energy equation may be expressed through the conservation of the specific entropy S, namely $S(\mathbf{X},t) = S_0(\mathbf{X})$.

Concerning the system (3.1), (3.2) we observe that the functions $\mathbf{x},\rho$, dependent on $\mathbf{X}$ and t, are the unknowns for the problem under consideration whereas the functions $p(\rho,S)$, $\rho_0(\mathbf{X})$, $S_0(\mathbf{X})$ are assigned. Letting u be the pair $(\mathbf{x},\rho)$, the system (3.1), (3.2) may be given the form $N(u) = 0$ thereby defining the differential operator N. It is a routine matter to check that N is not potential, namely it does not meet (2.8) with respect to the pairing (2.1), as it is readily recognized by

using the explicit formulas (A2). However, putting $p' = \partial p(\rho, S_0)/\partial\rho$, the analysis of (A2) in connection with the system (3.1), (3.2) suggests that we adopt the equivalent form

$$\rho_0 x_{a,tt} + J p_{,M} X_{Ma} = 0, \tag{3.3}$$

$$p'(\rho_0/\rho) - p' J = 0, \tag{3.4}$$

which defines a potential operator. Then, on choosing $u_0 = (\mathbf{0}, \hat{\rho})$, the relation (2.6) yields the Lagrangian

$$\begin{aligned} L = {} & \tfrac{1}{2}\rho_0 x_a x_{a,tt} + x_a \int_0^1 J(\lambda x_{bQ}) \\ & \times p_{,M}(\tilde{\rho}, S_0) X_{Ma}(\lambda x_{bQ}) d\lambda \\ & + (\rho - \hat{\rho}) \int_0^1 \frac{\rho_0}{\tilde{\rho}} p'(\tilde{\rho}, S_0) d\lambda \\ & - (\rho - \hat{\rho}) \int_0^1 p'(\tilde{\rho}, S_0) J(\lambda x_{bQ}) d\lambda, \end{aligned}$$

where $\tilde{\rho} = \hat{\rho} + \lambda(\rho - \hat{\rho})$. Now, on account of the obvious relations

$$J(\lambda x_{bQ}) = \lambda^n J(x_{bQ}), \quad X_{Ma}(\lambda x_{bQ}) = \lambda^{-1} X_{Ma}(x_{bQ}),$$

and of the identity[18,19]

$$(J X_{Ma})_{,M} = 0, \tag{3.5}$$

up to boundary terms the Lagrangian L becomes

$$\begin{aligned} L = {} & -\tfrac{1}{2}\rho_0 x_{a,t} x_{a,t} + \rho_0 \int_{\hat{\rho}}^{\rho} (p'(r, S_0)/r)\, dr \\ & - J x_{aM} X_{Ma} \int_0^1 \lambda^{n-1} p(\tilde{\rho}, S_0)\, d\lambda \\ & - (\rho - \tilde{\rho}) J \int_0^1 \lambda^n p'(\tilde{\rho}, S_0)\, d\lambda, \end{aligned} \tag{3.6}$$

the dependence on $u = (\mathbf{x}, \rho)$ being understood. Observe now that, on the basis of the relationship between the pressure p and the internal energy E, namely $p = \rho^2 \partial E/\partial\rho$, integration by parts gives

$$\begin{aligned} \int_{\hat{\rho}}^{\rho} \frac{p'(r, S_0)}{r}\, dr = {} & \frac{p(\rho, S_0)}{\rho} + E(\rho, S_0) \\ & - \left(\frac{p(\hat{\rho}, S_0)}{\hat{\rho}} + E(\hat{\rho}, S_0) \right). \end{aligned} \tag{3.7}$$

Also, an integration by parts yields

$$\begin{aligned} & (\rho - \hat{\rho}) \int_0^1 \lambda^n p'(\tilde{\rho}, S_0)\, d\lambda \\ & = p(\rho, S_0) - \int_0^1 n \lambda^{n-1} p(\tilde{\rho}, S_0)\, d\lambda. \end{aligned} \tag{3.8}$$

Then, because $x_{aM} X_{Ma} = n$, substitution of (3.7) and (3.8) into (3.6) allows the Lagrangian to be written in the equivalent form

$$\begin{aligned} L(x, \rho) = {} & \tfrac{1}{2}\rho_0 x_{a,t} x_{a,t} - \rho_0 E(\rho, S_0) \\ & + [J - (\rho_0/\rho)]\, p(\rho, S_0). \end{aligned} \tag{3.9}$$

Often the literature bears evidence of different approaches to the variational description of fluid dynamics. It is then of interest to establish precise connections between these approaches and ours. In essence one approach consists in embodying the continuity equation into the equation of motion thus making the latter equation the unique one for the problem at hand. Specifically, substitution of $\rho = \rho_0/J$ (and $S = S_0$) into (3.1) gives

$$\rho_0 x_{a,tt} + J X_{Ma} p_{,M} = 0, \tag{3.10}$$

where p must be regarded as a function on $\mathbf{x}_{,M}$ (and $\mathbf{X}$), namely $p = p(\rho_0/J, S_0)$. Letting $u = \mathbf{x}$, the equation (3.10) may be written as the operator equation $N(u) = 0$; it turns out that the operator N so defined is potential. Then, on setting $u_0 = \hat{\mathbf{x}} \neq \mathbf{0}$, we find the Lagrangian

$$\begin{aligned} L = {} & \rho_0 (x_a - \hat{x}_a) \int_0^1 \tilde{x}_{a,tt}\, d\lambda + (x_a - \hat{x}_a) \\ & \times \int_0^1 J(\tilde{x}_{bQ}) X_{Ma}(\tilde{x}_{bQ}) p_{,M}(\rho_0 J^{-1}(\tilde{x}_{bQ}), S_0)\, d\lambda, \end{aligned}$$

where $\tilde{\mathbf{x}} = \hat{\mathbf{x}} + \lambda(\mathbf{x} - \hat{\mathbf{x}})$. On evaluating the first integral and using the identity (3.5) in connection with the second integral, up to boundary terms (and up to the sign) L takes the form

$$\begin{aligned} L = {} & \tfrac{1}{2}\rho_0 x_{a,t} x_{a,t} + (x_a - \hat{x}_a)_{,M} \\ & \times \int_0^1 J(\tilde{x}_{bQ}) X_{Ma}(\tilde{x}_{bQ}) p(\rho_0 J^{-1}(\tilde{x}_{bQ}), S_0)\, d\lambda. \end{aligned}$$

Observe now that

$$J X_{Ma} = \frac{\partial J}{\partial x_{aM}} \tag{3.11}$$

and then that

$$(x_a - \hat{x}_a)_{,M} J(\tilde{x}_{bQ}) X_{Ma}(\tilde{x}_{bQ}) = \frac{\partial J}{\partial \lambda};$$

accordingly

$$\begin{aligned} & \int_0^1 (x_a - \hat{x}_a)_{,M} J(\tilde{x}_{bQ}) X_{Ma}(\tilde{x}_{bQ}) p(\rho_0 J^{-1}(\tilde{x}_{bQ}), S_0)\, d\lambda \\ & = \rho_0 \int_0^1 p(r(\lambda), S_0) \frac{\partial}{\partial\lambda}(r^{-1}(\lambda))\, d\lambda =: \bar{I}, \end{aligned}$$

where $r = \rho_0/J$. Because

$$\bar{I} = \rho_0 \int_{\hat{\rho}}^{\rho} \frac{p(r, S_0)}{r^2}\, dr,$$

where $\hat{\rho} = \rho_0/J(\hat{x}_{bQ})$ and $\rho = \rho_0/J(x_{bQ})$, and integration by parts and the relationship $p = \rho^2\, \partial E/\partial\rho$ give

$$\bar{I} = \rho_0 [E(\rho, S_0) - E(\hat{\rho}, S_0)].$$

Hence L may be written in the form

$$L(\mathbf{x}) = \tfrac{1}{2}\rho_0 x_{a,t} x_{a,t} - \rho_0 E(\rho_0 J^{-1}(x_{bQ}), S_0) \tag{3.12}$$

which is the one usually dealt with in the literature.

The second approach originates from the following question: What happens if the continuity equation is regarded as a constraint from the variational viewpoint? The fact that (3.2) is a variational constraint leads us to modify the Lagrangian (3.12) in

$$L(\mathbf{x}, \rho, \mu) = \tfrac{1}{2}\rho_0 x_{a,t} x_{a,t} - \rho_0 E(\rho, S_0) + \mu(J - \rho_0/\rho), \tag{3.13}$$

$\mu = \mu(\mathbf{X})$ being the Lagrange multiplier. The unknown functions are x_a, ρ, μ; in view of the identities (3.5), (3.6) it follows at once that the corresponding Euler–Lagrange equations are

$$\rho_0 x_{a,tt} + J X_{Ma}\,\mu_{,M} = 0, \tag{3.14}$$

$$\mu - \rho^2 \frac{\partial E}{\partial \rho} = 0, \tag{3.15}$$

$$J - \rho_0/\rho = 0. \tag{3.16}$$

As we should expect, the system (3.14)–(3.16) is equivalent to the system (3.1), (3.2), which proves that (3.13) accounts properly for the constraint (3.2) within a variational approach. Moreover (3.15) shows that the Lagrange multiplier μ is just the pressure p. That the Lagrange multiplier μ associated with the continuity equation constraint is the pressure, was proved by Lanczos,[20] and later by Eckart,[21] in the case of incompressible fluids and also by Bedford and Drumheller[22] in connection with mixtures of incompressible fluids.

In a sense it could seem that the change from (3.12) to (3.13) consists in the addition of a natural condition in accordance with the Courant–Hilbert general principle[23]: If a variational problem for a given functional is changed by the explicit addition of one or more natural conditions to the set of constraints, the stationary character of the functional is not affected. However such is not the case because $J - \rho_0/\rho = 0$ is not a consequence of the variational problem associated with (3.12). Yet, direct connections exist between the variational problems related to (3.9), (3.12), and (3.13). Precisely, (3.15) gives $\mu = p(\rho, S_0)$; substitution into (3.13) yields the Lagrangian (3.9). If, instead, we substitute (3.16), namely $\rho = \rho_0/J$, into (3.13)—or into (3.9) as well—we obtain the Lagrangian (3.12). In conclusion we have found a hierarchy between variational formulations through the following procedure: The substitution of a natural condition into the corresponding stationary functional, in such a way that the number of unknowns is reduced, leads to a functional having as Euler–Lagrange equations a proper subset of the previous Euler–Lagrange equations.

4. ALTERNATIVE VARIATIONAL FORMULATIONS OF FLUID DYNAMICS

Since the appearance of Lichtenstein's book[24] in 1929, a number of works concerning variational principles in fluid dynamics have been performed. First Taub[25] and Herivel[26] improved Lichtenstein's formulation by accounting also for the conservation of energy. Later Serrin[27] revisited the subject and emphasized a method of Lin involving Lagrange multipliers; the method was subsequently applied by Lin himself in connection with liquid helium.[28]

Briefly, the main idea introduced by Herivel is that variational formulations, based on the Eulerian description of fluid dynamics, may be set up provided the mass conservation and the (isentropic) energy equation are accounted for through Lagrange multipliers. Herivel's scheme however is restricted to special flows only; for example, if $S_{,M} = 0$ then $\mathbf{v} = \mathbf{x}_{,t}$ is required to be irrotational. Lin's improvement consists in the addition of three constraints, expressing the conservation of the identity of particles, thus avoiding any restriction on the type of flow under consideration.

In 1968, a paper of Seliger and Whitham[29] appeared, which is important both for the thoroughness of the approach and for the influence on the subsequent development of variational approaches in continuum mechanics. Among other topics, such a paper shows how to reduce Lin's additional constraints to one only without any loss of generality. Specifically, Seliger and Whitham's approach is based on the Lagrangian

$$L = \tfrac{1}{2}\rho v^2 - \rho E(\rho, S) + \phi\left(\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho \mathbf{v})\right) + \eta\left(\frac{\partial(\rho S)}{\partial t} + \nabla\cdot(\rho \mathbf{v} S)\right) + \beta\left(\frac{\partial(\rho\alpha)}{\partial t} + \nabla\cdot(\rho \mathbf{v}\alpha)\right), \tag{4.1}$$

where the unknowns $\rho, S, \mathbf{v}, \alpha, \phi, \eta, \beta$ are viewed as functions on the present position $\mathbf{x}$ and the time t—here $\nabla f := \partial f(\mathbf{x},t)/\partial \mathbf{x}$, $\partial f/\partial t := \partial f(\mathbf{x},t)/\partial t$. The variations with respect to $\mathbf{v}, \rho, S, \alpha$ yield, respectively,

$$\mathbf{v} = \nabla\phi + S\nabla\eta + \alpha\nabla\beta, \tag{4.2}$$

$$\frac{1}{2}v^2 - \frac{\partial(\rho E)}{\partial \rho} = \left(\frac{\partial \phi}{\partial t} + \mathbf{v}\cdot\nabla\phi\right) + S\left(\frac{\partial \eta}{\partial t} + \mathbf{v}\cdot\nabla\eta\right) + \alpha\left(\frac{\partial \beta}{\partial t} + \mathbf{v}\cdot\nabla\beta\right), \tag{4.3}$$

$$\frac{\partial E}{\partial S} = -\frac{\partial \eta}{\partial t} - \mathbf{v}\cdot\nabla\eta, \tag{4.4}$$

$$\frac{\partial \beta}{\partial t} + \mathbf{v}\cdot\nabla\beta = 0, \tag{4.5}$$

while the variations with respect to ϕ, η, β give the side (constraint) conditions. Taking the material time derivative of (4.2) and accounting for (4.3)–(4.5) lead to the usual Euler equation of fluid dynamics.[29–31]

As remarked by Bretherton,[32] although it describes completely the dynamics of the fluid, Seliger and Whitham's approach is not always very convenient because the potentials involved suffer from indeterminacies and redundancies in their definition and are not endowed with a clear physical meaning. To overcome this drawback, Bretherton himself set up a hybrid approach which is based on the Eulerian description of motion but regards the variations of the fields at a fixed particle as the independent variations of the problem. With the same purpose, Wilhelm[33] has considered the equations of fluid dynamics in the form

$$\frac{\partial(nm\mathbf{v})}{\partial t} + \nabla\cdot(nm\mathbf{v}\mathbf{v}) + \nabla p + n\nabla\Phi = \mathbf{0}, \tag{4.6}$$

$$\frac{\partial n}{\partial t} + \nabla\cdot(n\mathbf{v}) = 0, \tag{4.7}$$

$$\frac{\partial p}{\partial t} + \nabla\cdot(p\mathbf{v}) + (\gamma - 1)p\nabla\cdot\mathbf{v} = 0, \tag{4.8}$$

where n is the particle density, $nm = \rho$, and Φ is the potential of the external field while Eq. (4.8) is a formal extension of the adiabatic law. As it stands, the system (4.6)–(4.8) does not admit a variational formulation. This gives reason for two Wilhelm's results. First, a variational derivation of Eq. (4.6) only, Eqs. (4.7), (4.8) occurring as side conditions. Second, a variational derivation of the system (4.6)–(4.8) when written in terms of the new canonical fields $\mathbf{p} = m\mathbf{v}$ and $\mathbf{q}$, defined by $\partial\mathbf{q}/\partial t = n\mathbf{v}$; in such a case a Lagrangian $L(\mathbf{q})$ is

found.

Usually the Lagrangian description of motion allows a more direct approach to variational formulations. This assertion is substantiated by the papers of Eckart[21] and Leech.[2] Unlike ours, their procedures do not lead to the continuity equation as an Euler–Lagrange equation; indeed their schemes are closely related to the one characterized by the Lagrangian (3.12).

A noticeable bridge between variational formulations, based on Lagrangian and Eulerian descriptions, has been accomplished by Van Saarloos.[31] Specifically, on looking at the position vector $\mathbf{x}$ as the only unknown function of the problem, by means of a canonical transformation the variational principle of Seliger and Whitham for the Eulerian description is derived from the variational principle, for the Lagrangian description, corresponding to the Lagrangian (3.12). Since the derivation is based on the use of Hamiltonian variables, Van Saarloos-like procedures fail when also the continuity equation is regarded as an Euler–Lagrange equation merely because the Lagrangian is independent of $\rho_{,t}$ [as it happens for (3.9) and (3.13)] which makes the associated conjugate momentum vanish.

Based on the analysis of the literature outlined so far, the main result of our variational approach turns out to be the feature that the continuity equation is obtained as an Euler–Lagrange equation without having recourse to Lagrange multipliers. In fact, this result has been arrived at by looking at the equations of fluid dynamics as a system of equations and applying systematically Vainberg's theorem.

In ending this section, we point out that according to some claims a misunderstanding might arise about the existence of variational principles for viscous fluids. For example in Refs. 2 and 34, the authors assert to yield variational principles for the time-dependent viscous Navier–Stokes equation in terms of the Eulerian description. In fact, they merely write as a variational principle a differential expression which is not the variation of any functional. On the one hand, the lack of a functional does not permit the recourse to fruitful techniques such as direct methods of the variational calculus. On the other hand, use of a differential expression is consistent with the fact that, as Vainberg's theorem allows us to prove, a functional cannot be found which admits the customary viscous Navier–Stokes equation as Euler-Lagrange equation provided supplementary, unphysical, variables are not introduced. A detailed proof of such a nonexistence property will be presented in a forthcoming paper; here we mention that Vainberg's theorem allowed Finlayson[35] to shorten Millikan's proof whereby the steady state Navier–Stokes equation for an incompressible fluid does not admit a variational principle unless either $(\mathbf{v}\cdot\nabla)\mathbf{v}=\mathbf{0}$ or $\mathbf{v}\times(\nabla\times\mathbf{v})=\mathbf{0}$.

5. VARIATIONAL FORMULATIONS IN CONTINUUM MECHANICS

In order to show evidence of the utility of Vainberg's theorem, here we apply the theory elaborated in Sec. 2 so as to arrive at variational formulations for a prominent set of partial differential equations concerning various branches of continuum mechanics. Of course, likewise in Sec. 3, the check on the potentialness of operators defined by such equations is performed via the conditions (A2) delivered in the Appendix.

Look first at some equations occuring in fluid dynamics. The Korteweg–de Vries (KdV) equation, accounting for the behavior of weakly dispersive and weakly nonlinear water waves, may be given the form

$$u_{,t}+u_{,x}+uu_{,x}+u_{,xxx}=0, \tag{5.1}$$

$u=u(x,t)$ being the unknown function. It is a simple matter to see that the operator N for(5.1) is not a potential operator and that, moreover, this is due to the presence of a third order derivative. This feature suggests that we put $u=\theta_{,x}$ or $u=\theta_{,t}$. If $u=\theta_{,x}$ then Eq. (5.1) becomes

$$\theta_{,xt}+\theta_{,xx}+\theta_{,x}\,\theta_{,xx}+\theta_{,xxxx}=0$$

and the associated operator N turns out to be a potential operator. Accordingly, in view of (2.7), which for one unknown function θ reads

$$L(\theta)=\theta\int_0^1 N(\lambda\theta)\,d\lambda, \tag{5.2}$$

we find the Lagrangian

$$L(\theta)=\tfrac{1}{2}\theta\theta_{,xt}+\tfrac{1}{2}\theta\theta_{,xx}+\tfrac{1}{3}\theta\theta_{,x}\,\theta_{,xx}+\tfrac{1}{2}\theta\theta_{,xxxx} \tag{5.3}$$

which is equivalent to

$$L(\theta)=\tfrac{1}{2}\theta_{,x}\,\theta_{,t}+\tfrac{1}{2}(\theta_{,x})^2+\tfrac{1}{6}(\theta_{,x})^3+\theta_{,x}\,\theta_{,xxx}+\tfrac{1}{2}(\theta_{,xx})^2. \tag{5.4}$$

It is worth mentioning that substituting $\theta_{,xx}=\chi$ into (5.4) yields a first-order Lagrangian which traces back to Whitham.[36]

As to the choice $u=\theta_{,t}$, instead, it follows that the corresponding equation singles out an operator N which does not admit a variational formulation.

In spite of the many impressive properties of solutions to the KdV equation, there are grave technical difficulties associated with the problem of the existence of the solution. Besides this, the physical assumptions leading to the KdV equation equally well justify the Benjamin, Bona, and Mahony (BBM) equation

$$u_{,t}+u_{,x}+uu_{,x}-u_{,xxt}=0 \tag{5.5}$$

as modeling long water waves.[30,37] Based on these aspects, Benjamin, Bona, and Mahony advocated (5.5) as a better founded model than (5.1). Owing again to the presence of a third-order derivative, Eq. (5.5) does not admit a variational formulation. Upon substituting $u=\theta_{,x}$ Eq. (5.5) is changed into

$$\theta_{,xt}+\theta_{,xx}+\theta_{,x}\,\theta_{,xx}-\theta_{,xxxt}=0 \tag{5.6}$$

which is associated with a potential operator N; the use of (5.2) leads to the Lagrangian

$$L(\theta)=\tfrac{1}{2}\theta\theta_{,xt}+\tfrac{1}{2}\theta\theta_{,xx}+\tfrac{1}{3}\theta\theta_{,x}\,\theta_{,xx}-\tfrac{1}{2}\theta\theta_{,xxxt}\,. \tag{5.7}$$

Lately a generalization of the BBM equation in higher dimensions has been suggested and investigated by Goldstein and Wichnoski[38]; their GBBM equation reads

$$u_{,t}-\nabla^2 u_{,t}+\nabla\cdot[\phi(u)]=0 \tag{5.8}$$

∇ being now the gradient operator in d dimensions. As it stands, Eq. (5.8) does not admit a variational formulation again because of a third-order derivative ($\nabla^2 u_{,t}$). Then, by analogy with the previous cases, we let $u = \Sigma_1^d{}_i\, \theta_{,i}$ and write (5.8) in the form

$$\sum_1^d{}_i\, [\theta_{,it} - \nabla^2 \theta_{,it} + \nabla\theta_{,i}\cdot\boldsymbol{\phi}'] = 0, \tag{5.9}$$

where $\boldsymbol{\phi}'$ is the derivative of $\boldsymbol{\phi}$ with respect to its argument $\Sigma_1^d{}_k\, \theta_{,k}$. In view of (5.2) the potential operator N defined by (5.9) allows (5.9) itself to be the Euler–Lagrange equation of

$$L(\theta) = \sum_1^d{}_i\, \Big[\tfrac{1}{2}\theta_{,i}\,\theta_{,t} + \tfrac{1}{2}\theta_{,it}\nabla^2\theta - -\theta\nabla\theta_{,i}\cdot\int_0^1 \lambda\boldsymbol{\phi}'\Big(\lambda\sum_1^d{}_i\,\theta_{,k}\Big)\,d\lambda\Big]. \tag{5.10}$$

On the basis of argument similar to those of Benjamin, Bona, and Mahony, Jeffrey[39] advocated the J equation

$$u_{,t} + u_{,x} + uu_{,x} + u_{,xtt} = 0. \tag{5.11}$$

Again it is convenient to set $u = \theta_{,x}$; this makes (5.11) into the equation

$$\theta_{,xt} + \theta_{,xx} + \theta_{,x}\,\theta_{,xx} + \theta_{,xxtt} = 0$$

which is the Euler–Lagrange equation of

$$L(\theta) = \tfrac{1}{2}\theta_{,x}\,\theta_{,t} + \tfrac{1}{2}(\theta_{,x})^2 + \tfrac{1}{6}(\theta_{,x})^3 + \theta_{,t}\,\theta_{,xxt} + \tfrac{1}{2}(\theta_{,xt})^2. \tag{5.12}$$

In a sense, the equation

$$u_{,t} + f(u)\,u_{,x} + u_{,xxx} = 0 \tag{5.13}$$

may be viewed as a particular case of (5.8). Nevertheless it deserves our attention for many respects. Specifically, if $f(u) = u^2$ then (5.13) models the motion of anharmonic discrete–mass strings.[40] Moreover, if $f(u) = -u^2$ and the new function v is introduced through the Miura transformation[41]

$$v = u^2 + \sqrt{6}\,u_{,x}$$

then (5.13) becomes just the KdV equation. Again put $u = \theta_{,x}$; Eq. (5.13) becomes

$$\theta_{,xt} + f(\theta_{,x})\,\theta_{,xx} + \theta_{,xxxx} = 0.$$

It is a routine matter to arrive at the corresponding Lagrangian

$$L(\theta) = -\tfrac{1}{2}\theta_{,x}\,\theta_{,t} + \tfrac{1}{2}(\theta_{,xx})^2 + \theta\theta_{,xx}\int_0^1 \lambda f(\lambda\theta_{,x})\,d\lambda.$$

Consider now some equations modeling elastic media. To begin with, look at an infinite beam of mass density ρ and bending stiffness B laterally supported by a distributed spring of spring constant K and compressed by the axial load P. Its motion is governed by[42]

$$\rho u_{,tt} + Ku + Pu_{,xx} + Bu_{,xxxx} = 0. \tag{5.14}$$

The operator N defined by (5.14) turns out to be potential; on applying (5.2) we arrive at the corresponding Lagrangian

$$L(u) = \tfrac{1}{2}\,[\,\rho(u_{,t})^2 - Ku^2 + P(u_{,x})^2 - B(u_{,xx})^2\,].$$

A second example is given by Love's equation for waves in rods, namely

$$u_{,tt} - u_{,xx} - u_{,xxtt} = 0;$$

this equation models also shallow-water waves (linear Boussinesq equation). On account of (5.2) we find the Lagrangian

$$L(u) = \tfrac{1}{2}\,[(u_{,t})^2 - (u_{,x})^2 + (u_{,xt})^2].$$

A third example has the remarkable feature that viscous damping does not prevent a variational formulation. Specifically, waves on an elastically supported string damped by air friction are described by[43]

$$u_{,tt} - u_{,xx} + u + 2\sigma u_{,t} = 0, \tag{5.15}$$

σ being the constant damping coefficient. As it stands, Eq. (5.15) does not admit a variational formulation. Now multiply (5.15) by the integrating factor $f(t)$; we find that the new equation corresponds to a potential operator if $f(t) = \exp(2\sigma t)$. In such a case we arrive at the Lagrangian

$$L(u) = \tfrac{1}{2}\exp(2\sigma t)\,[(u_{,t})^2 - (u_{,x})^2 - u^2]\,. \tag{5.16}$$

It is worth observing that, owing to the identity

$$[\exp(\sigma t)\,u_{,t})^2]$$
$$= \{[\exp(\sigma t)\,u]_{,t}\}^2 - \sigma\,[\exp(2\sigma t)\,u^2]_{,t} + \sigma^2\,[\exp(\sigma t)\,u]^2,$$

on letting $\psi = \exp(\sigma t)\,u$, the Lagrangian (5.16) may be written as

$$L(\psi) = \tfrac{1}{2}\,[(\psi_{,t})^2 - (\psi_{,x})^2 - (1-\sigma^2)\,\psi^2]\,,$$

which is the well-known Lagrangian for the Klein–Gordon equation.

A further example, arising from quite a different context, consists in an equation concerning nonstationary heat conduction in rigid bodies. To evade the drawback due to the parabolic character of the standard heat equation, Fourier's law has been retouched to read

$$\tau\mathbf{q}_{,t} + \mathbf{q} + \kappa\nabla T = \mathbf{0}.$$

Then, letting $\mathbf{H}_{,t} = \mathbf{q}$, the heat conduction turns out to be described by the system[44]

$$\begin{aligned} &u + \nabla\cdot\mathbf{H} = 0,\\ &\tau\mathbf{H}_{,tt} + \mathbf{H}_{,t} + \kappa\nabla T = \mathbf{0}, \end{aligned} \tag{5.17}$$

in the unknowns T, $\mathbf{H}$, while u, κ are known functions on T. To adhere to physical reality the relaxation time τ as well should be a function on T; however, for the sake of simplicity, τ is assumed to be a constant. A direct inspection shows that the system (5.17) does not satisfy the conditions (A2) for the existence of a variational formulation. Meanwhile, the inspection indicates that equations (5.17) could satisfy the required conditions via suitable integrating factors, namely $-\kappa\exp(t/\tau)$ and $\exp(t/\tau)$, respectively. Then application of (2.7) and some rearrangements yield the Lagrangian

$$L(T,\mathbf{H}) = \tau\kappa\exp(t/\tau)\Big(uT_{,t} + \frac{1}{\tau}\,\mathbf{H}\cdot\nabla T - \frac{1}{2\kappa}\,\mathbf{H}_{,t}\cdot\mathbf{H}_{,t}\Big).$$

We end this section by examining a system of third order differential equations describing vectorial solitons in anharmonic lattices[45]; this system reads

$$\begin{aligned} &u_{,t} + uu_{,x} + \beta vv_{,x} - \alpha u_{,xxx} = 0,\\ &\epsilon v_{,t} - \gamma v_{,x} + \beta(uv_{,x} + u_{,x}v) - \alpha v_{,xxx} = 0, \end{aligned}$$

where α, β, γ, ϵ are constants and u, v are the unknown

functions. Likewise for KdV equation, this system, as it stands, does not meet the potentialness conditions. However, letting $u = \theta_{,x}$ and $v = \phi_{,x}$, we obtain the system

$$\theta_{,xt} + \theta_{,x}\,\theta_{,xx} + \beta\phi_{,x}\,\phi_{,xx} - \alpha\theta_{,xxxx} = 0,$$
$$\epsilon\phi_{,xt} - \gamma\phi_{,xx} + \beta(\theta_{,x}\,\phi_{,xx} + \theta_{,xx}\,\phi_{,x}) - \alpha\phi_{,xxxx} = 0,$$

in the unknowns θ,ϕ, which complies with the conditions (A2) and then it allows for a variational formulation. Indeed, use of (2.7) yields the Lagrangian

$$L(\theta,\phi) = \tfrac{1}{2}\theta_{,x}\,\theta_{,t} + \tfrac{1}{6}(\theta_{,x})^3 + \tfrac{1}{2}\alpha(\theta_{,xx})^2 + \tfrac{1}{2}\beta(\phi_{,x})^2\,\theta_{,x} + \tfrac{1}{2}\epsilon\phi_{,x}\,\phi_{,t} - \tfrac{1}{2}\gamma(\phi_{,x})^2 + \tfrac{1}{2}\alpha(\phi_{,xx})^2.$$

6. VARIATIONAL FORMULATION FOR ELECTROMAGENTISM

Several variational formulations for electromagnetism both in vacuum and in matter have been established (see, e.g., Refs. 46, 47 and references therein); here we look again at electromagnetism in vacuum with the purpose of setting up new formulations and of relating them with old ones.

When dealing with electromagnetism it is a crucial point that Maxwell's equations are eight equations in the six unknowns $\mathbf{E}$, $\mathbf{B}$ on $(\mathbf{x},t)$; this implies that, as they stand, Maxwell's equations cannot be framed in a variational formulation. A number of procedures overcome this difficulty.

First observe that, owing to the continuity equation

$$\nabla\cdot\mathbf{J} + \rho_{,t} = 0, \tag{6.1}$$

the scalar equations

$$\nabla\cdot\mathbf{E} = 4\pi\rho, \tag{6.2a}$$
$$\nabla\cdot\mathbf{B} = 0 \tag{6.2b}$$

hold at any time t provided only that they hold on the initial data.[48,49] This allows us to confine our attention to the two vector equations

$$\nabla\times\mathbf{B} - (1/c)\,\mathbf{E}_{,t} = (4\pi/c)\,\mathbf{J}, \tag{6.3a}$$
$$\nabla\times\mathbf{E} + (1/c)\,\mathbf{B}_{,t} = 0 \tag{6.3b}$$

in the two unknown vectors $\mathbf{E}$, $\mathbf{B}$. The equations (6.3) are easily recognized to be associated with a first order potential operator; hence use of (2.7) leads to the Lagrangian

$$L(\mathbf{E},\mathbf{B}) = (1/c)\mathbf{E}\cdot\mathbf{B}_{,t} + \tfrac{1}{2}\mathbf{E}\cdot\nabla\times\mathbf{E} + \tfrac{1}{2}\mathbf{B}\cdot\nabla\times\mathbf{B} - (4\pi/c)\mathbf{J}\cdot\mathbf{B} \tag{6.4}$$

A second procedure renders the number of unknowns equal to the number of the equations through the introduction of additional unknowns. Specifically, as is well-known, Eqs. (6.2b) and (6.3b) amount to expressing $\mathbf{E}$ and $\mathbf{B}$ in terms of the potentials $\mathbf{A}$ and ϕ. Accordingly, the complete system of equations reads

$$-\mathbf{E} - (1/c)\,\mathbf{A}_{,t} - \nabla\phi = \mathbf{0}, \tag{6.5a}$$
$$\mathbf{B} - \nabla\times\mathbf{A} = \mathbf{0}, \tag{6.5b}$$
$$(1/c)\,\mathbf{E}_{,t} - \nabla\times\mathbf{B} + (4\pi/c)\,\mathbf{J} = \mathbf{0}, \tag{6.5c}$$
$$\nabla\cdot\mathbf{E} - 4\pi\rho = 0. \tag{6.5d}$$

An immediate check shows that the system (6.5) is associated with a potential operator; then, by means of (2.7), we arrive at the Lagrangian

$$L(\mathbf{E},\mathbf{B},\mathbf{A},\phi) = \tfrac{1}{2}(B^2 - E^2) - \mathbf{E}\cdot\left(\frac{1}{c}\mathbf{A}_{,t} + \nabla\phi\right) - \mathbf{B}\cdot\nabla\times\mathbf{A} + 4\pi\left(\frac{1}{c}\mathbf{J}\cdot\mathbf{A} - \rho\phi\right). \tag{6.6}$$

We mention that Seliger and Whitham[29] obtained the Lagrangian (6.6) through a different procedure involving (6.2b) and (6.3b) as constraints on $\mathbf{E}$ and $\mathbf{B}$.

By analogy with Sec. 3, here we point out a hierarchy between variational formulations. Specifically, in view of (6.5a,b) we replace (6.5c,d) and (6.6) with

$$\frac{1}{c}\left(\frac{1}{c}\mathbf{A}_{,t} + \nabla\phi\right)_{,t} + \nabla\times(\nabla\times\mathbf{A}) - \frac{4\pi}{c}\mathbf{J} = \mathbf{0}, \tag{6.7}$$

$$\nabla\cdot\left(\frac{1}{c}\mathbf{A}_{,t} + \nabla\phi\right) + 4\pi\rho = 0, \tag{6.8}$$

and

$$L(\mathbf{A},\phi) = \frac{1}{2}\left(\frac{1}{c}\mathbf{A}_{,t} + \nabla\phi\right)^2 - \frac{1}{2}(\nabla\times\mathbf{A})^2 + 4\pi\left(\frac{1}{c}\mathbf{J}\cdot\mathbf{A} - \rho\phi\right), \tag{6.9}$$

respectively. It is a trivial matter to ascertain that (6.7) and (6.8) are the Euler–Lagrange equations of the well-known Lagrangian (6.9).

Owing to its extensive use, the Lorentz gauge

$$\nabla\cdot\mathbf{A} + (1/c)\,\phi_{,t} = 0 \tag{6.10}$$

deserves our attention. Observe first that

$$\tfrac{1}{2}(\nabla\times\mathbf{A})^2 = \nabla\mathbf{A}:\nabla\mathbf{A} - \nabla\mathbf{A}:(\nabla\mathbf{A})^{\mathrm{T}} \tag{6.11}$$

where $\nabla\mathbf{A}:\nabla\mathbf{A} = A_{j,i}\,A_{j,i}$, and that, up to boundary terms,

$$\frac{2}{c}\mathbf{A}_{,t}\cdot\nabla\phi = b.t. - \mathbf{A}\cdot\nabla\left(\frac{1}{c}\phi_{,t}\right) - \frac{1}{c}\phi\,(\nabla\cdot\mathbf{A})_{,t}\,. \tag{6.12}$$

Returning now to the Lagrangian (6.9), application of (6.10)–(6.12) and some rearrangements yield

$$L(A,\phi) = \frac{1}{2}\left(\frac{1}{c^2}\mathbf{A}_{,t}\cdot\mathbf{A}_{,t} - \nabla\mathbf{A}:\nabla\mathbf{A} + \nabla\phi\cdot\nabla\phi - \frac{1}{c^2}(\phi_{,t})^2\right) + 4\pi\left(\frac{1}{c}\mathbf{J}\cdot\mathbf{A} - \rho\phi\right). \tag{6.13}$$

The Euler–Lagrange equations associated with (6.13) are the usual equations for the potentials $\mathbf{A}$ and ϕ in the Lorentz gauge.

Analogous procedures may be performed in other gauges (such as the Coulomb gauge $\nabla\cdot\mathbf{A} = 0$ or the gauge $\phi = 0$).

APPENDIX

Here we derive explicit conditions for an operator N to be potential with respect to the pairing (2.1), namely

$$\langle h,k\rangle = \int_{\mathscr{D}} h(x)\cdot k(x)\, d\mathscr{V}.$$

Specifically, we look at the system of fourth-order differential equations

$$f_A(u_B,\ u_{B,p}\ u_{B,pq}, u_{B,pqr}, u_{B,pqrs}) = 0 \tag{A1}$$

in the unknown functions u_B on the n variables $x_1,\ldots,x_n$, where A and B run over a suitable set of indices; for example, $A = 1,\ldots,m$ or $A = (i,j)$, $i,j = 1,\ldots,m$. According to Vainberg's theorem, a Gâteaux differentiable operator $N(u)$ is potential if and only if

$$\langle DN(u|h), k\rangle = \langle DN(u|k), h\rangle$$

for arbitrary test functions h, k. On applying the definition (2.3) to the operator N defined by the system (A1) we have

$$\langle Df_A(u_B|\, h_B), k_A\rangle = \int_{\mathscr{D}} \left[\frac{\partial f_A}{\partial u_B} h_B + \frac{\partial f_A}{\partial u_{B,p}} h_{B,p} + \frac{\partial f_A}{\partial u_{B,pq}} h_{B,pq} + \frac{\partial f_A}{\partial u_{B,pqr}} h_{B,pqr} + \frac{\partial f_A}{\partial u_{B,pqrs}} h_{B,pqrs} \right] k_A\, d\mathscr{V}.$$

An analogous expression holds for $\langle Df_B(u_A|\, h_A), k_B\rangle$. Then, on performing a suitable sequence of integrations by parts and appealing to the arbitrariness of the test functions h_A, k_B we can assert that

$$\langle Df_A(u_B|h_B), k_A\rangle = \langle Df_B(u_A|k_A), h_B\rangle$$

is true if and only if the conditions

$$\frac{\partial f_A}{\partial u_{B,pqrs}} = \frac{\partial f_B}{\partial u_{A,pqrs}}, \tag{A2a}$$

$$\frac{\partial f_A}{\partial u_{B,pqr}} = -\frac{\partial f_B}{\partial u_{A,pqr}} + 4\left(\frac{\partial f_B}{\partial u_{A,pqrs}}\right)_{,s}, \tag{A2b}$$

$$\frac{\partial f_A}{\partial u_{B,pq}} = \frac{\partial f_B}{\partial u_{A,pq}} - 3\left(\frac{\partial f_B}{\partial u_{A,pqr}}\right)_{,r} + 6\left(\frac{\partial f_B}{\partial u_{A,pqrs}}\right)_{,rs}, \tag{A2c}$$

$$\frac{\partial f_A}{\partial u_{B,p}} = -\frac{\partial f_B}{\partial u_{A,p}} + 2\left(\frac{\partial f_B}{\partial u_{A,pq}}\right)_{,q} - 3\left(\frac{\partial f_B}{\partial u_{A,pqr}}\right)_{,qr} + 4\left(\frac{\partial f_B}{\partial u_{A,pqrs}}\right)_{,qrs}, \tag{A2d}$$

$$\frac{\partial f_A}{\partial u_B} = \frac{\partial f_B}{\partial u_A} - \left(\frac{\partial f_B}{\partial u_{A,p}}\right)_{,p} + \left(\frac{\partial f_B}{\partial u_{A,pq}}\right)_{,pq} - \left(\frac{\partial f_B}{\partial u_{A,pqr}}\right)_{,pqr} + \left(\frac{\partial f_B}{\partial u_{A,pqrs}}\right)_{,pqrs}, \tag{A2e}$$

are satisfied.

Observe that, upon disregarding the left-hand side of these relations, each column involves derivatives of f_B with respect to derivatives of u_A of a particular order, say α, and that the sign of the coefficients of such a column is $(-1)^\alpha$. Apart from the sign so determined, the entire set of coefficients results in Pascal's (or Tartaglia's) triangle. With these rules it is immediate to write explicitly necessary and sufficient conditions for a differential operator of any order to be potential.

A comment is now in order. When f_A and u_B represent in fact one equation, $f = 0$, in one unknown, u, some of the conditions (A2) become very powerful. First, if $f = 0$ is an odd-order differential equation then the condition involving the highest order derivative, namely

$$\frac{\partial f}{\partial u_{,pqr\ldots.}} = -\frac{\partial f}{\partial u_{,pqr\ldots.}}$$

implies that no variational formulation is possible. As an immediate consequence, the KdV equation in its original form does not admit a variational formulation. Second, if $f(u) := au_{,xx} + bu_{,x} + g(u,x)$, where u, a, and b are functions on x only, the condition (A2d) shows that the equation

$$\mu(x) f(u) = 0$$

does always admit a variational formulation provided $\mu = \exp[\int (b/a)\, dx]$.

We note in passing that the check of the conditions (A2) for a system of equations requires a preliminary labeling of the equations and of the unknowns. Accordingly, the fact that the given system of equations is or not a system of Euler–Lagrange equations may depend on the labeling.

Finally we mention that when the number of equations is different from the number of unknowns then no variational formulation can be obtained merely because the range and the domain of the corresponding differential operator N are different and hence N cannot be the derivative (gradient) of a functional.

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Maximum of the spin-flip cross section from unitarity and four constraints[a)]

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(Received 3 June 1982; accepted for publication 23 July 1982)

The upper bound on the spin-flip cross section is improved by adding a fourth constraint in a variational calculus. The total cross section, elastic cross section, the forward slope, and the backward slope of the imaginary part of the amplitude form the equality constraints. In addition the unitarity of the partial waves gives inequality constraints.

PACS numbers: 02.30.Wd, 11.80.Et

I. INTRODUCTION

The application of the variational calculus to scattering problems in particle physics[1,2] was generalized to cases with spin, in Refs.[3–5] The results of those papers were applied to spin (1/2)-spin 0 cases to find numerical solutions. Thus, the cases $\pi^+ p$ and $K^+ p$ were investigated[6,7] with only two constraints, namely, the forward slope and the total cross section. For this, the phase shifts of several groups were used.[8–10] One totally unexpected result of this study was the wide discrepancy between the predictions of different phase shift sets for the spin-flip cross section. Apparently this quantity had never been tested with phase shifts before. They differed by as much as a factor of 6. Still, the bounds found with two constraints were weak. In the best cases they were larger by a factor of 8 and in many cases more than a factor of 10. When we added a third constraint, namely the elastic total cross section, the bounds improved greatly. In general they were now larger by only a factor of 2 and in some cases even smaller.

In this paper we add a fourth constraint, the backward slope of the imaginary part of the amplitude. The complication introduced by this new constraint is the separation of the partial waves into even and odd l types. Also a fourth l-independent Lagrange multiplier appears. The forms of the partial waves depend now on four Lagrange parameters. However, since the fourth constraint we are adding is linear in imaginary parts of the partial waves the new multiplier appears, unlike the third one, on equal footing with the multipliers corresponding to the first two constraints. The third constraint, that is the elastic cross section, was quadratic in the real and imaginary parts of the partial waves. As a consequence of this its Lagrange parameter had appeared in the denominators of the partial waves.[5] This feature had made the problem of fitting the constraints a nonlinear problem. It still remains nonlinear, but now we have to fit four constraints with four parameters to maximize the spin-flip cross section.

In Sec. II we define our constraints and the quantity to be maximized. We write the Lagrange function and taking its second derivatives we find the maximum conditions. Spins of the particles are taken fully into account by defining four classes for this spin (1/2)-spin 0 case according to the elasticity of the partial waves.

In Sec. III we find, using the consequences of inequality constraints satisfied by the partial waves in different classes, the explicit forms of the partial waves in terms of the l-independent Lagrange parameters.

In the conclusion we outline the formalism used to maximize the spin-flip cross section subject to the given four constraints using the forms of the partial waves in different classes. We also summarize and discuss our results.

II. FOUR CONSTRAINTS AND UNITARITY

In order not to carry the multiplicative factors in the calculations we define instead of $\sigma_{SF}, \sigma^T, \sigma^E, (dA/dt)|_{z=1}, (dA/dt)|_{z=-1}$ the quantities G, A_0, E, S, and T.

$$G = \frac{k^2}{2\pi}\sigma_{SF} = \sum \frac{2l(l+1)}{2l+1}\left[(a_{l+} - a_{l-})^2 + (r_{l+} - r_{l-})^2\right], \tag{1}$$

$$A_0 = \frac{k^2}{4\pi}\sigma^T = \sum \left[(l+1)\,a_{l+} + l a_{l-}\right], \tag{2}$$

$$E = \frac{k^2}{4\pi}\sigma^E = \sum \left[(l+1)(a_{l+}^2 + r_{l+}^2) + l(a_{l-}^2 + r_{l-}^2)\right], \tag{3}$$

$$S = 4k^2 \frac{k}{\sqrt{s}}\frac{dA}{dt}\bigg|_{z=1} = \sum l(l+1)\left[(l+1)\,a_{l+} + l a_{l-}\right], \tag{4}$$

$$T = 4k^2 \frac{k}{\sqrt{s}}\frac{dA}{dt}\bigg|_{z=-1} = \sum l(l+1)\left[(l+1)a_{l+} + l a_{l-}\right](-1)^{l+1}. \tag{5}$$

Here σ_{SF} is the spin-flip cross section, σ^T the total cross section, σ^E elastic cross section, A the imaginary part of the scattering amplitude, $dA/dt|_{z=1}$ its derivative in the forward direction and $dA/dt|_{z=-1}$ the derivative in the backward direction. k is the c.m. momentum, $a_{l+}, a_{l-}, r_{l+}, r_{l-}$ are the imaginary and real parts of the partial waves.

Unitarity gives the following inequality constraints:

$$u_l = a_{l+} - a_{l+}^2 - r_{l+}^2 \geqslant 0, \tag{6}$$

$$v_l = a_{l-} - a_{l-}^2 - r_{l-}^2 \geqslant 0. \tag{7}$$

We want to maximize G subject to constraints (2)–(7).

[a)] Research supported by the Natural Sciences and Engineering Research Council (NSERC).

 0022-2488/82/122322-06$02.50

The Lagrange function is

$$L = G + \alpha A_0 + \gamma E + \beta S + \delta T + \sum (l+1)\lambda_l u_l + \sum l \mu_l v_l. \tag{8}$$

The Lagrange multipliers λ_l and μ_l associated with the inequality constraints satisfy

$$\lambda_l \geqslant 0, \quad \mu_l \geqslant 0.$$

The factors $(l+1)$ and l in the series are chosen for convenience. We also define the frequently appearing combinations:

$$B \equiv \frac{2l}{2l+1}, \quad D \equiv \frac{2(l+1)}{(2l+1)}. \tag{9}$$

Differentiating the Lagrange function with respect to different variables we find $(\partial L / \partial a_{l+}) = 0$ gives

$$(B+\gamma-\lambda_l)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \lambda_l] = 0, \tag{10}$$

$(\partial L / \partial a_{l-}) = 0$ gives

$$Da_{l+} - (D+\gamma-\mu_l)a_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \mu_l] = 0, \tag{11}$$

$(\partial L / \partial r_{l+}) = 0$ gives

$$(B+\gamma-\lambda_l)r_{l+} - Br_{l-} = 0, \tag{12}$$

$(\partial L / \partial r_{l-}) = 0$ gives

$$Dr_{l+} - (D+\gamma-\mu_l)r_{l-} = 0. \tag{13}$$

For a given value of l there are two amplitudes f_{l+} and f_{l-}. A pair of partial wave amplitudes belong to one and only one of the following four classes:

$$I^+I^- = \{l \,|\, u_l > 0, v_l > 0\}, \quad \lambda_l = 0, \ \mu_l = 0, \tag{14}$$

$$I^+B^- = \{l \,|\, u_l > 0, v_l = 0\}, \quad \lambda_l = 0, \ \mu_l \geqslant 0, \tag{15}$$

$$I^-B^+ = \{l \,|\, u_l = 0, v_l > 0\}, \quad \lambda_l \geqslant 0, \ \mu_l = 0, \tag{16}$$

$$B^+B^- = \{l \,|\, u_l = 0, v_l = 0\}, \quad \lambda_l \geqslant 0, \ \mu_l \geqslant 0. \tag{17}$$

Maximum conditions are found from the second derivatives of L.

$$\frac{\partial^2 L}{\partial a_{l+}^2} = 2(l+1)(B+\gamma-\lambda_l), \tag{18}$$

$$\frac{\partial^2 L}{\partial a_{l+}\partial a_{l-}} = -BD(2l+1), \tag{19}$$

$$\frac{\partial^2 L}{\partial r_{l+}^2} = 2(l+1)(B+\gamma-\lambda_l), \tag{20}$$

$$\frac{\partial^2 L}{\partial r_{l+}\partial r_{l-}} = -BD(2l+1), \tag{21}$$

$$\frac{\partial^2 L}{\partial a_{l-}^2} = 2l(D+\gamma-\mu_l), \tag{22}$$

$$\frac{\partial^2 L}{\partial r_{l-}^2} = 2l(D+\gamma-\mu_l). \tag{23}$$

These conditions have not changed from the three constraint case by adding the fourth constraint T, because T is linear in a_{l+} and a_{l-}. For maxima, the condition that second derivatives be negative give

$$B+\gamma-\lambda_l \leqslant 0, \tag{24}$$

$$D+\gamma-\mu_l \leqslant 0. \tag{25}$$

III. PARTIAL WAVES IN FOUR CLASSES

Class I^+I^-: In this class $\lambda_l = 0$, $\mu_l = 0$. Hence Eqs. (10) and (11) become

$$(B+\gamma)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] = 0, \tag{26}$$

$$Da_{l+} - (D+\gamma)a_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] = 0. \tag{27}$$

Unless the determinant

$$\begin{vmatrix} B+\gamma & -B \\ D & -(D+\gamma) \end{vmatrix}$$

vanishes, that is unless $2+\gamma = 0$, we have

$$a_{l+} = a_{l-} = -(1/2\gamma)[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}]. \tag{28}$$

Unitarity gives

$$0 \leqslant -(1/2\gamma)[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] \leqslant 1. \tag{29}$$

With $\lambda_l = \mu_l = 0$ in this class, the maximum conditions (24), (25) become

$$B+\gamma \leqslant 0, \tag{30}$$

$$D+\gamma \leqslant 0, \tag{31}$$

γ being l-independent only certain values of l will satisfy these inequalities.

In this class Eqs. (12) and (13) take the forms

$$(B+\gamma)r_{l+} - Br_{l-} = 0, \tag{32}$$

$$Dr_{l+} - (D+\gamma)r_{l-} = 0, \tag{33}$$

r_{l+} and r_{l-} are different from zero only if the determinant vanishes, e.g.,

$$\gamma = -2. \tag{34}$$

When $2+\gamma = 0$ the inhomogeneous Eqs. (26) and (27) are consistent. That is

$$\frac{B+\gamma}{D} = \frac{B}{D+\gamma} = -1. \tag{35}$$

The real and imaginary parts of the partial waves then satisfy

$$(B-2)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] = 0, \tag{36}$$

$$(B-2)r_{l+} - Br_{l-} = 0, \tag{37}$$

$$a_{l+} - a_{l+}^2 - r_{l+}^2 > 0, \tag{38}$$

$$a_{l-} - a_{l-}^2 - r_{l-}^2 > 0. \tag{39}$$

If the determinant does not vanish, that is, if $2+\gamma \neq 0$ we have

$$r_{l+} = r_{l-} = 0. \tag{40}$$

Class I^+B^-: In this class $\lambda_l = 0, \mu_l \geqslant 0$. The Eqs. (10)–(13) become

$$(B+\gamma)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] = 0, \tag{41}$$

$$Da_{l+} - (D+\gamma-\mu_l)a_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \mu_l] = 0, \tag{42}$$

$$(B+\gamma)r_{l+} - Br_{l-} = 0, \tag{43}$$

$$Dr_{l+} - (D+\gamma-\mu_l)r_{l-} = 0. \tag{44}$$

Again in order that r_{l+} and r_{l-} be different from zero the determinant of Eqs. (43) and (44) mush vanish. This gives

$$\mu_l(B+\gamma) = \gamma(\gamma+2). \tag{45}$$

Equation (45) can be satisfied only by certain values of l. When the determinant is zero, the other two determinants of the inhomogeneous equations (41) and (42) also must vanish. Or

$$\frac{B+\gamma}{D} = \frac{B}{D+\gamma-\mu_l} = -\frac{\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}}{\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \mu_l}. \tag{46}$$

For this equation to be satisfied we must have either

$$\gamma + 2 = \mu_l = 0, \tag{47}$$

or

$$\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma = 0. \tag{48}$$

As we have $\lambda_l = 0$ in I^+B^-, the first case is similar to the class I^+I^-, except that $v_l = 0$.

The second possibility $l(l+1) = -[(\alpha+\gamma)/(\beta+\delta(-1)^{l+1})]$ can be satisfied by at most one l value if the right-hand side is a positive integer.

In the first case the equations satisfied by the partial waves are identical with the Eqs. (36)–(39), except that (39) is now an equality.

In the second case, they are

$$(B+\gamma)a_{l+} - Ba_{l-} - \tfrac{1}{2}\gamma = 0, \tag{49}$$

$$(B+\gamma)r_{l+} - Br_{l-} = 0, \tag{50}$$

$$a_{l+} - a_{l+}^2 - r_{l+}^2 > 0, \tag{51}$$

$$a_{l-} - a_{l-}^2 - r_{l-}^2 = 0. \tag{52}$$

When the determinant is different from zero, we have

$$r_{l+} = r_{l-} = 0.$$

In this class

$$v_l = a_{l-} - a_{l-}^2 - r_{l-}^2 = 0.$$

Hence, except for the values of l which might satisfy Eq. (45) we have in general

$$v_l = a_{l-} - a_{l-}^2 = 0.$$

Thus

$$a_{l-} = \begin{cases} 1 \\ 0 \end{cases}.$$

(1) If $a_{l-} = 1$, we find from Eq. (41) for a_{l+}

$$a_{l+} = \frac{1}{B+\gamma}\{B - \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}]\}. \tag{53}$$

Equation (42) gives

$$\mu_l = \frac{2+\gamma}{B+\gamma}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + 2\gamma]. \tag{54}$$

We impose the unitarity condition $0 \leqslant a_{l+} \leqslant 1$ on Eq. (53). Together with the maximum condition (24) this gives

$$2B \leqslant \alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} \leqslant -2\gamma. \tag{55}$$

The maximum condition (25) imposed on (54), together with Eq. (55) and Eq. (24) gives

$$\gamma \geqslant -2 \tag{56}$$

and

$$\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} \leqslant \frac{BD}{2+\gamma} - \gamma. \tag{57}$$

(2) If $a_{l-} = 0$, we find from Eq. (41),

$$a_{l+} = -\frac{1}{2(B+\gamma)}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}]. \tag{58}$$

From Eq. (42) we find

$$\mu_l = -\frac{2+\gamma}{B+\gamma}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}]. \tag{59}$$

The unitary condition

$$0 \leqslant a_{l+} \leqslant 1,$$

imposed on (58), together with the maximum condition (24), gives

$$0 \leqslant \alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} \leqslant -2(B+\gamma). \tag{60}$$

The maximum condition (25) imposed on (59) together with $\mu_l \geqslant 0$, Eq. (60), and $B+\gamma \leqslant 0$ gives

$$\gamma + 2 \geqslant 0, \tag{61}$$

and

$$\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} \geqslant -\frac{BD}{2+\gamma} - \gamma. \tag{62}$$

The contributions of the partial waves of the form (53) or (58) to G, A_0, S, E, and T cannot be summed in closed form as was the case with two constraints. The reason for this is the presence of γ in the denominators of these two formulas. However, in practical calculations[6,7] this has no effect since a finite numer of partial waves are summed numerically.

Class I^-B^+: In this class $\lambda_l \geqslant 0$, $\mu_l = 0$. The Eqs. (10)–(13) become

$$(B+\gamma-\lambda_l)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \lambda_l] = 0, \tag{63}$$

$$Da_{l+} - (D+\gamma)a_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] = 0, \tag{64}$$

$$(B+\gamma-\lambda_l)r_{l+} - Br_{l-} = 0, \tag{65}$$

$$Dr_{l+} - (D+\gamma)r_{l-} = 0. \tag{66}$$

For r_{l+} and r_{l-} to be different from zero the determinant of the Eqs. (65) and (66) must vanish. This condition gives

$$\lambda_l(D+\gamma)=\gamma(\gamma+2). \tag{67}$$

Since γ is l-independent only certain l values will satisfy this equation. When the determinant of the homogeneous Eqs. (65) and (66) vanishes, the two other determinants of the inhomogeneous Eqs. (63) and (64) must vanish. Hence

$$\frac{B+\gamma-\lambda_l}{D}=\frac{B}{D+\gamma}$$
$$=-\frac{\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}+\lambda_l}{\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}}. \tag{68}$$

These equations give either

$$\gamma+2=\lambda_l=0, \tag{69}$$

or

$$\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}+\gamma=0. \tag{70}$$

Since in the class $I^-B^+\mu_l=0$, the first case is similar to the class I^+I^- except that $u_l=0$. Writing Eq. (70) in the form

$$l(l+1)=-\frac{\alpha+\gamma}{\beta+\delta(-1)^{l+1}},$$

one can see that this relation can be satisfied at most by one positive integer l if the right-hand side is a positive integer.

In the first case (69) Eqs. (36)–(39) remain the same except that Eq. (38) is now an equality.

In the second case (70) they become

$$Da_{l+}-(D+\gamma)a_{l-}+\tfrac{1}{2}\gamma=0, \tag{71}$$
$$Dr_{l+}-(D+\gamma)r_{l-}=0, \tag{72}$$
$$a_{l+}-a_{l+}^2-r_{l+}^2=0, \tag{73}$$
$$a_{l-}-a_{l-}^2-r_{l-}^2>0. \tag{74}$$

When the determinant of Eqs. (65) and (66) is different from zero,

$$r_{l+}=r_{l-}=0.$$

Except for the special values of l which might satisfy Eq. (67) we have in general

$$u_l=a_{l+}-a_{l+}^2=0.$$

Hence

$$a_{l+}=\begin{cases}1\\0\end{cases}.$$

(1) If $a_{l+}=1$, we find from Eq. (64),

$$a_{l-}=\frac{1}{D+\gamma}\{D-\tfrac{1}{2}[\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}]\}. \tag{75}$$

Equation (63) gives

$$\lambda_l=\frac{2+\gamma}{D+\gamma}\{\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}+2\gamma\}. \tag{76}$$

We impose the unitarity condition,

$$0\leqslant a_{l-}\leqslant 1$$

on Eq. (75). Together with the maximum condition (25) this gives

$$2D\leqslant\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}\leqslant-2\gamma. \tag{77}$$

The maximum condition (24) imposed on (76), together with $\lambda_l\geqslant 0$, Eq. (77), and

$$D+\gamma\leqslant 0,$$

gives

$$2+\gamma\geqslant 0, \tag{78}$$

and

$$\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}\leqslant\frac{BD}{2+\gamma}-\gamma. \tag{79}$$

(2) If $a_{l+}=0$, we find from Eq. (64),

$$a_{l-}=-\frac{1}{2(D+\gamma)}[\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}]. \tag{80}$$

Equation (63) gives

$$\lambda_l=-\frac{2+\gamma}{D+\gamma}[\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}]. \tag{81}$$

We impose the unitarity condition $0\leqslant a_{l-}\leqslant 1$, on Eq. (80). Together with the maximum condition (25) this gives

$$0\leqslant\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}\leqslant-2(D+\gamma). \tag{82}$$

The maximum condition (24) imposed on (81), together with $\lambda_l\geqslant 0$, Eq. (82), and $D+\gamma\leqslant 0$,

gives

$$2+\gamma\geqslant 0, \tag{83}$$

and

$$\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}\geqslant-\frac{BD}{2+\gamma}-\gamma. \tag{84}$$

The remarks about summing the series G, A_0, E, S, and T with partial waves given by their forms in the class I^+B^- apply also to the class I^-B^+.

Class B^+B^-: In this class neither λ_l nor μ_l is zero. As before we have to solve Eqs. (10)–(13). We also note that the determinant of the homogeneous Eqs. (12) and (13) is the same as the determinant of the inhomogeneous Eqs. (10) and (11). If this determinant does not vanish the solutions of Eqs. (12) and (13) are trivial:

$$r_{l+}=r_{l-}=0.$$

Since in the class B^+B^-, $u_l=0$ and $v_l=0$, we have

$$a_{l+}=\begin{cases}1\\0\end{cases}\text{ and }a_{l-}=\begin{cases}1\\0\end{cases}.$$

This leads to four possibilities:

(1) When $a_{l+}=a_{l-}=0$,

$$\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}+\lambda_l=0,$$
$$\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}+\mu_l=0.$$

Hence

$$\lambda_l=-[\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}]\geqslant 0,$$
$$\mu_l=-[\alpha+l(l+1)\beta+l(l+1)\delta(-1)^{l+1}]\geqslant 0. \tag{85}$$

Obviously this case does not contribute to G, A_0, E, S, or T.

(2) When $a_{l+}=0$, $a_{l-}=1$ Eqs. (10) and (11) give

$$\lambda_l = 2B - [\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] \geqslant 0, \tag{86}$$

$$\mu_l = 2(D+\gamma) + [\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] \geqslant 0. \tag{87}$$

The analysis of these inequalities as function of l is different from the two (A_0,S) or three (A_0,S,E) constraint cases. In the relation

$$y = \alpha + l(l+1)[\beta + \delta(-1)^{l+1}],$$

analytic continuation from integer values of l to a real variable is made difficult by the factor $(-1)^{l+1}$.

We should therefore define two continuations, one for even and the other for odd l:

$$y_+ = \alpha + l(l+1)(\beta - \delta),$$
$$y_- = \alpha + l(l+1)(\beta + \delta).$$

These are two parabolas in the variable l with their extrema at $l = -\frac{1}{2}$. The sign of $(\beta - \delta)$ or $(\beta + \delta)$ determines whether this extremum is a maximum or minimum. B and D as defined by Eqs. (9) are, respectively, monotonically increasing or decreasing functions of l, asymptotically approaching 1.

(3) When $a_{l+} = 1, a_{l-} = 0$, Eqs. (10) and (11) give

$$\lambda_l = 2(B+\gamma) + [\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] \geqslant 0, \tag{88}$$

$$\mu_l = 2D - [\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] \geqslant 0. \tag{89}$$

With Eqs. (24) and (25) we also find from (88) and (89),

$$\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma \geqslant -B, \tag{88a}$$

$$\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma \leqslant D. \tag{89a}$$

(4) When $a_{l+} = 1, a_{l-} = 1$, Eqs. (10) and (11) give

$$\lambda_l = \mu_l = 2\gamma + [\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1}] \geqslant 0. \tag{90}$$

Again using the Eqs. (24) and (25) we find from (90),

$$\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma \geqslant B, \tag{90a}$$

$$\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma \geqslant D. \tag{90b}$$

We note that this case does not contribute to G, even though it contributes to A_0, E, S, and T.

(5) Finally there is a fifth case for the class B^+B^-. This is when the determinant of the homogeneous Eqs. (12) and (13) vanishes. In this case the remaining two determinants of the Eqs. (10) and (11) also vanish. We can then write

$$\frac{B+\gamma-\lambda_l}{D} = \frac{B}{D+\gamma-\mu_l} = -\frac{\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \lambda_l}{\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \mu_l}. \tag{91}$$

These equations are satisfied for

$$\lambda_l = \mu_l = 2 + \gamma. \tag{92}$$

In this case Eq. (10) is proportional to (11) and Eq. (12) proportional to (13). The partial waves are given by the solutions of the following set:

$$Da_{l+} + Ba_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + 2 + \gamma] = 0, \tag{93}$$

$$Dr_{l+} + Br_{l-} = 0, \tag{94}$$

$$a_{l+} - a_{l+}^2 - r_{l+}^2 = 0, \tag{95}$$

$$a_{l-} - a_{l-}^2 - r_{l-}^2 = 0. \tag{96}$$

The solutions of these equations are

$$a_{l+} = \frac{1}{4}\frac{\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma + 2}{[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma]D}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma + D - B], \tag{97}$$

$$a_{l-} = \frac{1}{4}\frac{\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma + 2}{[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma]B}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma + B - D], \tag{98}$$

$$r_{l+}^2 = \frac{1}{16}\frac{\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma + 2}{[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma]^2 D^2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma + D - B] \times [B^2 - (\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma - D)^2], \tag{99}$$

$$r_{l-}^2 = \frac{1}{16}\frac{\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma + 2}{[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma]^2 B^2}[\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma + B - D] \times [D^2 - (\alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma - B)^2]. \tag{100}$$

Here because of the positivity of λ_l and μ_l and Eq. (92),

$$\gamma + 2 \geqslant 0.$$

Unitarity imposed on (97) and (98) gives two possible domains both for a_{l+} and a_{l-}. They are

$$[2/(2l+1)] \leqslant \alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma \leqslant 2, \tag{101}$$

or

$$-2 \leqslant \alpha + l(l+1)\beta + l(l+1)\delta(-1)^{l+1} + \gamma \leqslant -[2/(2l+1)]. \quad (102)$$

Since in the class B^+B^- both partial waves are elastic their contributions to E and A_0 will be equal as was the case with three constraints.

IV. CONCLUSION

We extended the application of the variational calculus to scattering problems to the cases with spin. As an example the spin-flip cross section G was maximized with four constraints A_0, E, S, and T. The unitarity of partial waves gives additional restrictions in the form of inequality constraints. In a scattering problem for particles with spin there will be a certain number of partial waves. To handle the spin we defined classes according to the elasticity or inelasticity of the partial waves such as to exhaust the possible combinations. From the theory of inequality constraints the l-dependent Lagrange multipliers vanish whenever a partial wave is inelastic. This property assigns to partial waves well defined forms in different classes in terms of l-independent Lagrange parameters and l.

In the spin $\frac{1}{2}$-spin 0 case there are two partial waves f_{l+} and f_{l-} and four classes in which both waves are elastic, both inelastic, one elastic the other inelastic, and vice versa. We found in those classes expressions for a_{l+}, a_{l-}, r_{l+}, and r_{l-}. In some cases they are simple, like $a_{l\pm} = 1$ or $r_{l\pm} = 0$. In other classes like in B^+B^- the expressions were fairly complicated.

To maximize G one selects partial waves from different classes and expresses the four constraints with these waves. The four unknown Lagrange multipliers are thus determined with these four relations. Hence the numerical values of the partial waves are found. However, the right form of the partial waves and fitting of the constraints does not yet guarantee the solutions. Because the unitarity and the maximum conditions obtained from the second derivatives of the Lagrange function impose further restrictions on the partial waves in the form of inequalities. Therefore, all sets of partial waves which fit the constraints must be tested against those inequality conditions. The solutions which satisfy these conditions will give us a maximum. In general there are more than one, but a small number of, solutions because we are working in an infinite dimensional space. Among those we choose the one which gives the largest spin-flip cross section. In the numerical applications we have numbered the possible forms of the partial waves. Even though there are only four classes, there may be more than one form in a given class consistent with the conditions of this class. For the three constraints case nine different forms can contribute to the solutions. We therefore gave the solutions in the form of a set of numbers like 9, 9, 2, 8 for example. This means that the $l = 1$ partial waves are of the form labeled 9, $l = 2$ partial waves are of the form labeled 9, $l = 3$ partial waves are of the form labeled 2 and so on.

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Renormalized Lie perturbation theory

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(Received 29 April 1981; accepted for publication 23 July 1982)

A Lie operator method for constructing action-angle transformations continuously connected to the identity is developed for area preserving mappings. By a simple change of variable from action to angular frequency, a perturbation expansion is obtained in which the small denominators have been renormalized. The method is shown to lead to the same series as the Lagrangian perturbation method of Greene and Percival, which converges on KAM surfaces. The method is not superconvergent but yields simple recursion relations which allow automatic algebraic manipulation techniques to be used to develop the series to high order. It is argued that the operator method can be justified by *analytically continuing* from the complex angular frequency plane onto the real line. The resulting picture is one where preserved primary KAM surfaces are continuously connected to one another.

PACS numbers: 02.40. + m, 02.30. + g, 02.50.Ey

I. INTRODUCTION

The construction of action-angle transformations[1] for Hamiltonian systems is an important goal since it represents an essentially complete solution of the dynamics. An integrable system is one where these transformations are defined almost everywhere in phase space, with the possible exception of the separatrices between regions where the topologies of the orbits are different (in general a set of zero measure).

The Kolmogorov–Arnold–Moser theorem[2] guarantees that for a wide class of nonintegrable systems sufficiently close to integrability a privileged set of invariant surfaces exists (the KAM surfaces). This set is of finite measure, and on each KAM surface a form of action-angle variables is well defined.[3,4] As we increase the perturbation parameter which takes us away from integrability, the isolating integrals (actions) cease to exist locally. Accordingly, KAM surfaces are broken when action is no longer well defined.[5] When, in a given region of phase space, the last KAM surface with the same topology as the unperturbed surfaces is broken, connected stochasticity prevails throughout that region. The purpose of this paper is to examine methods that make use of the notion of action as an isolating integral. Our aim is to develop perturbative methods that will be *practical* tools for determining the transition to stochastic behavior, but with a more solid foundation than the empirical observations that lead to the "overlap-of-resonances" criterion.[8] The transition to global stochasticity can be determined if we have a method for calculating the action-angle transformation and a rule for selecting the most robust surfaces.

In this paper we compare two perturbative approaches to the problem of constructing action-angle variables on the primary KAM surfaces. We limit ourselves to iterated two-dimensional area-preserving mappings, in particular to the Standard mapping of Chirikov and Taylor and a variant, the Semistandard mapping of Greene and Percival.[5] These mappings can be regarded as return maps or surfaces of section of Hamiltonian flows. The perturbative approach can be readily extended to continuous flows and systems of dimensionality higher than two.

In Sec. II we set up the general problem of computing the action-angle transformation for primary KAM curves. The first method we examine is based on the assumption that there exists a global canonical transformation continuously connected to the identity, such that the primary KAM surfaces (KAM curves in 2D) are reduced to straight lines. Lie methods are used to construct a formal power series in the perturbation parameter, ϵ,[7–10] which is justified by an argument based on analytic continuation in the complex action plane. In Sec. III we review the Lie transform formalism. In Sec. IV we generate a perturbation theory in the canonical action-angle variables using Lie methods. The theory is affected by the well known problem of small denominators, even on preserved KAM surfaces, and therefore can provide only an asymptotic series.

In Sec. V we review a different approach, the Lagrangian perturbation theory of Greene and Percival. The theory has the remarkable property of avoiding resonant denominators on primary KAM surfaces. In fact, this Lagrangian theory is *convergent* on a strip around the real axis of the angle variable, for small enough ϵ. We call such a theory a *renormalized* theory.

In Sec. VI we alter the theory of Sec. IV to avoid the resonant denominators through the use of a noncanonical set of variables. We thus construct a *renormalized Lie perturbation theory* which shares the advantages of the Lagrangian renormalized method while being of wider applicability than it. In Sec. VII we show that the perturbation method can be used to provide an alternative and more justifiable version of the overlap of resonances picture.[6] In Sec. VIII we examine the convergence of the perturbation series, while in Sec. IX we use the Fourier convergence method of Greene and Percival to map out the region of convergence in the complex angular frequency plane.

II. ACTION-ANGLE TRANSFORMATIONS FOR PRIMARY KAM CURVES

Suppose we have an area preserving $T:\mathbb{R}^2 \to \mathbb{R}^2$ (i.e., of a 2D real vector space onto itself). We denote the nth iterate

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 0022-2488/82/122328-11$02.50

of the 2-vector (θ_0, I_0) by (θ_n, I_n). That is

$$(\theta_n, I_n) = \mathbf{T}(\theta_{n-1}, I_{n-1}) = \mathbf{T}\circ\mathbf{T}(\theta_{n-2}, I_{n-2}) = \cdots, \quad (1)$$

where $f\circ g(x) \equiv f(g(x))$ denotes the composition of any two functions f and g.

We assume $\mathbf{T}$ to be analytic in both θ and I, so that it may be extended to a complex mapping $\mathbf{T}:\mathbb{C}\to\mathbb{C}^2$, where $\mathbb{C}^2$ is a 2D complex vector space. By the area preserving property, the Jacobian of $\mathbf{T}$ is unity on $\mathbb{R}^2$, and hence on $\mathbb{C}^2$ by analytic continuation:

$$\frac{\partial\theta_{n+1}}{\partial\theta_n}\frac{\partial I_{n+1}}{\partial I_n} - \frac{\partial\theta_{n+1}}{\partial I_n}\frac{\partial I_{n+1}}{\partial\theta_n} = 1\,. \quad (2)$$

Suppose further that $\mathbf{T}$ is the vector sum of an unperturbed part $\mathbf{T}_0$ and a perturbation $\epsilon\mathbf{T}_1$, where ϵ is a continuously variable parameter. We assume that (θ,I) are action-angle variables for the unperturbed mapping, i.e.,

$$\mathbf{T}_0(\theta,I) = (\theta + \Omega_0(I), I)\,. \quad (3)$$

We also assume $\mathbf{T}_1$ to be 2π-periodic in θ.

In this paper we shall be applying the formalisms to an especially simple class of mappings whose unperturbed angular frequency is given by

$$\Omega_0(I) = I\,. \quad (4)$$

The perturbed part of the mapping is assumed to be derivable from a potential, i.e.,

$$\mathbf{T}_1(\theta, I) = -V'(\theta)\cdot(1,1)\,. \quad (5)$$

Chirikov[6] gives physical motivations for discussing this class, and has termed the choice

$$V(\theta) = -\cos\theta\,, \quad (6)$$

the Standard mapping (we have changed the sign to put the potential well at $\theta = 0$). This is the potential which describes, in a continuous time formulation, the motion of a particle in an electrostatic wave; in this case, the action-angle transformation can be called an oscillation-center transformation.[7]

The slow transition to ergodic behavior that the KAM theorem implies occurs only for potentials whose Fourier expansion $\Sigma_m V_m \exp(im\theta)$ decays rapidly (e.g. exponentially) as $m\to\infty$. For less smooth potentials, KAM curves may not exist at all for nonzero ϵ.[11] The standard mapping has a finite Fourier series, and is therefore a good case to study.

An even simpler representative of this class is obtained by deleting the $m = -1$ component of $\cos\theta$:

$$V(\theta) = -\tfrac{1}{2}e^{i\theta}\,. \quad (7)$$

This has been called the Semistandard mapping by Greene and Percival,[5] and has a meaning only within the context of mappings on $\mathbb{C}^2$.

The mapping $\mathbf{T} = \mathbf{T}_0 + \epsilon\mathbf{T}_1$ is said to be *integrable* if phase space is covered with curves invariant under the application of $\mathbf{T}$. In this case the invariant curves can be labelled by a new action, J, constant on each curve, and parametrized along their length by a new angle Θ, so that

$$(\theta, I) = \mathbf{C}(\Theta, J)\,, \quad (8)$$

where $\mathbf{C}$ is a canonical (unit Jacobian) transformation 2π-periodic in Θ. Since we are interested in constructing $\mathbf{C}$ by a perturbation expansion in ϵ, we require $\mathbf{C}:\mathbb{C}^2\to\mathbb{C}^2$ to lie within the group of canonical transformations containing the identity. We also assume the inverse transformation to exist:

$$(\Theta, J) = \mathbf{C}^{-1}(\theta, I)\,, \quad (9)$$

and assume $\mathbf{C}$ and $\mathbf{C}^{-1}$ to be differentiable. That is, $\mathbf{C}$ is a *diffeomorphism*. These restrictions on $\mathbf{C}$ mean that Θ and J will correspond to action-angle variables, as ordinarily understood, only when the invariant curves $J = \text{const.}$ have the same topology as the unperturbed curves $I = \text{const.}$ For example, in the case of the physical pendulum, with gravity regarded as the perturbation, $\mathbf{C}$ is an ordinary action-angle transformation only in the region of phase space corresponding to rotational motion.[1] The interpretation of $\mathbf{C}$ for libratory motion will be discussed elsewhere.

In the new action-angle representation, the nth iterate of the point (Θ_0, J_0) is given by composing n times a mapping $\mathbf{S}$, which is similar to $\mathbf{T}_0$, but with a different angular frequency function $\Omega(J)$. That is:

$$(\Theta_n, J_n) = \mathbf{S}(\Theta_{n-1}, J_{n-1})\,, \quad (10)$$

$$\mathbf{S}(\Theta, J) = (\Theta + \Omega(J,\epsilon), J)\,. \quad (11)$$

From Eqs. (1), (4), and (6) we see that

$$\mathbf{T} = \mathbf{C}\circ\mathbf{S}\circ\mathbf{C}^{-1}\,. \quad (12)$$

The relation between $\mathbf{T}$ and $\mathbf{S}$ is represented by the following commutative diagram:

$$\begin{array}{ccccccc} \begin{pmatrix}\theta_0\\ I_0\end{pmatrix} & \overset{\mathbf{T}}{\mapsto} & \begin{pmatrix}\theta_1\\ I_1\end{pmatrix} & \overset{\mathbf{T}}{\mapsto} & \cdots & \overset{\mathbf{T}}{\mapsto} & \begin{pmatrix}\theta_n\\ I_n\end{pmatrix} \\ \updownarrow\mathbf{C} & & \updownarrow\mathbf{C} & & & & \updownarrow\mathbf{C} \\ \begin{pmatrix}\Theta_0\\ J_0\end{pmatrix} & \underset{\mathbf{S}}{\mapsto} & \begin{pmatrix}\Theta_1\\ J_1\end{pmatrix} & \underset{\mathbf{S}}{\mapsto} & \cdots & \underset{\mathbf{S}}{\mapsto} & \begin{pmatrix}\Theta_n\\ J_n\end{pmatrix} \end{array}$$

In this diagram horizontal direction corresponds to the discrete "time" flow, while the vertical direction corresponds to a continuous flow in ϵ.

The case when $\mathbf{T}$ is integrable for finite ϵ is highly exceptional; in general, no $\mathbf{C}$ exists such that $\mathbf{S}$ is everywhere of the form given by Eq. (11). However, the KAM theorem, for sufficiently small ϵ there remains an infinity of invariant curves characterized by Eq. (11) with $J = \text{const.}$[2] Because $\mathbf{C}$ is a diffeomorphism, these invariant KAM surfaces are topologically equivalent to the straight line invariant curves of $\mathbf{T}_0$. We term these the *primary* KAM curves to distinguish them from other invariant curves surrounding elliptic fixed points of $\mathbf{T}$.

In Sec. IV we construct a perturbation theory using ϵ as an expansion parameter by proceeding formally as if $\mathbf{T}$ were integrable. If $\mathbf{T}$ is restricted to $\mathbb{R}^2$ this expansion can at best converge only for values of J on the primary KAM curves. Unfortunately, there is no way of telling *a priori* which values of J to examine, since KAM curves are actually characterized by an irrational value of the winding number $2\pi/\Omega(J,\epsilon)$. We follow Greene[12] in assuming that the most robust KAM surfaces, those which disrupt last as ϵ increases, are those possessing inverse winding numbers which we can call *generalized golden means*. That is, the most robust surfaces

will be those with values of Ω whose partial fraction expansion is terminated by an infinite number of ones, i.e.,

$$\Omega = 2\pi[a,b,...,y,z,1,1,1,...], \tag{13}$$

with $a,b,...,y,z$ integers. Since Ω selects the most stable KAM surfaces, it would seem preferable to treat Ω, rather than J, as the independent variable. Two such methods are discussed in Secs. V and VI.

From the above discussion it would appear that **C** is defined only on a highly pathological, perhaps not even dense, set of values of J or Ω on which differentiation cannot be defined. This is true if Ω is restricted to be real, but by continuing **T** and **C** into $\mathbb{C}^2$, we shall find that **C** is analytic in a large connected region of the complex Ω plane. By proceeding formally on the assumption that **C** exists we are implicitly working in $\mathbb{C}^2$. The transformation is obtained on primary KAM curves by analytic continuation back to the real Ω axis. The analytic continuation across the real Ω axis is justified by the theory of monogenic functions.[13]

III. LIE THEORY

There is a one to one correspondence between canonical transformations, such as **T** and **C** which map phase space onto itself, and certain unitary operators which map the space of functions defined on phase space onto itself.[14] For instance, given the transformation **A**, we define the corresponding unitary operator A by

$$Af(\Theta, J) = f(\mathbf{A}(\Theta, J)), \tag{14}$$

where f is any function on phase space. $Af(\Theta, J)$ is known as the *pullback* of f under **A**.[15]

Note that **A** is a nonlinear, vector-valued function of a vector, whereas A is a linear, scalar operator defined on functions of Θ and J. Given A, we can conversely construct **A**, since

$$\mathbf{A}(\Theta, J) = (A\Theta, AJ). \tag{15}$$

We denote this one-to-one correspondence thus: $A \leftrightarrow \mathbf{A}$. Consider now a function $f(\mathbf{A}\circ\mathbf{B}(\Theta, J)) = f(\mathbf{A}(\mathbf{B}(\Theta, J)))$. According to Eq. (14) we get:

$$f(\mathbf{A}\circ\mathbf{B}(\Theta, J)) = (Af)(\mathbf{B}(\Theta, J)) = BAf(\Theta, J),$$

from where the composition rule for unitary operators is given by

$$AB \leftrightarrow \mathbf{B}\circ\mathbf{A}. \tag{16}$$

Similarly, $ABC \leftrightarrow \mathbf{C}\circ\mathbf{B}\circ\mathbf{A}$, and so on. In particular, the operator equation corresponding to Eq. (12) is

$$T = C^{-1}SC. \tag{17}$$

It is well known that a Hamiltonian flow generates a family of canonical transformations parametrized by the time variable. Analogously, by inventing a suitable generator W which plays the role of the Hamiltonian, we can obtain any canonical transformation that is continuously connected to the identity by "advancing" the coordinates in a new variable which plays the role of time (the Lie parameter, ϵ). The canonical transformation **C** is thus forced to be continuously connected to the identity at $\epsilon = 0$, while **T** and **S** are assumed to be continuously connected to the unperturbed mapping, i.e., $\mathbf{T}_0 = \mathbf{T}(\epsilon = 0) = \mathbf{S}(\epsilon = 0)$. Following Dewar[7] we seek "Lie generating functions" $U(\Theta, J,\epsilon), V(\Theta, J,\epsilon)$, and $W(\Theta, J,\epsilon)$ such that the unitary operators S, T, and C obey the following operator equations and boundary conditions:

$$\partial_\epsilon T = L_V T, \quad T(\epsilon = 0) = T_0, \tag{18}$$

$$\partial_\epsilon S = L_U S, \quad S(\epsilon = 0) = T_0, \tag{19}$$

$$\partial_\epsilon C = L_W C, \quad C(\epsilon = 0) = 1, \tag{20}$$

where $\partial_\epsilon \equiv \partial/\partial\epsilon$. L_W denotes the Lie derivative or Poisson bracket operator:

$$L_W \equiv (\partial_J W)\partial_\Theta - (\partial_\Theta W)\partial_J, \tag{21}$$

and T_0 is the operator $\exp[\Omega_0(J)\partial_\Theta]$. Similarly, by Eq. (11)

$$S = \exp[\Omega(J,\epsilon)\partial_\Theta]. \tag{22}$$

Comparing Eqs. (19), (21) and (22) we see that $U \equiv U(J,\epsilon)$ such that

$$\Omega(J,\epsilon) = \Omega_0(J) + \int_0^\epsilon d\epsilon' \partial_J U(J,\epsilon'). \tag{23}$$

In similar fashion, we can determine V, since T is associated with the prescribed mapping **T**. For instance, in the special case of mappings defined by Eqs. (6) and (7), the generating function V is readily verified to be the potential $V(\Theta)$. What we need now is to find equations for W and U. We take the ϵ derivative of Eq. (17), and using Eqs. (18)–(20) and the expression[7]:

$$\partial_\epsilon C^{-1} = -C^{-1}L_W, \tag{24}$$

we get

$$-C^{-1}L_W SC + C^{-1}L_U SC + C^{-1}SL_W C = L_V T. \tag{25}$$

As Dewar[7] shows, the identities

$$C^{-1}L_f C = L_{C^{-1}f}, \quad SL_f S^{-1} = L_{Sf}, \tag{26}$$

are obeyed for any function f. By inserting the identity operator in the forms CC^{-1} and $S^{-1}S$ in the proper places in Eq. (25), Eqs. (26) can be used to show that

$$-L_{C^{-1}W} T + L_{C^{-1}U} T + L_{C^{-1}SW} T = L_V T,$$

which can be satisfied by choosing the generating function W and an arbitrary constant in U so that

$$(S - 1)W = CV - U. \tag{27}$$

This is the analogue of the "Hamilton–Jacobi equation for the Lie generating function" derived previously for continuous Hamiltonian flows,[7] with U playing the role of the "new Hamiltonian," K. In order to determine $U(J,\epsilon)$, observe that

$$\langle (S - 1)W \rangle = (S - 1)\langle W \rangle = 0,$$

where the averaging operation $\langle\ \rangle$ is defined for any f by

$$\langle f \rangle \equiv \frac{1}{2\pi}\int_0^{2\pi} d\Theta f.$$

The average of Eq. (27) yields

$$U = \langle CV \rangle. \tag{28}$$

Eq. (28) ensures that W will be a generator for an action-angle transformation, but it is still not unique, since we have

not yet specified $\langle W\rangle$. The simplest choice is to take $\langle W\rangle = 0$; instead, to facilitate comparison with the Lagrangian perturbation theory, we can require

$$\langle C\Theta - \theta\rangle = 0\,. \tag{29}$$

This is not necessarily equivalent to specifying $\langle W\rangle = 0$, but the difference corresponds simply to a trivial action-dependent phase shift in the Θ coordinate. In the case of the Standard and Semistandard mappings, Eq. (29) is equivalent to $\langle W\rangle = 0$.

IV. CANONICAL PERTURBATION THEORY

Adding $(T_0 - S)W$ to both sides of Eq. (27) we write it in the form:

$$(T_0 - 1)W = CV + (T_0 - S)W - U\,. \tag{30}$$

Since $(T_0 - 1)$ is independent of ϵ, Eq. (30) is in a form amenable to solution by simple power-series expansion of $W(\Theta, J, \epsilon)$ which we term a *primitive* perturbation expansion.

In order to avoid working with operators, it is convenient to define auxiliary variables:

$$v \equiv CV\,, \tag{31}$$

$$\theta \equiv C\Theta\,, \tag{32}$$

$$w \equiv (T_0 - S)W\,. \tag{33}$$

The variable $\theta(\Theta, J, \epsilon)$ is simply the old angle in terms of the new phase space coordinates Θ and J. It is needed to implement Eq. (29). The auxiliary variable $v(\Theta, J, \epsilon)$ is simply $V(\theta)$ in the case of the mappings defined by Eqs. (6) and (7).

We now expand W and U according to the convention:

$$W = \sum_{n=0}^{\infty} W_{n+1}\,\epsilon^n\,, \tag{34}$$

$$U = \sum_{n=1}^{\infty} U_{n+1}\,\epsilon^n \tag{35}$$

(we assume $\langle V\rangle = 0$ so that Eq. (28) implies $U_1 = 0$). The convention for v is

$$v = \sum_{n=0}^{\infty} v_n\,\epsilon^n\,, \tag{36}$$

and similarly for θ and w. Differentiating Eqs. (31) and (32) with respect to ϵ, using Eq. (20), and equating coefficients of different powers of ϵ, we find the following simple nonlinear recursion relations for $n \geqslant 1$:

$$v_n = \frac{1}{n}\sum_{m=1}^{n} \{v_{n-m}, W_m\}\,, \tag{37}$$

$$\theta_n = \frac{1}{n}\sum_{m=1}^{n} \{\theta_{n-m}, W_m\}\,, \tag{38}$$

where $\{f, g\}$ denotes the Poisson bracket $L_g f$, and the recursion is initialized with

$$v_0 = V(\Theta)\,, \tag{39}$$

$$\theta_0 = \Theta\,. \tag{40}$$

The recursion for w_n is much more complicated:

$$w_n = -T_0 \sum_{k=1}^{[n/2]} \sum_{l=0}^{[n/2-m]} \frac{C_{l,k}}{k!}\,\partial_\Theta^k\, W_{n-2k-2l+1}\,, \tag{41}$$

where

$$C_{l,k} = \frac{1}{lA_0}\sum_{\nu=1}^{l} (\nu k - l + \nu) A_\nu C_{l-\nu} \quad \text{for } l > 0\,,$$

$$C_{0,k} = A_0^k\,, \tag{42}$$

$$A_\nu = [1/2(\nu+1)]\,\partial_J\, U_{2(\nu+1)}\,,$$

and $[f]$ denotes the integer part of f. We have assumed that V involves only odd Fourier components (as for the Standard and Semistandard map cases), so that $U_{2n+1} = 0$ for all integers n. The coefficients $C_{l,k}$ are independent of Θ, so Eq. (41) does not couple Fourier components.

Denoting $(f - \langle f\rangle)$ by $\tilde{f}$, we split Eq. (30) into its average and fluctuating parts, and equating powers of ϵ, we obtain two more recurrence relations:

$$U_{n+1} = \langle v_n\rangle\,, \tag{43}$$

$$\tilde{W}_{n+1} = (T_0 - 1)^{-1}(\tilde{v}_n + \tilde{w}_n)\,. \tag{44}$$

By Eqs. (29) and (40) we require

$$\langle\theta_n\rangle = 0 \quad \text{for } n \geqslant 1\,.$$

Equation (38) then gives a recursion relation for $\langle W_{n+1}\rangle$:

$$\partial_J \langle W_{n+1}\rangle = -\sum_{m=1}^{n} \langle\{\theta_{n+1-m}, \tilde{W}_m\}\rangle\,. \tag{45}$$

Equations (37), (41)–(45) make up a complete set of recurrence relations for all unknowns. The inversion of $T_0 - 1$ in Eq. (44) is most easily accomplished in Fourier space:

$$W_{n+1}^m = [(v_n^m + w_n^m)/(\exp[im\Omega_0(J)] - 1)]\,, \tag{46}$$

for $m \neq 0$. Here, and in the following sections, the Fourier representation f^m of any function $f(\Theta)$ is defined by:

$$f(\Theta) = \sum_{m=-\infty}^{\infty} f^m \exp im\Theta\,. \tag{47}$$

Clearly, Eq. (46) will be undefined for some value of m whenever $\Omega_0(J)/2\pi$ is a rational fraction. Since $\Omega_0(J) \neq \Omega(J, \epsilon)$ in general, we can expect this primitive perturbation series to be divergent even if J is chosen so that Ω is a "generalized golden mean". Also, the complicated nature of the recursion for w_n suggests that adding $(T_0 - S)W$ to Eq. (27) was not the best thing to do. In Sec. VI we present a method which allows $(S - 1)$ to be inverted directly.

V. LAGRANGIAN PERTURBATION THEORY

The work of Greene and Percival,[5] based on the averaged Lagrangian variational principle of Percival[3] shows that there is indeed an alternative and simple perturbation method for primary KAM surfaces; this method is convergent (for ϵ small enough) within a strip containing the real axis in the complex angle variable (Θ) plane. Their starting point is the discretization of the Lagrangian differential equations of motion. The use of canonical variables and Poisson brackets is avoided, simplifying the recursion relations significantly. The method does not give rise in general to simple recursion relations. For this reason, we restrict ourselves in this section to an examination of the Standard and the Semistandard maps.

From Eqs. (1)–(5) and (8)–(11) we can show that:

$$\delta^2\theta \equiv \theta(\Theta + \Omega) - 2\theta(\Theta) + \theta(\Theta - \Omega) = -\epsilon V'(\theta)\,. \tag{48}$$

Since J and ϵ can be regarded as constants in Eq. (48), we have suppressed the last two arguments of $\theta(\Theta, J, \epsilon)$.

For a concrete example let us consider the Standard mapping, given by Eq. (6). Defining auxiliary variables:

$$f(\theta,\Omega,\epsilon) = -V'(\theta) = -\sin\theta\,, \tag{49}$$

and

$$v(\theta,\Omega,\epsilon) = V(\theta) = -\cos\theta\,, \tag{50}$$

we get

$$\partial_\epsilon f = -v\partial_\epsilon\,\theta, \quad \partial_\epsilon\, v = f\partial_\epsilon\theta\,. \tag{51}$$

The derivatives with respect to ϵ are taken at fixed Ω, rather than at fixed J. We now assume that ϵ is a small parameter, and expand f, v and θ as in Eq. (36). From Eqs. (48) and (51), by equating powers of ϵ, we obtain simple nonlinear recursion relations [c.f. Eqs. (37)–(44)]:

$$\begin{aligned} nv_n &= \sum_{\nu=1}^{n} \nu f_{n-\nu}\,\theta_\nu\,, \\ nf_n &= -\sum_{\nu=1}^{n} \nu v_{n-\nu}\,\theta_\nu\,, \\ \delta^2\theta_n &= f_{n-1}\,. \end{aligned} \tag{52}$$

Note that the existence of a finite set of quadratically nonlinear recursion relations is critically dependent on the specific form of V, in contrast to the canonical perturbation theory.

The second difference operator is inverted by Fourier expanding θ_j, v_j and f_j in Θ, getting:

$$\begin{aligned} v_n^m &= \frac{1}{n}\sum_{\nu=1}^{n}\sum_{\mu=-\infty}^{\infty} \nu f_{n-\nu}^{m-\mu}\,\theta_\nu^\mu\,, \\ f_n^m &= -\frac{1}{n}\sum_{\nu=1}^{n}\sum_{\mu=-\infty}^{\infty} \nu v_{n-\nu}^{m-\mu}\,\theta_\nu^\mu\,, \\ \theta_n^m &= -\frac{\exp im\Omega}{2(\exp[im\Omega\,]-1)^2} f_{n-1}^m\,. \end{aligned} \tag{53}$$

Equations (53) furnish us with a closed recursion procedure, provided we start with finite Fourier series in Θ for f_0 and v_0, because the μ summations truncate after a finite number of terms. Note that the recursion formulas are completely algebraic in nature, involving no differential operators. In particular, for the Standard mapping we start with:

$$\begin{aligned} &f_0^1 = (1/2i), \quad f_0^{-1} = -(1/2i), \\ &v_0^1 = (1/2), \quad v_0^{-1} = (1/2)\,, \end{aligned} \tag{54}$$

and $f_0^m = v_0^m = 0$ for $m \neq 1, -1$. The Fourier–power coefficients form a triangular array, such that the nth power in ϵ contains Fourier modes ranging from $-n$ through n, and only those terms where n has the same parity as m are nonzero, i.e.,

$$\begin{array}{ccccccc} & & \theta_1^1 & 0 & \theta_1^{-1} & & \\ & \theta_2^2 & 0 & \theta_2^0 & 0 & \theta_2^{-2} & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \theta_m^m & 0 & \theta_m^{m2} & \cdots & \theta_m^{m+2} & 0 & \theta_m^{-m} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{array} \tag{55}$$

and similarly for f and v.

A similar procedure can be followed for the Semistandard mapping. In this case, all harmonic coupling raises the Fourier index; the only terms that survive in the Fourier-power coefficient matrix are those on the left edge of the triangular array (55). Remarkably, for this case *the Fourier series is the perturbation series*. This allows for a very efficient recursion procedure.

VI. RENORMALIZED CANONICAL PERTURBATION THEORY

A simple renormalization of the resonant denominators in Eq. (46) can be effected by changing from the canonical set $\{\Theta, J, \epsilon\}$ to the noncanonical set $\{\Theta, \Omega, \epsilon\}$ of independent variables.[16] The procedure amounts to a simple change of variables. Therefore ∂_ϵ and ∂_Θ *will henceforth imply that* Ω, *rather than* J, *is to be held fixed*. Where ∂_ϵ and ∂_J occurred previously, they must be replaced according to the rule:

$$\partial_J \to (\partial_\Omega J)^{-1}\partial_\Omega\,, \tag{56}$$

$$\partial_\epsilon \to (\partial_\Omega J)^{-1}[(\partial_\Omega J)\partial_\epsilon - (\partial_\epsilon J)\partial_\Omega\,]\,. \tag{57}$$

We again need the auxiliary variables v and θ, but w does not have to be used since $S - 1$ is now independent of ϵ, and Eq. (27) is now in suitable form for recursively generating $W(\Theta,\Omega,\epsilon)$, again assuming power series expansions of the forms in Eqs. (34) and (36).

An equation for v is obtained by taking the ϵ derivative of Eq. (31) at constant J and using Eqs. (20), (56) and (57):

$$[(\partial_\Omega J)\partial_\epsilon - (\partial_\epsilon J)\partial_\Omega\,]v = [\![v, W]\!]\,. \tag{58}$$

where $[\![,]\!]$ denotes the *modified Poisson bracket*

$$[\![f, g]\!] = (\partial_\Theta f)(\partial_\Omega g) - (\partial_\Omega f)(\partial_\Theta g)\,. \tag{59}$$

Similarly, θ obeys

$$[(\partial_\Omega J)\partial_\epsilon - (\partial_\epsilon J)\partial_\Omega\,]\,\theta = [\![\theta, W]\!]\,. \tag{60}$$

An equation for J is obtained by differentiating Eq. (23) with respect to ϵ at constant J and using Eqs. (56) and (57):

$$J(\Omega,\epsilon) = J_0(\Omega\,) - \int_0^\epsilon d\epsilon'\partial_\Omega\, U(\Omega,\epsilon')\,, \tag{61}$$

where $J_0(\Omega\,)$ is the solution of the equation

$$\Omega_0(J_0) = \Omega\,. \tag{62}$$

We insert Eq. (61) in Eq. (58) having expanded all functions as in Eqs. (34)–(36) and the additional expansions:

$$J = J_0(\Omega\,) + \sum_{n=1}^{\infty} J_n\,\epsilon^n\,, \tag{63}$$

$$\theta = \Theta + \sum_{n=1}^{\infty} \theta_n\,\epsilon^n\,. \tag{64}$$

After expanding all functions in Fourier series over Θ we obtain a recursive expression for the coefficients of the double expansion for v, given by Eqs. (36) and (47):

$$\begin{aligned} v_n^j = \frac{1}{n}\sum_{m=0}^{n-1}\Bigg(\sum_\nu i(j-\nu)\,[v_{n-m}^{j-\nu}\,\partial_\Omega\, W_{m+1}^\nu \\ - \partial_\Omega\, v_{n-m}^\nu\, W_{m+1}^{j-\nu}\,] \\ - \partial_\Omega\, v_{n-m}^j\,\partial_\Omega\, U_m + \frac{n-m+1}{m} v_{n-m}^j\,\partial_\Omega^2\, U_m\Bigg)\,. \end{aligned} \tag{65}$$

The Fourier analysis in Θ permits the explicit evaluation of $(S-1)W$ in the fluctuating part of Eq. (27), yielding

$$W^m_{n+1} = \begin{cases} \dfrac{v^m_n}{\exp(im\Omega)-1}, & m \neq 0, \\ 0, & m = 0 \text{ (by assumption)}, \end{cases} \tag{66}$$

Eqs. (65)–(66) constitute a closed set of recursion formulas, since U is given by the average of v.

Similarly, starting from Eq. (60), we find that θ can be computed from

$$\theta^j_n = \frac{1}{n}\sum_{m=0}^{n-1}\Bigg(\sum_\nu i(j-\nu)\,[\theta^{j-\nu}_{n-m}\,\partial_\Omega\, W^\nu_{m+1} - \partial_\Omega\,\theta^\nu_{n-m}\, W^{j-\nu}_{m+1}] - \partial_\Omega\,\theta^j_{n-m}\,\partial_\Omega U_m + \frac{n-m+1}{m}\theta^j_{n-m}\,\partial^2_\Omega\, U_m\Bigg). \tag{67}$$

The recursion formulas are fairly straightforward, and the resonant denominators now involve only Ω directly. This achieves the desired renormalization. In fact, Eq. (67) reproduces the results of the Lagrangian theory of Sec. V for the Standard and Semistandard mappings.

VII. PERTURBATION SERIES AND A RESONANCE OVERLAP CRITERION

We have constructed different perturbation theories which share certain characteristics: they are recursive, do not involve any approximations beyond those inherent in the perturbative formulation itself, and have relatively simple recursion formulas. Their practical value depends strongly on our ability to obtain high-order results. The recursion relations we have described so far are simple enough to permit this, in contrast to other possible avenues of attack, such as superconvergent expansions.[2]

The primitive perturbation theory yields, at best, an asymptotic series. While reasonable results can often be otained from such series,[17] a convergent series is clearly preferable (for the special case of the Semistandard mapping, the primitive perturbation theory is equivalent to the renormalized theory, since in this case $J=\Omega$ identically). The renormalized theory is simple and convergent on KAM surfaces for small enough values of ϵ, in both its canonical and Lagrangian formulations. The formulas of the renormalized canonical theory are of wider applicability than those of the Lagrangian formulation, since the recursion relations are closed through the use of a generating function instead of the properties of the potentials used. We pay a price for this, however: the canonical theory is more difficult to use, because it involves differential operators in its recursion formulas, as opposed to purely algebraic recursive relations for the Lagrangian theory.

The recursive formulations of perturbation theories are ideally suited to computer implementation. We can obtain analytic results to relatively high order in ϵ through the use of an automatic algebraic manipulator.[18] We have used MACSYMA to obtain results to order ϵ^{10} before the complexity of the expressions involved made it impractical to proceed further. The analytic results provide us with significant insight into the resonance-resonance interaction mechanism. The first few orders in the primitive perturbation theory for W and U are given by

$$W = \epsilon\frac{\Xi}{2(\Upsilon-1)} + \epsilon^2\frac{\Xi^2}{4(\Upsilon-1)^3(\Upsilon+1)} + \epsilon^3\left(\frac{\Upsilon(\Upsilon^2+1)(\Upsilon^2+3\Upsilon+1)\Xi}{16(\Upsilon-1)^5(\Upsilon+1)^2} + \frac{\Upsilon^2(\Upsilon^2+4\Upsilon+1)\Xi^3}{16(\Upsilon-1)^5(\Upsilon+1)^2(\Upsilon^2+\Upsilon+1)}\right) + O(\epsilon^4), \tag{68}$$

$$U = -\frac{\epsilon\Upsilon}{2(\Upsilon-1)^2} - \frac{\epsilon^3\Upsilon^2(\Upsilon^4+2\Upsilon^3+4\Upsilon^2+2\Upsilon+1)}{8(\Upsilon-1)^6(\Upsilon+1)^2} + O(\epsilon^5), \tag{69}$$

where $\Xi \equiv \exp(i\Theta)$ and $\Upsilon \equiv \exp(iJ)$. By using Eq. (23) we can attempt to determine the angular frequency for a given value of J, but the denominators in U will produce undefined values at the resonances. A selective ressumation of the primitive perturbation series could provide us with an alternative renormalization,[19] but that requires a much better picture of the structure of the series than that which we have been able to obtain analytically.

In contrast to the primitive theory, the renormalized perturbation theory in either its Lagrangian or canonical formulations uses Ω as the expansion variable. The resonant denominators in the renormalized theory will never be zero provided we choose an irrational value for $\Omega/2\pi$. The perturbation theory will converge for small enough ϵ on a surface characterized by one such value. As ϵ is increased a point will be reached where the perturbation series will cease to converge. This point marks the destruction of the particular KAM surface corresponding to the chosen value of Ω. It is sufficient to consider the perturbation series for W, since if W diverges, so will all other quantities.[8]

The perturbation theories can provide information about the local properties of the mapping close to a resonance. By expanding every term in the ϵ series for W in partial fractions, we obtain a series whose general form is

$$W = \sum_\mu W_\mu,$$

with

$$W_\mu = \sum_n\sum_m \epsilon^n \exp(im\Theta)\sum_{\nu=0}^{\nu_{\max}} \frac{a_{nm\mu\nu}}{(Y-Y_\mu)^\nu}, \tag{70}$$

where $Y \equiv \exp(i\Omega)$, $\nu_{\max}$ is an integer which depends on n, m and μ, $a_{nm\mu\nu}$ is some constant, and $Y_\mu = \exp(2i\pi\mu)$ for $\mu = q/p$, where q and p are any two mutually prime integers such that $0 \leqslant \mu < 1$. Y_μ is termed a *primitive pth root of unity*.[20] We approximate W_μ by retaining only the most divergent terms, $\nu = \nu_{\max}$, and get an approximation which is good near the $Y = Y_\mu$ resonance

$$W_\mu \approx \sum_m\sum_n \frac{a_{nm\mu}\,\epsilon^n \exp(im\Theta)}{(Y-Y_\mu)^{\nu_{\max}}}. \tag{71}$$

To examine a simple case, we restrict ourselves to the Semistandard map, since in this case $a_{nm\mu\nu} = a'_{n\mu\nu}\,\delta^m_n$; we thus get:

TABLE I. Local approximations to the generating function W for the Semistandard mapping at selected resonances. Notation corresponds to Eq. (72).

n	$M_\mu =$ $\nu_{\max}$	1 $\alpha'_{n\mu}$	$Y_\mu =$ $\nu_{\max}$	-1 $\alpha'_{n\mu}$	$Y_\mu =$ $\nu_{\max}$	$e^{(2i\pi/3)}$ $\alpha'_{n\mu}$	$Y_\mu =$ $\nu_{\max}$	i $\alpha'_{n\mu}$
1	1	$\frac{-1}{2}$						
2	3	$\frac{1}{8}$	1	$\frac{1}{32}$				
3	5	$\frac{-1}{32}$	2	$\frac{-1}{256}$	1	$\frac{-e^{i\pi/3}+1}{144}$		
4	7	$\frac{1}{128}$	3	$\frac{-1}{2048}$	2	$\frac{2e^{i\pi/3}-1}{2592}$	1	$\frac{-5i}{1538}$
5	9	$\frac{-1}{512}$	4	$\frac{1}{16384}$	2	$\frac{e^{i\pi/3}+1}{7776}$	2	$\frac{-5i-5}{24576}$
6	11	$\frac{1}{2048}$	5	$\frac{1}{131072}$	3	$\frac{1}{41472}$	2	$\frac{5}{49152}$
7	13	$\frac{-1}{8192}$	6	$\frac{-1}{1048076}$	4	$\frac{-5(e^{i\pi/3}+1)^{-1}}{1492992}$	2	$\frac{-5i+5}{131072}$
8	15	$\frac{1}{32768}$	7	$\frac{-1}{8388608}$	4	$\frac{7e^{i\pi/3}}{448976(e^{i\pi/3}+2)}$	3	$\frac{-25i}{4718592}$
9	17	$\frac{-1}{13172}$	8	$\frac{1}{67108864}$	5	$\frac{-(e^{i\pi/3}-1)^{-1}}{11943936}$	4	$\frac{-25}{50331648(i-1)}$

$$W_\mu \approx \sum_n \frac{\alpha'_{n\mu}\epsilon^n \exp(in\theta)}{(Y-Y_\mu)^{\nu_{\max}}}. \tag{72}$$

A table of $\alpha'_{n\mu}$ and $\nu_{\max}$ for the Semistandard map is shown in Table I, while Table II shows the values for the coefficients $a_{nm\mu\nu}$ for one particular resonance, $\mu = 0$. A more refined approximation than Eq. (71) can be obtained by considering more terms in Eq. (70) than those with $\nu = \nu_{\max}$ (cf. Table II).

The "*radius of divergence*" of the W_μ series in the complex Y-plane can be determined by taking ratios of terms in Eq. (71) for a fixed value of ϵ. The detailed scaling of the size of the divergent regions can be extracted from Table I. We take ratios of those terms in Eq. (72) where the differences in $\nu_{\max}$ are 2. By following this procedure, we obtain fixed ratios for each resonance, from which we can conclude that the radius of divergence at $Y = Y_\mu$ scales as $\epsilon^{\lambda/2}$, where λ is the order in ϵ at which the resonance at Y_μ first appears. This means that the size of the resonance at $Y = 1$ scales at $\sqrt{\epsilon}$, at $Y = -1$ it scales as ϵ, etc.; this is the scaling we would expect from direct mode-coupling between the primary resonances.

The partial fraction decomposition provides a more rigorous version of the overlapping resonances picture of the breakup of KAM surfaces than does Chirikov's criterion.[6] Consider an irrational value of $\Omega/2\pi$. Define $\rho_n(\Omega)$ as the "radius of divergence" associated with the nth convergent of $\Omega/2\pi$, $\mu_n \equiv q_n/p_n$ [Ref. 21] (nth order truncations of the continued fraction expansion). The invariant curve associated with Ω will be preserved only if $\rho_n(\Omega) \to 0$ faster than $q_n/p_n \to \Omega/2\pi$ as $n \to \infty$. As ϵ is increased, $\rho_n(\Omega)$ ceases to be a rapidly decreasing function of n as $n \to \infty$, and there-

TABLE II. Coefficients for the partial fraction expansion of W near the primary resonance ($Y_\mu = 1$) for the Semistandard map. Notation corresponds to Eq. (70).

n	$\alpha_{nm0\nu}$ $\nu = 1$	2	3	4	5	6	7	8	9	10	11
1	$-\frac{1}{2}$										
2	$-\frac{1}{32}$	$\frac{1}{16}$	$\frac{1}{8}$								
3	$\frac{-23}{4608}$	0	$\frac{5}{384}$	$-\frac{1}{32}$	$-\frac{1}{32}$						
4	$\frac{-125}{165888}$	$\frac{-313}{110592}$	$\frac{313}{55296}$	$-\frac{1}{256}$	$-\frac{1}{256}$	$\frac{3}{256}$	$\frac{1}{128}$				
5	$\frac{3973}{9830400}$	$\frac{-481}{165888}$	$\frac{481}{165888}$	0	$\frac{-3457}{1105920}$	$\frac{3}{1024}$	$\frac{1}{1024}$	$\frac{-1}{256}$	$\frac{-1}{512}$		
6	$\frac{28561931}{21233664000}$	$\frac{-12186443}{3538944000}$	$\frac{9927143}{5308416000}$	$\frac{7531}{5894240}$	$\frac{-7531}{9949120}$	$\frac{31}{32768}$	$\frac{1}{768}$	$\frac{-25}{16384}$	$\frac{-5}{24576}$	$\frac{5}{4096}$	$\frac{1}{2048}$

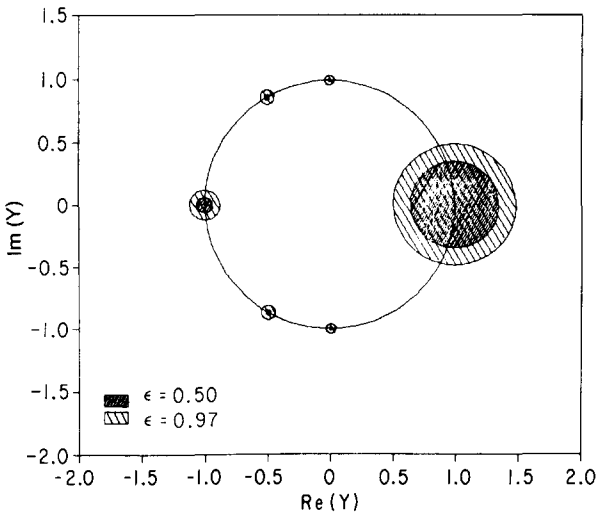

FIG. 1. Regions of divergence of the renormalized perturbation theory around selected resonances for the Semistandard Mapping. The shaded areas denote the regions of divergence in the $Y \equiv \exp(i\Omega)$ complex plane.

fore the invariant curve will be destroyed when ϵ is greater than $\epsilon_{\text{crit}}(\Omega)$, the value at which $\rho_n(\Omega)$ and $\Omega - 2\pi\mu_n$ approach 0 at the same asymptotic rate. Even if an invariant curve is destroyed on the real Ω axis, "surfaces" will still be preserved for complex Ω's far enough away from the axis, to avoid being overlapped by any of the circles of divergence (see Fig. 1). Because $\rho_n(\Omega)$ decreases rapidly with n, the region of convergence will have "tendrils", touching the real line at the preserved primary KAM curves, if any of them are left. An alternative method for extrapolating the behavior of $\rho_n(\Omega)$ at infinitely high order has been suggested by Escande and Doveil,[22] through the use of renormalization group techniques.

VIII. CONVERGENCE OF THE ϵ POWER SERIES

In either the Lagrangian or the canonical perturbation theory, the functions of interest are expressed as a double series: a power series in ϵ and a Fourier series in Θ. Greene and Percival[5] examine the convergence of the Fourier series to determine analyticity of their perturbation theory. This assumes that the power series expansion for each Fourier mode converges. We shall examine the convergence of the Fourier series in Sec. IX, but it is necessary to examine the ϵ power series for convergence first.

For the semistandard mapping the double summation collapses into a single sum. For this case the convergence study is reduced to a determination of the convergence of the Fourier series (see Sec. IX). Regretfully, this cannot be done for the Standard mapping, where the assumption of convergence of the ϵ power series must be justified.

Figure 2(a) shows a plot of the magnitude of the coefficients θ_n^m of the Lagrangian theory [see Eqs. (53)] for $m = 1$, $\Omega/2\pi = (\sqrt{5} - 1)/2$ as a function of the ϵ power index n. The general features of this plot are obtained for other harmonics as well. The magnitude of the coefficients has a ragged behavior, which will be explained in Sec. IX. However, the general trend is for these coefficients to decay rapidly for

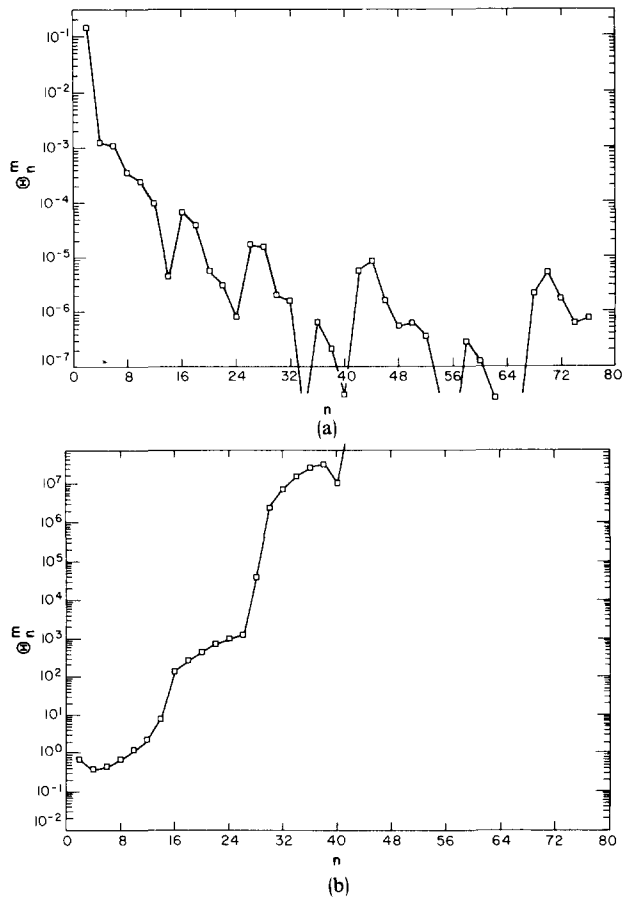

FIG. 2. Magnitude of the power series coefficients for the $m = 1$ mode of the Standard Mapping obtained from the Lagrangian perturbation theory for $\Omega/2\pi = (\sqrt{5} - 1)/2$. The behavior shown is typical of all modes.

small n, and then more and more slowly as n increases. In this case, the first few terms of the ϵ-series give a good approximation to each Fourier coefficient, even when the series is not absolutely convergent.

In contrast, Fig. 2(b) shows the same plot for a surface that breaks very early, $\Omega/2\pi = \pi - 3$. Now the coefficients grow exponentially. For a sufficiently small value of ϵ, however, the exponential growth can be overcome. For this value of Ω, we estimate that the power series for each Fourier mode can be majorized by a convergent geometric series if $\epsilon \lesssim 0.465 \pm 0.02$. For this particular value of $\Omega/2\pi$, it is difficult to insure that the majorization will persist beyond the point where the recursive calculation was stopped. This is due to the peculiar continued-fraction expansion that the number $\pi - 3$ possesses. In general, for nonquadratic irrational values of $\Omega/2\pi$, we can safely establish values of ϵ beyond which the power series is guaranteed to diverge, but it appears hazardous to claim that the power series would converge for ϵ less than a specific number. Note that this qualification is unnecessary for quadratic irrational values of $\Omega/2\pi$.

In the next section we will discuss the analyticity of the Fourier series. For this analysis, we will assume that the power series for each Fourier mode converges, at least up to $\epsilon_{\text{crit}}(\Omega)$, the critical value at which the Fourier series ceases to converge uniformly for real Θ. We have examined the

perturbation theories for several different values of $\Omega/2\pi$. For all quadratic irrational values of $\Omega/2\pi$ examined the empirical evidence is that each ϵ series has a radius of convergence approximately equal to $\epsilon_{\text{crit}}(\Omega)$. The agreement is to within 2% or better with a computational horizon (i.e. the value of n at which we stop our calculation) of $n = 80$. Thus to get very accurate values for the Fourier coefficients near $\epsilon = \epsilon_{\text{crit}}(\Omega)$ we would need a large number of terms in the ϵ series. The study of convergence properties of the power series defining one Fourier coefficient can be a more sensitive diagnostic of convergence than the study of the complete Fourier series for $\epsilon \simeq \epsilon_{\text{crit}}(\Omega)$. Because of the finite computational horizon we may see no apparent divergence in the Fourier series up to this horizon while the power series convergence estimate indicates that the double series is indeed diverging. It becomes apparent that the analyses described herein are valid provided we choose a large enough horizon to be able to discern some self-similar behavior, thus justifying the extrapolations used. This can be done by examining the continued fraction decompositions of $\Omega/2\pi$, which will also be done in the next section. Since nonquadratic irrational values of $\Omega/2\pi$ do not exhibit self-similar behavior in their continued fraction expansions, one can safely infer only that $\epsilon < \epsilon_{\text{crit}}(\Omega)$ is a necessary but not sufficient condition for the convergence of the series.

The difficulties of principle in determining convergence do not appear when using superconvergent expansions.[2] Indeed, for a rigorous proof of convergence one probably has to resort to these expansions at the expense of increased complexity of the perturbation series. For practical work a simple perturbation theory is sufficient to furnish reasonably high-precision quantitative results.

IX. THE STRUCTURE OF THE FOURIER SERIES

Assuming that the ϵ series for the Fourier coefficients converges, and summing over different orders in ϵ, we can examine the existence of the transformation by studying the convergence of the Fourier series, without using the partial fraction decomposition. This is the approach used by Greene and Percival.[5] Because of the superposition of all the different resonances, the Fourier coefficients have a very irregular dependence on m, the mode index, necessitating the calculation of the series to very high order. The Lagrangian formulation seems ideally suited to this task, because the algebraic nature of its recursion relations permits us to obtain extremely high order results [$O(\epsilon^{2000})$ for the Semistandard mapping] in a purely numerical fashion.

The coefficients of the Fourier series must decay exponentially if the series is to converge. We can estimate the decay rate of the Fourier coefficients by least-squares fits of exponentials or exponential-polynomial products to the values of the coefficients of the series for θ obtained from the perturbation theory. This yields the value for the critical ϵ needed to break the golden-mean surface [$\Omega/2\pi = (\sqrt{5}-1)/2$] to within 1% of the value Greene[12] obtained for the Standard map ($\epsilon_{\text{crit}} = 0.97$), considering only the first 80 Fourier coefficients. Figure 3 shows a least squares fit of $\alpha m^{\beta}\ \exp m\gamma$ to the Fourier coefficients for the Standard mapping for the

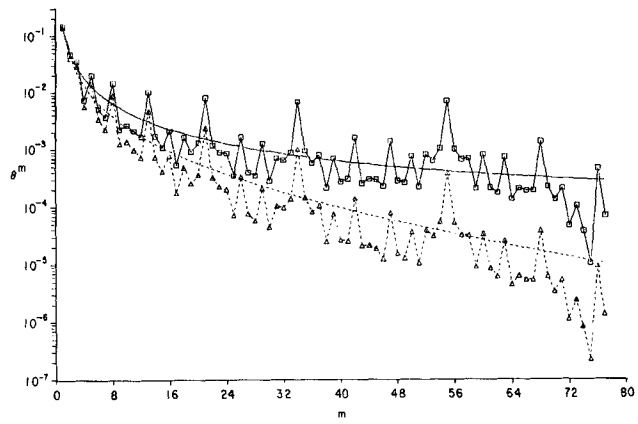

FIG. 3. Fourier coefficients for the Standard Mapping obtained from the Lagrangian perturbation theory, summed up to order 78 in the perturbation theory. Least-squares fits of $\alpha m^{\beta}\ \exp m\gamma$ are shown for two different values of ϵ, before ($\epsilon = 0.95$, dashed curve) and after breakage ($\epsilon = 0.95$, solid curve) of the KAM surface at the golden mean, $\Omega/2\pi = (\sqrt{5}-1)/2$.

golden mean, where we adjust α, β, and γ. We show two such fits, for different values of ϵ; γ changes sign for $\epsilon = 0.96\ldots$, which marks the point where the Fourier series starts to diverge. Higher accuracy can be obtained simply by considering a larger number of Fourier coefficients.

The Fourier coefficients for both the Standard and the Semistandard maps show some very interesting structure for real Ω. The structure is a direct consequence of the resonant denominators. If we construct the convergents[21] q_n/p_n of any irrational value of Ω, we can see that the Fourier coefficients with mode index $m = p_n$ are the slowest decaying ones. Further subsequences can be picked by a simple algorithm. It is easy to see that the subsequence $m = p_n + p_{n-1}$ again decays slowly, though not as slow as the subsequence $m = p_n$. In general, coefficients with mode index corresponding to linear combinations of p_n's with integer coefficients form slowly decaying subsequences, as can again be expected from mode beating arguments. Subsequences formed by modes where m cannot be expressed as one such linear combination will decay the fastest, and in general

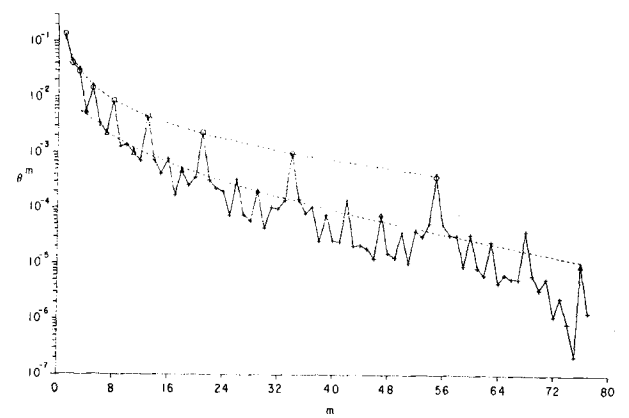

FIG. 4. Smoothly decaying subsequences for the Standard Mapping. We show a case for $\Omega/2\pi = 2/(3+\sqrt{5}) = [0.2,1,1,1,\ldots]$. Compare the positions of the peaks with those in Fig. 3, where $\Omega/2\pi = [0,1,1,1,\ldots]$. The dashed curves pass through two "slowly decaying" subsequences of Fourier coefficients.

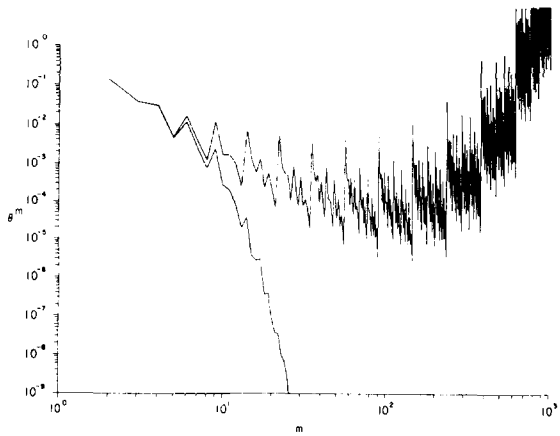

FIG. 5. Comparison of the Semistandard Mapping's Fourier coefficients on and off the real Ω axis for a $\epsilon = 1$; the Fourier series diverges on the real axis but converges away from it. The top curve corresponds to $\Omega / 2\pi = (\sqrt{5} - 1)/2$, while the bottom $\Omega /2\pi = (\sqrt{5} - 1)/2 + 0.01i$.

three-mode combinations decay faster than two-mode combinations. It is sufficient to fit exponential-polynomial decay curves to those coefficients decaying the slowest to determine convergence or divergence of the whole series. Figure 4 shows the absolute value of the Fourier coefficients of θ for the Semistandard mapping. The exponential-power fit to each subsequence is now much better than in Fig. 3.

When we analytically continue the mappings into the complex Ω plane, the spiky structure of the Fourier coefficients is preserved close to the real axis. As we get farther from the real axis and the resonances therein, the magnitude of the Fourier coefficients begins to drop dramatically, again showing the convergence of the Fourier expansion in the same domain where the ϵ expansion converges. Figure 5 shows a comparison of the Fourier coefficients on and off the real axis.

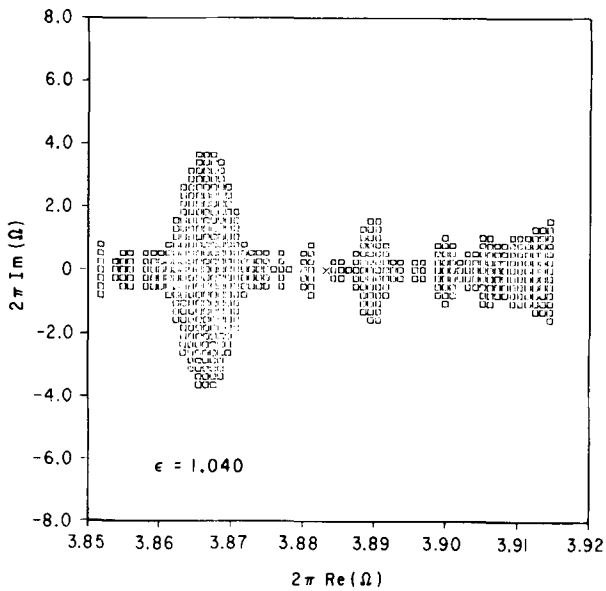

FIG. 6. Numerical scan about $\Omega /2\pi = (\sqrt{5} - 1)/2$. The dots correspond to cases where the numerical fit of exponential decay curves to the Fourier coefficients of the Semistandard Mapping indicate divergence of the perturbation series, using $O(\epsilon^{100})$ perturbation theory. Tendrils of convergence can be seen reaching down to the real axis at the preserved KAM surfaces.

By scanning over complex values of Ω, we determine numerically the regions of divergence of the Fourier series for fixed values of ϵ by looking at the exponential decay of the Fourier coefficients. Figure 6 shows such a scan for the Semistandard mapping, for Ω in the vicinity of the golden mean. The "tendrils" structure is again obtained. In the case of the Semistandard map this is not surprising, since the Fourier series is equivalent to the perturbation series in ϵ; this is not true in the Standard mapping case, where the convergence studies can be carried out independently of each other.

X. SUMMARY

The renormalized perturbation theory, both in its Lagrangian and in its canonical formulation appears to be a much more rigorous tool to study nonintegrable mappings than many others hitherto used. The theory is convergent on KAM surfaces and is remarkably useful both for understanding the analytical structure of resonance-resonance interactions as well as for obtaining numerical estimates (such as critical values for the breakup of the KAM surfaces).

The canonical formulation has a simpler recursive structure in general than the Lagrangian theory, but it involves differential operators that limit its use. Even though these differential operators are normal to the KAM surfaces, their presence is not of great concern because they can be understood as derivatives taken in the complex Ω plane; since a "tendril" of analyticity reaches down to a preserved KAM surface, the differential operators can be thought of as the analytic continuation to the real line of well defined operators in the complex plane.

The process of analytic continuation allows us to understand the process of the breakup of KAM surfaces. Since we can compute the size of the divergent regions in the complex angular frequency plane, we can see clearly that KAM surfaces are destroyed by an overlapping process reminiscent of that of Chirikov.[6] In contrast to the Chirikov picture, however, the resonances that ultimately destroy a given KAM surfaces *are not the primary resonances*; they are the high-order resonances lying nearby. The scaling of the widths of these resonances with ϵ seems to be consistent with a picture where the primary resonances beat directly against each other, i.e., where we neglect the interaction between resonances that have themselves been generated by beating. This fact is substantiated by a comparison between the divergent regions predicted by the Fourier series convergence studies and the analytical estimations of the radii of divergence of the perturbation series.

The values of the perturbation parameters necessary to break any given KAM surface can be obtained with arbitrary accuracy given enough computer time, using the theories described in this paper to compute the regions of divergence associated with high-order resonances. This is a significant achievement for a perturbation theory, since, as discussed above, the existence of KAM surfaces is determined by the interaction of resonances of arbitrarily high order.

A study of the libratory motion of the physical pendulum, to be reported elsewhere, suggests that secondary (is-

land-like) KAM surfaces correspond to certain complex values of Ω. If this is true as well for nonintegrable systems, then the perturbative theories, coupled with the analytic continuation methods, may allow us to explore the nature of stochastic motion in a region where the quasilinear diffusion approximation fails.[23]

ACKNOWLEDGMENTS

We gratefully acknowledge useful discussions with Dr. J. M. Greene, Dr. Y. C. Lee and Dr. D. Escande. This work was supported by the United States Department of Energy under contract number DE-AC02-76-CH03073. The high order calculations were done with the aid of MACSYMA, a large symbolic manipulation program developed at the MIT Laboratory for Computer Science and supported by the National Aeronautics and Space Administration under grant NSG 1323, by the Office of Naval Research under grant N00014-77-C-0641, by the U. S. Department of Energy under grant ET-78-C-02-4687, and by the U. S. Air Force under grant F49620-79-C-020.

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The complexification of a nonrotating sphere: An extension of the Newman–Janis algorithm

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(Received 18 January 1982; accepted for publication 30 June 1982)

A procedure given by Newman and Janis, to obtain the exterior Kerr metric from the exterior Schwarzschild metric by performing a complex coordinate transformation, is applied to an interior spherically symmetric metric. The resulting metric can be matched to the exterior Kerr metric on the boundary of the source which is chosen to be an oblate spheroid. A specific example of an interior solution for which the energy density is positive is given in detail.

PACS numbers: 02.40.Ky, 04.20. − q

I. INTRODUCTION

Since the discovery of the Kerr[1] metric there have been many attempts[2–6] to find a matter distribution that could be matched to it. With this aim we shall employ a procedure given by Newman and Janis,[7] by means of which one "derive" the Kerr metric from the Schwarzschild metric. The reason for the success of the Newman–Janis algorithm is quite obscure; it may be merely an accident. However, we feel it is worth exploring in a variety of circumstances to see if there is any method behind it, and if its uses can be extended to other cases.

The procedure mentioned above is applied to a spherical symmetric metric which contains the internal Schwarzschild solution for a perfect fluid as a special case. The new metric can be matched at the surface of the source to the exterior Kerr metric. The spin coefficients and the scalars corresponding to the traceless Ricci tensor are calculated (see Appendix A). An inspection of the components of the energy–momentum tensor in the spherically symmetric limit, for the specific example given below, allows us to show that the energy density is everywhere positive for, at least, small values of the parameter a.

In Sec. II we shall briefly recall the Newman–Janis procedure. The new metric is given in Sec. III. In Sec. IV a discussion of the boundary conditions, and the matching of the solution is presented.

A specific example is analyzed in Sec. V to illustrate the method.

Finally a discussion of the results is given in the conclusions.

II. THE NEWMAN–JANIS ALGORITHM

For sake of completeness we shall very briefly recall how to obtain the Kerr (exterior) metric from the Schwarzschild exterior metric following the algorithm indicated by Newman and Janis.[7]

We start with the complex null tetrad associated to the Schwarzschild exterior metric.

$$l^{\mu}=\delta^{\mu}_{1},\quad n^{\mu}=\delta^{\mu}_{0}-\tfrac{1}{2}(1-r_0/r)\delta^{\mu}_{1},$$
$$m^{\mu}=\frac{1}{\sqrt{2}r}\left(\delta^{\mu}_{2}+\frac{i}{\sin\theta}\delta^{\mu}_{3}\right),$$
$$\bar{m}^{\mu}=\frac{1}{\sqrt{2}r}\left(\delta^{\mu}_{2}-\frac{i}{\sin\theta}\delta^{\mu}_{3}\right),$$

where the bar indicate complex conjugation, r_0 is the gravitational radius, and the coordinates are $X^0\equiv u$ a timelike coordinate such that $u=$ const defines a null cone open to the future, $X^1\equiv r$ a null radial coordinate, and $X^{2,3}\equiv\theta,\phi$ two angle variables.

Now, the coordinate r is allowed to take complex values and the tetrad is rewritten in the form

$$l^{\mu}=\delta^{\mu}_{1};\ n^{\mu}=\delta^{\mu}_{0}-\tfrac{1}{2}\left[1-\frac{r_0}{2}\left(\frac{1}{r}+\frac{1}{\bar{r}}\right)\right]\delta^{\mu}_{1},$$
$$m^{\mu}=\frac{1}{\sqrt{2}\bar{r}}\left(\delta^{\mu}_{2}+\frac{i}{\sin\theta}\delta^{\mu}_{3}\right);$$
$$\bar{m}^{\mu}=\frac{1}{\sqrt{2}r}\left(\delta^{\mu}_{2}-\frac{i}{\sin\theta}\delta^{\mu}_{3}\right).$$

Next, one performs the complex coordinate transformation

$$r'=r+ia\cos\theta,\qquad \theta'=\theta,$$
$$u'=u'-ia\cos\theta,\quad \phi'=\phi.$$

Finally, one allows r' and u' to be real, and obtains

$$l'^{\mu}=\delta^{\mu}_{1};\ n'^{\mu}=\delta^{\mu}_{0}-\tfrac{1}{2}\{1-r_0[r'/(r'^2+a^2\cos^2\theta)]\}\delta^{\mu}_{1},$$
$$m'^{\mu}=[\sqrt{2}(r'+ia\cos\theta)]^{-1}$$
$$\times[ia\sin\theta(\delta^{\mu}_{0}-\delta^{\mu}_{1})+\delta^{\mu}_{2}+(i/\sin\theta)\delta^{\mu}_{3}]. \qquad (1)$$

Now, it can be shown that the metric associated to this tetrad is the Kerr metric.

In the next section a similar algorithm will be applied to a spherical symmetric metric which contain as special case the internal Schwarzschild metric.

III. SOURCE CONSTRUCTION

Let us start with the following metric;

$$ds^2=(Ve^{2b}/r)\,du^2+2e^{2b}du\,dr-r^2(d\theta^2+\sin^2\theta\,d\phi^2) \qquad (2)$$

with

$$e^{2b}=\frac{A-B(1-r^2/R^2)^{1/2}}{(1-r^2/R^2)^{1/2}},$$
$$Ve^{2b}/r=[A-B(1-r^2/R^2)^{1/2}]^2,$$

and the coordinates the same as in the Sec. II.

If one chooses

$$A=\tfrac{3}{2}(1-2M/r_1)^{1/2},\quad B=\tfrac{1}{2}$$

and $R^2=r_1^3/2M$, then the metric (2) becomes the usual

[a] Supported in part by C.O.N.I.C.I.T., Caracas, Venezuela.

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Schwarzschild interior solution for a sphere of radius r_1 filled with a perfect fluid of density $\rho = 3/8\pi R^2$. The null tetrad associated with the metric (2) is

$$l^\mu = e^{-2b}\delta^\mu_1, \quad n^\mu = \delta^\mu_0 - (V/2r)\delta^\mu_1,$$
$$m^\mu = \frac{1}{r\sqrt{2}}\left(\delta^\mu_2 + \frac{i}{\sin\theta}\delta^\mu_3\right), \tag{3}$$

or in covariant components,

$$l_\mu = \delta^0_\mu, \quad n_\mu = (Ve^{2b}/r)\delta^0_\mu + e^{2b}\delta^1_\mu,$$
$$m_\mu = -(r/\sqrt{2})(\delta^2_\mu + i\sin\theta\delta^3_\mu). \tag{3'}$$

At this point it is worthwhile to make the following remark: We shall complexify the metric (2), with A, B, and R as arbitrary functions of r (after the complexification they become functions of θ and r'), and not the interior Schwarzschild metric. This is due to the fact that using the interior Schwarzschild solution, one is led to a metric that cannot be matched to the exterior Kerr metric on the boundary. Actually it is impossible to choose an appropriate boundary for the source in that case. The reason for this could be found in the fact that the values of A, B, and R are closely related to the conditions on the boundary, which of course are different in the spherical and nonspherical case.

Let us now come back to our tetrad field (3). Assuming the coordinate r is allowed to take complex values, the tetrad is rewritten in the form

$$l^\mu = e^{-2b}\delta^\mu_1, \quad n^\mu = \delta^\mu_0 - \tfrac{1}{2}W\delta^\mu_1,$$
$$m^\mu = \frac{1}{\bar{r}\sqrt{2}}(\delta^\mu_2 + i\cos\theta\delta^\mu_3)$$

with

$$e^{2b} = \frac{A - B\left(1 - \dfrac{r^2+\bar{r}^2}{2R^2}\right)^{1/2}}{\left(1 - \dfrac{r^2+\bar{r}^2}{2R^2}\right)^{1/2}},$$
$$W = \left(1 - \frac{r^2+\bar{r}^2}{2R^2}\right)^{1/2}\left[A - B\left(1 - \frac{r^2+\bar{r}^2}{2R^2}\right)^{1/2}\right].$$

Performing the complex transformation

$$r' = r + ia\cos\theta, \quad \theta' = \theta,$$
$$u' = u - ia\cos\theta, \quad \phi' = \phi,$$

one is led to (dropping primes)

$$l^\mu = e^{-2b}\delta^\mu_1 = (X/Y)\delta^\mu_1,$$
$$n^\mu = \delta^\mu_0 - \tfrac{1}{2}XY\delta^\mu_1, \tag{4}$$
$$m^\mu = \frac{1}{\sqrt{2}(r + ia\cos\theta)} \times [ia\sin\theta(\delta^\mu_0 - \delta^\mu_1) + \delta^\mu_2 + i\csc\theta\delta^\mu_3]$$

and

$$l_\mu = \delta^0_\mu - a\sin^2\theta\delta^3_\mu, \tag{4'}$$
$$n_\mu = \frac{Y^2}{2}\delta^\mu_0 + \frac{Y}{X}\delta^1_\mu + a\sin^2\theta\left(\frac{Y}{X} - \frac{Y^2}{2}\right)\delta^3_\mu,$$
$$m_\mu = -\frac{(r - ia\cos\theta)}{\sqrt{2}}(\delta^2_\mu + i\sin\theta\delta^3_\mu),$$

where

$$X \equiv \left(1 - \frac{r^2 - a^2\cos^2\theta}{R^2}\right)^{1/2},$$
$$Y \equiv A - BX$$

(note that A, B, and R are now functions of r and θ). We shall assume that a is a function of r, such that $a(r) \equiv a, da(r)/dr = 0$ at the surface, and $a(r=0) = 0$. This freedom (letting a be a function) will be very helpful to avoid the presence of singularities at the center ($r = 0$). Thus, the metric is

$$ds^2 = Y^2\,du^2 + 2(Y/X)\,du\,dr + 2a\sin^2\theta(Y/X - Y^2)\,du\,d\phi - 2a\sin^2\theta(Y/X)\,dr\,d\phi - (r^2 + a^2\cos^2\theta)\,d\theta^2 - [(r^2 + a^2\cos^2\theta)\sin^2\theta + 2a^2\sin^4\theta(Y/X - Y^2/2)]\,d\phi^2. \tag{5}$$

Now, the spin coefficients, the scalars corresponding to the traceless Ricci tensor, the curvature scalars, and the components of the energy–momentum tensor can be obtained[8,9] (see Appendix A).

IV. THE BOUNDARY CONDITIONS

In order to consider the energy–momentum tensor given by (A9) as a source of the Kerr metric, we should be able, on one hand, to match the metric (5) with the Kerr metric on the boundary of the source, and on the other hand, to satisfy certain physical requirements (e.g., that the energy density be nonnegative, that the stresses be not too large compared to the energy density, etc.).

In this section we shall concentrate on the problem of matching the metric (5) to the Kerr metric. With this aim, let us start by choosing the equation of the boundary separating the interior and the exterior solutions. We shall choose as the equation of the boundary

$$r = r_1 = \text{const.} \tag{6}$$

We make this choice both by simplicity and because in the coordinate system we are working with, Eq. (6) defines an oblate spheroid (at least in the weak field approximation). Oblatness, is of course an expected property of a rotating axially symmetric body. To see this, consider the flat space limit of the metric (5).

$$ds^2 = du^2 + 2\,du\,dr - 2a\sin^2\theta\,dr\,d\phi - (r^2 + a^2\cos^2\theta)\,d\theta^2 - (r^2 + a^2)\sin^2\theta\,d\phi^2. \tag{7}$$

Expression (7) can be transformed to the Minkowskian line element in Cartesian coordinates by means of the transformation

$$t = u + r,$$
$$x = (r\cos\phi + a\sin\phi)\sin\theta,$$
$$y = (r\sin\phi - a\cos\phi)\sin\theta, \tag{8}$$
$$z = r\cos\theta.$$

Now it is easy to see from (8) that

$$\frac{x^2}{r^2 + a^2} + \frac{y^2}{r^2 + a^2} + \frac{z^2}{r^2} = 1. \tag{9}$$

For each value of $r = \text{const}$, Eq. (8) defines an oblate sphere.

Next, in order to guarantee that the Lichnerowicz boundary conditions[10] hold in some coordinate system, it is sufficient to require that the first fundamental form

$$I = (g_{\mu\nu}dx^{\mu}dx^{\nu})_{r=r_1} \tag{10}$$

and the second fundamental form

$$II = (-n_{\mu;\nu}dx^{\mu}dx^{\nu})_{r=r_1} \tag{11}$$

(where n_{μ} is the unit vector normal to the boundary), be continuous across the boundary. We start with condition (10), which implies (in Appendix B we give the line element and the spin coefficients for the exterior Kerr metric in the coordinate system we are working with)

$$e^{2b}|_{r=r_1} = 1 \tag{12}$$

and

$$W|_{r=r_1} = \left[1 - \frac{2Mr}{r^2 + a^2\cos^2}\right]_{r=r_1}. \tag{13}$$

Equations (12) and (13) are equivalent to

$$\left[\frac{A - B(1 - (r^2 - a^2\cos^2\theta)/R^2)^{1/2}}{(1 - (r^2 - a^2\cos^2\theta)/R^2)^{1/2}}\right]_{r=r_1} = 1 \tag{14}$$

and

$$\left[\frac{r^2 - a^2\cos^2\theta}{R^2}\right]_{r=r_1} = \left[\frac{2Mr}{r^2 + a^2\cos^2\theta}\right]_{r=r_1}. \tag{15}$$

Finally (14) and (15) can be combined, to give

$$(r^4 - a^4\cos^4\theta)_{r=r_1} = (2MrR^2)_{r=r_1} \tag{16}$$

and

$$\left[\frac{2Mr}{r^2 + a^2\cos^2\theta}\right]_{r=r_1} = 1 - \left(\frac{A}{1+B}\right)^2_{r=r_1}. \tag{17}$$

Next, instead of (11) we shall satisfy a more stringent condition, namely, all the spin coefficients are continuous across the surface $r = r_1$ (it is not difficult to convince oneself that the latter condition implies (11). It can be seen very easily that in this particular example both conditions are equivalent.

Now, the continuity of τ, which guarantees the continuity of λ, α, β, and π, implies, using (12), (7) and (B2), (B3),

$$(X_2)_{r=r_1} = (Y_2)_{r=r_1}, \tag{18}$$

$$(X_1)_{r=r_1} = (Y_1)_{r=r_1}, \tag{19}$$

and the continuity of ν leads, together with (18) and (19) to

$$(R_2)_{r=r_1} = \left(\frac{a^4\cos^3\theta\sin\theta}{Rmr}\right)_{r=r_1}, \tag{20}$$

$$(R_1)_{r=r_1} = \left(\frac{3r^4 + a^4\cos^2\theta}{4mr^2R}\right)_{r=r_1}. \tag{21}$$

Finally, the continuity of γ is assured if (12), (13) and (18), (19) are satisfied.

V. AN EXAMPLE OF AN INTERIOR SOLUTION

We shall now give an example which satisfies the boundary conditions and whose energy density is everywhere positive for, at least, small values of the parameter a.[11]

Let us take

$$X = \left[1 - \frac{2Mr\sin^2\beta r}{r^2 + a^2\cos^2\theta + \sigma(r - r_1)^2 r}\right]^{1/2}, \tag{22}$$

$$Y = X + \frac{\gamma r\cos^2\beta r}{r^2 + a^2\cos^2\theta + \frac{1}{2}\sigma(r - r_1)^2 r}, \tag{23}$$

where

$$\sigma \equiv \frac{1}{r_1}, \quad \beta \equiv \frac{\pi}{2r_1},$$

$r = r_1$ defines the boundary of the source. The constant γ is arbitrary, and its value can be chosen so that the stresses vanish at the surface of the sphere. However, with this choice of γ, the stresses will be larger than the energy density inside the sphere. For this specific example it was impossible for the authors to find a γ such that both conditions (vanishing of the stresses at the surface and the energy density larger than the stresses inside) are satisfied.

It is very easy to check that all the boundary conditions are satisfied. In fact, (22) and (23) imply

$$B = -1, \quad A = \frac{r\cos^2\beta r}{r^2 + a^2\cos^2\theta + \frac{1}{2}\sigma(r - r_1)^2 r},$$

$$R^2 = \frac{(r^2 - a^2\cos^2\theta)[r^2 + a^2\cos^2\theta + (r - r_1)^2 r]}{2Mr\sin^2\beta r}.$$

And, a trivial calculation leads to conditions (16)–(21). Please, note that since $B + 1 = 0$, condition (17) should be written as

$$\left[1 - \frac{2Mr}{r^2 + a^2\cos^2\theta}\right]_{r=r_1}(1 + B)^2 = (A^2)_{r=r_1},$$

which is obviously true since $(A)_{r=r_1} = 0$.

Next, let us consider for a moment the nonrotating limit (spherical symmetric limit) of our metric (e.g., take $a = 0$).

In our coordinate system (see Ref. 12),

$$T_{00} = Y^2\rho, \tag{24}$$

where ρ is the energy density of the matter distribution, and from (A9),

$$T_{00} = 2\{\phi_{22} + \tfrac{1}{4}Y^4\phi_{00} + Y^2(\phi_{11} + 3\Lambda)\}. \tag{25}$$

Using (A2)–(A8) in (25) and comparing with (24) we get

$$\rho = \left(\frac{1 - X^2}{r^2} - \frac{2XX_1}{r}\right). \tag{26}$$

Next, using (22),

$$\rho = \frac{2M\sin^2\beta r}{r^2[r + \sigma(r - r_1)^2]}\left[1 - \frac{r}{r + \sigma(r - r_1)^2}\right] + \frac{4M\beta\sin\beta r\cos\beta r}{[r + \sigma(r - r_1)^2]r} + \frac{4M\sigma\sin^2\beta r(r_1 - r)}{r[r + \sigma(r - r_1)^2]^2}. \tag{27}$$

It is evident, that in the interval $0 \leqslant r \leqslant r_1$, the density ρ is positive. Thus, at least for small values of the parameter a the correct sign of the energy density is guaranteed.

In the same way we can obtain expressions for the radial and the tangential stresses (they are in general different).

Thus we get

$$P = \frac{2X^2}{r}\left(\frac{Y_1}{Y}\right) - \left(\frac{1 - X^2}{r^2}\right) \tag{28}$$

for the radial pressure, and

$$P_{\perp} = \frac{X}{Y}\left(X_1 Y_1 + XY_{11} + \frac{X_1 Y + XY_1}{r}\right) \tag{29}$$

for the tangential stresses. Both expressions, as well as the expression for the energy density are singularity-free in the region $0 \leqslant r \leqslant r_1$.

VI. CONCLUSIONS

We have seen so far that the metric (5) can be matched to the exterior Kerr metric provided the functions X and Y are chosen so as to satisfy the conditions (16)–(21).

Furthermore, the example given in Sec. V shows that a model with positive energy density is conceivable in the context of the method outlined above.

We realize of course that the example presented is still quite imperfect to be considered as "the interior Kerr metric." However, it is worthwhile to note that with a rather simple example [Eqs. (22) and (23)], the boundary conditions and the positiveness of the energy density are fulfilled. These resuls lead us to think that the application of the Newman–Janis procedure has some chances to be "the way" to the construction of a source for the Kerr metric.

It could be properly objected that the problem of the analyticity of the metric functions and the singular structure of the source have not been carefully analyzed. As a matter of fact the absence of singularities in the limit $a = 0$ does not say anything about the general $a \neq 0$ case. Concerning this point we just introduce, the function $a = a(r)$ such that in the flat space the equation $r = 0$ describes the origin in 3-space and not a disk, across which the coordinate θ will be discontinuous or multiple valued. [See Eq. (8).]

Since in our present example it is inconvenient that the interior stresses exceed the energy density, we did not present a careful analysis of this point.

It goes without saying that such analysis should be present in any attempt to construct a source for the Kerr metric.

Finally, a remark can be made which sheds some light on the nature of the source presented above. In the limit $a \to 0$, the expression for the energy–momentum tensor does not reduce to that of a perfect fluid. This result suggests that the stresses appearing in the source during the rotation do not vanish completely when the rotation stops. And the remaining object is a "solid" sphere in the limit $a \to 0$.

ACKNOWLEDGMENT

It is a pleasure to thank L. Witten for helpful discussions.

APPENDIX A

For the spin coefficients we get

$$\kappa = 0, \quad \rho = -\frac{r(X/Y) + ia\cos\theta}{(r^2 + a^2\cos^2\theta)}, \quad \lambda = 0,$$

$$\sigma = 0, \quad \tau = \frac{(X/Y)}{2\sqrt{2}(r + ia\cos\theta)} \times \left[\frac{ia\sin\theta(XY_1 - X_1Y) + (X_2Y - XY_2)}{X^2}\right],$$

$$\alpha = \frac{\bar{\tau}}{2} - \frac{\cot\theta}{2\sqrt{2}(r - ia\cos\theta)},$$

$$\beta = \frac{\tau}{2} + \frac{\cot\theta}{2\sqrt{2}(r + ia\cos\theta)}, \tag{A1}$$

$$\epsilon = \frac{ia\cos\theta}{2(r^2 + a^2\cos^2\theta)}\left(\frac{X}{Y} - 1\right), \quad \pi = -\bar{\tau},$$

$$\mu = \frac{XY}{2(r^2 + a^2\cos^2\theta)}\left[-r + ia\cos\theta\frac{Y}{X}\left(\frac{2}{XY} - 1\right)\right],$$

$$\gamma = \frac{XY}{2} + \frac{ia\cos\theta Y^2}{4(r^2 + a^2\cos^2\theta)}\left[\frac{2}{XY} - \frac{X}{Y} - 1\right],$$

$$\nu = \frac{Y}{\sqrt{2}(r - ia\cos\theta)}(ia\sin\theta Y_1 + Y_2) + Y^2\bar{\tau},$$

where the subscripts 1,2 indicate derivatives with respect to r and θ, respectively. Finally, the scalars corresponding to the traceless Ricci tensor and the curvature scalar are found from the Einstein equations (the notation is the same as in Ref. 8).

$$\Phi_{00} = D\rho - \bar{\delta}\kappa - (\rho^2 + \sigma\bar{\sigma}) - (\epsilon + \bar{\epsilon})\rho + \kappa\tau + \kappa(3\alpha + \bar{\beta} - \bar{\pi}) = D\rho - \rho^2$$

$$= \frac{r^2(X/Y)^2 + a^2\cos^2\theta}{(r^2 + a^2\cos^2\theta)^2} - \frac{(X/Y)^2}{(r^2 + a^2\cos^2\theta)}\left[1 + \frac{r(X_1Y - XY_1)}{XY}\right], \tag{A2}$$

$$\Phi_{10} = D\alpha - \bar{\delta}\epsilon - (\rho + \bar{\epsilon} - 2\epsilon)\alpha - \beta\bar{\sigma} + \beta\epsilon + \kappa\lambda + \bar{\kappa}\gamma - (\epsilon + \rho)\pi = D\alpha - \bar{\delta}\epsilon - (\rho + \bar{\epsilon} - 2\epsilon)\alpha + \bar{\beta}\epsilon - (\epsilon + \rho)\pi$$

$$= \frac{ia\sin\theta(X_{11}Y - XY_{11}) + (X_{21}Y - XY_{21} + X_2Y_1 - X_1Y_2)}{4\sqrt{2}(r - ia\cos\theta)Y^2} + \frac{ia\sin\theta(X_1Y - XY_1)^2 + (X_2Y - XY_2)(X_1Y - XY_1)}{4\sqrt{2}(r - ia\cos\theta)XY^3}$$

$$- \frac{ia\sin\theta(X_1Y - XY_1) + (X_2Y - XY_2)X_1}{2\sqrt{2}(r - ia\cos\theta)XY^2} - \frac{ia\sin\theta(X_1Y - XY_1) + (X_2Y - XY_2)}{4\sqrt{2}(r - ia\cos\theta)^2Y^2}$$

$$- ia\cos\theta\frac{[ia\sin\theta(X_1Y - XY_1) + (X_2Y - XY_2)]}{2\sqrt{2}(r - ia\cos\theta)(r^2 + a^2\cos^2\theta)Y^2} - \frac{[ia\sin\theta(X_1Y - XY_1) + (X_2Y - XY_2)]}{4\sqrt{2}(r - ia\cos\theta)(r^2 + a^2\cos^2\theta)XY}$$

$$\times\left[\left(\frac{X}{Y}\right)(r - 3ia\cos\theta) + 4ia\cos\theta\right] - \frac{ia\cos\theta\sin\theta}{2\sqrt{2}(r - ia\cos\theta)}\left(\frac{X}{Y} - 1\right)\frac{[a^2\cos^2\theta - r(r + ia\cos\theta)]}{(r^2 + a^2\cos^2\theta)^2}, \tag{A3}$$

$$\Phi_{20} = D\lambda - \bar{\delta}\pi - (\rho\lambda + \bar{\sigma}\mu) - \pi^2 - (\alpha - \bar{\beta})\pi - \nu\bar{\kappa} + (3\epsilon - \bar{\epsilon})\lambda = -\bar{\delta}\pi - \pi^2 - (\alpha - \bar{\beta})\pi = \bar{\delta}\bar{\tau} - \tau^2$$
$$- \frac{\cot\theta}{\sqrt{2}(r - ia\cos\theta)}\bar{\tau} = \frac{1}{\sqrt{2}(r - ia\cos\theta)} \times \left\{ \frac{ia\sin\theta}{2\sqrt{2}(r - ia\cos\theta)} \left[ia\sin\theta \left(\frac{X_{11}}{X} - \frac{Y_{11}}{Y} - \frac{X_1^2}{X^2} + \frac{Y_1^2}{Y} \right) \right.\right.$$
$$\left. + 2\left(\frac{X_{21}}{X} - \frac{Y_{21}}{Y} - \frac{X_2 X_1}{X^2} + \frac{Y_2 Y_1}{Y^2} \right)\right] + \frac{1}{2\sqrt{2}(r - ia\cos\theta)} \left(\frac{X_{22}}{X} - \frac{Y_{22}}{Y} - \frac{X_2^2}{X^2} + \frac{Y_2^2}{Y^2} \right)$$
$$- \frac{\cot\theta}{2\sqrt{2}(r - ia\cos\theta)} \left(\frac{X_2}{X} - \frac{Y_2}{Y} \right) - \frac{ia\sin\theta}{\sqrt{2}(r - ia\cos\theta)^2} \times \left[ia\sin\theta \left(\frac{X_1}{X} - \frac{Y_1}{Y} \right) + \left(\frac{X_2}{X} - \frac{Y_2}{Y} \right) \right] \Bigg\}$$
$$- \left\{ \frac{1}{2\sqrt{2}(r - ia\cos\theta)} \left| ia\sin\theta \left(\frac{X_1}{X} - \frac{Y_1}{Y} \right) + \left(\frac{X_2}{X} - \frac{Y_2}{Y} \right) \right| \right\}^2, \tag{A4}$$

$$\Phi_{22} = \delta\nu - \Delta\mu - \mu^2 - \mu(\gamma + \bar{\gamma}) + \bar{\nu}\pi - (\tau - 3\beta - \bar{\alpha})\nu = \frac{1}{4(r^2 + a^2\cos^2\theta)}$$
$$\times \frac{2Y}{X}(X_2 Y_2 + a^2\sin^2\theta X_1 Y_1) + Y_2^2 + a^2\sin^2\theta Y_1^2 + Y^2 \left[\left(\frac{X_{22}}{X} + \frac{Y_{22}}{Y} \right) + a^2\sin^2\theta \left(\frac{X_{11}}{X} + \frac{Y_{11}}{Y} \right) \right]$$
$$- \frac{Y^2}{X^2}(X_2^2 + a^2\sin^2\theta X_1^2) \Bigg\} + \frac{XY}{4(r^2 + a^2\cos^2\theta)} \left[XY \left(\frac{r^2 - a^2\cos^2\theta}{r^2 + a^2\cos^2\theta} \right) - r(X_1 Y + XY_1) \right]$$
$$+ \frac{XYr(XY_1)}{(r^2 + a^2\cos^2\theta)} - \frac{X^2 Y^2}{4(r^2 + a^2\cos^2\theta)^2} \left[r^2 - a^2\cos^2\theta \frac{Y^2}{X^2} \left(\frac{2}{XY} - 1 \right)^2 \right]$$
$$+ \frac{\cot\theta}{4(r^2 + a^2\cos^2\theta)} \left(\frac{Y}{X} \right)(X_2 Y + XY_2), \tag{A5}$$

$$\Phi_{11} = \tfrac{1}{2}\{D\gamma - \Delta\epsilon + \delta\alpha - \bar{\delta}\beta - (\tau + \bar{\pi})\alpha - (\bar{\tau} + \pi)\beta + (\epsilon + \bar{\epsilon})\gamma + \epsilon(\gamma + \bar{\gamma}) - \tau\pi - \nu\kappa - (\mu\rho - \lambda\sigma) - \alpha\bar{\alpha} - \beta\bar{\beta} + 2\alpha\beta$$
$$- \gamma(\rho - \bar{\rho}) - \epsilon(\mu - \bar{\mu})\} = \frac{1}{2}\left(\frac{X}{Y} \right)(X_1 Y_1 + XY_{11}) + \frac{\csc^2\theta}{4(r^2 + a^2\cos^2\theta)} + \frac{1}{16(r^2 + a^2\cos^2\theta)}$$
$$\times \left[\left(\frac{X_2}{X} - \frac{Y_2}{Y} \right)^2 + a^2\sin^2\theta \left(\frac{X_1}{X} - \frac{Y_1}{Y} \right)^2 \right] - \frac{XY}{4(r^2 + a^2\cos^2\theta)^2}$$
$$\times \left[r^2 \left(\frac{X}{Y} \right) + 3a^2\cos^2\theta \frac{Y}{X} \left(\frac{2}{XY} - 1 \right) \right] + \frac{a^2\cos^2\theta}{2(r^2 + a^2\cos^2\theta)^2}, \tag{A6}$$

$$\Phi_{12} = \delta\gamma - \Delta\beta + (\bar{\alpha} + \beta - \tau)\gamma - \mu\tau + \sigma\nu + \epsilon\bar{\nu} + \beta(\gamma - \bar{\gamma} - \mu) - \alpha\bar{\lambda} = \delta\gamma - \Delta\beta - \mu\tau + \epsilon\bar{\nu} + \frac{\beta XY}{2(r + ia\cos\theta)}$$
$$= \frac{(X_2 - ia\sin\theta X_1)Y_1 + (Y_{12} - ia\sin\theta Y_{11})X}{\sqrt{2}(r + ia\cos\theta)} + \frac{\left(\frac{2}{XY} - \frac{X}{Y} - 1 \right)}{2\sqrt{2}(r + ia\cos\theta)(r^2 + a^2\cos^2\theta)}$$
$$\times \left\{ a^2\sin\theta\cos\theta Y \left[Y_1 - \frac{Yr}{(r^2 + a^2\cos^2\theta)} \right] + ia\cos\theta \left[YY_2 + \frac{Y^2\tan\theta(a^2\cos^2\theta - r^2)}{2(r^2 + a^2\cos^2\theta)} \right] \right\}$$
$$+ \frac{ia\cos\theta}{4(r^2 + a^2\cos^2\theta)} \left\{ \left(1 - \frac{2}{X^2} \right)(XY_2 - X_2 Y) - ia\sin\theta \left[\left(1 - \frac{2}{X^2} \right)XY_1 + \left(1 + \frac{2}{X^2} \right)X_1 Y \right] \right\}$$
$$+ \frac{XY}{8\sqrt{2}(r + ia\cos\theta)} \left[\left(\frac{X_{21}}{X} - \frac{Y_{21}}{Y} \right) - \left(\frac{X_2 X_1}{X^2} - \frac{Y_2 Y_1}{Y^2} \right) - ia\sin\theta \left(\frac{X_{11}}{X} - \frac{Y_{11}}{Y} - \frac{X_1^2}{X^2} + \frac{Y_1^2}{Y^2} \right) \right]$$
$$+ \frac{XY}{4\sqrt{2}(r^2 + a^2\cos^2\theta)(r + ia\cos\theta)} \left\{ \left[r - ia\cos\theta \frac{Y}{X} \left(\frac{2}{XY} - 1 \right) \right] \right.$$
$$\times \left[\left(\frac{X_2}{X} - \frac{Y_2}{Y} \right) - ia\sin\theta \left(\frac{X_1}{X} - \frac{Y_1}{Y} \right) \right] + ia\cos\theta \left(1 - \frac{Y}{X} \right)$$
$$\left. \times \left[\left(\frac{X_2}{X} + \frac{Y_2}{Y} \right) - ia\sin\theta \left(\frac{X_1}{X} + \frac{Y_1}{Y} \right) \right] \right\}, \tag{A7}$$

$$\Lambda = \frac{1}{3}\{D\mu - \delta\pi - \delta\alpha - \bar{\delta}\beta - \mu(\rho + \bar{\rho}) - \gamma(\rho - \bar{\rho}) + \pi(\bar{\alpha} - \beta) + \nu\kappa + \bar{\epsilon}\mu + \epsilon\bar{\mu} - \alpha\bar{\alpha} - \beta\bar{\beta} - \pi\bar{\pi} - 2\alpha\beta - \Phi_{11}\}$$
$$= \frac{1}{3}\left\{ \frac{1}{4(r^2 + a^2\cos^2\theta)} \left[\left(\frac{X_{22}}{X} - \frac{Y_{22}}{Y} - \frac{X_2^2}{X^2} - \frac{Y_2^2}{Y^2} \right) + a^2\sin^2\theta \left(\frac{X_{11}}{X} - \frac{Y_{11}}{Y} - \frac{X_1^2}{X^2} - \frac{Y_1^2}{Y^2} \right) \right.\right.$$
$$+ \cot\theta \left(\frac{X_2}{X} - \frac{Y_2}{Y} \right) - \frac{1}{4}\left(\left(\frac{X_2}{X} - \frac{Y_2}{Y} \right)^2 + a^2\sin^2\theta \left(\frac{X_1}{X} - \frac{Y_1}{Y} \right)^2 \right) + \frac{a^2\cos^2\theta}{(r^2 + a^2\cos^2\theta)} Y^2 \left(\left(\frac{2}{XY} - 1 \right) \right.$$
$$\left. \times \left(2 - \frac{X}{Y} \right) - \frac{X}{Y} \right) + \frac{2XY}{(r^2 + a^2\cos^2\theta)} \left(- \frac{r^2 X}{Y} \right) + a^2\cos^2\theta \left(\frac{2}{XY} - 1 \right) \left(1 - \frac{Y}{2X} \right) + 1 \Bigg]$$
$$\left. - \frac{X}{2Y} \left[X_1 Y_1 + XY_{11} + \frac{r(X_1 Y + XY_1)}{(r^2 + a^2\cos^2\theta)} - XY \frac{(r^2 - a^2\cos^2\theta)}{(r^2 + a^2\cos^2\theta)^2} \right] \right\}, \tag{A8}$$

with

$$D=\frac{X}{Y}\partial_1,\quad \Delta=-\frac{XY}{2}\partial_1,\quad \delta=\frac{1}{\sqrt{2}(r+ia\cos\theta)}(\partial_2-ia\sin\theta\partial_1).$$

In terms of (A2)–(A8), the energy–momentum tensor of the source is

$$\begin{aligned}
T_{\mu\nu} &= 2\Phi_{22}l_\mu l_\nu+2\Phi_{00}n_\mu n_\nu+2\Phi_{20}m_\mu m_\nu+2\bar{\Phi}_{20}\bar{m}_\mu\bar{m}_\nu+4\Phi_{11}[\,l_{(\mu}n_{\nu)}+m_{(\mu}\bar{m}_{\nu)}\,]\\
&\quad-4\Phi_{21}l_{(\mu}m_{\nu)}-4\bar{\Phi}_{21}l_{(\mu}\bar{m}_{\nu)}-4\Phi_{10}n_{(\mu}m_{\nu)}-4\bar{\Phi}_{10}n_{(\mu}\bar{m}_{\nu)}+12\Lambda\,[\,l_{(\mu}n_{\nu)}-m_{(\mu}\bar{m}_{\nu)}\,]\\
&=2\left[\Phi_{22}+\frac{Y^4}{4}\Phi_{00}+Y^2(\Phi_{11}+3\Lambda)\right]\delta^0_\mu\delta^0_\nu+\left[\frac{Y^3}{X}\Phi_{00}+\frac{2Y}{X}(\Phi_{11}+3\Lambda)\right]\delta^0_\mu\delta^1_\nu\\
&\quad+\sqrt{2}\,\mathrm{Re}\{(r+ia\cos\theta)(2\Phi_{12}+Y^2\bar{\Phi}_{10})\}\,\delta^0_\mu\delta^2_\nu+2\left\{\frac{a\sin^2\theta Y^4}{4}\left(\frac{2}{XY}-1\right)\Phi_{00}-a\sin^2\theta\Phi_{22}\right.\\
&\quad\left.+\sqrt{2}\,\mathrm{Im}[\sin\theta(r+ia\cos\theta)\Phi_{12}]-\frac{Y^2}{\sqrt{2}}\mathrm{Im}[(r-ia\cos\theta)\sin\theta\Phi_{10}]+a\sin^2\theta Y^2\left(\frac{1}{XY}-1\right)(\Phi_{11}+3\Lambda)\right\}\delta^0_\mu\delta^3_\nu\\
&\quad+2\left(\frac{Y}{X}\right)^2\Phi_{00}\delta^1_\mu\delta^1_\nu+2\sqrt{2}\,\frac{Y}{X}\mathrm{Re}[\Phi_{10}(r-ia\cos\theta)]\delta^1_\mu\delta^2_\nu\\
&\quad+\frac{2Y}{X}\left\{\left(\frac{2}{XY}-1\right)\frac{Y^2}{2}\Phi_{00}-\sqrt{2}\sin\theta\,\mathrm{Im}[(r-ia\sin\theta)\Phi_{10}]-a\sin^2\theta(\Phi_{11}+3\Lambda)\right\}\delta^1_\mu\delta^3_\nu\\
&\quad+\{2\,\mathrm{Re}[\Phi_{20}(r-ia\cos\theta)^2]+2(r^2+a^+\cos^2\theta)(\Phi_{11}-3\Lambda)\}\,\delta^2_\mu\delta^2_\nu\\
&\quad+\left\{2\sin\theta\,\mathrm{Im}[\Phi_{20}(r+ia\cos\theta)^2]-2\sqrt{2}a\sin^2\theta\,\mathrm{Re}[\Phi_{21}(r-ia\cos\theta)]+\sqrt{2}a\sin^2\theta Y^2\right.\\
&\quad\left.\times\left(\frac{2}{XY}-1\right)\mathrm{Re}[\Phi_{10}(r-ia\cos\theta)]\right\}\delta^2_\mu\delta^3_\nu+\{2a^2\sin^4\theta\Phi_{22}\\
&\quad+\frac{a^2\sin^4\theta}{2}Y^4\left(\frac{2}{XY}-1\right)^2\Phi_{00}-2\,\mathrm{Re}[\Phi_{20}\sin^2\theta(r-ia\cos\theta)^2]+4\sqrt{2}a\sin^3\theta\,\mathrm{Im}[(r-ia\cos\theta)\Phi_{21}]\\
&\quad-2\sqrt{2}a\sin^3\theta Y^2\left(\frac{2}{XY}-1\right)\mathrm{Im}[\Phi_{10}(r-ia\cos\theta)]-2a^2\sin^4\theta Y^2\left(\frac{2}{XY}-1\right)\\
&\quad\times(\Phi_{11}+3\Lambda)+2\sin^2\theta(r^2+a^2\cos^2\theta)(\Phi_{11}-3\Lambda)\Big\}\delta^3_\mu\delta^3_\nu. \qquad \text{(A9)}
\end{aligned}$$

APPENDIX B

In the coordinate system we are working with, the exterior Kerr metric is given by

$$\begin{aligned}
ds^2&=\left(1-\frac{2Mr}{r^2+a^2\cos^2\theta}\right)du^2\\
&\quad+2\,du\,dr+\frac{4a\sin^2\theta Mr}{r^2+a^2\cos^2\theta}du\,d\phi\\
&\quad-2a\sin^2\theta\,dr\,d\phi-(r^2+a^2\cos^2\theta)\,d\theta^2\\
&\quad-\left[(r^2+a^2\cos^2\theta)\sin^2\theta+2a^2\sin^4\theta\right.\\
&\quad\left.\times\left(\frac{1}{2}+\frac{Mr}{r^2+a^2\cos^2\theta}\right)\right]d\phi^2, \qquad \text{(B1)}
\end{aligned}$$

and for the corresponding spin coefficients one has

$$\begin{aligned}
&\kappa'=\nu'=\sigma'=\lambda'=\epsilon'=0,\\
&\rho'=-(r-ia\cos\theta)^{-1},\\
&\tau'=-ia\sin\theta\rho\bar{\rho}/\sqrt{2},\\
&\pi'=ia\sin\theta\rho^2/\sqrt{2}, \qquad \text{(B2)}\\
&\beta'=-\cot\theta\bar{\rho}/2\sqrt{2},\\
&\alpha'=\pi'-\beta',\\
&\mu'=(r^2+a^2-2Mr)\rho^2\bar{\rho}/2,\\
&\gamma'=\mu'+(r-M)\rho\bar{\rho}/2,
\end{aligned}$$

where the primes indicate that these spin coefficients have been calculated with a tetrad field obtained from (1) by means of a null rotation about the vector l_μ,

$$g_1(z)=\begin{pmatrix}1&0\\z&1\end{pmatrix},$$

with

$$z=(ia\rho'\sin\theta)/\sqrt{2}.$$

The relationship between the two sets of spin coefficients is[13]

$$\begin{aligned}
&\rho'=\rho+z\kappa,\\
&\alpha'=\alpha+z(\rho+\epsilon)+z^2\kappa,\\
&\lambda'=\lambda+z(\pi+2\alpha)+z^2(\rho+2\epsilon)+z^3\kappa+\bar{\delta}z+zDz,\\
&\kappa'=\kappa,\\
&\epsilon'=\epsilon+z\kappa,\\
&\pi'=\pi+2z\epsilon+z^2\kappa+Dz,\\
&\sigma'=\sigma+\bar{z}\kappa,\\
&\beta'=\beta+z\sigma+\bar{z}\epsilon+z\bar{z}\kappa, \qquad \text{(B3)}\\
&\mu'=\mu+2z\beta+\bar{z}\pi+z^2\sigma+2z\bar{z}\epsilon+z^2\bar{z}\kappa+\delta z+\bar{z}Dz,\\
&\tau'=\tau+z\sigma+\bar{z}\rho+z\bar{z}\kappa,\\
&\gamma'=\gamma+z(\tau+\beta)+\bar{z}\alpha+z^2\sigma+z\bar{z}(\rho+\epsilon)+z^2\bar{z}\kappa,\\
&\nu'=\nu+z(\mu+2\gamma)+\bar{z}\lambda+z^2(2\beta+\tau)+z\bar{z}(2\alpha+\pi)\\
&\qquad+z^2\bar{z}(2\epsilon+\rho)+z^3\sigma+z^3\bar{z}\kappa+\Delta z+z\delta z+\overline{z\delta z}\\
&\qquad+z\bar{z}Dz.
\end{aligned}$$

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Geodesic deviation and first integrals of motion

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(Received 27 April 1982; accepted for publication 25 June 1982)

Generalized Killing tensors (GKT) and generalized conformal Killing tensors (GCKT) are defined as the class of totally symmetric tensor fields that generate solutions of a suitable inhomogeneous equation of geodesic deviation along arbitrary and null geodesics, respectively. A geometric interpretation of these fields as generators of Jacobi fields along arbitrary and null geodesics is also given. It is shown that well known fields such as Killing tensors, conformal Killing tensors, and geodesic collineations belong to the above classes. Finally, first integrals of geodesic motion concomitant with the existence of GKT's and GCKT's are determined.

PACS numbers: 02.40.Ky, 04.20.Me

1. INTRODUCTION

The knowledge of the geodesics in a given space–time manifold is of great interest in general relativity. In addition to the fundamental property of yielding the paths of freely falling particles, they are also involved, for instance, both in the determination of singular points and in the description of the global behavior of the given metric.[1,2]

The problem of solving the equation of the geodesics is considerably simplified when one knows first integrals (FI) of motion.[2,3] A remarkable class of such FI's, that may be written in the form of homogeneous polynomials in the tangent vector to the geodesic, in concomitant with the existence of Killing vectors (KV), Killing tensors (KT), and conformal Killing tensors (CKT).[2] In general, it follows that in principle there exists a whole class of such generators of FI's, but unfortunately this class is often empty, unless severe restrictions on the geometry are satisfied.[4]

To find a way out of these limitations, there have been attempts to extend the class of generators of FI's of motion. For instance, enlarged notions of symmetry related to the existence of projective collineations (PC) and homothetic motions (HM) have been used by various authors to derive additional FI's, provided that the manifold admits at least one generator of homogeneous polynomial FI's.[5–7] Following a different approach, Katzin and Levine have found necessary and sufficient conditions for the existence of geodesic FI's which are mth-order polynomials in the tangent vector and are assumed to depend explicitly on the path parameter.[8]

The aim of this paper is to present an alternative procedure leading to an extension of the concept of generator of FI's of geodesic motion. Our investigation is based on the following result. If $K_{a_1\cdots a_p}$ is a KT of order p and t^a is the tangent vector to an affinely parametrized geodesic γ, then the vector

$$X^a = K^a{}_{a_2\cdots a_p} t^{a_2}\cdots t^{a_p} \tag{1.1}$$

is a solution of the equation of geodesic deviation (egd) along γ.[9] Accordingly, we introduce the concept of GKT as a totally symmetric tensor field yielding solutions X^a of a suitably extended egd, through Eq. (1.1). The case of null geodesics is also examined in detail, leading to the definition of GCKT.

A geometric interpretation of GKT's (GCKT's) as generators of Jacobi fields (J fields) along arbitrary (null) geodesics is also given.

Morevoer, it is shown that already well known fields, such as KV's, KT's, and PC's, belong to the class of GKT's. In a similar way, it is proved that CKT's and conformal collineations (ConfC) satisfy the definition of GCKT.

In Sec. 3, we focus our attention on the determination of FI's of motion concomitant with the existence of GKT's (GCKT's). In this respect, we find sufficient conditions for the existence of FI's of motion related to a single GKT (GCKT). The connections with the above quoted recent results of Katzin and Levine are also briefly discussed.

In the last part of Sec. 3 we investigate the case when a pair of GKT's (GCKT's), say H and K, are given. We show that H, K and their covariant derivatives may always be combined to identify FI's of motion along arbitrary (null) geodesics. In turns out that this approach yields an extension of previously known procedures for deriving FI's of geodesics motion. Namely, it will be shown that our analysis recovers and unifies well known results concerning the Lie algebra of KT's and CKT's[10] and the so called "related integral theorems".[6]

A certain number of particular applications of our general statements will also be explicitly listed, in order to provide instructive examples of FI's of motion.

For generality in our analysis, we shall consider an n-dimensional indefinite Riemannian manifold of metric tensor g_{ab}. As far as notations are concerned, the action of the operator D^m/Ds^m on a tensor field is defined by

[a)] Work done under the auspices of the National Group for Mathematical Physics of C.N.R.

 0022-2488/82/122346-07$02.50

$$\frac{D^m}{Ds^m} = t^{a_1}\cdots t^{a_m}\nabla_{a_1}\cdots\nabla_{a_m},$$

where t^a is the tangent vector to a geodesic of affine parameter s. The following letter-saving conventions will also be employed: $t^{a_1}\cdots t^{a_p}$ will be denoted by $t^{a_1\cdots a_p}$; moreover the symbol K will be used to denote a tensor $K_{a_1\cdots a_p}$ when no possibility of misunderstanding arises.

2. GENERALIZED KILLING TENSORS

In a given manifold referred to local coordinates x^a $(a = 1,\ldots,n)$, consider a geodesic of equation $x^a = x^a(s)$, where s is an affine parameter, and denote by t its tangent vector.

We shall deal with the problem of determining a vector field $X^a = X^a(s)$ and a function $\psi = \psi(s)$ satisfying

$$\frac{D^2X^a}{Ds^2} + R^a{}_{bcd}\,t^b X^c t^d = 2\psi t^a, \tag{2.1}$$

where $R^a{}_{bcd}$ is, as usual, the curvature tensor.

In the case $\psi = 0$ Eq. (2.1) reduces to the well known egd, and the vector X is usually referred to as a J field.[11]

In general, every solution X of Eq. (2.1) may be decomposed as

$$X^a = \hat{X}^a + \int_{s_0}^{s}\left(\int_{s_0}^{\tau} 2\psi\, d\sigma\right)d\tau\, t^a, \tag{2.2}$$

where $\hat{X}$ is a J field. Therefore, every solution of Eq. (2.1) is very simply related to a corresponding J field defined along the geodesic, through Eq. (2.2). In this section, we shall be dealing with remarkable properties of solutions of Eq. (2.1). As a matter of fact, it could be shown that similar remarks hold, with slight modifications, for the solutions of any inhomogeneous extension of the egd. However, it will be shown that our particular choice turns out to be sufficiently general to lead to significant results and to avoid too much involved formal complexities.

As it was stated in the Introduction, we shall characterize the class of symmetric tensor fields that give rise to solutions of Eq. (2.1) along every geodesic. In this way we shall obtain an extension of the concept of KT's as generators of J fields, through Eq. (2.2). Furthermore, it will also be shown that such generalized KT's identify FI's of geodesic motion, as it was to be expected by a proper extension of a KT. Namely, we have the following theorem:

Theorem 2.1: Let K be a totally symmetric tensor of order p and let X be the vector defined by

$$X^a = K^a{}_{a_2\cdots a_p}\,t^{a_2\cdots a_p}, \quad \text{if } p > 1,$$
$$X^a = K^a, \quad \text{if } p = 1, \tag{2.3}$$

where K is restricted to the geodesic of tangent vector t. Then X is a solution of Eq. (2.1) along every geodesic iff there exists a totally symmetric tensor field k of order p such that

$$[(p+2)\nabla_{(b}\nabla_a K_{a_1\cdots a_p)} - 2\nabla_a\nabla_{(b}K_{a_1\cdots a_p)}]/p = g_{a(b}k_{a_1\cdots a_p)}. \tag{2.4}$$

Moreover, the function ψ is given by

$$\psi = \tfrac{1}{2}k_{a_1\cdots a_p}\,t^{a_1\cdots a_p}. \tag{2.5}$$

Furthermore, X is a J field along every geodesic iff $k = 0$, i.e., iff

$$\nabla_a\nabla_{(b}K_{a_1\cdots a_p)} = 0. \tag{2.6}$$

Proof: Using the Ricci identity and the symmetry of the field K, it follows that the vector X defined by Eq. (2.3) satisfies the identity

$$\frac{d^2X_a}{Ds^2} + R_{abcd}\,t^b X_c t^d = \frac{1}{p}[(p+1)\nabla_b\nabla_{(a}K_{a_1\cdots a_p)} - \nabla_a\nabla_{(b}K_{a_1\cdots a_p)}]\,t^{ba_1\cdots a_p}. \tag{2.7}$$

It is now more convenient to rewrite Eq. (2.7) in the equivalent form

$$\frac{D^2X_a}{Ds^2} + R_{abcd}\,t^b X^c t^d = \frac{1}{p}[(p+2)\nabla_{(b}\nabla_a K_{a_1\cdots a_p)} - 2\nabla_a\nabla_{(b}K_{a_1\cdots a_p)}]\,t^{ba_1\cdots a_p}. \tag{2.8}$$

Comparing Eq. (2.8) with Eq. (2.1), we find that the vector (2.3) satisfies Eq. (2.1) for each geodesic iff there exists a tensor field k such that Eq. (2.4) holds. In this case ψ is given by Eq. (2.5).

To prove the second part of the theorem, notice that from Eq. (2.4) it follows

$$\nabla_{(b}\nabla_a K_{a_1\cdots a_p)} = g_{(ab}k_{a_1\cdots a_p)}, \tag{2.9}$$

so that Eq. (2.4) is equivalent to

$$\nabla_a\nabla_{(b}K_{a_1\cdots a_p)} = \frac{p+2}{2}g_{(ab}k_{a_1\cdots a_p)} - \frac{p}{2}g_{a(b}k_{a_1\cdots a_p)}. \tag{2.10}$$

Moreover, X is a J field along every geodesic iff $\psi = 0$, that is iff $k = 0$, in view of Eq. (2.5). It follows from Eq. (2.10) that k vanishes iff Eq. (2.6) holds. Q.E.D.

Equation (2.4) may be regarded as a formal extension of the definition of KT

$$\nabla_{(a}K_{a_1\cdots a_p)} = 0. \tag{2.11}$$

Namely, Eq. (2.4) reduces to Eq. (2.6) if $k = 0$, and Eq. (2.6) is simply the covariant derivative of Eq. (2.11). Accordingly, we shall refer to a field K, which satisfies Eq. (2.4) for a suitable k, as a *generalized Killing tensor* of order p.

Denote by $K^{(0)}_a$ a vector field and denote by $K^{(m)}_{aa_1\cdots a_m}$ $(m = 1,\ldots,r)$ a class of totally symmetric tensor fields. GKT's may also be characterized[12] as the generators of polynomial solutions of Eq. (2.1) of the type

$$X^a = K^{(0)a} + \sum_{m=1}^{r} K^{(m)a}_{a_1\cdots a_m}\,t^{a_1\cdots a_m} \tag{2.12}$$

in the sense clarified by the following corollary.

Corollary 2.1: The field X defined by Eq. (2.12) is a solution of Eq. (2.1) along every geodesic if and only if both $K^{(0)}_a$ and $K^{(m)}_{aa_1\cdots a_m}$ $(m = 1,\ldots,r)$ are GKT's.

In order to obtain a further insight into the meaning of theorem 2.1, we recall that every GKT identifies a J field defined by Eq. (2.2) along every geodesic γ. Moreover, such a J field gives rise to a 1-parameter family of geodesics containing the given curve γ, i.e., to an infinitesimal variation of γ,

and conversely.[11] Accordingly, the previous discussion allows the geometrical interpretation of GKT's described in the following theorem:

Theorem 2.2: Every GKT defines an infinitesimal variation along every geodesic.

The above property applies directly to the vector defined by eq. (2.3) when K is a KT, and may be considered as an extension to arbitrary GKT's of a similar result holding for KV's.

We shall now analyze GKT's of order 1. Eq. (2.10), which is equivalent to Eq. (2.4), reduces to

$$\nabla_a \nabla_{(b} K_{c)} = \tfrac{3}{2} g_{(ab} K_{c)} - \tfrac{1}{2} g_{a(b} k_{c)}. \tag{2.13}$$

Equation (2.13) coincides with the definition[8] of PC. Furthermore, when k_a vanishes, Eq. (2.13) yields the well known definition of affine collineation[8] (AC). In other words, a PC is the most general vector field whose restriction to an arbitrary geodesic is a solution of Eq. (2.1). In particular, the restriction of a vector field to an arbitrary geodesic is a J field iff the vector field is an AC. The above remarks are summarized in the following corollary.

Corollary 2.2: The class of GKT's of order 1 coincides with the class of PC's. In particular, a GKT of order 1 is a solution of Eq. (2.6) iff it is an AC.

Notice also that, in view of Eq. (2.2), every PC yields a solution $\hat{X}$ of the egd. However, in general $\hat{X}$ does not identify a vector field of the given manifold, since it depends explicitly on the tangent vector of the geodesic.

The discussion that led to Theorem 2.1 may also be extended to the case of null geodesics, which is particularly relevant in view of possible applications to general relativity. To this aim, we notice that, going along the same lines already described in the proof of Theorem 2.1, we obtain the following result.

Theorem 2.3: Consider a totally symmetric tensor field K of order p and the vector X defined by Eq. (2.3), where t is the tangent vector to an arbitrary null geodesic and K is restricted to the geodesic. Then X is a solution of Eq. (2.1) whatever the choice of the null geodesic iff there exist tensor fields k and z of order p such that

$$(1/p)[(p+2)\nabla_{(b}\nabla_{a} K_{a_1\ldots a_p)} - 2\nabla_a \nabla_{(b} K_{a_1\ldots a_p)}] = g_{a(b} k_{a_1\ldots a_p)} + z_{a(a_1\ldots a_{p-1}} g_{a_p b)}. \tag{2.14}$$

The expression of ψ is given by Eq. (2.5). Moreover, X is a J field along every null geodesic iff $k = 0$, i.e., iff

$$\nabla_a \nabla_{(b} K_{a_1\ldots a_p)} = [(p+2)/2] z_{(a_1\ldots a_p} g_{ab)} - (p/2) z_{a(a_1\ldots a_{p-1}} g_{a_p b)}. \tag{2.15}$$

Equation (2.14) is to be regarded as the mathematical characterization of those totally symmetric tensor fields K yielding infinitesimal variations of null geodesics through Eqs. (2.3) and (2.2).

A remarkable class of solutions of Eq. (2.14) is given by CKT's which are defined as solutions of the equation

$$\nabla_{(b} K_{a_1\ldots a_p)} = g_{(ba_1} w_{a_2\ldots a_p)}, \tag{2.16}$$

where w is a suitable tensor field. Namely, we have the following theorem.

Theorem 2.4: Let K be a CKT of order p. Then Eq. (2.14) holds, with k and z given by

$$k_{a_1\ldots a_p} = (2/p)\nabla_{(a_1} w_{a_2\ldots a_p)}, \tag{2.17}$$

$$z_{a_1\ldots a_p} = (1/p)[(p-1)\nabla_{(a_p} w_{|a_1|a_2\ldots a_{p-1})} - \nabla_{a_1} w_{a_2\ldots a_p)}], \tag{2.18}$$

where w is defined by Eq. (2.16). Moreover, the following equation is satisfied along every geodesic of tangent vector t

$$\frac{D^2 X_a}{Ds^2} + R_{abcd} t^b X^c t^d = \left\{ \frac{2}{p} g_{ac} \nabla_b w_{a_2\ldots a_p} + \frac{1}{p} g_{bc} [(p-1)\nabla_{a_p} w_{aa_2\ldots a_{p-1}} - \nabla_a w_{a_2\ldots a_p}] \right\} t^{bca_2\ldots a_p}, \tag{2.19}$$

where X is defined by Eq. (2.3)

Proof: By taking the covariant derivative ∇_c of Eq. (2.16) and after some manipulations of the indices, we obtain the identity

$$(p+2)\nabla_{(b}\nabla_{a} K_{a_1\ldots a_p)} - 2\nabla_a \nabla_{(b} K_{a_1\ldots a_p)} = 2g_{a(b}\nabla_{a_1} w_{a_2\ldots a_p)} + (p-1)\nabla_{(b} w_{|a|a_1\ldots a_{p-2}} g_{a_{p-1} a_p)} - \nabla_a w_{(a_1\ldots a_{p-1}} g_{a_p b)}. \tag{2.20}$$

Comparing Eq. (2.20) with Eq. (2.14), we conclude that Eq. (2.14) is satisfied when k and z are defined by Eqs. (2.17) and (2.18). Substituting Eqs. (2.17) and (2.18) into Eq. (2.14), transvecting with $t^{a_1\ldots a_p b}$ and using Eqs. (2.3) and (2.8), we obtain Eq. (2.19). Q.E.D.

As suggested by the result of Theorem 2.4 every tensor field K *of order* p which is a solution of Eq. (2.14) will be referred to as *generalized conformal Killing tensor* or order p.

When we restrict our analysis to null geodesics, we may extend to GCKT's the remarks already made for GKT's. In particular, Corollary 2.1 and Theorem 2.2 are still valid if we substitute GCKT's for GKT's.

As far as the case $p = 1$ is concerned, referring to the diagrams of Katzin and Levine,[5,13] we have the following results.

Corollary 2.3: (i) Every PC is a GCKT; (ii) every ConfC is a GCKT; (iii) the restriction of a vector field X to an arbitrary null geodesic is a J field iff X is a null geodesic collineation (NC).

Proof: The proofs of the statements (i) and (ii) are trivial. To prove (iii) notice that, in the case $p = 1$, eq. (2.15) yields

$$\nabla_a \nabla_{(b} K_{c)} = g_{a(b} z_{c)}, \tag{2.21}$$

which coincides with the definition of NC.[5] Q.E.D.

We conclude this section with the following remarks. From the definitions (2.4) and (2.14) it follows that GKT's are a proper subclass of GCKT's. However, due to the different rôle played by these fields in the analysis of FI's of geodesic motion, we have introduced them in a separate way and with different notations. It will be understood that every result established for GCKT's also holds for GKT's. Moreover we shall refer for brevity to a solution of Eq. (2.6) [or (2.15)] as a homogeneous GKT (GCKT).

3. FIRST INTEGRALS OF GEODESIC MOTION

As it is well known, the fundamental motivation for the introduction of KT's or CKT's is given by the fact that they generate FI's of geodesic motion which are homogeneous polynomials in the tangent vector.

In the previous section, we introduced the definitions of GKT and GCKT as an extension of the concepts of KT and CKT. Then it seems worthwhile to see whether the new fields so defined could be generators of some type of geodesic FI's. We shall proceed to this investigation in two steps. Firstly, we derive FI's of geodesic motion which may be associated with a single solution of Eq. (2.4) or (2.14); then we study the FI's which are obtained from any two distinct solutions of the same equations. We shall also report here a certain number of already well known results which appear to have a common origin in this approach.

We start by giving a set of constants of geodesic motion which are a direct consequence of the definitions (2.4) and (2.14).

Lemma 3.1: Let K be a GKT of order p. Then we have

$$\nabla_a K_{a_1\ldots a_p} t^{aa_1\ldots a_p} - g_{ab} t^{ab} \int_{s_0}^{s} k_{a_1\ldots a_p} t^{a_1\ldots a_p}\, d\tau = c_1, \tag{3.1}$$

$$K_{a_1\ldots a_p} t^{a_1\ldots a_p} - g_{ab} t^{ab} \int_{s_0}^{s} \left(\int_{s_0}^{\sigma} k_{a_1\ldots a_p} t^{a_1\ldots a_p}\, d\tau \right) d\sigma$$

$$- s\left(\nabla_a K_{a_1\ldots a_p} t^{aa_1\ldots a_p} - g_{ab} t^{ab} \int_{s_0}^{s} k_{a_1\ldots a_p} t^{a_1\ldots a_p}\, d\tau\right) = c_2, \tag{3.2}$$

with c_1 and c_2 constant along every geodesic. If K is a GCKT, then Eqs. (3.1) and (3.2) hold along every null geodesic.

Proof: The proof follows easily by differentiating the left hand sides of Eqs. (3.1) and (3.2) along a geodesic and using Eq. (2.9). By a similar procedure it may be shown that the quantities (3.1) and (3.2) are constant along null geodesics if K is a GCKT. Q.E.D.

The conserved quantities defined by Eqs. (3.1) and (3.2) will be used to obtain an extension of known techniques for the generation of FI's of geodetic motion when K is properly chosen. Namely, we have the following results.

Theorem 3.1: If K is a GCKT of order p, then the field

$$\nabla_{(a} K_{a_1\ldots a_p)}, \tag{3.3}$$

is a CKT of order $p+1$, and the quantity

$$K_{a_1\ldots a_p} t^{a_1\ldots a_p} - s\nabla_a K_{a_1\ldots a_p} t^{aa_1\ldots a_p}, \tag{3.4}$$

is a FI of motion along null geodesics. Moreover, if K is a homogeneous GKT then the field (3.3) is a KT, and (3.4) is a FI along arbitrary geodesics.

As a particular case, notice that, given a GCKT (homogeneous GKT) of order 1, the FI (3.4) reduces to $K_a t^a - s\nabla_a K_b t^{ab}$ for t null (arbitrary). In view of Corollary 2.3, this result agrees with Theorem 7.1 (5.2) of a recent paper[8] by Katzin and Levine. Moreover, in all cases listed in Corollary 2.3 we obtain the well known result that the field $\nabla_{(a} K_{b)}$ is a CKT of order 2.

In general, an arbitrary GCKT identifies the FI of null geodesic motion described in Theorem 3.1. Further classes of FI's may be found when K is subject to suitable constraints. For instance, suppose that there exist an integer m and a field $\sigma_{a_1\ldots a_{m+p-2}}$ such that the field k defined in Eq. (2.14) satisfies the condition

$$\nabla_{(a_1}\ldots\nabla_{a_m} K_{a_{m+1}\ldots a_{m+p})} = g_{(a_1 a_2} \sigma_{a_3\ldots a_{m+p})}. \tag{3.5}$$

From Eq. (3.5) it follows that, along every null geodesic, we have

$$\frac{D^m}{Ds^m}\left(k_{a_1\ldots a_p} t^{a_1\ldots a_p}\right) = 0. \tag{3.6}$$

Then Eq. (3.6) implies that

$$k_{a_1\ldots a_p} t^{a_1\ldots a_p} = \sum_{j=0}^{m-1} \alpha_j s^j, \tag{3.7}$$

where the expressions for the constant coefficients α_j in terms of the covariant derivatives of k are given by

$$\alpha_j = \frac{1}{j!} \sum_{i=0}^{m-1-j} \frac{1}{i!} (-s)^i \frac{D^{i+j}}{Ds^{i+j}} \left(k_{a_1\ldots a_p} t^{a_1\ldots a_p}\right), \tag{3.8}$$

with $0 \leqslant j \leqslant m-1$. When j varies over the prescribed interval, Eq. (3.8) yields m FI's of null geodesic motion. Taking also into account the results of Theorem 3.1, we obtain two additional FI's of null geodesic motion. To summarize: every GCKT for which Eq. (3.5) holds, admits $m+2$ FI's of null geodesic motion.

If we fix our attention to arbitrary geodesics, we find a similar analysis holds, provided that the field k of Eq. (2.4) satisfies the supplementary condition

$$\nabla_{(a_1\ldots a_m} k_{a_{m+1}\ldots a_{m+p})} = 0 \tag{3.9}$$

for some integer m. The constraint (3.9) implies that Eq. (3.7) is satisfied along every geodesic. Then the FI's (3.8) hold for arbitrary geodesics. Moreover, in consequence of Lemma 3.1 and Eq. (3.7), the quantities

$$c_1 = \nabla_a K_{a_1\ldots a_p} t^{aa_1\ldots a_p} - g_{ab} t^{ab} \sum_{j=0}^{m-1} \alpha_j \frac{s^{j+1}}{j+1}, \tag{3.10}$$

$$c_2 = K_{a_1\ldots a_p} t^{a_1\ldots a_p} - s\nabla_a K_{a_1\ldots a_p} t^{aa_1\ldots a_p} + g_{ab} t^{ab} \sum_{j=0}^{m-1} \alpha_j \frac{s^{j+2}}{j+2}, \tag{3.11}$$

are constant along every geodesics. Recalling the relation (3.8) between the coefficients α_j and the covariant derivatives of k, we conclude that the quantities (3.10) and (3.11) are FI's of motion.

Equations of the form (3.9) have been found by Katzin and Levine[8] to be a necessary and sufficient condition for the existence of FI's of geodesic motion with explicit dependence on the path parameter s. These FI's are easily seen to be proportional to the α_j's given by Eq. (3.8). In view of Eqs. (3.10) and (3.11), we may comment on this fact by saying that the existence of a GKT K subject to the constraint (3.9) is a sufficient condition for increasing the number of FI's concomitant with k.

We shall now describe a class of FI's generated by pairs of GKT's or GCKT's. To this aim, we state a general result concerning constant of motion identified by solutions of Eq. (2.1).

Let us denote by (X, ψ) and (Y, ϕ) two solutions of Eq. (2.1), where the rhs is given by $2\psi t^a$ and $2\phi t^a$, respectively. Then we have the following theorem.

Theorem 3.2: Let (X, ψ), (Y, ϕ) be any two solutions of Eq. (2.1) on a given geodesic of tangent vector t. Then we have

$$X^a \frac{DY_a}{Ds} - Y^a \frac{DX_a}{Ds} - \int_{s_0}^{s} 2(\phi X_a t^a - \psi Y_a t^a)\, d\tau = c_3, \tag{3.12}$$

where c_3 is constant along the geodesic.

Proof: A direct proof follows easily by differentiating the l.h.s. of Eq. (3.12) along the geodesic and using the definitions of (X, ψ) and (Y, ϕ). Q.E.D.

Under the assumption that both X and Y are given by Eq. (2.3), Theorem 3.2 identifies FI's of motion that may be written in the form of homogeneous polynomials in the tangent vector to the geodesic. In other words, Theorem 3.2 will be used to generate KT's and CKT's. For instance, if $\psi = \phi = 0$, i.e., if both X and Y are J fields, Theorem 3.2 yields the following result.

Corollary 3.1: Let K and H be homogeneous GKT's of order p and q, respectively. Then the field

$$K_{a(a_2 \ldots a_p} \nabla_b H^a{}_{b_2 \ldots b_q)} - H_{a(b_2 \ldots b_q} \nabla_b K^a{}_{a_2 \ldots a_p)} \tag{3.13}$$

is a KT of order $p + q - 1$.

As an application of Corollary 3.1, notice that, if the fields K and H are AC's, then the field $K_a \nabla_b H^a - H_a \nabla_b K^a$ is a KV.

If we consider HM's, the last relation easily reduces to the already known result that the commutator of two HM's is a KV.[14]

The result given in Corollary 3.1 may be extended to the case of null geodesics as follows:

Corollary 3.2: Let K and H be homogeneous GCKT's of order p and q respectively. Then the tensor field (3.13) is a CKT of order $p + q - 1$.

In particular, two NC's identify a conformal Killing vector defined as $K_a \nabla_b H^a - H_a \nabla_b K^a$.

The constant of motion defined by Theorem 3.2 reduces to a well known FI when both K and H are KT's (CKT's), as it is shown by the following corollary.

Corollary 3.3: Let K and H be KT's (CKT's of order p and q, respectively. If X and Y are related to K and H by Eq. (2.3), then the constant of motion (3.12) coincides with the FI concomitant with the Schouten–Nijenhuis bracket[3,10] of K and H, up to a constant factor.

Proof: Let K and H be arbitrary CKT's satisfying the equations

$$\nabla_{(a} K_{a_1 \ldots a_p)} = g_{(aa_1} w_{a_2 \ldots a_p)}, \quad \nabla_{(a} H_{b_1 \ldots b_q)} = g_{(ab_1} v_{b_2 \ldots b_q)}, \tag{3.14}$$

for suitably defined w and v. Consider Eq. (3.12) and put

$$X^a = K^a{}_{a_2 \ldots a_p} t^{a_2 \ldots a_p}, \quad Y^a = H^a{}_{b_2 \ldots b_q} t^{b_2 \ldots b_q}. \tag{3.15}$$

From Eqs. (2.5) and (2.19) it follows that

$$\phi = \frac{1}{q} \frac{D}{Ds} (v_{b_2 \ldots b_q} t^{b_2 \ldots b_q}).$$

Since $X_a t^a$ is constant along null geodesics, we have

$$\int_{s_0}^{s} \phi X_a t^a \, d\tau = \frac{1}{q} K_{a_1 \ldots a_p} v_{b_2 \ldots b_q} t^{a_1 \ldots a_p b_2 \ldots b_q},$$

up to an additive constant. Writing down the analogous expression for $\int_{s_0}^{s} \psi Y_a t^a \, d\tau$ and substituting into Eq. (3.12) we obtain, in view of Eqs. (3.14),

$$\frac{1}{pq} [qH^b{}_{(b_2 \ldots b_q} \nabla_{|b|} K_{a_1 \ldots a_p)} - pK^b{}_{(a_1 \ldots a_{p-1}} \nabla_{|b|} H_{a_p b_2 \ldots b_q)}] t^{b_2 \ldots b_q a_1 \ldots a_p} = c_4, \tag{3.16}$$

with c_4 constant along every null geodesic. The CKT appearing in the square brackets of Eq. (3.16) coincides with the Schouten–Nijenhuis bracket of K and H.

The same procedure applies when K and H are KT's. In this case, noting that $\psi = \phi = 0$, we still obtain a FI described by an equation of the form (3.16), holding for arbitrary geodesic. Q.E.D.

In view of Corollary 3.3, the FI's obtained as a consequence of Theorem 3.2 may be regarded as extensions of the standard procedure for the generation of FI's based on the introduction of the Schouten–Nijenhuis bracket.

Theorem 3.2 may also be used to find a class of FI's of motion yielding an immediate extension of the so called "Related Integral Theorem".[6] Namely, by direct substitution into Eq. (3.12) and after some manipulation of the indices, we obtain the following results.

Corollary 3.4: Let H be a KT of order q. Then, denoting by $\mathcal{L}_K$ the Lie derivative with respect to the vector field K, we have:

(i) $\mathcal{L}_K H_{a_1 \ldots a_q}$ is a CKT if K is a NC,

(ii) $\mathcal{L}_K H_{a_1 \ldots a_q} - 2q\sigma H_{a_1 \ldots a_q}$ with $\sigma = \nabla_j K^j / n$ is a CKT if K is a ConfC,

(iii) $\mathcal{L}_K H_{a_1 \ldots a_q} - 2q\lambda H_{a_1 \ldots a_q}$ with $\lambda = \nabla_j K^j / (n+1)$ is a KT if K is a PC.

It is to be remarked that the statement (iii) coincides with the Related Integral Theorem. Moreover, the fields defined in (ii) and in (iii) reduce to the Schouten–Nijenhuis bracket of H and K if K degenerates into a conformal motion or into a motion, respectively.

The above discussion shows that the procedure for the construction of FI's based on Theorem 3.2 works also under the assumption that, by themselves, neither H or K give rise to FI's. However, each corollary has been proved under the assumption that the fields H and K, besides being GCKT's or GKT's, are subject to further supplementary conditions. We shall now deal with the problem of generating FI's from a more general viewpoint. It will be shown that the linear spaces of GCKT's and GKT's may be endowed with an algebra structure such that the properly defined product assumes values into the subalgebra of CKT's and KT's respectively.

Namely, as far as GCKT's are concerned, we state the following theorem that, recalling Theorem 3.1, may be proved by direct calculation.

Theorem 3.3: Let K and H be GCKT's of order p and q respectively. Then the field

$$K_{(a_1 \ldots a_p} \nabla_a H_{b_1 \ldots b_q)} - H_{(b_1 \ldots b_q} \nabla_a K_{a_1 \ldots a_p)} \tag{3.17}$$

is a CKT of order $p + q + 1$. In particular, when K and H are homogeneous GKT's the tensor field (3.17) is a KT.

For completeness, we list in detail the results obtained from Theorem 3.3 in the case $p = q = 1$. In view of Corollaries 2.2 and 2.3, we have the following statements.

Corollary 3.5: Consider the field

$$K_{(a} \nabla_b H_{c)} - H_{(a} \nabla_b K_{c)}. \tag{3.18}$$

(i) The field (3.18) is a CKT of order 3 if H and K, each independently of the other, are chosen in the set of PC's, of Conf C's, or of NC's. (ii) The field (3.18) is a KT of order 3 if both H and K are AC's.

The following theorem shows that there exists a FI of geodesic motion associated with every pair of GKT's.

Theorem 3.4: Suppose that K and H are GKT's of order p and q respectively. Then the field

$$g_{(a_1b_1}K^{a}{}_{a_2\ldots a_p}\nabla_b H_{|a|b_2\ldots b_q)} - g_{(a_1b_1}H^{a}{}_{b_2\ldots b_q}\nabla_b K_{|a|a_2\ldots a_p)} - K_{(a_1\ldots a_p}\nabla_b H_{b_1\ldots b_q)} + H_{(b_1\ldots b_q}\nabla_b K_{a_1\ldots a_p)} \tag{3.19}$$

is a KT of order $p+q+1$.

Proof: Consider the fields X and Y defined in Eqs. (3.15). On account of the fact that both vectors are solutions of Eq. (2.1), it follows that

$$\frac{D^2}{Ds^2}(X_a t^a) = 2\psi g_{ab}t^{ab}, \frac{D^2}{Ds^2}(Y_a t^a) = 2\phi g_{ab}t^{ab}. \tag{3.20}$$

Suppose the geodesic is non-null and consider the equation obtained by multiplying Eq. (3.12) by $g_{ab}t^{ab}$. Substituting Eqs. (3.20), it may be shown by a straightforward calculation that the following relation holds on every non-null geodesic:

$$[g_{a_1b_1}(X^a\nabla_b Y_a - Y^a\nabla_b X_a) - X_{a_1}\nabla_b Y_{b_1} + Y_{a_1}\nabla_b X_{b_1}]t^{a_1b_1b} = c_5, \tag{3.21}$$

with c_5 constant. Recalling the definitions (3.15) of X and Y, it follows from Eq. (3.21) that the quantity

$$[g_{a_1b_1}(K_{aa_2\ldots a_p}\nabla_b H^{a}{}_{b_2\ldots b_q} - H_{ab_2\ldots b_q}\nabla_b K^{a}{}_{a_2\ldots a_p}) - K_{a_1\ldots a_p}\nabla_b H_{b_1\ldots b_q} + H_{b_1\ldots b_q}\nabla_b K_{a_1\ldots a_p}] \times t^{a_1\ldots a_p bb_1\ldots b_q} \tag{3.22}$$

is constant on every non-null geodesic. In view of Theorem (3.3) the quantity (3.22) is a FI also along every null geodesic. Therefore we conclude that the field (3.19) is a KT. Q.E.D.

The content of Theorem 3.4 may be restated by saying that the operator defined by Eq. (3.19) assumes values into the class of KT's when acting on pairs of GKT's.

To complete our scheme, we describe some remarkable particular cases of Theorem 3.4 in the following corollary.

Corollary 3.6: (i) Let K and H be PC's. Then the field

$$H_a\nabla_{(c}K^{a}g_{bd)} - K_a\nabla_{(c}H^{a}g_{bd)} + K_{(b}\nabla_c H_{d)} - H_{(d}\nabla_c K_{b)} \tag{3.23}$$

is a KT of order 3.

(ii) Let H be a KT of order q, and let K be a PC. Then the field

$$g_{(ab}\mathcal{L}_K H_{a_1\ldots a_q)} - qH_{(a_1\ldots a_q}\nabla_b K_{a)} \tag{3.24}$$

is a KT of order $q+2$.

4. COMMENTS

In this work we have studied the so called GKT's (GCKT's) defined as the class of totally symmetric tensor fields that are generators of solutions of the inhomogeneous egd (2.1) along arbitrary (null) geodesics. We found the introduction of these fields to be of particular interest in two main respects. Firstly, we have shown that they provide a formal context for a unified treatment of the algebraic and geometric properties of some remarkable fields; like KT's, CKT's, and geodesic collineations. Secondly, they turn out to be among the most natural objects that can be used, either directly or combined in some way, for finding new FI's of geodesic motion.

From this point of view, the construction of FI's concomitant with GKT's and GCKT's is reduced to a straightforward calculation, applying the theorems presented in this paper, provided one knows the GKT's and the GCKT's admitted by a given metric.

Some application to general relativity of the techniques described in this paper may be found in a recent work[9] where the general integral of the egd is written down explicitly in a class of spherically symmetric space–times. The result is based on the fact that the metrics examined admit a sufficient number of KV's and KT's, i.e., of homogeneous GKT's.

As far as the existence of GKT's and GCKT's in generaly relativity is concerned, in the literature there are relatively few results related to KT's of order greater than one, while a considerable amount of information regarding GKT's and GCKT's of order one is available. For instance HM's, which belong to the class of GKT's, have been extensively studied.[14,15] In particular, it is well known that the only curvature collineations admitted by a vacuum space–time are HM's, unless the space is of Petrov type N.[14] In this case there exist also nontrivial conformal collineations.

The peculiar rôle played by the vacuum type N is due to its high degree of symmetry, and appears in some interesting respects also in connection with our problem. Vacuum type N space–times are probably the most natural support for the homogeneous GKT's, since the definition (2.6) of such tensors involves the existence of parallel fields. In connection with this point, it is to be noticed that, if one considers second order tensors, Eq. (2.6) is satisfied only by KT's in all vacuum space–times, again with the exclusion of Petrov type N.[9,16]

Having in mind this exception, it would be interesting to see whether such conclusions extend to symmetric tensors of any order, thus giving a unique characterization of KT's as generators of J fields for arbitrary geodesics.

Aside from these examples, no attempt has yet been made to give explicit solutions of Eqs. (2.4) and (2.14). The problem of finding nontrivial GCKT's in more general cases, which requires a study of the integrability conditions of these equations, is still a matter of investigation.

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[12]One has to make use of the following property. On an indefinite Riemannian manifold, consider a collection of tensor fields $A^{(m)}{}_{a_1\ldots a_m}$, $m = 1,\ldots,r$. An equation of the form

$$\sum_{m=1}^{r} A^{(m)}{}_{a_1\ldots a_m} t^{a_1\ldots a_m} = 0$$

holds for arbitrary (null) t iff $A^{(m)}{}_{a_1\ldots a_m} t^{a_1\ldots a_m} = 0$, for $1 \leqslant m \leqslant r$.
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Cascaded Poisson processes

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(Received 20 April 1982; accepted for publication 25 June 1982)

We investigate the counting statistics for stationary and nonstationary cascaded Poisson processes. A simple equation is obtained for the variance-to-mean ratio in the limit of long counting times. Explicit expressions for the forward-recurrence and inter-event-time probability density functions are also obtained. The results are expected to be of use in a number of areas of physics.

PACS numbers: 02.50. + s, 29.70. − e, 87.10. + e, 94.40.Pa

I. INTRODUCTION

Multiplication, reduction, and branching processes have been examined in a broad variety of contexts.[1–6] Applications range from astrophysics to biological information transmission. In the great majority of mathematical treatments, the multiplication or branching is treated as an instantaneous effect [see Fig. 1(a)]. However, in many physical systems, a random time delay (or spatial dispersion) is inherent in the multiplication process. In this paper, we carry out an analysis of a cascade of Poisson multiplications that includes such time effects [see Fig. 1(b)]. Our results reduce to previously known descriptions, in the limit of instantaneous multiplication.

In a recent series of papers, we examined the two-stage multiplicative-Poisson process with random time delay. The particular model that we analyzed is the shot-noise-driven doubly stochastic Poisson point process (SNDP), in which each event of a Poisson point process generates an inhomogeneous rate function which, in turn, generates a second Poisson process. The SNDP is a doubly stochastic Poisson point process (DSPP)[7,8]; it is also a special case of the Neyman–Scott cluster process.[9,10]

A number of results were established in our study. We showed that the theoretical count variance is proportional to the count mean for an arbitrary inhomogeneous rate function [we call this the impulse-response function $h(t)$]. For long counting times, the theoretical counting distribution was shown to be the Neyman Type-A,[11,12] and this distribution was experimentally measured for radioluminescence from glass.[13] The forward-recurrence-time and inter-event-time probability densities were obtained, both in the absence and in the presence of self-excitation (dead time or refractoriness).[14] The results were used to describe the detection of optical fluorescence or scintillation generated by ionizing radiation. They were also used to fit the maintained-discharge interspike-interval histograms recorded from a cat's on-center retinal ganglion cell in darkness.[15]

General expressions for the count mean and variance were also obtained in the presence of small dead time, and the results were experimentally verified for radioluminescence from several transparent materials.[16] We showed that self-excitation could be used to constructively enhance or diminish the effects of point processes that display clustering, according to whether they are signal or noise. Finally, general expressions for the single- and multifold counting and time statistics, as well as for the power spectrum, were obtained for many cases of interest.[17] We presented a broad review of the application of such multiplied-Poisson noise to many areas in physics, optics, and electrical engineering (e.g., cathodoluminescence, x-ray radiography).[17] The statistics for a nonstationary SNDP were also obtained, and the counting distribution was found to reduce to the Neyman Type-A for input signals of short duration.[18] In this paper, we extend many of these results to the multistage case.

The results of our cascade analysis are likely to find use in problems where a series of multiplicative effects occur. Examples are the behavior of photon and charged-particle detectors, the production of certain types of cosmic rays, and the transfer of neural information. In Sec. II, we briefly review the results for the case of instantaneous multiplication. In Sec. III, we obtain the cascade counting and time statistics, as well as the autocovariance function, in the more general case, when time effects are incorporated into the model. The behavior of the resulting counting statistics is discussed in Sec. IV, and the Conclusion is presented in Sec. V.

II. THE INSTANTANEOUS MULTIPLICATION PROCESS

We briefly discuss the instantaneous multiplication process. Let $p(n)$ represent the probability that an event at the mth generation creates n events at the $(m+1)$st generation. The quantity $G_m(z)$, which is the probability generating function for the total number of events produced at the mth

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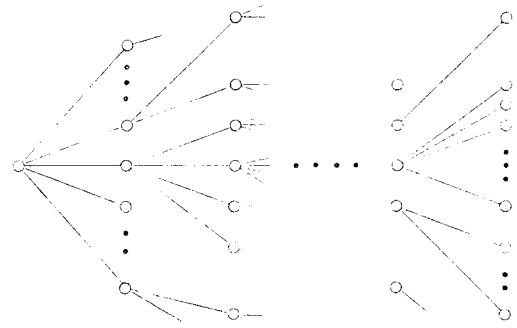
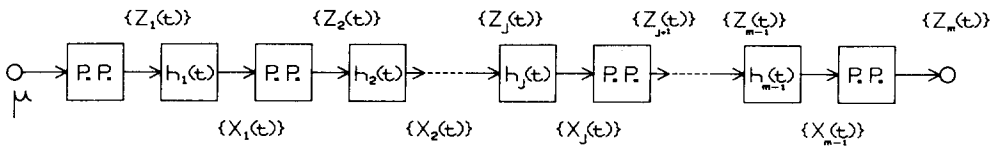


(a)



(b)

FIG. 1. Schematic representation of an m-stage cascaded system with Poisson multiplication at each stage. (a) Instantaneous multiplication; (b) time effects included. P. P. represents a Poisson process generator, whereas $h_j(t)$ represents a linear-filter impulse response function.

generation, is given by

$$G_m(z) = G_1(G_{m-1}(z)),$$

so that

$$G_m(z) = \underbrace{G_1(G_1(G_1(G_1\cdots G_1(z))))}_{m \text{ times}}. \tag{1}$$

Here

$$G_0(z) = z$$

and

$$G_1(z) = \sum_{n=0}^{\infty} z^n p(n).$$

Assuming that $p(n)$ is Poisson distributed with mean a, and substituting $z = \exp(-s)$ in (1), we obtain the moment generating function $Q_m(s)$ at the mth generation for the cascaded Poisson instantaneous multiplication process: that is,

$$Q_m(s) = Q_1(Q_{m-1}(s)),$$

or

$$Q_m(s) = \underbrace{Q_1(Q_1(Q_1(Q_1\cdots Q_1(s))))}_{m \text{ times}}. \tag{2}$$

Here

$$Q_0(s) = \exp(-s)$$

and

$$Q_1(s) = \exp(a(\exp(-s) - 1)).$$

III. POISSON MULTIPLICATION WITH TIME DELAY

As indicated in the Introduction, time delay can be an important effect in multiplication processes. In Subsec. A, we derive the counting-distribution moment generating function for an m-stage cascade of Poisson processes, for arbitrary T/τ_p. The quantity τ_p is the characteristic decay time of the inhomogeneous rate. This is followed by a calculation of the counting statistics for the single and multifold cases in Subsec. B and C, respectively. In Subsec. D, we derive the autocovariance function. The time statistics are obtained in Subsec. E. The counting statistics for the nonstationary case are considered in Subsec. F.

A. Moment generating function for the counting process at the mth stage

We consider the system illustrated in Fig. 1(b). The quantity μ is the initial deterministic driving rate, $\{Z_j(t)\}$ is a process of impulses corresponding to the point process at the jth stage, and $\{X_j(t)\}$ is the linearly filtered point process at the jth stage which, in turn, provides the driving rate process for the $(j+1)$st stage. The boxes labeled P.P. and $h_j(t)$ represent Poisson point process generators and linear filters, respectively. The moment generating functional for the filtered point process at the jth stage is defined by

$$L_{X_j}(s) \triangleq \left\langle \exp\left(-\int_{-\infty}^{\infty} s(t) X_j(t)\, dt \right) \right\rangle,$$
$$j = 1,2,\ldots,m-1. \tag{3}$$

It can be shown (see Appendix A) that (3) can be written as

$$L_{X_j}(s) = \left\langle \exp\left\{ \int_{-\infty}^{\infty} X_{j-1}(t) \times \left[\exp\left(-\int_{-\infty}^{\infty} h_j(\tau - t) s(\tau)\, d\tau \right) - 1 \right] dt \right\} \right\rangle. \tag{4}$$

If we replace $\exp(-\int_{-\infty}^{\infty} h_j(\tau - t) s(\tau)\, d\tau) - 1$ by $-s(t)$, the right-hand side of (4) is, by definition, the moment generating functional of the process $\{X_{j-1}(t)\}$; that is,

$$\left\langle \exp\left\{ \int_{-\infty}^{\infty} X_{j-1}(t) \left[\exp\left(-\int_{-\infty}^{\infty} h_j(\tau - t) s(\tau)\, d\tau \right) - 1 \right] dt \right\} \right\rangle$$
$$\Rightarrow \left\langle \exp\left(-\int_{-\infty}^{\infty} s(t) X_{j-1}(t)\, dt \right) \right\rangle = L_{X_{j-1}}(s). \tag{5}$$

Therefore, we have a recursive formula for the moment gen-

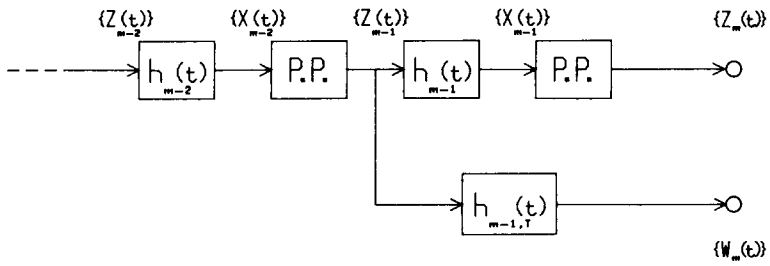


FIG. 2. Block diagram for generation of the integrated rate $\{W_m(t)\}$.

erating functional of the process $\{X_j(t)\}$,

$$L_{X_j}(s) = L_{X_{j-1}}\left\{1 - \exp\left(-\int_{-\infty}^{\infty} h_j(\tau - t)s(\tau)\,d\tau\right)\right\}, \quad (6)$$

where the moment generating functional of the first stage is

$$L_{X_1}(s) = \exp\left\{\mu\int_{-\infty}^{\infty}\left[\exp\left(-\int_{-\infty}^{\infty} h_1(\tau - t)s(\tau)\,d\tau\right) - 1\right]dt\right\}. \quad (7)$$

For convenience, we define the following operator:

$$q_j(\cdot) = \exp\left\{\int_{-\infty}^{\infty} h_j(t - t_j)[(\cdot) - 1]\,dt\right\},$$

$$j = 1,2,\ldots,m-1.$$

By using the above equations recursively, the moment generating functional for the process $\{X_{m-2}(t)\}$ becomes

$$L_{X_{m-2}}(s) = \exp\left\{\mu\int_{-\infty}^{\infty}\left[q_1\left(q_2\left(q_3\cdots\left(q_{m-3}\left(\exp\left(-\int_0^{\infty} h_{m-2}(t_{m-1} - t_{m-2})s(t_{m-1})\,dt_{m-1}\right)\right)\right)\cdots\right)\right) - 1\right]dt_1\right\}. \quad (8)$$

The integrated driving rate process at the mth stage is shown schematically in Fig. 2, and the moment generating functional for the process $\{W_m(t)\}$ is defined by

$$L_{W_m}(s) \triangleq \left\langle\exp\left(-\int_{-\infty}^{\infty} s(t)W_m(t)\,dt\right)\right\rangle. \quad (9)$$

It can be shown that the above equation can be written as

$$L_{W_m}(s) = \left\langle\exp\left\{\int_{-\infty}^{\infty} X_{m-2}(t)\times\left[\exp\left(-\int_{-\infty}^{\infty} h_{m-1,T}(\tau - t)s(\tau)\,d\tau\right) - 1\right]dt\right\}\right\rangle, \quad (10)$$

where the linear filter $h_{m-1,T}(t)$ is a convolution of $h_{m-1}(t)$ with an integrator (assumed to be noncausal for convenience) on the time interval $(0,T)$, i.e.,

$$h_{m-1,T}(t) = \int_0^T h_{m-1}(t + t')\,dt'. \quad (11)$$

To find the moment generating function of $\{W_m(t)\}$, we let $s(t) = s\delta(t)$ and we obtain

$$Q_{W_m}(s) = \left\langle\exp\left\{\int_{-\infty}^{\infty} X_{m-2}(t)[\exp(-sh_{m-1,T}(-t)) - 1]\,dt\right\}\right\rangle = L_{X_{m-2}}\{1 - \exp(-sh_{m-1,T}(-t))\}. \quad (12)$$

Combining (8) and (12) yields

$$Q_{W_m}(s) = \exp\left\{\mu\int_{-\infty}^{\infty}[q_1(q_2(q_3\cdots q_{m-2}(\exp(-sh_{m-1,T}(-t_{m-1})))\cdots)) - 1]\,dt_1\right\}. \quad (13)$$

This result will be used subsequently to find the counting and time statistics.

The moment generating function for the counting process at the mth stage is related to that of $\{W_m(t)\}$ by[19]

$$Q_{N_m}(s) = Q_{W_m}\{1 - \exp(-s)\}. \quad (14)$$

Inserting (13) into (14) then yields the final result

$$Q_{N_m}(s) = \exp\left\{\mu\int_{-\infty}^{\infty}[q_1(q_2(q_3\cdots q_{m-2}(\exp(1 - \exp(-s))\times h_{m-1,T}(-t_{m-1}))\cdots)) - 1\,dt_1\right\}. \quad (15)$$

B. Singlefold counting statistics at the mth stage

The probability distribution for the occurrence of n events in a fixed time interval $(0,T)$, at the mth stage, can be computed by using the formula[19]

$$p_m(n) = \frac{(-1)^n\partial^n}{n!\,\partial s^n} Q_{W_m}(s)\Big|_{s=1}. \quad (16)$$

With the help of the results derived in Appendix B, we have

$$p_m(0) = \exp\left\{\mu\int_{-\infty}^{\infty}[D_1^{(0)}(t) - 1]\,dt\right\}, \quad m \geqslant 2 \quad (17a)$$

and

$$(n+1)p_m(n+1) = \mu\sum_{k=0}^{n}\frac{(-1)^{k+1}}{k!}p_m(n-k)I^{(k+1)}, \quad m \geqslant 2, \quad (17b)$$

where

$$I^{(k+1)} = \int_{-\infty}^{\infty} D_1^{(k+1)}(t)\,dt, \quad k \geqslant 0,$$

$$D_j^{(k+1)}(t) = \sum_{r=0}^{k}\binom{k}{r}D_j^{(k-r)}(t) \times\int_{-\infty}^{\infty} h_j(\tau - t)D_{j+1}^{(r+1)}(\tau)\,d\tau, \quad k \geqslant 0,$$

$$j = 1,2,3,\ldots,m-2,$$

$$D_j^{(0)}(t)=\exp\left\{\int_{-\infty}^{\infty} h_j(\tau-t)[D_{j+1}^{(0)}(\tau)-1]\,d\tau\right\},$$
$$j=1,2,\ldots,m-2,$$
$$D_{m-1}^{(k)}(t)=\{-h_{m-1,T}(-t)\}^k\exp\{-h_{m-1,T}(-t)\},$$
$$m\geqslant 2,\quad k\geqslant 0,$$
$$D_j^{(k+1)}(t)=\frac{\partial^{k+1}}{\partial s^{k+1}}\exp(\theta_j(t,s))\Big|_{s=1},\qquad k\geqslant 0,$$
$$j=1,2,\ldots,m-2,$$
$$\theta_{m-1}(t,s)=-sh_{m-1,T}(-t),\qquad m\geqslant 2.$$

The count mean and variance at the mth stage can be derived by using the relations for the cumulant generating function[19]

$$\langle N_m(T)\rangle=-\frac{\partial}{\partial s}\ln Q_{N_m}(s)\Big|_{s=0} \tag{18a}$$

and

$$\mathrm{Var}(N_m(T))=\frac{\partial^2}{\partial s^2}\ln Q_{N_m}(s)\Big|_{s=0}. \tag{18b}$$

However, a moment's thought will demonstrate that the system in Fig. 3 is equivalent to the one in Fig. 1(b), as far as the first and the second moments are concerned. Here $\{V_0(t)\}$, $\{V_1(t)\},\ldots,\{V_{m-1}(t)\}$ are zero-mean, unit-variance white-processes, and the cross-correlation function of $\{V_i(t)\}$ and $\{V_j(t)\}$ is

$$R_{V_iV_j}(\tau)=\langle V_i(t+\tau)V_j(t)\rangle=\begin{cases}\delta(\tau) & \text{for } i=j,\\ 0 & \text{for } i\neq j.\end{cases} \tag{19}$$

The identity is provided by the theory of random processes in linear systems.[20,21] It can be shown that the mean and the autocorrelation function at the input to the mth stage are, respectively,

$$\langle X_{m-1}(t)\rangle=\mu\prod_{j=1}^{m-1}\alpha_j,\quad m\geqslant 2, \tag{20a}$$

and

$$R_{X_{m-1}}(\tau)=\mu^2\prod_{j=1}^{m-1}\alpha_j^2+\mu\sum_{i=1}^{m-1}\left\{\prod_{j=0}^{i-1}\alpha_j\mathop{*}_{k=i}^{m-1}g_k(\tau)\right\},\quad m\geqslant 2, \tag{20b}$$

where

$$\alpha_0=1,$$
$$\alpha_k\triangleq\int_{-\infty}^{\infty}h_k(t)\,dt,$$
$$g_k(\tau)\triangleq h_k(\tau)*h_k(-\tau),$$
$$\mathop{*}_{k=i}^{m-1}g_k(\tau)\triangleq g_i(\tau)*g_{i+1}(\tau)*\cdots*g_{m-1}(\tau).$$

The symbol $*$ indicates convolution. The counting statistics are easily derived by using the above equations.[19] The mean number of counts at the mth stage, in the counting interval $(0,T)$, is[22]

$$\langle N_m(T)\rangle=\langle W_m(T)\rangle=\left\langle\int_0^T X_{m-1}(t)\,dt\right\rangle=\mu T\prod_{j=1}^{m-1}\alpha_j. \tag{21}$$

The variance of the number of counts at the mth stage can be expressed as[19]

$$\mathrm{Var}(N_m(T))=\mu T\prod_{j=1}^{m-1}\alpha_j+\mu\sum_{i=1}^{m-1}\left\{\prod_{j=0}^{i-1}\alpha_j\int_{-T}^{T}(T-|\tau|)\left[\mathop{*}_{k=i}^{m-1}g_k(\tau)\right]d\tau\right\}. \tag{22}$$

In the limit of long counting times, which is a special case of substantial interest, the results can be found by substituting $\alpha_k\delta(t)$ for $h_k(t)$ in the above equations, which yields[22]

$$\mathrm{Var}(N_m(T))=\mu T\prod_{j=1}^{m-1}\alpha_j+\mu T\sum_{i=1}^{m-1}\left\{\prod_{j=0}^{i-1}\alpha_j\cdot\prod_{k=i}^{m-1}\alpha_k^2\right\}. \tag{23}$$

The variance-to-mean ratio (Fano factor) is then expressed quite simply as

$$F_m=\frac{\mathrm{Var}(N_m(T))}{\langle N_m(T)\rangle}=1+\sum_{i=1}^{m-1}\left\{\prod_{k=i}^{m-1}\alpha_k\right\},\quad m\geqslant 2. \tag{24a}$$

When all $\alpha_j=\alpha$, Eq. (24a) reduces to

$$F_m=1+\alpha[(1-\alpha^{m-1})/(1-\alpha)],\quad m\geqslant 1. \tag{24b}$$

For $m=1$ and $m=2$, we recover the usual expressions for the Poisson and Neyman Type-A distributions, respectively.

C. Multifold counting statistics at the mth stage

The joint probability for the number of counts N_j in L time intervals $[\tau_j,\tau_j+T_j]$, $j=1,2,3,\ldots,L$, for the m-stage cascaded Poisson system, can be written as[19]

$$p_m(\mathbf{n})=\prod_{j=1}^{L}\frac{(-1)^{n_j}\partial^{n_j}}{n_j!\,\partial s_j^{n_j}}Q_{\mathbf{W}_m}(\mathbf{s})\Big|_{\mathbf{s}=\mathbf{1}}, \tag{25}$$

where

$$\mathbf{n}=(n_1,n_2,\ldots,n_L),$$
$$\mathbf{s}=(s_1,s_2,\ldots,s_L),$$
$$\mathbf{1}=(1,1,\ldots,1),$$
$$\mathbf{W}_m=(W_{m_1},W_{m_2},\ldots,W_{m_L}),$$

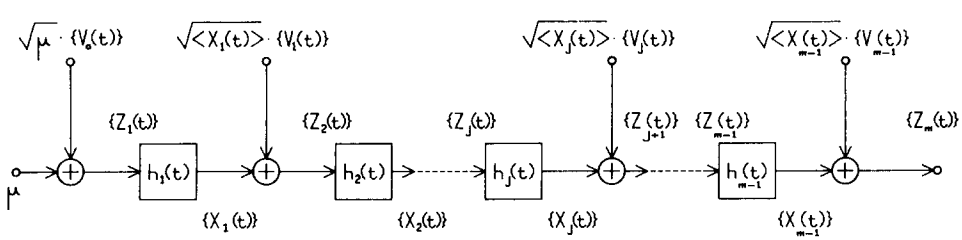


FIG. 3. Equivalent model to that presented in Fig. 1(b) as far as the count mean and variance are concerned. The $\{V_j(t)\}$ represent zero-mean unit-variance white processes.

provided that the integrated rate processes $\{W_{m_j}(t)\}$ at the mth stage are[17]

$$W_{m_j} = \int_{\tau_j}^{\tau_j + T_j} X_{m-1}(t)\,dt. \tag{26}$$

Here $Q_{\mathbf{W}_m}(\mathbf{s})$ is the L-dimensional multifold moment generating function of the integrated rate process at the mth stage, and can be expressed as

$$Q_{\mathbf{W}_m}(\mathbf{s}) = \exp\Bigg\{\mu\int_{-\infty}^{\infty}\Bigg[q_1\Bigg(q_2\Bigg(q_3\cdots q_{m-2}\Bigg(\exp\Bigg(-\sum_{j=1}^{L} s_j h_{m-1,T_j}(t_{m-1}+\tau_j)\Bigg)\Bigg)\cdots\Bigg)\Bigg)-1\Bigg]dt_1\Bigg\}. \tag{27}$$

However, it is quite difficult to obtain the joint probability distribution function using (25) and (27), and we therefore carry this result no further.

The L-dimensional multifold moment generating function for the counting process at the mth stage can be determined by using the formula[19]

$$Q_{\mathbf{N}_m}(\mathbf{s}) = Q_{\mathbf{W}_m}\{\mathbf{1} - \exp(-\mathbf{s})\}, \tag{28}$$

where

$$\mathbf{N}_m = (N_{m,1}, N_{m,2},\ldots,N_{m,L}),$$

$$\mathbf{1} - \exp(-\mathbf{s}) = (1-\exp(-s_1), 1-\exp(-s_2),\ldots, 1-\exp(-s_L)).$$

Finally, we obtain the general expression

$$Q_{\mathbf{N}_m}(s) = \exp\Bigg\{\mu\int_{-\infty}^{\infty}\Bigg[q_1\Bigg(q_2\Bigg(q_3\cdots q_{m-2}\Bigg(\exp\Bigg(-\sum_{j=1}^{L}(1-\exp(-s_j))h_{m-1,T_j}(t_{m-1}+\tau_j)\Bigg)\Bigg)\cdots\Bigg)\Bigg)-1\Bigg]dt\Bigg\}. \tag{29}$$

D. Autocovariance function at the mth stage

In this subsection we derive the autocovariance function for the number of counts N_m, registered in a time interval of duration T, for the m-stage cascaded Poisson process. The time separation between the intervals is $\tau = t_2 - t_1$. Using the definition of the autocovariance function and (29) we have

$$C_{N_m}(t_1,t_2) = \frac{\partial^2}{\partial s_1 \partial s_2} \ln Q_{N_m(t_1)N_m(t_2)}(s_1,s_2)\Big|_{s_1=s_2=0}$$

$$= \mu\int_{-\infty}^{\infty}\{U_{m-1}(t,t_1)U_{m-1}(t,t_2) + V_{m-1}(t,t_1,t_2)\}\,dt, \tag{30a}$$

where

$$U_k(t,t_j) = \int_{-\infty}^{\infty} h(\tau - t)U_{k-1}(\tau,t_j)\,d\tau, \quad k = 1,2,\ldots,m-1, \quad j = 1,2, \tag{30b}$$

$$U_0(t,t_1) = -[u(t-t_j) - u(t-t_j-T)], \quad j = 1,2, \tag{30c}$$

$$V_k(t,t_1,t_2) = \int_{-\infty}^{\infty} h(\tau - t)[U_{k-1}(\tau,t_1)U_{k-1}(\tau,t_2) + V_{k-1}(\tau,t_1,t_2)]\,d\tau, \quad k = 1,2,\ldots,m-1, \tag{30d}$$

$$V_0(t,t_1,t_2) = 0. \tag{30e}$$

It can be shown (see Appendix C) that, when all stages are identical, (30a) can be rewritten as

$$C_{N_m}(\tau) = \mu T\int_{-\infty}^{\infty}\Bigg\{\alpha\Bigg[\frac{|H(\omega)|^{2(m-1)} - \alpha^{m-1}}{|H(\omega)|^2 - \alpha}\Bigg] + |H(\omega)|^{2(m-1)}\Bigg\}\Phi_T(\omega)e^{j\omega\tau}\frac{d\omega}{2\pi}, \tag{31}$$

where

$$\tau = t_2 - t_1, \quad \alpha = \int_{-\infty}^{\infty} h(t)\,dt,$$

$$H(\omega) = \text{F.T. of } h(t), \quad \Phi_T(\omega) = T\Bigg[\frac{\sin(\omega T/2)}{(\omega T/2)}\Bigg]^2.$$

From (31), we can obtain the variance of the counting process by simply setting $\tau = 0$, so that

$$\mathrm{Var}(N_m(T)) = \mu T\alpha^{m-1} + \mu\sum_{i=1}^{m-1}\Bigg\{\alpha^{i-1}\int_{-T}^{T}(T-|\tau|)\Big[\overset{m-i}{*}\, g(\tau)\Big]\,d\tau\Bigg\}. \tag{32}$$

Equation (32) can also be obtained from (22), and the definition of $g_k(\tau)$ given in (20b), by substituting $h_k(t) = h(t)$ for all k. The power spectral density for the process is obtained by taking the Fourier transform of (31).

E. Time statistics at the mth stage

The forward-recurrence-time probability density $P_m^{(1)}(t)$ and the inter-event-time probability density $P_m^{(2)}(t)$, for the m-stage cascaded Poisson system can be derived from the explicit expression for $Q_{W_m}(s)$.[19] The calculations are straightforward and lead to

$$P_m^{(1)}(T) = -\frac{\partial}{\partial T}Q_{W_m}(1)$$

$$= \mu Q_{W_m}(1)\underbrace{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}}_{(m-1)\text{-fold integrals}} h_{m-1}(t_{m-1}+T)\times h_{m-2}(t_{m-1}-t_{m-2})\cdots h_2(t_3-t_2)h_1(t_2-t_1)\exp\Bigg\{\sum_{j=1}^{m-1}\theta_j(t_j)\Bigg\}\times dt_1\,dt_2\cdots dt_{m-1}, \tag{33}$$

and

$$P_m^{(2)}(T) = \frac{-1}{\langle X_{m-1}(t)\rangle}\frac{\partial}{\partial T}P_m^{(1)}(T)$$

$$= \Bigg(Q_{W_m}(1)\Big/\prod_{j=1}^{m-1}\alpha_j\Bigg)\Bigg[\mu\Bigg\{\underbrace{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}}_{(m-1)\text{-fold integrals}} h_{m-1}(t_{m-1}+T)\times h_{m-2}(t_{m-1}-t_{m-2})\cdots h_2(t_3-t_2)h_1(t_2-t_1)\exp\Bigg\{\sum_{j=1}^{m-1}\theta_j(t_j)\Bigg\}dt_1\,dt_2\cdots dt_{m-1}\Bigg\}^2$$

$$-\underbrace{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}}_{(m-1)\text{-fold integrals}}\Bigg\{h_{m-1}(t_{m-1}+T)\times\frac{\partial}{\partial T}\sum_{j=1}^{m-1}\theta_j(t_j) + \frac{\partial}{\partial T}h_{m-1}(t_{m-1}+T)\Bigg\}\times h_{m-2}(t_{m-1}-t_{m-2})\cdots h_2(t_3-t_2)h_1(t_2-t_1)\times\exp\Bigg\{\sum_{j=1}^{m-1}\theta_j(t_j)\Bigg\}dt_1\,dt_2\cdots dt_{m-1}\Bigg], \tag{34}$$

where

$$Q_{W_m}(1) = [\text{Eq. (13)}]|_{s=1},$$

$$\theta_j(t) = \int_{-\infty}^{\infty} h_j(\tau - t)[\exp(\theta_{j+1}(\tau)) - 1]\, d\tau, \qquad j = 1,2,\ldots,m-1,$$

$$\theta_{m-2}(t) = -h_{m-1,T}(-t).$$

F. Counting statistics for the nonstationary case

In this section, we obtain the moment generating function for the counting statistics, together with its mean and variance, for a nonstationary cascaded Poisson process (i.e., μ is a function of time).

A schematic diagram illustrating the generation of the process can be obtained by replacing μ by $\mu(t)$ in Fig. 1(b). The moment generating function for the m-stage integrated rate process $\{W_m(t,T)\}$ can be found by using a similar approach to that used in Subsec. A, giving rise to

$$Q_{W_m(t,T)}(s) = \exp\left\{\int_{-\infty}^{\infty} \mu(t-t_1)[q_1(q_2(q_3 \cdots q_{m-2}(\exp(-sh_{m-1,T}(-t_{m-1})))\cdots)) - 1]\, dt_1\right\}, \quad (35)$$

where

$$q_j(\cdot) = \exp\left\{\int_{-\infty}^{\infty} h_j(t-t_j)[(\cdot) - 1]\, dt\right\}.$$

Given the statistics of the integrated rate process $\{W_m(t,T)\}$, we readily obtain the statistics of the mth stage counting process. The mean and variance are, respectively,

$$\langle N_m(t,T)\rangle = \mu(t) * h_{m-1,T}(t) \overset{m-2}{\underset{j=1}{*}} h_j(t), \quad (36)$$

$$\mathrm{Var}(N_m(t,T)) = \mu(t) * h_{m-1,T}(t) \overset{m-2}{\underset{j=1}{*}} h_j(t) + \sum_{k=1}^{m-1} \mu(t) \overset{k-1}{\underset{j=1}{*}} h_j(t) * \left[h_{m-1,T}(t) \overset{m-2}{\underset{r=k}{*}} h_r(t)\right]^2. \quad (37)$$

Here

$$\overset{j}{\underset{r=i}{*}} h_r(t) = \delta(t) \quad \text{for } j < i,$$

and the moment generating function is

$$Q_{N_m(t,T)}(s) = \exp\left\{\int_{-\infty}^{\infty} \mu(t-t_1)[q_1(q_2(q_3 \cdots q_{m-2}(\exp(1-\exp(-s)) \times h_{m-1,T}(-t_{m-1}))\cdots)) - 1]\, dt_1\right\}. \quad (38)$$

Note that (35), (36), (37), and (38) are identical to (13), (21), (22), and (15), where $\mu(t)$ is not a function of time.

The L-dimensional multifold moment generating functions of the integrated rate process and the counting process at the mth stage are easily obtained, and they are, respectively,

$$Q_{\mathbf{W}_m(t,T)}(\mathbf{s}) = \exp\left\{\int_{-\infty}^{\infty} \mu(t-t_1)\left[q_1\left(q_2\left(q_3 \cdots q_{m-2}\left(\exp\left(-\sum_{j=1}^{L} s_j h_{m-1,T_j}(t_{m-1} + \tau_j)\right)\right)\cdots\right)\right) - 1\right] dt_1\right\}, \quad (39)$$

and

$$Q_{\mathbf{N}_m(t,T)}(\mathbf{s}) = \exp\left\{\int_{-\infty}^{\infty} \mu(t-t_1)\left[q_1\left(q_2\left(q_3 \cdots q_{m-2}\left(\exp\left(-\sum_{j=1}^{L}(1-\exp(-s_j)) \times h_{m-1,T_j}(t_{m-1}+\tau_j)\right)\right)\cdots\right)\right) - 1\right] dt_1\right\}. \quad (40)$$

These equations correspond to (27) and (29), respectively.

We now consider an important limiting case in which the rate $\mu(t)$ has a time course τ_s that is very short in duration, compared with the counting time T, added to the total linear filter correlation time $(m-1)\tau_c$ ($\tau_s \ll T + (m-1)\tau_c$). In that case, the quantity $\mu(t)$ can be mathematically represented by the limiting distribution

$$\mu(t) = E\delta(t), \quad (41)$$

where E is the strength of the excitation (number of points) and $\delta(t)$ is the Dirac delta function. Substituting (41) in (36)

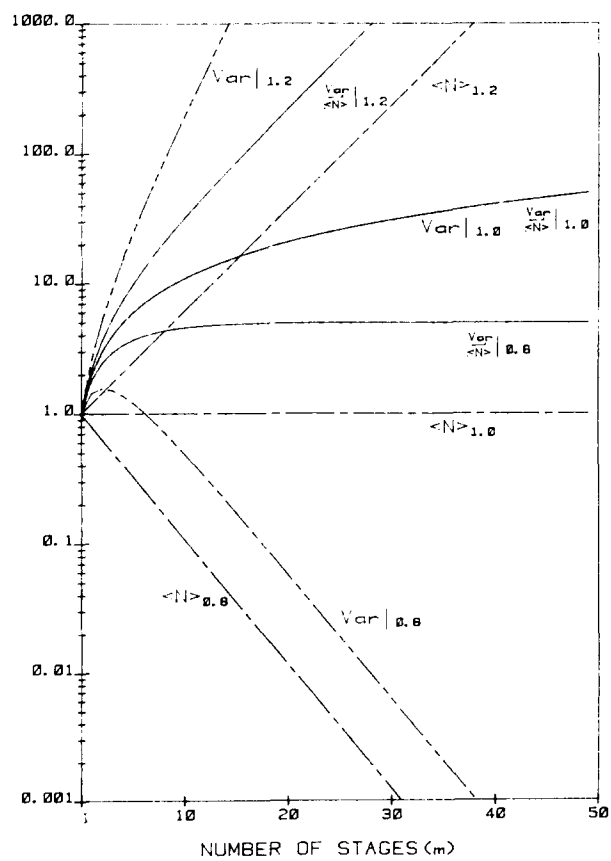
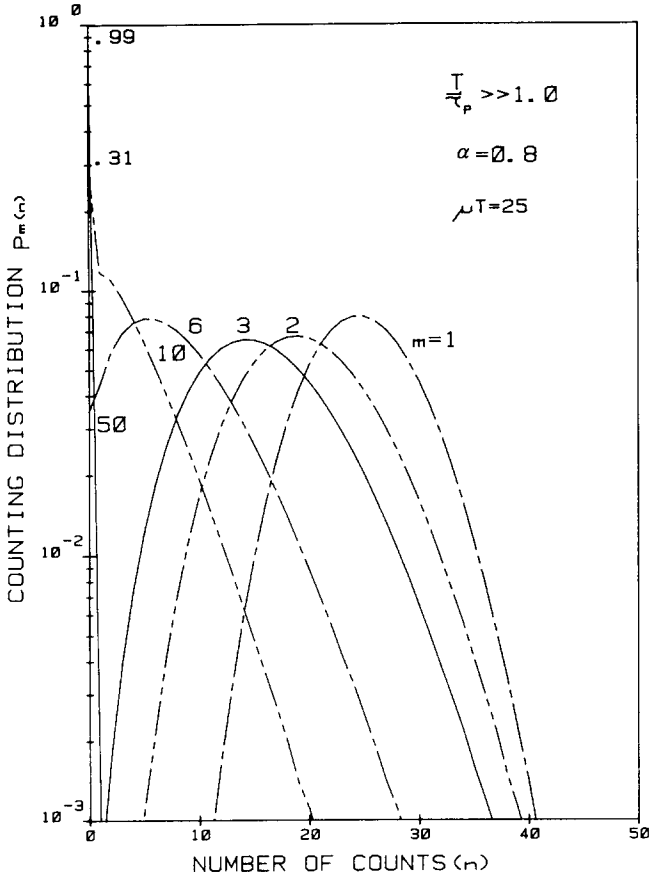
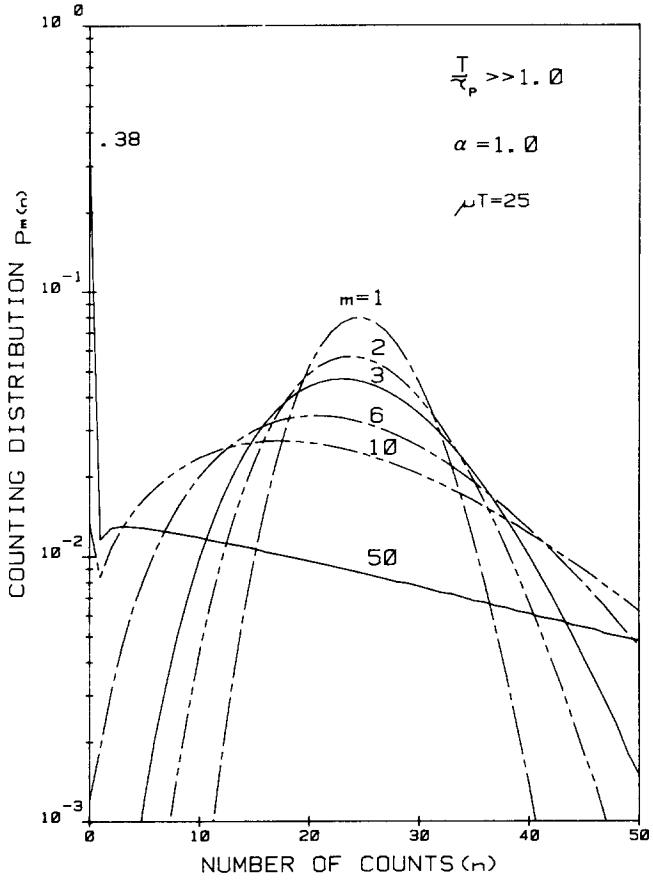


FIG. 4. Count mean $\langle N_m(T)\rangle$, count variance $\mathrm{Var}(N_m(T))$, and variance-to-mean ratio $\mathrm{Var}(N_m(T))/\langle N_m(T)\rangle$, vs number of stages m, with α as a parameter.



(a)



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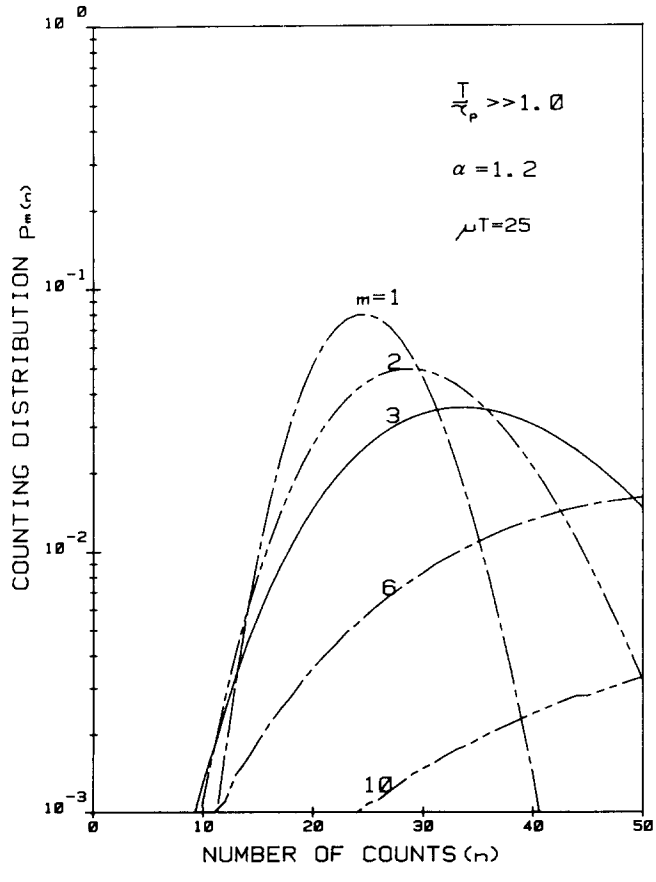


(c)

FIG. 5. Counting distribution $p_m(n)$ vs count number n for $T/\tau_p \gg 1.0$, $\mu T = 25$, and $m = 1,2,3,6,10$, and 50. (a) $\alpha = 0.8$; (b) $\alpha = 1.0$; (c) $\alpha = 1.2$.

and (37) yields the mean and variance

$$\langle N_m(t,T)\rangle = Eh_{m-1,T}(t) \overset{m-2}{\underset{j=1}{*}} h_j(t), \tag{42}$$

$$\mathrm{Var}(N_m(t,T)) = Eh_{m-1,T}(t) \overset{m-2}{\underset{j=1}{*}} h_j(t) + E\sum_{k=1}^{m-1} \overset{k-1}{\underset{j=1}{*}} h_j(t) * \left[h_{m-1,T}(t) \overset{m-2}{\underset{r=k}{*}} h_r(t)\right]^2. \tag{43}$$

The variance-to-mean ratio (Fano factor) is

$$F_m = 1 + \left\{\sum_{k=1}^{m-1} \overset{k-1}{\underset{j=1}{*}} h_j(t) * \left[h_{m-1,T}(t) \overset{m-2}{\underset{r=k}{*}} h_r(t)\right]^2 \Big/ h_{m-1,T}(t) \overset{m-2}{\underset{j=1}{*}} h_j(t)\right\}. \tag{44}$$

IV. BEHAVIOR OF THE COUNTING STATISTICS

In this section, we discuss the behavior of the counting distributions given by (17). For simplicity, we assume that the impulse response functions for all stages are identical exponential functions with areas α and time constants $\tau_p/2$, so that

$$h(t) = (2\alpha/\tau_p)\exp(-2t/\tau_p)u(t). \tag{45}$$

Here $u(t)$ is the unit step function.

In Fig. 4, we plot the count mean $\langle N_m(T)\rangle$, the count variance $\mathrm{Var}(N_m(t))$, and the ratio $F_m = \mathrm{Var}(N_m(T))/\langle N_m(T)\rangle$ versus the number of stages m, with α as a parameter, when $T/\tau_p \gg 1.0$. For $\alpha = 0.8\ (< 1.0)$, $\langle N_m(T)\rangle$ and $\mathrm{Var}(N_m(T))$ have exponentially decaying behavior for large m; however, the ratio F_m approaches a constant as m becomes large, as is evident from (24). This is the same as for the SNDP, or in fact for any two-stage multiplied process in which the first stage is Poisson.[6,17] This is clearly a result of the decrease in mean and variance at each stage.

For $\alpha = 1.0$, $\langle N_m(t)\rangle$ is independent of m, but $\mathrm{Var}(N_m(T))$ and F_m are identical, monotonically increasing functions of m, thereby transparently reflecting the broadening of the distributions as the number of stages increases. For $\alpha = 1.2$, the three functions, $\langle N_m(T)\rangle$, $\mathrm{Var}(N_m(T))$, and F_m are dramatically increasing functions of m, as expected from (21), (23), and (24).

In Fig. 5, we exhibit the behavior of the counting distributions at the output of the mth stage ($m = 1,2,3,6,10$, and 50), with $T/\tau_p \gg 1.0$, for three different values of α, with μT constant. In Fig. 5(a) ($\alpha = 0.8$), the distributions move to the left as the mean decreases, and the variance also decreases as m increases. This is apparent from (21) and (23). In Fig. 5(b) ($\alpha = 1.0$), the mean remains fixed, but the character of the distributions changes dramatically as the number of stages increases. This reflects the accentuation of the clustering in the process by increasing m. If we consider the curves for $m = 10$ and 50 in Fig. 5(b), small dips around $n = 1$ can be observed. It can be shown that under certain conditions for μ, T, α, and m, $p_m(1) < p_m(0)$ and $p_m(1) < p_m(2)$. In Fig. 5(c) ($\alpha = 1.2$), the distributions move to the right, and the variances increase as m increases (the case for $m = 50$ is not shown). This can be understood from (21) and (23).

The counting distributions for a large number of stages ($m = 50$) is shown in Fig. 6, when $T/\tau_p \gg 1.0$. The mean of the output count is fixed at 10, and α is a parameter. An increasingly flat counting distribution for $n \neq 0$.

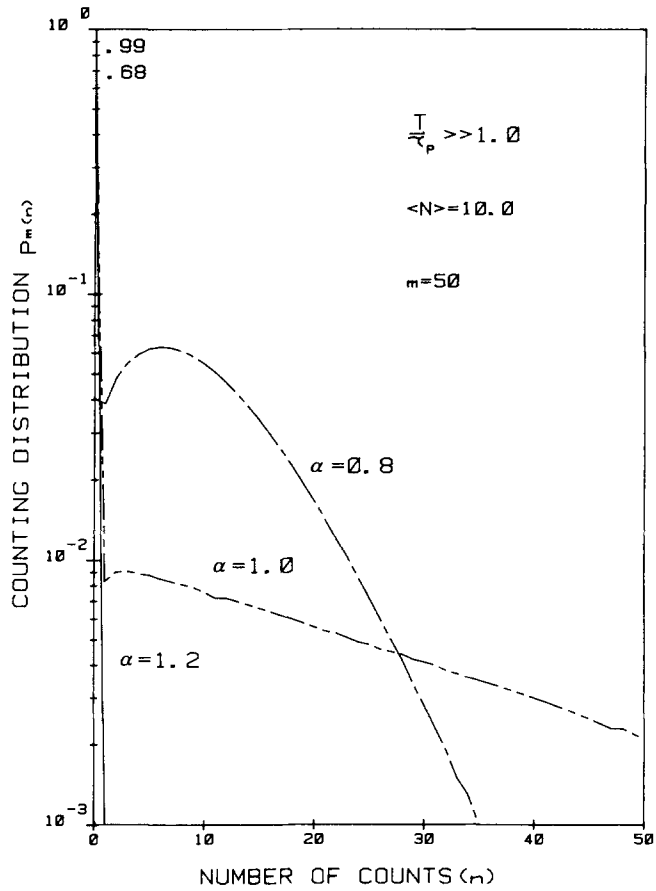


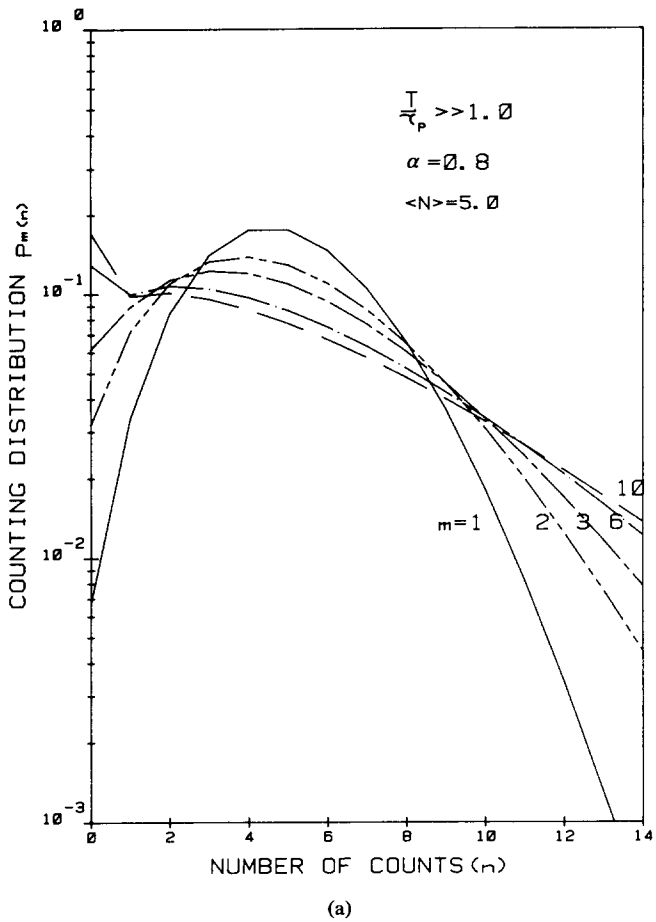
FIG. 6. Counting distribution $p_m(n)$ vs count number n for $m = 50$, $T/\tau_p \gg 1.0$, and $\langle N_m(T)\rangle = 10$.

In Fig. 7, we display the counting distributions for large T/τ_p with the output count mean $\langle N_m(T)\rangle$ fixed at 5, and with α as a parameter. Note that for fixed m, the distributions broaden as α increases. The distribution for large m and large α assumes a character resembling a delta function at $n = 0$,together with a flat component.

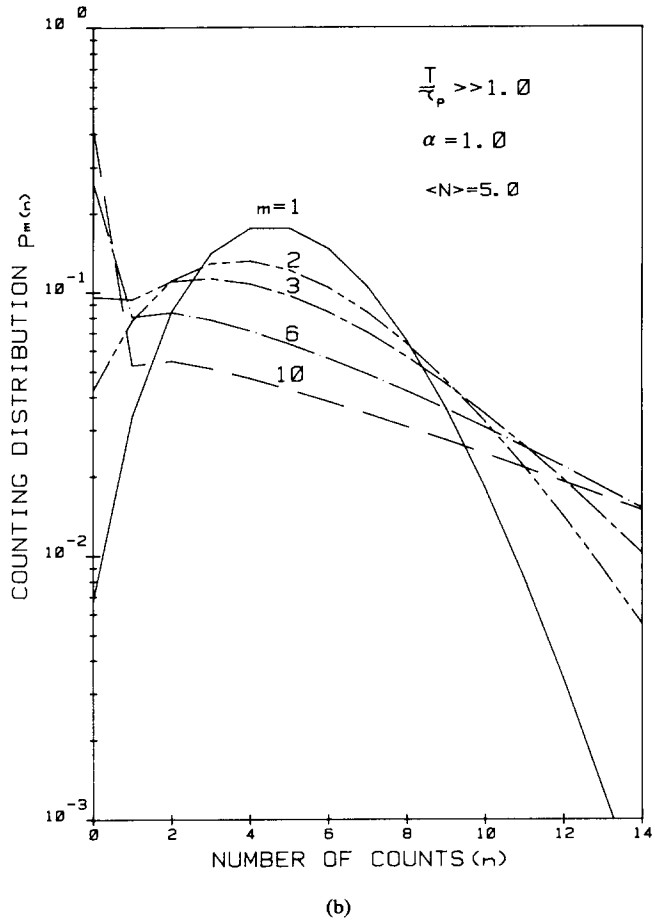
In Fig. 8, we display the dependence of the counting distributions on the ratio T/τ_p, the number of stages m, and the area of the impulse response function α. For all cases, the average number of counts $\langle N_m(T)\rangle$ is fixed at 5. In the limit where $\alpha T/\tau_p \ll 1.0$ and $T/\tau_p \ll 1.0$, the output of the first stage will be Poisson[13] so that, by induction, it is clear that the output of the cascade is also Poisson. Because of cumulative truncation and integration errors in the numerical calculations, it is quite difficult to obtain accurate counting statistics for arbitrary T/τ_p, for $m > 4$.

V. CONCLUSION

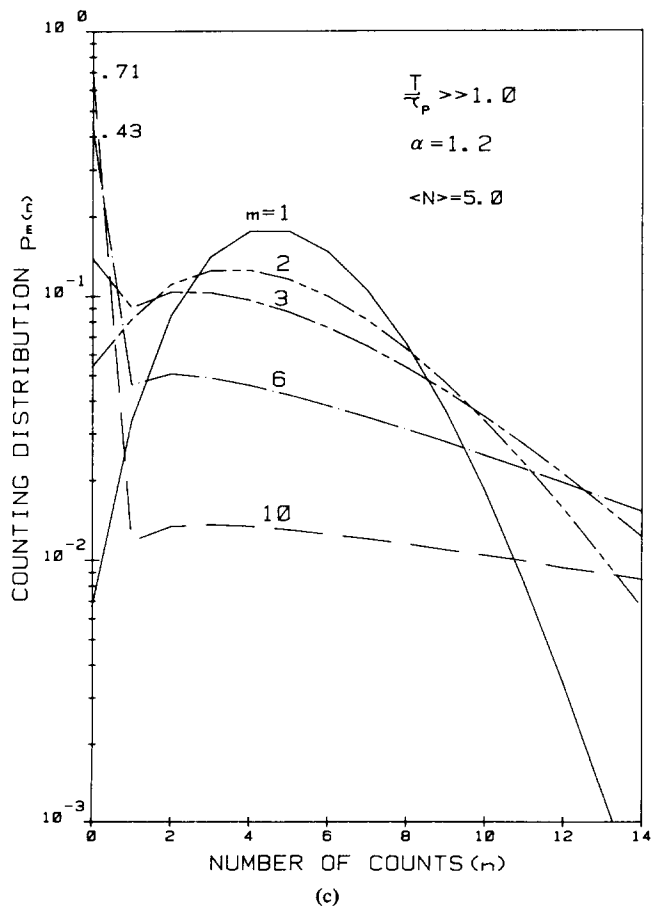
We have developed the statistics of a point process generated by a cascade of independent Poisson processes, and have found the moment generating function, as well as the counting and time statistics when dynamics are included.



(a)

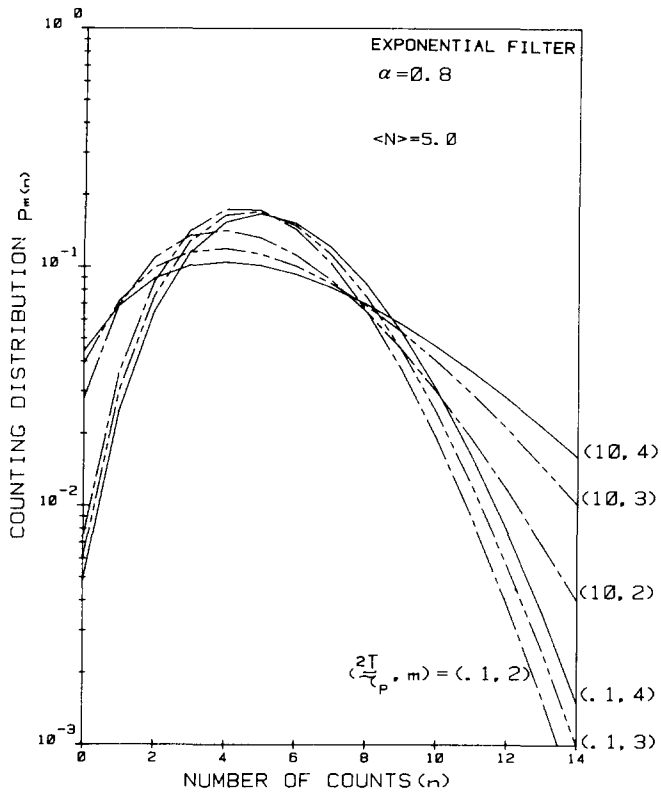


(b)

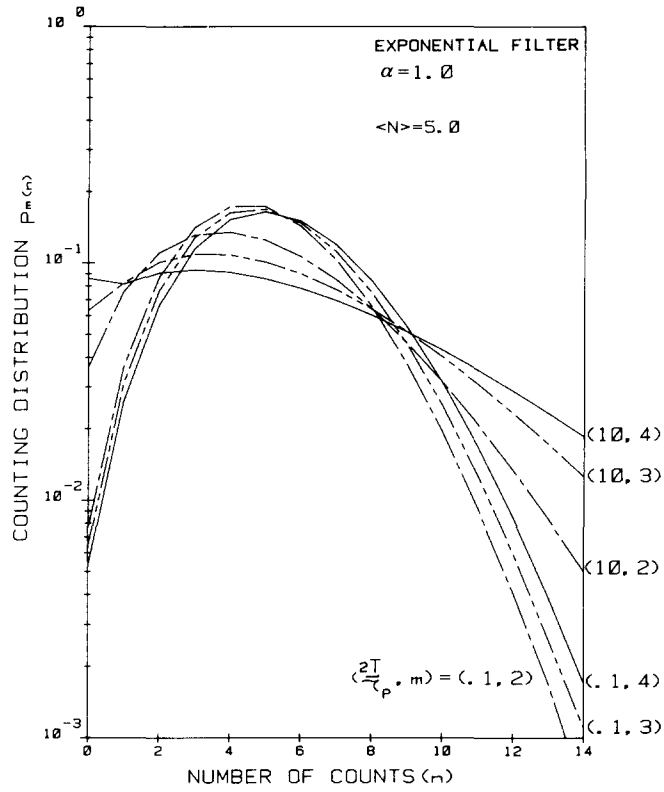


(c)

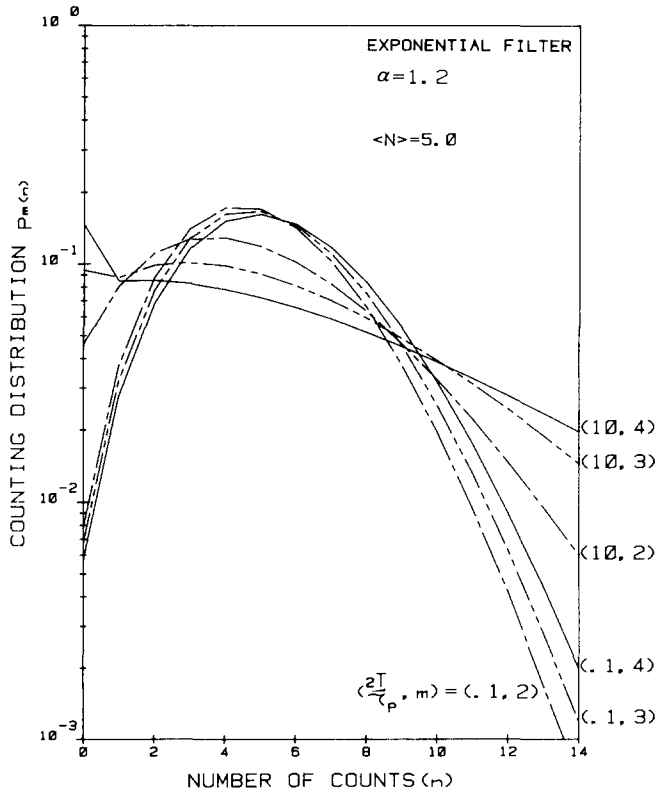
FIG. 7. Counting distribution $p_m(n)$ vs count number n for $T/\tau_p \gg 1.0$, $\langle N_m(T)\rangle = 5$, and $m = 1,2,3,6$, and 10. (a) $\alpha = 0.8$; (b) $\alpha = 1.0$; (c) $\alpha = 1.2$.



(a)



(b)



(c)

FIG. 8. Counting distribution $p_m(n)$ vs count number n with $2T/\tau_p$, m, and α as parameters. The impulse response function $h(t)$ is exponential with characteristic decay time $\tau_p/2$, and the mean count $\langle N_m(T)\rangle = 5.0$ for all cases. In the limit $T/\tau_p \to 0$, the counting distributions approach the Poisson, independent of m and α, whereas in the limit $T/\tau_p \to \infty$, the counting distributions approach those derived with instantaneous multiplication. (a) $\alpha = 0.8$; (b) $\alpha = 1.0$; (c) $\alpha = 1.2$.

Both the stationary and nonstationary cases have been considered. A simple expression for the variance-to-mean ratio at the mth stage has been obtained. We have carried out a parametric study of the counting distributions, by employing the DEC PDP 11/60 and IBM 4341 computers.

In some of the aforementioned applications of cascaded Poisson processes, a statistically independent additive Poisson point process may also be present, representing for example, broadband background light and/or thermionic emission in a photomultiplier tube. The counting statistics

for the superposition process can be simply determined by the use of numerical discrete convolution. Our approach may be useful for describing the detection of light by the human visual system at threshold.[23,24] We have applied a similar analysis to branching Poisson processes, in which all initiating events are included in the final point process. The results of this study will be reported shortly.[25]

ACKNOWLEDGMENTS

This work was supported by the Joint Services Electronics Program (U.S. Army, U.S. Navy, and U.S. Air Force) under Contract DAAG29-82-K-0080, and by the National Science Foundation under Grant ENG78-26498.

APPENDIX A: DERIVATION OF THE MOMENT GENERATING FUNCTIONAL FOR A FILTERED POISSON PROCESS AT THE jth STAGE

Let $\{X_j(t)\}$ be a filtered Poisson process in which points occur with intensity $\{X_{j-1}(t)\}$. The moment generating functional in the interval $(0,T)$ is given by[21]

$$L_{X_j}(s) \triangleq \left\langle \exp\left(-\int_0^T s(t) X_j(t)\, dt \right) \right\rangle, \tag{A1}$$

which is evaluated to be

$$L_{X_j}(s) = \left\langle \exp\left\{ \int_0^T X_{j-1}(t) \times \left[\exp\left(-\int_0^T h_j(\tau - t) s(\tau)\, d\tau \right) - 1 \right] dt \right\} \right\rangle. \tag{A2}$$

Proof: By using the conditional expectation and the property of the Poisson process, we have

$$L_{X_j|X_{j-1}}(s) = \text{the moment generating functional of } \{X_j(t)\} \text{ conditioned on the driving process } \{X_{j-1}(t)\}$$

$$= \text{Prob}(N_T = 0) + \sum_{k=1}^{\infty} \text{Prob}(N_T = k) \times \left\langle \exp\left\{ -\sum_{n=1}^{k} \int_0^T h_j(t - \tau_n) s(t)\, dt \right\} \middle| N_T = k \right\rangle, \tag{A3}$$

where $\text{Prob}(N_T = k)$ is the probability of having k events in $0 < t < T$. The summation within the expectation is unchanged by a random reordering of the occurrence times, $\tau_1, \tau_2, \ldots, \tau_k$. With this reordering, the occurrence times, given $N_T = k$, are independent and identically distributed, and the common density is

$$P_{\tau_n}(\tau) = X_{j-1}(\tau) \Big/ \int_0^T X_{j-1}(t)\, dt, \quad n = 1,2,\ldots,k.$$

Thus we obtain

$$\left\langle \exp\left\{ -\sum_{n=1}^{k} \int_0^T h_j(t - \tau_n) s(t)\, dt \right\} \middle| N_T = k \right\rangle = \left\{ \int_0^T X_j(\tau) \exp\left(-\int_0^T h_j(t - \tau) s(t)\, dt \right) d\tau \Big/ \int_0^T X_{j-1}(t)\, dt \right\}^k.$$

Substituting this expression into (A3), and using a straightforward calculation with the Poisson distribution provides

$$L_{X_j|X_{j-1}}(s) = \exp\left\{ \int_0^T X_{j-1}(t) \times \left[\exp\left(-\int_0^T h_j(\tau - t) s(\tau)\, d\tau \right) - 1 \right] dt \right\}. \tag{A4}$$

To remove the conditioning of the process $\{X_j(t)\}$, we average (A4) over $\{X_{j-1}(t)\}$, to obtain (A2). Finally, setting $t = -\infty$ (assuming the process starts at $-\infty$) and $T = \infty$, we have

$$L_{X_j}(s) = \left\langle \exp\left\{ \int_{-\infty}^{\infty} X_{j-1}(t) \times \left[\exp\left(-\int_{-\infty}^{\infty} h_j(\tau - t) s(\tau)\, d\tau \right) - 1 \right] dt \right\} \right\rangle. \tag{A5}$$

APPENDIX B: DERIVATION OF THE COUNTING DISTRIBUTION AT THE mth STAGE

Examining (13), we perform the following substitutions:

$$\theta_{m-1}(t,s) = -s h_{m-1,T}(-t), \quad m \geqslant 2 \tag{B1a}$$

and

$$\theta_j(t,s) = \int_{-\infty}^{\infty} h_j(\tau - t) [\exp(\theta_{j+1}(\tau,s)) - 1]\, d\tau, \quad j = 1,2,\ldots,m-2. \tag{B1b}$$

Then (13) becomes

$$Q_{W_m}(s) = \exp\left\{ \mu \int_{-\infty}^{\infty} [\exp(\theta_1(t,s)) - 1]\, dt \right\}. \tag{B2}$$

Taking the $(n+1)$st derivative, with respect to s, on both sides of (B2) yields

$$\frac{\partial^{n+1}}{\partial s^{n+1}} Q_{W_m}(s) = \mu \sum_{k=0}^{n} \binom{n}{k} \frac{\partial^{n-k}}{\partial s^{n-k}} Q_{W_m}(s) \times \frac{\partial^{k+1}}{\partial s^{k+1}} \int_{-\infty}^{\infty} \exp(\theta_1(t,s))\, dt. \tag{B3}$$

Using (16), together with the substitution

$$I^{(k+1)} = \frac{\partial^{k+1}}{\partial s^{k+1}} \int_{-\infty}^{\infty} \exp(\theta_1(t,s))\, dt \Big|_{s=1}, \tag{B4}$$

leads to a recurrence relation for the counting distribution at the mth stage, given by

$$(n+1) p_m(n+1) = \mu \sum_{k=0}^{n} \frac{(-1)^k}{k!} p_m(n-k) I^{(k+1)},$$

$$p_m(0) = Q_{W_m}(s)|_{s=1} = \exp\left\{ \mu \int_{-\infty}^{\infty} [\exp(\theta_1(t,s)) - 1]\, dt \right\} \Big|_{s=1}. \tag{B5}$$

Equation (B4) can be rewritten as

$$I^{(k+1)} = \frac{\partial^{k+1}}{\partial s^{k+1}} \int_{-\infty}^{\infty} \exp(\theta_1(t,s))\, dt \Big|_{s=1} = \int_{-\infty}^{\infty} \frac{\partial^{k+1}}{\partial s^{k+1}} \exp(\theta_1(t,s))\, dt \Big|_{s=1} = \int_{-\infty}^{\infty} D_1^{(k+1)}(t)\, dt. \tag{B6}$$

We have assumed that the order of integration and differentiation can be interchanged, and we have used the substitution

$$D_1^{(k+1)}(t) = \frac{\partial^{k+1}}{\partial s^{k+1}} \exp(\theta_1(t,s))\Big|_{s=1}. \tag{B7}$$

The $(k+1)$st derivative of the exponential function of (B1b) for $j=1$ yields

$$\frac{\partial^{k+1}}{\partial s^{k+1}} \exp(\theta_1(t,s)) = \sum_{r=0}^{k} \binom{k}{r} \frac{\partial^{k-r}}{\partial s^{k-r}} \exp(\theta_1(t,s)) \times \int_{-\infty}^{\infty} h_1(\tau - t) \frac{\partial^{r+1}}{\partial s^{r+1}} \exp(\theta_2(\tau,s))\, d\tau. \tag{B8}$$

Substituting (B8) into (B7) gives rise to

$$D_1^{(k+1)}(t) = \sum_{r=0}^{k} \binom{k}{r} D_1^{(k-r)}(t) \times \int_{-\infty}^{\infty} h_1(\tau - t) D_2^{(r+1)}(\tau)\, d\tau. \tag{B9}$$

Similarly

$$D_j^{(k+1)}(t) = \sum_{r=0}^{k} \binom{k}{r} D_j^{(k-1)}(t) \int_{-\infty}^{\infty} h_j(\tau - t) D_{j+1}^{(r+1)}(\tau)\, d\tau, \quad j = 1,2,\ldots,m-2, \tag{B10}$$

and

$$D_{m-1}^{(k)}(t) = \frac{\partial^k}{\partial s^k} \exp(\theta_{m-1}(t,s))\Big|_{s=1} = \{-h_{m-1,T}(-t)\}^k \exp\{-h_{m-1,T}(-t)\}. \tag{B11}$$

APPENDIX C: DERIVATION OF THE AUTOCOVARIANCE FUNCTION

From the Fourier transform (F.T.) of (30b) and (30c), we obtain

$$\tilde{U}_k(\omega,t_j) = [H^*(\omega)]^k \tilde{U}_0(\omega,t_j), \quad j = 1,2, \tag{C1}$$

where

$$\tilde{U}_0(\omega,t_j) = \text{F.T. of } U_0(t,t_j).$$

Similarly, the Fourier transform of (30d) and (30e) yields

$$\tilde{V}_k(\omega,t_1,t_2) = \sum_{r=0}^{k-1} \tilde{\psi}_r(\omega,t_1,t_2)[H^*(\omega)]^{k-r}, \tag{C2}$$

where

$$\tilde{\psi}_r(\omega,t_1,t_2) = \tilde{U}_r(\omega,t_1) * \tilde{U}_r^*(\omega,t_2).$$

Taking the inverse Fourier transform of (C1) and (C2), and substituting into (30a), results in (31).

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A generating integral for matrix elements of the Coulomb Green's function

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(Received 22 January 1982; accepted for publication 18 June 1982)

The generating integral $I_l(\lambda,\lambda';E) = \int d^3\mathbf{r}\, d^3\mathbf{r}' \exp(-\lambda r - \lambda' r')(rr')^{l-1}\, \overline{Y_{l,m}(\theta,\phi)}\, G(\mathbf{r},\mathbf{r}';E) \times Y_{l,m}(\theta',\phi')$ is evaluated, where the Coulomb Green's function G is the inverse $(E-H)^{-1}$ with H the hydrogenic Hamiltonian $-\frac{1}{2}\nabla^2 - Zr^{-1}$ and $Y_{l,m}$ is a spherical harmonic. The result can be used for the evaluation of matrix elements of G with respect to wave functions of the form $Y_{l,m}(\theta,\phi) f_{l,p}^{(\alpha)}(r)$ where $f_{l,p}^{(\alpha)}(r) = N_{l,p}^{(\alpha)} \exp(-ar/2)(ar)^l L_p^{(\alpha)}(ar)$ with $L_p^{(\alpha)}$ a Laguerre polynomial and $N_{l,p}^{(\alpha)}$ a normalizing factor. For general E the result is given in terms of a special case of the hypergeometric function which satisfies an inhomogeneous linear first-order ordinary differential equation. For $E = E_n$ where $E_n = -Z^2/(2n^2)$ is a hydrogenic bound state energy, G is replaced by the generalized Green's function (generalized inverse) and the results are given in closed form in terms of elementary functions.

PACS numbers: 02.70 + d, 32.90. + a

I. INTRODUCTION

A. Statement of the problem

The present work was motivated by the need to compute matrix elements of the generalized Coulomb Green's function (also known as the reduced Coulomb Green's function) for use in the computation of lower bounds to the eigenvalues of atomic Hamiltonians. The desired matrix elements were of the form

$$\int d^3\mathbf{r}\, d^3\mathbf{r}'\, \overline{\Psi_{l,m,p}^{(\alpha)}(\mathbf{r})} G(\mathbf{r},\mathbf{r}';E) \Psi_{l',m',p'}^{(\alpha)}(\mathbf{r}'), \tag{1.1}$$

where the Coulomb Green's function G is the inverse $(E-H)^{-1}$ with H the hydrogenic Hamiltonian

$$H = -\tfrac{1}{2}\nabla^2 - Zr^{-1}. \tag{1.2}$$

When $E = E_n$, where

$$E_n = -Z^2/(2n^2) \tag{1.3}$$

is an eigenvalue of H, G is the generalized inverse (generalized Green's function). The basis functions with respect to which matrix elements were needed are

$$\Psi_{l,m,p}^{(\alpha)}(\mathbf{r}) = Y_{l,m}(\theta,\phi) f_{l,p}^{(\alpha)}(r), \tag{1.4}$$

with

$$f_{l,p}^{(\alpha)}(r) = N_{l,p}^{(\alpha)} \exp(-ar/2)(ar)^l L_p^{(\alpha)}(ar), \tag{1.5}$$

where $Y_{l,m}$ is a spherical harmonic, $L_p^{(\alpha)}$ is a generalized Laguerre polynomial, and $N_{l,p}^{(\alpha)}$ is a normalizing factor.

B. Outline

Matrix elements of the form (1.1) can be evaluated from the generating integral

$$I_l(\lambda,\lambda';E) = \int d^3\mathbf{r}\, d^3\mathbf{r}' \exp(-\lambda r - \lambda' r') \times (rr')^{l-1}\, \overline{Y_{l,m}(\theta,\phi)} G(\mathbf{r},\mathbf{r}';E) Y_{l,m}(\theta',\phi') \tag{1.6}$$

by using the generating function

$$(1-\omega)^{-\alpha-1} \exp[-\eta\omega/(1-\omega)] = \sum_{p=0}^{\infty} \omega^p L_p^{(\alpha)}(\eta) \tag{1.7}$$

for the generalized Laguerre polynomials. The generating integral in (1.6) is essentially a Laplace transform of the radial Coulomb Green's function g_l, which appears in the partial wave expansion

$$G(\mathbf{r},\mathbf{r}';E) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{l,m}(\theta,\phi)\, \overline{Y_{l,m}(\theta',\phi')} g_l(r,r';E) \tag{1.8}$$

and satisfies the radial equation

$$(H_l - E) g_l(r,r';E) = -(rr')^{-1}\delta(r-r') \tag{1.9}$$

with H_l the radial Hamiltonian

$$H_l = -\frac{1}{2r}\frac{\partial^2}{\partial r^2} r + \frac{l(l+1)}{2r^2} - \frac{Z}{r}. \tag{1.10}$$

The differential operator H_l has a regular singular point at $r = 0$ and an irregular singular point at $r = \infty$; the solution of (1.9) is made unique by the boundary conditions

$$g_l(r,r';E) = O(r^l), \quad r \to 0 \tag{1.11}$$

and

$$g_l(r,r';E) = O(r^{-1+Z/\alpha} \exp(-\alpha r)), \quad \alpha = (-2E)^{1/2}, \quad r \to \infty. \tag{1.12}$$

The use of (1.8) in (1.6) yields

$$I_l(\lambda,\lambda';E) = \int_0^{\infty} dr \int_0^{\infty} dr' \times \exp(-\lambda r - \lambda' r')(rr')^{l+1} g_l(r,r';E), \tag{1.13}$$

which shows that I_l is the (double) Laplace transform of $(rr')^{l+1} g_l(r,r';E)$. Our results for I_l are obtained by Laplace transforming the differential equation (1.9) in r and r' to obtain an equation which can be solved (with appropriate boundary conditions) by solving a linear first-order ordinary differential equation. Results for the generalized Green's function which occurs when $E = E_n$ are obtained via a limiting procedure from the result for general E. Make the defini-

[a)] Work done in partial fulfillment of the requirements for the B. S. Degree with Distinction.

 0022-2488/82/122365-06$02.50

tions

$$g_{n,l}(r,r') \equiv \left[\frac{\partial}{\partial E}(E-E_n)g_l(r,r';E)\right]_{E=E_n} \tag{1.14}$$

and

$$I_{n,l}(\lambda,\lambda') \equiv \int_0^\infty dr \int_0^\infty dr' \times \exp(-\lambda r - \lambda' r')(rr')^{l+1} g_{n,l}(r,r'). \tag{1.15}$$

For $l \geqslant n$, $g_{n,l}(r,r')$ is just the ordinary radial Green's function $g_l(r,r';E_n)$ which satisfies (1.9), (1.11), and (1.12), with $E = E_n$. For $l \leqslant n-1$, the prescription (1.14) gives the generalized radial Green's function which satisfies

$$(H_l - E_n)g_{n,l}(r,r') = -(rr')^{-1}\delta(r-r') + R_{n,l}(r)R_{n,l}(r'), \tag{1.16}$$

the boundary conditions (1.11) and (1.12), and the orthogonality condition

$$\int_0^\infty R_{n,l}(r)g_{n,l}(r,r')r^2 dr = 0, \tag{1.17}$$

where the $R_{n,l}(r)$, given by

$$R_{n,l}(r) = 2Zn^{-2}[(n-l-1)!Z/(n+l)!]^{1/2} \times \exp(-Zr/n)(2Zr/n)^l L_{n-l-1}^{(2l+1)}(2Zr/n), \tag{1.18}$$

are the normalized bound state eigenfunctions of H_l. It follows from the prescription (1.14) for $g_{n,l}$ that

$$I_{n,l}(\lambda,\lambda') = \left[\frac{\partial}{\partial E}(E-E_n)I_l(\lambda,\lambda';E)\right]_{E=E_n}. \tag{1.19}$$

Equation (1.19) is the basis of the limiting procedure used when $E = E_n$. Section II records the general result for $I_l(\lambda,\lambda';E)$ and closed-form results for $I_{n,l}(\lambda,\lambda')$ for both the case $l \geqslant n$, where $g_{n,l}$ is the ordinary radial Green's function, and the case $l \leqslant n-1$, where $g_{n,l}$ is the generalized radial Green's function. Section III sketches the details of the computations.

C. Relation to previous work

Recent work of Johnson and Hirschfelder,[1] which was in turn based on earlier work by Hameka,[2] Hostler,[3] Sherstyuk,[4] and Laurenzi and Flamberg[5] showed that general closed-form expressions could be obtained for the $g_{n,l}(r,r')$. Closed-form expressions for $I_{n,l}(\lambda,\lambda')$ can be obtained from the Johnson–Hirschfelder[1] results for the $g_{n,l}$; in fact the result (2.6) for $I_{n,l}(\lambda,\lambda')$ when $l \geqslant n$ given in Sec. II was initially obtained, after a long and tedious calculation, from Johnson and Hirschfelder's Eq. (2.13). A few special cases of the general result (2.7) for $I_{n,l}(\lambda,\lambda')$ when $l \leqslant n-1$ were also obtained from Johnson and Hirschfelder's equation (2.18). We have, however, found it easier to obtain general results for $I_{n,l}(\lambda,\lambda')$ from (1.19), with $I_l(\lambda,\lambda';E)$ obtained by Laplace transforming the differential equation (1.9) for $g_l(r,r';E)$. The Johnson–Hirschfelder work was nevertheless an important starting point for us, because their results made it clear that a closed-form evaluation of $I_{n,l}$ is possible. The notation of the present paper is consistent with the notation of Johnson and Hirschfelder.

We are grateful to an unknown referee for pointing out that our general result (2.1) for I_l has been obtained previously by Zon, Manakov, and Rapoport[6] via a different method. Their $g_l(E;r,r')$ is the same as our $g_l(r,r';E)$ if one sets $m = d = 1$ in their formulas and uses their (4) to define g_l. Their result (8) then agrees with our (2.1). There is a sign discrepancy among their Eqs. (2), (3), and (4). The closed form results (2.6) and (2.7) for $\nu = n$ are, we believe, new. Related work by Maquet[7] and by Suffczynski and Swierkowski[8] was also called to our attention by the referee.

II. RESULTS

The general result for I_l is

$$I_l(\lambda,\lambda';E) = -2(2l+1)!(l-\nu+1)^{-1}[\nu/(2Z)]^{2l+3} \times [(\nu\lambda+Z)(\nu\lambda'+Z)/(4Z^2)]^{-2l-2} \times {}_2F_1(2l+2,l-\nu+1;l-\nu+2;1-\zeta), \tag{2.1}$$

$$\nu = Z(-2E)^{-1/2} \tag{2.2}$$

and

$$\zeta = 2\nu Z(\lambda+\lambda')[(\nu\lambda+Z)(\nu\lambda'+Z)]^{-1}, \tag{2.3}$$

with ${}_2F_1$ the hypergeometric function in standard notation. The integral representation

$${}_2F_1(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 t^{b-1} \times (1-t)^{c-b-1}(1-tz)^{-a}dt, \tag{2.4}$$

$\mathrm{Re}\, c > \mathrm{Re}\, b > 0$, $|\arg(1-z)| < \pi$, is a convenient definition of ${}_2F_1$ for our purposes. The inhomogeneous first-order differential equation

$$\left[(1-\zeta)\frac{d}{d\zeta} - (l-\nu+1)\right] \times {}_2F_1(2l+2,l-\nu+1;-l+2;1-\zeta) = -(l-\nu+1)\zeta^{-2l-2} \tag{2.5}$$

can be useful for the recursive computation of derivatives of I_l with respect to λ and/or λ'.

If E is an eigenvalue E_n, then $\nu = n$. When $\nu = n$ with $l \geqslant n$, the closed form result

$$I_{n,l}(\lambda,\lambda') = -2[n/(2Z)]^{2l+3}[(n\lambda+Z)(n\lambda'+Z)/(2Z)^2]^{-2l-2}(n+l)! \times \sum_{k=0}^{n+l}\frac{(k+l-n)!}{k!}\zeta^{n-k-l-1} \tag{2.6}$$

is obtained, with ζ given by (2.3) with $\nu = n$. When $\nu = n$ with $l \leqslant n-1$, the closed form result

$$I_{n,l}(\lambda,\lambda') = 2[n/(2Z)]^{2l+3}\frac{(l+n)!}{(n-l-1)!} \times \left\{[(n\lambda+Z)(n\lambda'+Z)/(4Z^2)]^{-2l-2} \times \left[-\frac{(n+l+1)}{2n}(1-\zeta)^{n-l} + \left(l n\zeta + \Psi(n+l+1) - \Psi(n-l) - \frac{(2l+3)}{2n}\right)(1-\zeta)^{n-l-1} + \frac{(n-l-1)}{2n}(1-\zeta)^{n-l-2}\right.\right.$$

$$+\sum_{k=0}^{n-l-2}\frac{(1-\zeta)^k}{n-l-1-k}$$
$$-(n-l-1)!$$
$$\times\sum_{k=0}^{2l}\frac{(2l-k)!}{(n+l-k)!}\zeta^{-2l-1+k}\Bigg]$$
$$+[(n\lambda+Z)(n\lambda'+Z)/(4Z^2)]^{-2l-3}$$
$$\times\Bigg[\frac{(n+l+1)}{2n}(1-\zeta)^{n-l-1}$$
$$-\frac{(n-l-1)}{2n}(1-\zeta)^{n-l-2}\Bigg]\Bigg\} \tag{2.7}$$

is obtained, with ζ again given by (2.3) with $\nu=n$. Ψ is the logarithmic derivative of the gamma function.

III. DETAILS

The derivation of the result (2.1), from which the other results follow, begins with the changes of variable

$$\xi\equiv 2Zr/\nu,\quad \xi'\equiv 2Zr'/\nu, \tag{3.1}$$

where ν is given by (2.2). For $E=E_n$, $\nu=n$ is used. Make the definitions

$$\gamma_l(\beta,\beta';E)\equiv\int_0^\infty d\xi\int_0^\infty d\xi'\exp(-\beta\xi-\beta'\xi')$$
$$\times(\xi\xi')^{l+1}g_l\left(\frac{\nu\xi}{2Z},\frac{\nu\xi'}{2Z};E\right), \tag{3.2}$$
$$\gamma_{n,l}(\beta,\beta')\equiv\int_0^\infty d\xi\int_0^\infty d\xi'\exp(-\beta\xi-\beta'\xi')$$
$$\times(\xi\xi')^{l+1}g_{n,l}\left(\frac{n\xi}{2Z},\frac{n\xi}{2Z}\right), \tag{3.3}$$

and

$$\rho_{n,l}(\beta)\equiv\int_0^\infty d\xi\,\xi^{l+1}\exp(-\beta\xi)R_{n,l}(n\xi/2Z). \tag{3.4}$$

It follows that the generating integrals I_l and $I_{n,l}$ are given by

$$I_l(\lambda,\lambda';E)=\left(\frac{\nu}{2Z}\right)^{2l+4}\gamma_l\left(\frac{\nu\lambda}{2Z},\frac{\nu\lambda'}{2Z};E\right) \tag{3.5}$$

and

$$I_{n,l}(\lambda,\lambda')=\left(\frac{n}{2Z}\right)^{2l+4}\gamma_{n,l}\left(\frac{n\lambda}{2Z},\frac{n\lambda'}{2Z}\right). \tag{3.6}$$

The formula (1.18) for obtaining $I_{n,l}$ from I_l becomes

$$\gamma_{n,l}\left(\frac{n\lambda}{2Z},\frac{n\lambda'}{2Z}\right)=\Bigg\{\Bigg[\frac{\beta}{n}\left(\frac{\partial}{\partial\beta}\right)_{\beta',\nu}+\frac{\beta'}{n}\left(\frac{\partial}{\partial\beta'}\right)_{\beta,\nu}$$
$$+\left(\frac{\partial}{\partial\nu}\right)_{\beta,\beta'}+\frac{4l+5}{2n}\Bigg]$$
$$\times\left[(\nu-n)\gamma_l\left(\beta,\beta';-\frac{Z^2}{2\nu^2}\right)\right]\Bigg\}_{\nu=n}. \tag{3.7}$$

Here $\nu=n$ implies that β and β' are to be evaluated at $\beta=n\lambda/(2Z)$, $\beta'=n\lambda'/(2Z)$.

We will now characterize γ_l and $\gamma_{n,l}$ by a differential equation. Define the differential operator $K_\beta(\nu)$ by

$$K_\beta(\nu)\equiv(\beta^2-\tfrac14)\frac{\partial^2}{\partial\beta^2}$$
$$+[2(l+2)\beta-\nu]\frac{\partial}{\partial\beta}+2(l+1). \tag{3.8}$$

It follows from (3.2), (3.8), and the differential equation (1.12) for g_l that γ_l satisfies the differential equation

$$K_\beta(\nu)\gamma_l\left(\beta,\beta';-\frac{Z^2}{2\nu^2}\right)=\frac{4Z(2l+2)!}{\nu(\beta+\beta')^{2l+3}}. \tag{3.9}$$

For $l\geqslant n$, $\gamma_{n,l}(\beta,\beta')=\gamma_l(\beta,\beta';-Z^2/(2n^2))$ satisfies the differential equation (3.9) with $\nu=n$. For $l\leqslant n-1$, (3.3), (3.4), (3.8), and the differential equation (1.16) for $g_{n,l}$ imply that $\gamma_{n,l}$ satisfies the differential equation

$$K_\beta(n)\gamma_{n,l}(\beta,\beta')=\frac{4Z(2l+2)!}{n(\beta+\beta')^{2l+3}}$$
$$-\frac{n^2}{2Z^2}\frac{\partial^2\rho(\beta)}{\partial\beta^2}\rho(\beta'). \tag{3.10}$$

Similarly it can be shown that

$$K_\beta(n)\rho_{n,l}(\beta)=0. \tag{3.11}$$

The orthogonality condition (1.17), which is needed to uniquely determine the generalized Green's function $g_{n,l}$ for $l\leqslant n-1$, implies that

$$\int_{-i\infty}^{i\infty}\sigma_{n,l}(-\beta)\gamma_{n,l}(\beta,\beta')d\beta=0, \tag{3.12}$$

where $\sigma_{n,l}(z)$ is determined by

$$\sigma_{n,l}(z)=\int_0^\infty\exp[-(z+\tfrac12)\xi]L_{n-l-1}^{(2l+1)}(\xi)\xi\,d\xi. \tag{3.13}$$

The contour is (3.12) runs along the imaginary axis. The generating function (1.7) for the generalized Laguerre polynomials can be used to show that

$$\sigma_{n,0}(z)=n(z+\tfrac12)^{-2}[(z-\tfrac12)/(z+\tfrac12)]^{n-1} \tag{3.14}$$

and that

$$\sigma_{n,l}(z)=(z+\tfrac12)^{-2}$$
$$\times\sum_{k=0}^{n-l-1}\binom{n+l-2-k}{n-l-1-k}(k+1)\left(\frac{z-\frac12}{z+\frac12}\right)^k,\quad l>1, \tag{3.15}$$

where

$$\binom{p}{q}\equiv p(p-1)(p-2)\ldots(p-q+1)/q! \tag{3.16}$$

is a binomial coefficient.

Boundary conditions are needed to make the solutions to (3.9)–(3.11) unique. The differential operator $K_\beta(\nu)$ has regular singular points at $\beta=-\frac12$, at $\beta=\frac12$, and at $\beta=\infty$, and can, if desired, be transformed into the hypergeometric operator. We will impose boundary conditions at $\beta=\frac12$ and at $\beta=\infty$. The method of Frobenius shows that the homogeneous equation

$$K_\beta(\nu)y(\beta)=0 \tag{3.17}$$

has solutions $y_1(\beta)$, $y_2(\beta)$ in the neighborhood of $\beta=\frac12$ with the behaviors

$$y_1(\beta)=O(1),\quad y_2(\beta)=O((\beta-1/2)^{-l+\nu-1}) \tag{3.18a}$$

for $\beta\to\frac12$ and solutions $y_3(\beta)$, $y_4(\beta)$ in the neighborhood of $\beta=\infty$ with the behaviors

$$y_3(\beta)=O(\beta^{-1}),\quad y_4(\beta)=O(\beta^{-2l-2}) \tag{3.18b}$$

for $\beta\to\infty$. We will show that y_2 and y_3 are not allowed; the

solutions of (3.9)–(3.11) must behave like y_1 for $\beta \to \frac{1}{2}$ and like y_4 for $\beta \to \infty$.

The Laplace transforms (3.2)–(3.4) define analytic functions of β in the domain in which the integrals converge. The boundary condition (1.14), which holds for $R_{n,l}(r)$ as well as $g_l(r,r';E)$, implies that $\rho_{n,l}(\beta)$ is an analytic function of β for $\mathrm{Re}\beta > -\frac{1}{2}$. For both r and r' large and $r \geqslant r'$, the boundary condition (1.14) plus the fact that the exponentially increasing solution is $O(r^{-1-Z/\alpha}\exp(\alpha r))$ for large r implies that

$$g_l(r,r';E) = O((rr')^{-1}(r/r')^{Z/\alpha}\exp[-\alpha(r-r')]), \quad r\to\infty, r'\to\infty, r\geqslant r'. \tag{3.19}$$

The generalized radial Green's function $g_{n,l}(r,r')$ also has the behavior (3.19) for large r and r'. It follows that $\gamma_l(\beta,\beta';E)$ and $\gamma_{n,l}(\beta,\beta')$ are analytic functions of β for $\mathrm{Re}\beta > \max(-\frac{1}{2}, -\mathrm{Re}\beta')$. In particular, $\rho_{n,l}$ is analytic at $\beta = \frac{1}{2}$, and γ_l and $\gamma_{n,l}$ are analytic at $\beta = \frac{1}{2}$ for $\mathrm{Re}\beta' > 0$. It follows that a solution which behaves likely $y_2(\beta)$, which is not analytic at $\beta = \frac{1}{2}$ except when $\nu = n$ with $n \geqslant l+1$, is not acceptable.

According to Watson's lemma,[9] the behavior of the Laplace transforms (3.2)–(3.4) for large β (large β') is determined by the behavior of g_l, $g_{n,l}$, and $\rho_{n,l}$ for small r (small r'), and may be computed by inserting a small r expansion (small r' expansion) and integrating term by term. This works because the factor $\exp(-\beta\xi)[\exp(-\beta'\xi')]$ cuts off the integral very rapidly for large β (large β'), so that only small ξ (small ξ') matters. For both r and r' small and $r \leqslant r'$, the boundary condition (1.13) plus the fact that the increasing solution is $O(r^{-l-1})$ for small r implies that

$$g_l(r,r';E) = O(r^l r'^{-l-1}), \quad r\to 0, r'\to 0, \quad r\leqslant r'. \tag{3.20}$$

It follows that

$$\gamma_l(\beta,\beta';E) = O((\beta\beta')^{-1}(\beta+\beta')^{-2l-1}),$$
$$\gamma_{n,l}(\beta,\beta') = O((\beta\beta')^{-1}(\beta+\beta')^{-2l-1}), \tag{3.21}$$
$$\beta\to\infty,\ \beta'\to\infty,$$

and that

$$\rho_{n,l}(\beta) = O(\beta^{-2l-2}), \quad \beta\to\infty. \tag{3.22}$$

It follows that a solution which behaves like $y_3(\beta)$ for $\beta \to \infty$ is not acceptable.

It will now be shown that the boundary conditions of (1) analyticity at $\beta = 1/2$ and (2) large β behavior given by (3.21) and (3.22) are enough to uniquely determine the solution γ_l to (3.9) except when $\nu = n$ with $n \geqslant l+1$, in which case these boundary conditions plus (3.12) uniquely determine the solution $\gamma_{n,l}$ to (3.10). The solution $y_1(\beta)$ to the homogeneous equation (3.17) can be taken to be

$$y_1(\beta) = C(\beta+\tfrac{1}{2})^{-1}{}_2F_1(-\nu-l,1;l-\nu+2; (\beta-\tfrac{1}{2})/(\beta+\tfrac{1}{2})), \tag{3.23}$$

where C is an arbitrary constant. The behavior of this y_1 for β large follows from the formula

$${}_2F_1(a,b;c;1) = \Gamma(c)\Gamma(c-a-b)[\Gamma(c-a)\Gamma(c-b)]^{-1}, \quad \mathrm{Re}(a+b-c)<0, \quad c\neq 0,-1,-2,..., \tag{3.24}$$

which implies that

$$y_1(\beta) = 0(\beta^{-1}), \quad \beta\to\infty \tag{3.25}$$

except when $\nu = n$ with $n \geqslant l+1$. It follows that γ_l is uniquely determined by (3.9) plus the boundary conditions (1) and (2) except when $\nu = n$ with $n \geqslant l+1$. When $\nu = n$ with $n \geqslant l+1$, the only solution to the homogeneous Eq. (3.17) which satisfies boundary conditions (1) and (2) is $C\rho_{n,l}(\beta)$ with C an arbitrary constant. The condition (3.12) fixes the amount of the homogeneous solution $\rho_{n,l}$ which can be added to a particular solution of (3.10) which satisfies the boundary conditions. It follows that $\gamma_{n,l}$ for $n \geqslant l+1$ is uniquely determined by (3.10), (3.12), and the boundary conditions (1) and (2).

We now look for a particular solution to (3.9) in the form

$$\gamma_l(\beta,\beta';E) = [(\beta+\tfrac{1}{2})(\beta'+\tfrac{1}{2})]^{-2l-2}F_{\nu,l}(\zeta) \tag{3.26}$$

with ζ given by

$$\zeta = (\beta+\beta')/[(\beta+\tfrac{1}{2})(\beta'+\tfrac{1}{2})]. \tag{3.27}$$

It is straightforward to show that (3.9) will be satisfied if

$$\left[(1-\zeta)\frac{d}{d\zeta} - (l-\nu+1)\right]F_{\nu,l}(\zeta) = \frac{4Z(2l+1)!}{\nu\zeta^{2l+2}}. \tag{3.28}$$

The boundary conditions of analyticity at $\beta = \frac{1}{2}$ and β^{-2l-2} fall-off at infinity will be satisfied if $F_{\nu,l}(\zeta)$ is analytic at $\zeta = 1$. The solution of the homogeneous version of (3.28) is $(1-\zeta)^{\nu-l-1}$, which is analytic at $\zeta = 1$ only if $\nu = n$ with $n \geqslant l+1$. The standard method for the solution of linear first-order ordinary differential equations then shows that the unique solution of (3.28) analytic at $\zeta = 1$ is

$$F_{\nu,l}(\zeta) = \frac{4Z}{\nu}(2l+1)!(1-\zeta)^{\nu-l-1} \times\int_1^\zeta \omega^{-2l-2}(1-\omega)^{l-\nu}d\omega. \tag{3.29}$$

The change of variables $\omega = 1 - t + \zeta t$ brings this to the form

$$F_{\nu,l}(\zeta) = -\frac{4Z}{\nu}(2l+1)!\int_0^1 t^{l-\nu}(1-t+\zeta t)^{-2l-2}dt. \tag{3.30}$$

The solution (3.29), or equivalently (3.30), is valid only for $\mathrm{Re}\,\nu < l+1$, because the integral diverges at $\omega = 1$ (at $t = 0$) for $\mathrm{Re}\,\nu \geqslant l+1$. The integral representations (3.29) and (3.30) can, however, be extended via analytic continuation in ν to obtain a solution of (3.28), analytic in ζ at $\zeta = 1$, for all complex ν except $\nu = n$ with $n \geqslant l+1$, where the analytic continuation in ν of $F_{\nu,l}$ has poles [as must happen because $g_l(r,r';E)$ has poles at $E = E_n$, i.e., at $\nu = n$, for $n \geqslant l+1$]. Comparison of (3.30) with (2.4) shows that

$$F_{\nu,l}(\zeta) = -4Z(2l+1)![\nu(l-\nu+1)]^{-1} \times{}_2F_1(2l+2,l-\nu+1;l-\nu+2;1-\zeta). \tag{3.31}$$

The general result (2.1) for I_l with ζ given by (2.3) now follows from (3.2), (3.26), (3.27), and (3.31). The differential equation (3.28) is equivalent to (2.5).

The results (2.6) and (2.7) for $\nu = n$ can be obtained from suitable transformations of $F_{\nu,l}(\zeta)$. The change of variables $t = (1+\zeta x)^{-1}$ in (3.30) brings it to the form

$$F_{\nu,l}(\zeta) = -\frac{4Z}{\nu}(2l+1)!\zeta^{-2l-1} \times \int_0^\infty (1+\zeta x)^{l+\nu}(1+x)^{-2l-2}dx. \quad (3.32)$$

Repeated integration by parts, which integrates $(1+x)^{-2l-3+k}$ and differentiates $(1+\zeta x)^{l+\nu-1+k}$ at the k th step, yields

$$F_{\nu,l}(\zeta) = -\left\{\sum_{j=0}^{2l}\frac{(2l-j)!\Gamma(l+\nu+1)}{\Gamma(l+\nu-j+1)}\zeta^{j-2l-1} + \frac{\Gamma(l+\nu+1)}{\Gamma(\nu-l)}J_{\nu,l}(\zeta)\right\}, \text{Re}\,\nu < l+1, \quad (3.33)$$

where $J_{\nu,l}(\zeta)$ is defined by

$$J_{\nu,l}(\zeta) = \int_0^\infty (1+\zeta x)^{\nu-l-1}(1+x)^{-1}dx. \quad (3.34)$$

For $\nu = n$ with $n \leqslant l$, the formula (3.33) reduces to

$$F_{n,l}(\zeta) = -\frac{4Z}{n}\sum_{j=0}^{n+l}\frac{(2l-j)!(l+n)!}{(l+n-j)!}\zeta^{j-2l-1}, \quad n \leqslant l. \quad (3.35)$$

The result (2.6) now follows from (3.5), (3.26), (3.27), and (3.35).

The case $\nu = n$ with $n \geqslant l+1$ requires additional work. The desired results can be obtained by analytic continuation of the integral representation (3.34) in ν. Use the change of variables $1+\zeta x = t^{-1}$ to bring (3.34) to the form

$$J_{\nu,l}(\zeta) = \int_0^1 t^{l-\nu}[1+(\zeta-1)t]^{-1}dt. \quad (3.36)$$

Make the definitions

$$\phi_{0,\nu}(t) = t^{l-\nu}, \quad (3.37)$$

$$\phi_{k,\nu}(t) \equiv \frac{t^{l+k-\nu}}{\prod_{j=1}^{k}(\nu-l-j)} - \sum_{j=0}^{k-1}\frac{(-t)^j}{j!(k-j-1)!(\nu-l-k+j)}, \quad k \geqslant 1. \quad (3.38)$$

With the aid of the partial fraction expansion

$$\frac{1}{\prod_{j=1}^{k}(\nu-l-j)} = \sum_{j=0}^{k-1}\frac{(-1)^j}{j!(k-j-1)!(\nu-l-k+j)} \quad (3.39)$$

it can be shown that

$$\int_t^1 \phi_{k,\nu}(t')dt' = \phi_{k+1,\nu}(t), \quad k \geqslant 0, \quad (3.40)$$

that

$$\phi_{k,\nu}(1) = 0, \quad k \geqslant 1, \quad (3.41)$$

and that $\phi_{k,\nu}(t)$ is an analytic function of ν at $\nu = l+j$, $1 \leqslant j \leqslant k$ despite the apparent poles at these values of ν. It can also be shown from (3.38) that

$$\phi_{k,\nu}(0) = -[(k-1)!(\nu-l-k)]^{-1}, \quad k \geqslant 1. \quad (3.42)$$

Repeated integration by parts which uses (3.37) and (3.40)–(3.42) and which always integrates $\phi_{k,\nu}(t)$ and differentiates $[1+(\zeta-1)t]^{-k-1}$ brings (3.36) to the form

$$J_{\nu,l}(\zeta) = -\sum_{j=1}^{n-l}\frac{(1-\zeta)^{j-1}}{\nu-l-j} + (n-l)!(l-\zeta)^{n-l}\int_0^1 \phi_{n-l,\nu}(t) \times [1+(\zeta-1)t]^{-n+l-1}dt, \quad n \geqslant l+1. \quad (3.43)$$

The formula (3.43) provides the analytic continuation in ν of $J_{\nu,l}(\zeta)$ from the domain $\text{Re}\,\nu < l+1$ in which (3.36) is valid to the larger domain $\text{Re}\,\nu < n+1$. It follows from (3.33) and (3.43) that, for $n \geqslant l+1$,

$$\lim_{\nu\to n}(\nu-n)F_{\nu,l}(\zeta) = \frac{4Z(n+l)!}{n(n-l-1)!}(1-\zeta)^{n-l-1} \quad (3.44)$$

and that

$$\lim_{\nu\to n}\frac{\partial}{\partial\nu}[(\nu-n)F_{\nu,l}(\zeta)] = \frac{4Z}{n}\left\{-(n+l)!\sum_{j=0}^{2l}\frac{(2l-j)!}{(n+l-j)!}\zeta^{-2l-1+j} + \frac{(n+l)!}{(n-l-1)!}(l-\zeta)^{n-l-1}[K_{n,l}(\zeta) + \Psi(n+l+1) - \Psi(n-l) - n^{-1}] + \frac{(n+l)!}{(n-l-1)!}\sum_{j=0}^{n-l-2}\frac{(1-\zeta)^j}{n-l-1-j}\right\}, \quad (3.45)$$

where

$$K_{n,l}(\zeta) \equiv (n-l)!(\zeta-1)\int_0^1 \phi_{n-l,n}(t) \times [1+(\zeta-1)t]^{-n+l-1}dt. \quad (3.46)$$

Here

$$\phi_{n-l,n}(t) = \lim_{\nu\to n}\phi_{n-l,\nu}(t) = -\frac{1}{(n-l-1)!}\left\{\ln t + \sum_{j=1}^{n-l-1}\left[j^{-1} + \binom{n-l-1}{j}\frac{(-t)^j}{j}\right]\right\}. \quad (3.47)$$

The sum in (3.47) is to be counted as zero for $n = l+1$.

It can be shown from (3.47) that

$$\phi_{n-l,n}(t) = -\frac{1}{(n-l-1)!}\left[\ln t + \sum_{j=1}^{n-l-1}\frac{(1-t)^j}{j}\right]. \quad (3.48)$$

It can be shown from either (3.47) or (3.48) that

$$\frac{d\phi_{n-l,n}(t)}{dt} = -\frac{(1-t)^{n-l-1}}{(n-l-1)!t}. \quad (3.49)$$

An integration by parts which uses (3.48) to show that $\phi_{n-l,n}(1)$ is zero brings (3.46) to the form

$$K_{n,l}(\zeta) = (n-l-1)!\int_0^1 \{[1+(\zeta-1)t]^{-n+l} - 1\} \times \frac{d\phi_{n-l,n}(t)}{dt}dt. \quad (3.50)$$

It follows from (3.49) and (3.50) that

$$\frac{dK_{n,l}(\zeta)}{d\zeta} = (n-l)\int_0^1 (1-t)^{n-l-1}[1+(\zeta-1)t]^{-n+l-1}dt$$

$$= \left\{ -\frac{1}{\zeta}\left[\frac{1-t}{1+(\zeta-1)t}\right]^{n-l} \right\}_{t=0}^{t=1} = \frac{1}{\zeta}, \tag{3.51}$$

and that

$$K_{n,l}(1) = 0. \tag{3.52}$$

Integrating (3.51) with the initial condition (3.52) yields

$$K_{n,l}(\zeta) = \ln\zeta. \tag{3.53}$$

The result (2.7) for $\nu = n$ with $n \geqslant l + 1$ now follows from (3.6), (3.7), (3.26), (3.27), (3.44), (3.45), and (3.53). The result obtained from (3.7) for $\gamma_{n,l}(\beta,\beta')$ with $n \geqslant l + 1$ has been checked by verifying that (3.10), (3.12), and the boundary conditions are all satisfied.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation under Grants No. PHY-7906936 and PHY-8106771 (Robert Nyden Hill) and under Grant No. SPI-8025439 Undergraduate Research Participation (Barton D. Huxtable).

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A direct approach to finding exact invariants for one-dimensional time-dependent classical Hamiltonians

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(Received 30 March 1982; accepted for publication 18 June 1982)

For a classical Hamiltonian $H = (1/2)p^2 + V(q,t)$ with an arbitrary time-dependent potential $V(q,t)$, exact invariants that can be expressed as series in positive powers of p, $I(q,p,t) = \Sigma_{n=0}^{\infty} p^n f_n(q,t)$, are examined. The method is based on direct use of the equation $dI/dt = \partial I/\partial t + [I,H] = 0$. A recursion relation for the coefficients $f_n(q,t)$ is obtained. All potentials that admit an invariant quadratic in p are found and, for those potentials, all invariants quadratic in p are determined. The feasibility of extending the analysis to find invariants that are polynomials in p of higher degree than quadratic is discussed. The systems for which invariants quadratic in p have been found are transformed to autonomous systems by a canonical transformation.

PACS numbers: 03.20. + i

I. INTRODUCTION

Time-dependent linear systems with Hamiltonians of the form

$$H = \tfrac{1}{2}p^2 + V(q,t) \tag{1.1}$$

are of considerable interest in various fields, for example in plasma physics. The degree of interest may be gauged by the number of workers who have searched by various means for invariants for systems of the type described by (1.1). To mention but a few, reference is made to the works of Lutzky,[1] Sarlet,[2–4] Sarlet and Bahar,[5,6] Ray,[7,8] Ray and Reid,[9,10] and Prince and Eliezer,[11] as well as to some contributions by the present writers: Lewis,[12–14] Leach,[15–17] and Lewis and Leach.[18,19]

Recently there has been some criticism[6] of the practice of determining invariants (used throughout this note solely in the sense of first integral or constant of the motion) via the generators of symmetry transformations, which is the case when Noether's theorem or the method of the Lie theory of extended groups is employed. The basis of the criticism is that such a procedure is roundabout. Certainly this is so if there is no interest in the associated algebra of the group of generators of symmetry transformations or if the group is of no interest in itself.

In this paper we discuss a direct method for constructing invariants for systems of the type (1.1) and, in Secs. II and III, we apply the method to find explicitly all invariants that are either linear or quadratic in the momentum p. Only certain potentials $V(q,t)$ admit such invariants, and we determine those potentials explicitly. In Sec. IV, we give some examples of invariants quadratic in p and we comment on the case of polynomial invariants in p of degree higher than two in Sec. V. In Sec. VI, we use a canonical transformation to transform the systems for which we have invariants quadratic in p into autonomous systems. We present some concluding remarks in Sec. VII.

Any invariant satisfies the fundamental defining equation

$$\frac{dI}{dt} = \frac{\partial I}{\partial t} + [I,H] = \frac{\partial I}{\partial t} + \frac{\partial I}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial I}{\partial p}\frac{\partial H}{\partial q} = 0. \tag{1.2}$$

We assume a formal power series expansion in p of the invariant,

$$I(q,p,t) = \sum_{n=0}^{\infty} p^n f_n(q,t). \tag{1.3}$$

In general, such a series would not have an infinite radius of convergence in p. The functions $f_n(q,t)$ are determined by the conditions obtained by substituting (1.3) into the defining equation (1.2) and setting the coefficient of p^n equal to zero for each n. This yields a system of differential equations that the functions $f_n(q,t)$ must satisfy:

$$\frac{\partial f_n}{\partial t} + \frac{\partial f_{n-1}}{\partial q} - (n+1)f_{n+1}\frac{\partial V}{\partial q} = 0. \tag{1.4}$$

Equation (1.4) may be considered as a recursion relation,

$$f_{n+1} = \frac{\dfrac{\partial f_n}{\partial t} + \dfrac{\partial f_{n-1}}{\partial q}}{(n+1)\dfrac{\partial V}{\partial q}}, \tag{1.5}$$

from which in principle each f_n, for $n > 0$, could be calculated in terms of f_0 and its derivatives. This point of view has not been productive.

In the present application, we concentrate on the cases in which the series for $I(q,p,t)$ terminates to give an invariant that is either linear in p or quadratic in p. Some consideration is given to the case in which the invariant is a polynomial in p of degree higher than two. It turns out that $I(q,p,t)$ can be linear in p only if $V(q,t)$ is quadratic in q; a much wider class of potentials can be treated if the invariant is allowed to be quadratic in p.

The Hamiltonian (1.1) is sufficient for treating all Hamiltonians of the form

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$$H = a(t)p^2 + b(q,t)p + c(q,t) \tag{1.6}$$

because (1.1) may be obtained from (1.6) by the generalized canonical transformation[20]

$$Q = q, \quad P = p + \frac{b}{2a}, \quad T = \int^t a(t')dt', \tag{1.7}$$

provided that T is monotonic. By discussing the general case (1.6) through the simpler intermediate case (1.1), the calculations are simplified.

II. INVARIANTS LINEAR IN p

If the invariant is linear in p,

$$I(q,p,t) = pf_1(q,t) + f_0(q,t), \tag{2.1}$$

then, with H as given in (1.1), the equation defining the invariant, Eq. (1.2), becomes

$$p^2\frac{\partial f_1}{\partial q} + p\left(\frac{\partial f_0}{\partial q} + \frac{\partial f_1}{\partial t}\right) + \frac{\partial f_0}{\partial t} - f_1\frac{\partial V}{\partial q} = 0. \tag{2.2}$$

The coefficient of each power of p may be equated to zero to give the system of partial differential equations

$$\frac{\partial f_1}{\partial q} = 0, \tag{2.3}$$

$$\frac{\partial f_0}{\partial q} + \frac{\partial f_1}{\partial t} = 0, \tag{2.4}$$

$$\frac{\partial f_0}{\partial t} - f_1\frac{\partial V}{\partial q} = 0. \tag{2.5}$$

From (2.3),

$$f_1 = a(t), \tag{2.6}$$

where, because of the assumed form of I, $a(t)$ is not identically zero. By substituting this into (2.4), we obtain

$$f_0 = b(t) - \dot{a}q, \tag{2.7}$$

whence (2.5) becomes

$$\dot{b} - \ddot{a}q - a\frac{\partial V}{\partial q} = 0. \tag{2.8}$$

By integrating this last equation with respect to q, we find that the potential must be

$$V(q,t) = c(t) + \frac{\dot{b}q}{a} - \frac{\ddot{a}q^2}{2a}. \tag{2.9}$$

The additive function of time $c(t)$ may be ignored, and we can state the result for invariants linear in p as follows. The Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{\dot{b}q}{a} - \frac{\ddot{a}q^2}{2a} \tag{2.10}$$

has the invariant linear in p given by

$$I = ap + b - \dot{a}q, \tag{2.11}$$

and this Hamiltonian is the only one that possesses an invariant linear in p.

As a simple example of a Hamiltonian of this type, we consider the time-dependent linear oscillator,

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2(t)q^2. \tag{2.12}$$

Comparing (2.12) with (2.10) we see that b is identically zero and that

$$\ddot{a} + \omega^2(t)a = 0. \tag{2.13}$$

From (2.13) it is evident that there are two linearly independent solutions for $a(t)$. In terms of the solution[21] of an auxiliary equation

$$\ddot{\rho} + \omega^2(t)\rho = 1/\rho^3, \tag{2.14}$$

the solution set for (2.13) is

$$\left\{a(t) = \rho\sin T, \rho\cos T; T = \int^t \rho^{-2}(t')dt'\right\}. \tag{2.15}$$

Thus, there are two linearly independent invariants of the form (2.11), viz.,

$$I_1 = p\rho\cos T - \left(\dot{\rho}\cos T - \frac{1}{\rho}\sin T\right)q, \tag{2.16}$$

$$I_2 = p\rho\sin T - \left(\dot{\rho}\sin T + \frac{1}{\rho}\cos T\right)q. \tag{2.17}$$

Because these expressions can be inverted to give

$$q = I_1\rho\sin T - I_2\rho\cos T, \tag{2.18}$$

$$p = I_1\left(\dot{\rho}\sin T + \frac{1}{\rho}\cos T\right) - I_2\left(\dot{\rho}\cos T - \frac{1}{\rho}\sin T\right), \tag{2.19}$$

I_1 and I_2 clearly relate to the initial conditions and (2.16) and (2.17) may be called the initial condition integrals. It is evident that a similar result applies to the general potential (2.9).

III. INVARIANTS QUADRATIC IN p

We now assume the invariant to be quadratic in p,

$$I(q,p,t) = p^2f_2(q,t) + pf_1(q,t) + f_0(q,t). \tag{3.1}$$

Following the same procedure as in Sec. II for invariants linear in p, we find that the functions f_0, f_1, f_2, and V are required to satisfy the system of partial differential equations

$$\frac{\partial f_2}{\partial q} = 0, \tag{3.2}$$

$$\frac{\partial f_1}{\partial q} + \frac{\partial f_2}{\partial t} = 0, \tag{3.3}$$

$$\frac{\partial f_0}{\partial q} - 2f_2\frac{\partial V}{\partial q} + \frac{\partial f_1}{\partial t} = 0, \tag{3.4}$$

$$-f_1\frac{\partial V}{\partial q} + \frac{\partial f_0}{\partial t} = 0. \tag{3.5}$$

From (3.2) and (3.3) we find

$$f_2 = 2a(t), \quad f_1 = b(t) - 2\dot{a}(t)q, \tag{3.6}$$

where $a(t)$ and $b(t)$ are arbitrary functions. Substituting for f_2 and f_1 in (3.4) we obtain

$$\frac{\partial f_0}{\partial q} - 4a\frac{\partial V}{\partial q} + \dot{b} - 2\ddot{a}q = 0, \tag{3.7}$$

which can be integrated immediately to give

$$V(q,t) = \frac{1}{4a}\left[f_0(q,t) - \ddot{a}q^2 + \dot{b}q\right] + g(t), \tag{3.8}$$

where $g(t)$ is an arbitrary function. Thus (3.5) becomes

$$(2\dot{a}q - b)\left(\frac{\partial f_0}{\partial q} - 2\ddot{a}q + \dot{b}\right) + 4a\frac{\partial f_0}{\partial t} = 0. \tag{3.9}$$

Equation (3.9) is a linear, first-order, partial differential equation for f_0 whose characteristic equations are

$$\frac{dq}{dt} = \frac{1}{4a}(2\dot{a}q - b), \tag{3.10}$$

$$\frac{df_0}{dt} = \frac{(2\dot{a}q - b)(2\ddot{a}q - \dot{b})}{4a} = \frac{d}{dt}\left[\frac{1}{2a}\left(\dot{a}q - \frac{1}{2}b\right)^2\right]. \tag{3.11}$$

The solution of the characteristic equations is

$$u = \frac{q}{a^{1/2}} + \frac{1}{4}\int^t \frac{b(t')}{a^{3/2}(t')}dt', \tag{3.12}$$

$$v = f_0(q,t) - \frac{1}{2a}\left(\dot{a}q - \frac{1}{2}b\right)^2, \tag{3.13}$$

where u and v are constant along the characteristics. Therefore, the general solution of (3.9) is

$$f_0(q,t) = G\left(\frac{q}{a^{1/2}} + \frac{1}{4}\int^t \frac{b(t')}{a^{3/2}(t')}dt'\right) + \frac{1}{2a}(\dot{a}q - \tfrac{1}{2}b)^2, \tag{3.14}$$

where G is an arbitrary function.

Now we have determined the potentials for which an invariant quadratic in p exists and we have determined the invariants. A convenient way of expressing the result is in terms of functions ρ, α, and $\tilde{G}$ defined by

$$\rho = 2a^{1/2}, \tag{3.15}$$

$$-\frac{\alpha}{\rho} = \frac{1}{8}\int^t \frac{b(t')}{a^{3/2}(t')}dt', \tag{3.16}$$

$$\tilde{G}(x) = G(2x). \tag{3.17}$$

The result is that an invariant quadratic in p exists if and only if the potential is of the form

$$V(q,t) = \left(\frac{\ddot{\rho}\alpha}{\rho} - \ddot{\alpha}\right)q - \frac{1}{2}\frac{\ddot{\rho}}{\rho}q^2 + \frac{1}{\rho^2}\tilde{G}\left(\frac{q-\alpha}{\rho}\right), \tag{3.18}$$

where ρ, α and $\tilde{G}$ are arbitrary functions of their arguments. We have chosen the irrelevant function $g(t)$ such that no additive function of t appears in the potential. The invariant quadratic in p that is associated with this potential is

$$I(q,p,t) = \frac{1}{2}[\rho(p - \dot{\alpha}) - \dot{\rho}(q - \alpha)]^2 + \tilde{G}\left(\frac{q-\alpha}{\rho}\right). \tag{3.19}$$

Another convenient way of expressing the result is the following. The potentials for which there exists an invariant quadratic in p have the form

$$V(q,t) = -F(t)q + \tfrac{1}{2}\Omega^2(t)q^2 + \frac{1}{\rho^2}U\left(\frac{q-\alpha}{\rho}\right), \tag{3.20}$$

where U is an arbitrary function of its argument, and where F, Ω^2, ρ, and α are arbitrary functions that satisfy

$$\ddot{\rho} + \Omega^2(t)\rho - \frac{k}{\rho^3} = 0, \tag{3.21}$$

$$\ddot{\alpha} + \Omega^2(t)\alpha = F(t), \tag{3.22}$$

and k is an arbitrary constant. Now we have chosen the irrelevant function $g(t)$ such that no additive function of t appears in this form of the potential. The invariant quadratic in p that is associated with this potential is

$$I(q,p,t) = \tfrac{1}{2}[\rho(p - \dot{\alpha}) - \dot{\rho}(q - \alpha)]^2 + \frac{1}{2}k\left(\frac{q-\alpha}{\rho}\right)^2 + U\left(\frac{q-\alpha}{\rho}\right). \tag{3.23}$$

This invariant is more general in form than those reported in Refs. 1–18. The main reason for this greater generality is that there are two arbitrary time-dependent functions, $\rho(t)$ and $\alpha(t)$. The invariant (3.23) for the potential (3.20) can also be obtained by considering a certain transformed Ermakov system.[22]

The result can be viewed in two ways. The first is, given a potential, can it be written in the form (3.20) or (3.18)? If so, then our invariant applies. The second is constructive in nature: given functions ρ, α, and U, the invariant can be constructed and the associated Hamiltonian deduced.

IV. SOME EXAMPLES OF INVARIANTS QUADRATIC IN p

Before considering the problem of finding invariants that are polynomials in p of higher degree than two, it will be instructive to consider some examples. First we take the case of the time-dependent linear oscillator whose Hamiltonian is

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\omega^2(t)q^2; \tag{4.1}$$

this problem has been of great interest. We can obtain (4.1) from (3.18) by taking α equal to zero and

$$\tilde{G}(x) = \tfrac{1}{2}x^2. \tag{4.2}$$

This leads to the familiar differential equation for $\rho(t)$,

$$\ddot{\rho} + \omega^2(t)\rho - 1/\rho^3 = 0. \tag{4.3}$$

A closely related problem is the time-dependent linear oscillator to which has been added a centrifugal force. The Hamiltonian is

$$H = \tfrac{1}{2}p^2 + \omega^2(t)q^2 + K/q^2, \tag{4.4}$$

where K is a constant. We can obtain this by taking α equal to zero and

$$\tilde{G}(x) = \tfrac{1}{2}x^2 + K/x^2. \tag{4.5}$$

Again ρ satisfies (4.3).

As an example of a problem that is not some variant of the harmonic oscillator, we consider the Emden equation,

$$\ddot{x} + \frac{2}{t}\dot{x} + x^5 = 0. \tag{4.6}$$

This can be converted to the reduced form

$$\ddot{q} + q^5/t^4 = 0 \tag{4.7}$$

by the transformation

$$q = tx. \tag{4.8}$$

A Hamiltonian for (4.7) is

$$H = \tfrac{1}{2}p^2 + q^6/6t^4. \tag{4.9}$$

We can obtain this Hamiltonian by taking α equal to zero and choosing

$$\tilde{G}(x) = \tfrac{1}{2}kx^2 + \beta x^6, \tag{4.10}$$

where $\rho(t)$ and the constants k and β must satisfy

$$\rho\ddot{\rho} - k/\rho^2 = 0, \tag{4.11}$$

$$\beta\rho^{-8} = 1/6t^4. \tag{4.12}$$

These conditions can be satisfied by choosing

$$\beta = \tfrac{1}{6}, \quad \rho^{-2} = t, \quad k = -\tfrac{1}{4}. \tag{4.13}$$

From (3.19), the invariant is

$$I(q,p,t) = \tfrac{1}{2}[tp^2 - pq + q^6/3t^3], \tag{4.14}$$

in agreement with the result given by Sarlet and Bahar.[5]

V. POLYNOMIAL INVARIANTS IN p OF HIGHER DEGREE

It would be useful to have invariants for a wider class of potentials than we have been able to treat with invariants quadratic in p. All invariants that are polynomials in p are determined by (1.3) and (1.4). For a polynomial of a given degree, one can obtain expressions for all of the functions $f_n(q,t)$ in terms of $V(q,t)$ and its integrals, arbitrary functions of t, and powers of q by integrating with respect to q the equations (1.4) for which $n \neq 0$. Substitution of the expression for f_1 and f_0 into the equation (1.4) for which $n = 0$,

$$\frac{\partial f_0}{\partial t} - f_1 \frac{\partial V}{\partial q} = 0, \tag{5.1}$$

yields a consistency relation that $V(q,t)$ must satisfy in order that there exist an invariant that is a polynomial in p of the given degree. Unlike the cases in which the invariant is linear or quadratic in p, this consistency relation is nonlinear, the amount of nonlinearity increasing with the degree. Explicit formulas analogous to those given in Secs. II and III have not been obtained.

VI. CANONICAL TRANSFORMATION INTERPRETATION FOR INVARIANTS QUADRATIC IN p

We can transform the systems for which we have invariants quadratic in p into autonomous systems as follows. We make the canonical transformation specified by

$$Q = \frac{q - \alpha}{\rho}, \tag{6.1}$$

$$P = [\rho(p - \dot{\alpha}) - \dot{\rho}(q - \alpha)]. \tag{6.2}$$

With this canonical transformation, which is given in terms of the old variables and time, the new Hamiltonian K is given by[18]

$$K = H + P\frac{\partial Q}{\partial t} + \frac{\partial F}{\partial t}. \tag{6.3}$$

A generating function F for this transformation is

$$F(q,t) = \frac{1}{2}\frac{\dot{\rho}}{\rho}q^2 + \left(\dot{\alpha} - \frac{\dot{\rho}}{\rho}\alpha\right)q. \tag{6.4}$$

The new Hamiltonian may be taken to be

$$K = \frac{1}{\rho^2}\left[\frac{1}{2}P^2 + \tilde{G}(Q)\right], \tag{6.5}$$

where we have dropped an irrelevant function of t alone. If we further transform the time variable from t to T according to

$$T = \int^t \rho^{-2}(t')dt', \tag{6.6}$$

then the Hamiltonian becomes

$$K(Q,P,T) = \tfrac{1}{2}P^2 + \tilde{G}(Q), \tag{6.7}$$

which is exactly the invariant (3.19) written in terms of the new variables. It is interesting to note that the coordinate transformation is a linear point transformation and that the momentum transformation is that which is induced by the (q,t) to (Q,T) transformation.

VII. CONCLUSION

We have investigated potentials for which there exist invariants that are polynomials in the momentum by direct application of the fundamental definition of an invariant, (1.2). We have found the class of potentials for which there exists an invariant that is linear or quadratic in the momentum. For those potentials we have also found the invariants explicitly. The case of invariants that are polynomials in the momentum of degree higher than two has not been solved explicitly. Finally, for the case of invariants quadratic in the momentum, we have found a canonical transformation that transforms the system to an autonomous system.

ACKNOWLEDGMENT

This work was performed under the auspices of the United States Department of Energy.

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Linear Hamiltonian systems are integrable with quadratics

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(Received 16 December 1981; accepted for publication 30 June 1982)

A new proof of a theorem of Williamson on the complete integrability of time-independent, real, linear Hamiltonian differential equations with quadratic integrals is given. The sets where these integrals are functionally dependent are explicitly found.

PACS numbers: 03.20. + i, 02.20.Sv, 02.30.Hq

I. INTRODUCTION

In spite of its long and colorful history, classical mechanics has been unable either to solve the system of differential equations or completely describe the behavior of solutions of general mechanical problems. The only exceptions are the well-known completely integrable systems like the heavy symmetric spinning top, the problem of attraction by two fixed centers, etc.[1,2]

Complete integrability is the exception rather than the rule; in fact, such systems are not generic in the set of all Hamiltonian systems.[3] Nevertheless, during the past several years there has been a surge of activity and excitement as new completely integrable systems were discovered. This interest heightened when seemingly unrelated examples like the Toda lattice, the geodesic flow on semisimple Lie groups and the infinite-dimensional Hamiltonian system of the Korteweg–de Vries equation could be treated uniformly.[4]

In the light of these new developments it is natural to reconsider the question of complete integrability of linear Hamiltonian differential equations. Since linear differential equations can be readily solved, it is hardly surprising that they are completely integrable. In 1930 Wintner conjectured that they are integrable with *quadratic* functions and this was proved by Williamson in 1940.[5]

The real symplectic group acts on its Lie algebra naturally by conjugation, called the adjoint action, as follows:

$$\mathrm{Sp}(n,\mathbb{R})\times sp(n,\mathbb{R}) \to sp(n,\mathbb{R}),$$
$$(P,A) \mapsto P^{-1}AP.$$

Equivalence classes of time-independent, real, linear Hamiltonian systems up to canonical transformations can be identified with the orbits of this adjoint action. Representatives of these orbits are called normal forms. It suffices to prove the complete integrability of systems in normal form only.

After giving a precise formulation of the normal form problem, we present a complete list of normal forms specifically designed for our purposes. Since Williamson the normal form question has been studied by many authors; the interested reader is referred to Refs. 5–7. We conclude with a new proof of the theorem of Williamson by explicitly exhibiting a sufficient number of quadratic integrals and determining the sets on which they are functionally dependent.

II. THE NORMAL FORM PROBLEM

In this section we give an invariant characterization of real, linear, time-independent Hamiltonian differential equations and a precise algebraic statement of the normal form problem.

Let V be an n-dimensional vector space over the real numbers $\mathbb{R}$. The group of all linear automorphisms of V, under composition, is called the general linear group $\mathrm{GL}(n,\mathbb{R})$. Its Lie algebra, the general linear algebra $gl(n,\mathbb{R})$, is the set of all endomorphisms of V with Lie bracket given by $[A,B] = A\circ B - B\circ A$ for $A,B \in gl(n,\mathbb{R})$.

A bilinear mapping $\omega: V\times V \to \mathbb{R}$ is called *symplectic* if for all $x, y \in V$ it has the properties

(i) $\omega(x,y) = -\omega(y,x)$, that is, ω is skew symmetric;

(ii) the linear mapping

$$\omega^{\#}: V \to V^{*} : x \mapsto \omega(x,\cdot)$$

is an isomorphism, that is, ω is nondegenerate, where V^{*} denotes the dual space of V.

Note that the nondegeneracy of ω forces V to be even dimensional. The pair (V,ω) is called a symplectic vector space.

The *real symplectic group* $\mathrm{Sp}(n,\mathbb{R})$ is defined to be the subgroup of $\mathrm{GL}(2n,\mathbb{R})$ of all elements which leave ω invariant, that is,

$$\omega(Ax,Ay) = \omega(x,y). \tag{1}$$

Similarly, the Lie subalgebra of $gl(2n,\mathbb{R})$ of all elements satisfying

$$\omega(Ax,y) + \omega(x,Ay) = 0 \tag{2}$$

is called the *real symplectic algebra* $sp(n,\mathbb{R})$. The elements of $\mathrm{Sp}(n,\mathbb{R})$ and of $sp(n,\mathbb{R})$ are called, respectively, *symplectic* and *infinitesimally symplectic* linear mappings. The matrix analogs of the defining equations (1) and (2) can be written as

$$\hat{A}\,{}^{t}\omega^{\#}A = \omega^{\#}, \tag{3}$$

$$\hat{A}\,{}^{t}\omega^{\#} + \omega^{\#}A = 0 \tag{4}$$

and the matrix of $\omega^{\#}$ can be chosen to be

$$\begin{bmatrix} 0 & -I_n \\ +I_n & 0 \end{bmatrix},$$

where I_n is the $n\times n$ identity matrix in an appropriate basis of V, called a *symplectic basis*.

Let $H: V \to \mathbb{R}$ be a quadratic form on (V,ω) given by $H(x) = \frac{1}{2}\tilde{H}(x,x)$ where $\tilde{H}$ is a symmetric bilinear form. Differentiating H gives a linear mapping $DH: V \to V^{*}$ defined by $x \mapsto \tilde{H}(x,\cdot)$, which is symmetric. The symplectic gradient of H is the real linear map

$$X_H: V \to V : x \mapsto (\omega^{\#})^{-1}DH(x)$$

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on (V,ω); it is the real linear Hamiltonian vector field associated to H. A curve $\gamma:\mathbb{R}\to V$ is an integral curve of this Hamiltonian vector field if and only if, for $t\in\mathbb{R}$,

$$\frac{d}{dt}\gamma(t)=X_H(\gamma(t)). \tag{5}$$

In a symplectic basis of V if we let $x=(p,q)$ with $x\in V$ and p,q are n-vectors, then Eq. (5) can be written as

$$\frac{d}{dt}\begin{bmatrix}p\\q\end{bmatrix}=\begin{bmatrix}0 & I_n\\ -I_n & 0\end{bmatrix}\begin{bmatrix}D_1H(p,q)\\D_2H(p,q)\end{bmatrix}, \tag{6}$$

where $(D_1H(p,q), D_2H(p,q))$ is the matrix of $DH(p,q)$. The system of differential equations (6) is the usual form of Hamilton's equations.

Proposition 2.1[6]: Let $Q(V,\mathbb{R})$ be the vector space of quadratic functions on V, a $2n$-dimensional real vector space. The map

$$K: sp(n,\mathbb{R})\to Q(V,\mathbb{R}): A\mapsto K(A),$$
$$K(A)x=\omega(Ax,x)$$

is an isomorphism of vector spaces and its inverse is given by

$$K^{-1}: Q(V,\mathbb{R})\to sp(n,\mathbb{R}): H\mapsto X_H.$$

Example: Let $x=(x_1,x_2,x_3,x_4)$ and $H(x)=\frac{1}{2}x_2^2+x_1x_4$. The associated Hamiltonian vector field X_H at x is given by

$$X_H(x)=(\omega^{\#})^{-1}DH(x)$$
$$=\left[\begin{array}{ccc|c}&&&1\\&&&0\quad 1\\\hline -1&&&\\0&-1&&\end{array}\right]\begin{bmatrix}x_4\\x_2\\0\\x_1\end{bmatrix}=\left[\begin{array}{c}0\\x_1\\\hline -x_4\\-x_2\end{array}\right].$$

The matrix of the linear transformation $x\mapsto X_H(x)$ is the infinitesimally symplectic matrix corresponding to H and it is equal to

$$X_H=\left[\begin{array}{ccc|ccc}0&&&&&\\1&0&&&&\\\hline 0&&&0&-1&\\0&-1&&&0&\end{array}\right].$$

Conversely, we can recover H from X_H as follows:

$$H(x)=\tfrac{1}{2}x\omega^{\#}X_Hx^t$$
$$=\tfrac{1}{2}[x_1,x_2,x_3,x_4]\left[\begin{array}{ccc|c}&&&-1\\&&&0\quad -1\\\hline 1&&&\\0&1&&\end{array}\right]$$
$$\cdot\left[\begin{array}{ccc|c}0&&&\\1&0&&\\\hline 0&&0&-1\\0&-1&&0\end{array}\right]\begin{bmatrix}x_1\\x_2\\x_3\\x_4\end{bmatrix}$$
$$=\tfrac{1}{2}x_2^2+x_1x_4.$$

Proposition 2.2[6]: The elements of $\mathrm{Sp}(n,\mathbb{R})$ are the canonical transformations of real linear Hamiltonian systems $sp(n,\mathbb{R})$ and

$$P^{-1}X_H\,P=X_{H\circ P},$$

where $H\circ P$: $V\to\mathbb{R}: x\mapsto H(Px)$.

Two elements X_H and $X_{H'}$ of $sp(n,\mathbb{R})$ are said to be *symplectically* conjugate if there exists a $P\in\mathrm{Sp}(n,\mathbb{R})$ such that $P^{-1}X_H\,P=X_{H'}$. Symplectic conjugacy is an equivalence relation and determining a representative of each equivalence class is the normal form problem for real linear Hamiltonian differential equations.

III. LIST OF NORMAL FORMS

This section contains the statement of the normal form theorem along with a list of normal forms. To facilitate the presentation we begin with several algebraic concepts.[6]

Consider the pair $(A\,|\,W,W)$ where $A\in sp(n,\mathbb{R})$ and W is an ω-nondegenerate, A-invariant subspace of a $2n$-dimensional symplectic vector space (V,ω). Two pairs $(A_1|W_1,W_1)$ and $(A_2|W_2,W_2)$ are *equivalent* if and only if there is a real symplectic mapping $P\in\mathrm{Sp}(n,\mathbb{R})$ such that $P(W_2)=W_1$ and $(P^{-1}A_1P)|W_2=A_2|W_2$. An equivalence class of pairs is called a *type*.

Suppose that the pair $(A\,|\,W,W)$ is an element of the type, say Δ, and there are proper A-invariant, ω-nondegenerate, ω-orthogonal subspaces W_1 and W_2 such that $W=W_1\oplus W_2$. Then we write $\Delta=\Delta_1+\Delta_2$ where $(A\,|\,W_i,W_i)\in\Delta_i$ for $i=1,2$. A type Δ is an *indecomposable* type if it cannot be written as the sum of two types.

Theorem 3.1: Every type is the sum of indecomposable types which are uniquely determined up to the order of the summands. Furthermore, List I contains all possible indecomposable types.

For the proof of this theorem, which is rather long and intricate linear algebra, the reader is referred to Burgoyne and Cushman[6] and Kocak.[7]

In order to simplify the later matrix computations, a little more linear algebra is needed.

A linear endomorphism S of V is called *semisimple* if for every S-invariant subspace U of V there is an S-invariant subspace W such that $V=U\oplus W$. Since the field of real numbers is not algebraically closed semisimple linear transformations, in general, are not diagonalizable. A linear endomorphism N of V is called *nilpotent of index m* if $N^m\neq 0$ on V, but $N^{m+1}=0$.

Proposition 3.2[8]: Let $A\in\mathrm{End}(V)$, the set of linear endomorphisms of V. Then,

(i) There exist *unique* $S,N\in\mathrm{End}(V)$ satisfying the conditions $A=S+N$, S is semisimple, N is nilpotent, S and N commute.

(ii) There exist polynomials p, q in one indeterminate, without constant terms, such that $S=p(A)$ and $N=q(A)$. In particular, S and N commute with any endomorphism which commutes with A.

The decomposition $A=S+N$ is called the (additive) *Jordan–Chavelley decomposition* of A; S and N are called, respectively, the semisimple and the nilpotent parts of A. If A is infinitesimally symplectic, so are its semisimple and nilpotent parts.[6]

If $A=N+S$ with N having index of nilpotency m, then m is called the *height* of $(A,V)\in\Delta$ and it is an invariant of the type Δ.

If λ is an eigenvalue of $A\in sp(n,\mathbb{R})$, then $-\lambda$, $\bar{\lambda}$, and $-\bar{\lambda}$ are also eigenvalues of A. This fact is called the infini-

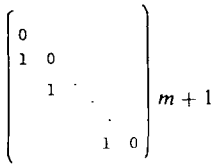
tesimally symplectic eigenvalue theorem.[1]

Finally, ϵ is a parameter with possible values $+1$ or -1.

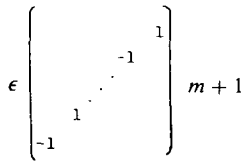
In local problems of Hamiltonian mechanics the standard form of the symplectic form is almost sacred. Unfortunately, in the symplectic basis most of the necessary matrix computations become unmanageably cumbersome. In order to overcome these problems, in the following list the bases of the underlying vector spaces are chosen so that matrices of nilpotent parts become the classical Jordan normal form and the matrices of semisimple parts are piecewise diagonal. In these new bases the matrix of the symplectic form ω is no longer the standard one. Matrices of the new symplectic form are included in the list as well. If necessary, using the results of Kocak[7] the theorems we prove can be pulled back to the standard symplectic basis.

LIST I. Indecomposable types of linear Hamiltonian systems

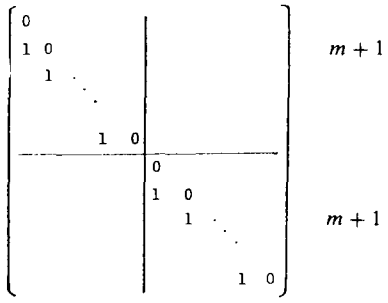
(1) *Eigenvalue*: 0 (zero),
Height: m, odd,
Jordan–Chavelley decomposition: $A = N$ (no semisimple part),



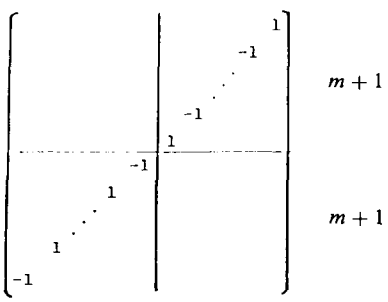
Matrix of ω:



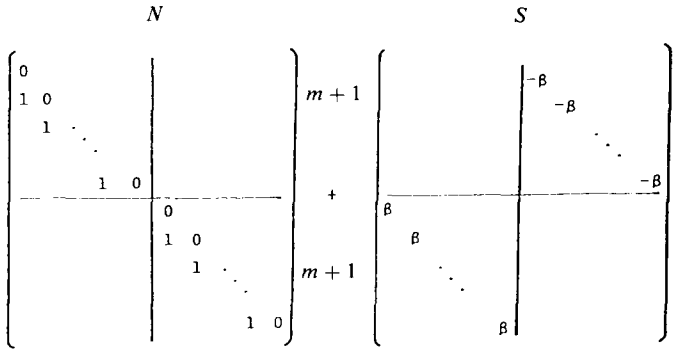
(2) *Eigenvalue*: 0 (zero),
Height: m, even,
Jordan–Chavelley decomposition: $A = N$ (no semisimple part),



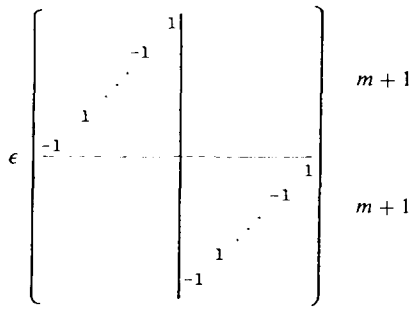
Matrix of ω:



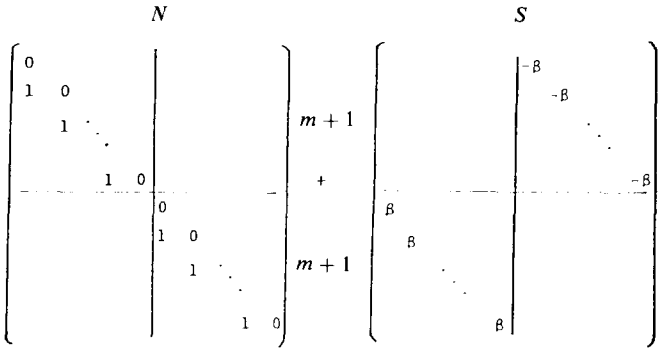
(3) *Eigenvalues*: $i\beta$, $-i\beta$ ($\beta > 0$, real),
Height: m, odd,
Jordan–Chavelley decomposition: $A = N + S$,



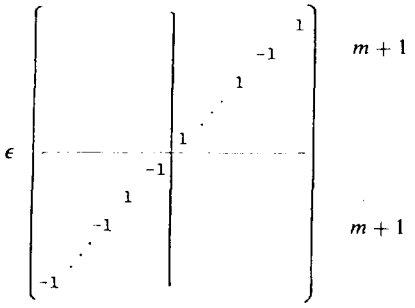
Matrix of ω:



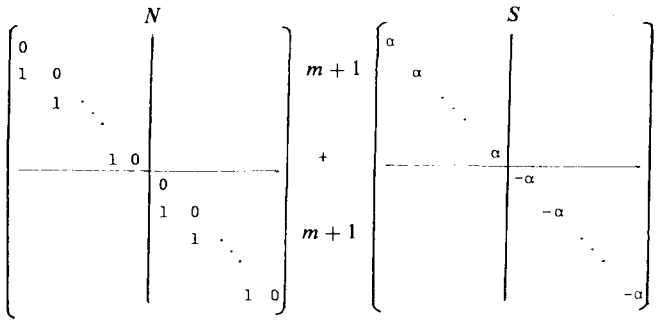
(4) *Eigenvalues*: $i\beta$, $-i\beta$ ($\beta > 0$, real),
Height: m, even,
Jordan–Chavelley decomposition: $A = N + S$



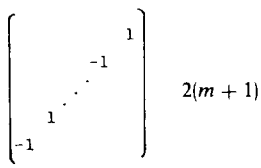
Matrix of ω:



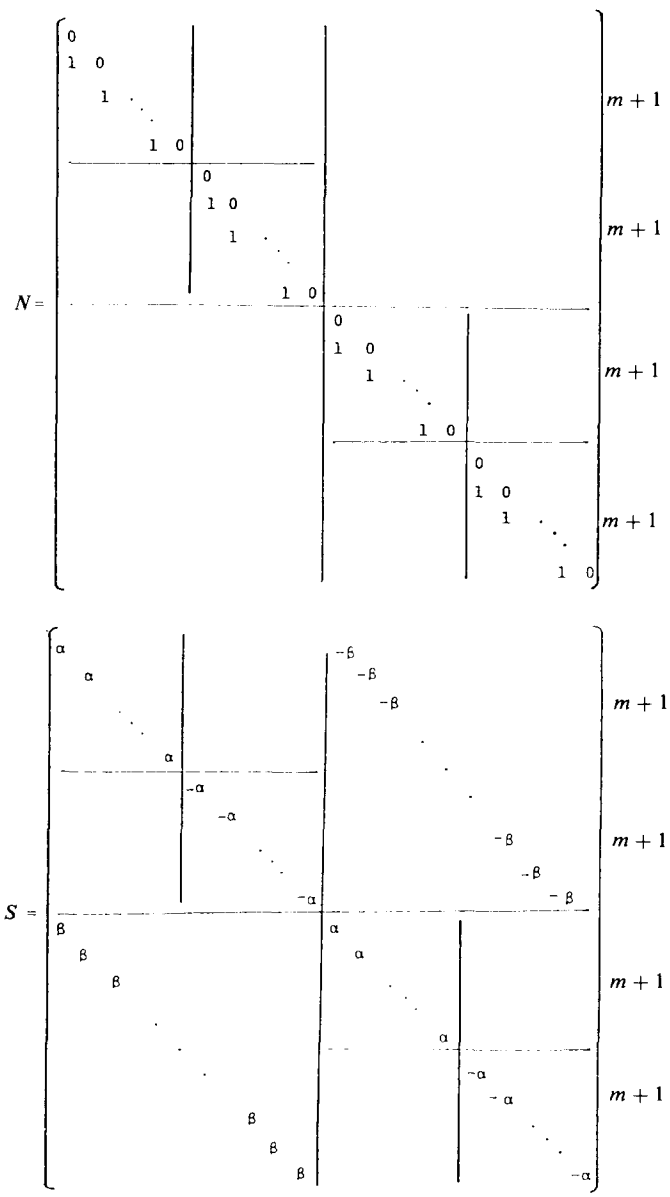
(5) *Eigenvalues*: α, $-\alpha$ ($\alpha > 0$, real),
Height: m (odd or even),
Jordan–Chavelley decomposition: $A = N + S$,



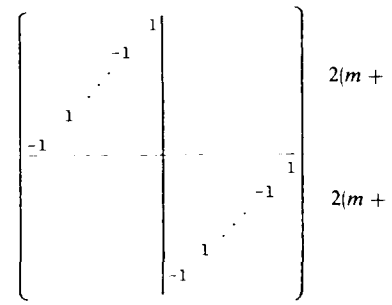
Matrix of ω:



(6) *Eigenvalues*: $\alpha + i\beta, \alpha - i\beta, -\alpha - i\beta, -\alpha + i\beta\ (\alpha > 0, \beta > 0)$,
Height: m (odd or even),
Jordan–Chavelley decomposition: $A = N + S$,



Matrix of ω:



It is evident from the previous list that an indecomposable type is determined by three invariants (m,λ,ϵ) where m is the height, λ is an eigenvalue, and ϵ is ± 1. Since from Theorem 3.1 every type can be uniquely written as the sum of indecomposable types, the unordered sequence $\{(m_i,\lambda_i,\epsilon_i)\}$ is a complete set of invariants for the conjugacy class of $A \in sp(n,\mathbb{R})$ and we say that A is of type $\{(m_i,\lambda_i,\epsilon_i)\}$. In practice, however, one usually deals with a specific Hamiltonian and faces the problem of conjugating it to a normal form given in List I. Burgoyne and Cushman[6] devised a constructive algorithm to resolve this question.

IV. COMPLETE INTEGRABILITY

This section contains a brief account of the notion of complete integrability in Hamiltonian mechanics adapted to our purposes. For a general discussion of this topic in a global and more geometric setting the interested reader is referred to the Refs. 1 and 2.

The *Poisson bracket* $\{H,F\}$ of two real-valued differentiable functions on (V,ω), a symplectic real vector space of dimension $2n$, is another such function given by

$$\{H,F\} = dH \cdot X_F.$$

Let $F_1,\ldots,F_k$ be *first integrals* of the motion of the Hamiltonian H, that is $\{H,F_i\} = 0$ for all $1 \leqslant i \leqslant k$. The set of real-valued differentiable functions $F_1,\ldots,F_k$ on (V,ω) is said to be in *involution* if $\{F_i,F_j\} = 0$ for all $i,j, 1 \leqslant i,j \leqslant k$.

The set of functions $F_1,\ldots,F_k$ is said to be *functionally independent* if the set of critical points of the function $F = F_1 \times \cdots \times F_k$; in other words the set where the rank of dF is strictly less than k, has measure zero.

A Hamiltonian function H or the associated vector field X_H on (V,ω) is called *completely integrable* or just *integrable* if there exists $n = \frac{1}{2}$ (dimension of V) functionally independent first integrals of the motion of H which are in involution.

V. WILLIAMSON'S THEOREM

Theorem 5.1: Any real-valued homogeneous quadratic Hamiltonian function on a symplectic vector space (V,ω), or equivalently the associated real linear time-independent Hamiltonian differential equations, is completely integrable with *quadratic* functions.[5]

Before we embark on the proof of the theorem above we

present the specialization of the concepts of involution and functional independence to quadratic functions.

Under the Poisson bracket the set of quadratic functions on (V,ω), $Q(V,\mathbb{R})$, becomes a Lie algebra. The map

$$Q(V,\mathbb{R}) \to sp(n,\mathbb{R}) : H \to X_H$$

is a Lie algebra isomorphism. Therefore, we have

$$\{H,F\} \mapsto [X_H, X_F],$$

where $H,F \in Q(V,\mathbb{R})$ and the square brackets on the right are Lie brackets, or the commutator, in $sp(n,\mathbb{R})$. In particular, we have the following lemma.[9]

Lemma 5.2: If $H,F \in Q(V,\mathbb{R})$, then $\{H,F\} = 0$ if and only if $[X_H, X_F] = 0$.

Because of Lemma 5.2 to show that $X_H \in sp(n,\mathbb{R})$ has n quadratic first integrals in involution it suffices to exhibit an n-dimensional abelian subalgebra of $sp(n,\mathbb{R})$ containing X_H. The following notation will be used to describe the abelian subalgebras. Let T^m, ${}^mT$, U^m, and V^m be of size $m \times m$, square, lower triangular matrices with entries lying on a line parallel to the main diagonal having the same value.

The entries of ${}^mT$ are the same as those of T^m except that starting with the diagonal the entries on every other line parallel to the main diagonal have opposite sign from those of T^m.

The entries of U^m are 0 on every other line parallel to the diagonal starting with the (zero) diagonal.

The entries of V^m are 0 on every other line parallel to the diagonal starting with the (zero) subdiagonal.

Lower case latin letters will be arbitrary real numbers and in each case they will be assumed to be unrelated even if we use the same letters.

For example, if $m = 5$ then

$$T^5 = \begin{pmatrix} a & & & & \\ b & a & & & \\ c & b & a & & \\ d & c & b & a & \\ e & d & c & b & a \end{pmatrix},$$

$${}^5T = \begin{pmatrix} -a & & & & \\ b & -a & & & \\ -c & b & -a & & \\ d & -c & b & -a & \\ -e & d & -c & b & -a \end{pmatrix},$$

$$U^5 = \begin{pmatrix} 0 & & & & \\ f & 0 & & & \\ 0 & f & 0 & & \\ g & 0 & f & 0 & \\ 0 & g & 0 & f & 0 \end{pmatrix},$$

$$V^5 = \begin{pmatrix} h & & & & \\ 0 & h & & & \\ i & 0 & h & & \\ 0 & i & 0 & h & \\ j & 0 & i & 0 & h \end{pmatrix}.$$

Suppose that $X_{F_1},\ldots,X_{F_n}$ form a basis of an abelian subalgebra of $sp(n,\mathbb{R})$. Since $(\omega^\#)^{-1}$ is nonsingular, to prove that the corresponding quadratic first integrals $F_1,\ldots,F_n$ in involution are functionally independent it is enough to show that the matrix

$$(\omega^\#)^{-1} dF(x) = (X_{F_1}(x),\ldots,X_{F_n}(x)),$$

where $F = F_1 \times \cdots \times F_n$, has rank n for all $x = (x_1,\ldots,x_{2n}) \in V$ except a set of measure zero in V.

Proof of Theorem 5.1: Without loss of generality we may assume that X_H is in normal form. For each indecomposable type in List I we will exhibit an abelian subalgebra containing it, and if X_H is a sum of given indecomposable types then an abelian subalgebra containing X_H is simply the direct sum of the abelian subalgebras of the indecomposable summands of X_H.

Abelian subalgebras will be described in terms of T^m, ${}^mT$, U^m, and V^m as given above. Bases of abelian subalgebras can be obtained by setting one of the parameters to 1, the others to 0 in T^m, ${}^mT$, U^m, V^m and running through all the parameters. Routine matrix multiplications show that these basis elements commute.[10,11] The basis elements are the linear Hamiltonian vector fields in involution and the corresponding quadratic first integrals can be obtained from Proposition 2.1. In the cases (iii) and (iv) below X_H will not be one of the basis elements just described. Although it is not required in the definition of complete integrability we will modify the basis in such a way that X_H becomes one of the basis elements.

(i) Suppose that X_H is the indecomposable of type (1) of List I, i.e., nilpotent of height m(odd) or equivalently of size $(m+1)\times(m+1)$. An abelian subalgebra containing X_H is U^{m+1}. Let $n = \frac{1}{2}(m+1)$. It is easy to choose and $n \times n$ triangular submatrix of $(\omega^\#)^{-1} dF(x)$ with determinant x_1^n. Therefore, the rank of $(\omega^\#)^{-1} dF(x)$ is equal to n except when $x_1 = 0$ which is a measure zero subset of V. For example, let $m+1 = 6$, $n = 3$. Then

$$X_H = X_{F_1} = \begin{pmatrix} 0 & & & & & \\ 1 & 0 & & & & \\ & 1 & 0 & & & \\ & & 1 & 0 & & \\ & & & 1 & 0 & \\ & & & & 1 & 0 \end{pmatrix},$$

$$U^{m+1} = \begin{pmatrix} 0 & & & & & \\ a & 0 & & & & \\ 0 & a & 0 & & & \\ b & 0 & a & 0 & & \\ 0 & b & 0 & a & 0 & \\ c & 0 & b & 0 & a & 0 \end{pmatrix},$$

$$X_{F_2} = \begin{pmatrix} 0 & & & & & \\ 0 & & & & & \\ 0 & & & & & \\ 1 & & & & & \\ 0 & 1 & & & & \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix},$$

$$X_{F_1} = \begin{pmatrix} 0 & & & & & \\ 0 & & & & & \\ 0 & & & & & \\ 0 & & & & & \\ 0 & & & & & \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

and

$$(\omega^{\#})^{-1} dF(x) = \begin{pmatrix} 0 & & \\ x_1 & & \\ x_2 & & \\ x_3 & x_1 & \\ x_4 & x_2 & \\ x_5 & x_3 & x_1 \end{pmatrix}. \tag{1}$$

The determinant of the 3×3 submatrix consisting of the second, fourth, and sixth rows of (1) is equal to x_1^3. Hence (1) has rank 3 unless $x_1 = 0$ which is a measure zero subset of $\mathbb{R}^6$.

(ii) Suppose that X_H is indecomposable of type (2) or (5) in List I, i.e., either nilpotent of even height m or has real eigenvalues. Then an abelian subalgebra containing X_H is

$$\left(\begin{array}{c|c} T^{m+1} & \\ \hline & {}^{m+1}T \end{array}\right).$$

Functional independence is proved as in the case (i) by taking $n = m + 1$.

(iii) Suppose that X_H is indecomposable type (3) or (4) of List I, i.e., it has purely imaginary eigenvalues $\pm i\beta, \beta \neq 0$, and of height m. Let $n = m + 1$. Then an abelian subalgebra containing X_H is

$$\left(\begin{array}{c|c} U^n & -V^n \\ \hline V^n & U^n \end{array}\right).$$

If we take $X_{F_1} = X_H$, and $X_{F_2}, \ldots, X_{F_n}$ are obtained by setting one parameter in U^n or V^n to 1, all the others to 0 and running through all the parameters except the one on the diagonal entries of V^n, we get a basis of the abelian subalgebra above.

By row operations it is easy to choose an $n\times n$ submatrix of $(\omega^{\#})^{-1} dF(x)$ with determinant $\beta \cdot x_{n+1}^{n/2} \cdot x_1^{n/2}$ if n is even and $\beta \cdot x_{n+1}^{(n-1)/2} \cdot x_1^{(n+1)/2}$ if n is odd. So the rank of $(\omega^{\#})^{-1} dF(x)$ is equal to n except when $x_1 = 0$ and/or $x_{n+1} = 0$ which is a measure zero subset of $\mathbb{R}^{2n}$, thus establishing the functional independence of the quadratic first integrals described above.

(iv) Suppose that X_H is the indecomposable type (6) of List I, i.e., it has complex eigenvalues $\pm\alpha \pm i\beta, \alpha, \beta \neq 0$, and is of height m. Let $n = 2(m + 1)$. Then an abelian subalgebra containing X_H is

$$\left(\begin{array}{c|c|c|c} T_1^n & & T_2^n & \\ \hline & {}^nT_1 & & -{}^nT_2 \\ \hline -T_2^n & & T_1^n & \\ \hline & {}^nT_2 & & {}^nT_1 \end{array}\right).$$

If we take $X_H = X_{F_1}$, and $X_{F_2}, \ldots, X_{F_n}$ are obtained by setting one parameter in T_1^n (hence in ${}^nT_1$) or T_2^n (hence in ${}^nT_2$) to 1, all the others to 0 and running through all the parameters except the one on the diagonal entries of T_1^n and ${}^nT_1$, we get a basis of the abelian subalgebra above.

By row operations one can choose an $n\times n$ submatrix of $(\omega^{\#})^{-1} dF(x)$ with determinant $\alpha(x_1^2 + x_{n+1}^2)^n$. Therefore, the n quadratic first integrals described by the abelian subalgebra above are functionally independent except when $x_1 = x_{n+1} = 0$.

It appears that the quadratic integrals we have constructed are useful in the theory of global action-angle coordinates of linear Hamiltonian systems.[12] We will report on this in a subsequent paper.

ACKNOWLEDGMENTS

We are grateful to Professor Al Kelley and Professor Richard Cushman for their guidance and the CSUC for the Faculty Development Award. A critical reading of the manuscript by Professor Jurgen Moser saved us from some erroneous statements.

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Measurements, Hilbert space and quantum logics

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(Received 12 May 1982; accepted for publication 11 August 1982)

We consider single and multiple measurements on a quantum logic (P,S) as well as states and propositions conditioned by a measurement. We show that corresponding to any measurement A, there is a canonically associated Hilbert space H_A. Algebraic and statistical properties of (P,S) that are preserved in H_A are found. We then study the problem of embedding a quantum logic in Hilbert space.

PACS numbers: 03.65. – w

1. INTRODUCTION

According to one interpretation of the quantum logic approach, if $\mathscr{S}$ is a physical system, the set of states S of $\mathscr{S}$ represents the set of preparation procedures for $\mathscr{S}$ and the set of propositions P represents the set of physical yes-no experiments for $\mathscr{S}$. Mathematically P is a σ-orthocomplete orthomodular poset and S is a set of countably additive probability measures on P.[1]

We define a measurement (or operation[2]) to be a maximal orthogonal subset of P. For example, suppose the measuring apparatus consists of a finite sequence of n counters with mutually disjoint volumes of sensitivity. Then the measurement consists of mutually orthogonal yes-no experiments $a_1,a_2,\ldots,a_n,b$ [the ith counter clicks (a_i), no counter clicks (b)]. Or suppose the output of the measuring apparatus is a dial reading. A corresponding measurement would be a partition of the scale on the dial face. In any case, the result of a measurement consists of a set of mutually exclusive alternatives one of which always holds.

The physical system $\mathscr{S}$ can be thought of as a black box whose structure we seek to determine. We can prepare the box in various states and we may then subject the box to various measurements $\mathscr{M}$. By repeating preparations of $\mathscr{S}$ in the state $\alpha\in S$ each followed by a performance of the measurement $\{a_i\}\in\mathscr{M}$, we obtain a probability distribution $\{\alpha(a_i)\}$. These probability distributions give the only information about $\mathscr{S}$ available to us. The corresponding sequences $\{\alpha(a_i)^{1/2}\}$ generate a Hilbert space which will play a central role in our study.

In this article we shall consider single and multiple measurements. We shall also study states and propositions conditioned by a measurement. We observe that corresponding to any measurement A, there is a canonically associated Hilbert space H_A. We shall study to what extent the algebraic and statistical properties of (P,S) are preserved in $\{H_A : A\in\mathscr{M}\}$. Finally we consider the problem of embedding a quantum logic in Hilbert space.

[a)] This author wishes to thank the University of Denver for the hospitality extended to him during a quarter's visit during which this paper was begun.

2. MEASUREMENTS

In the sequel P will denote a *σ-orthocomplete orthomodular poset*. From now on we shall make the physically plausible assumption that P is *separable*, that is, every orthogonal set of elements of P is at most countable. Recall that a subset M of P is a *Boolean subσ-algebra* of P in case (i) M, with the ordering the orthocomplementation induced from P, is a Boolean σ-algebra and (ii) the countable joins in M function as joins in P. We say that a set $A\subseteq P$ is *compatible* if A is contained in a Boolean subσ-algebra of P, and in this case we denote the Boolean subσ-algebra generated by A by $\mathscr{B}(A)$. We say that $A,B\subseteq P$ are *compatible* (written $A\leftrightarrow B$) if $A\cup B$ is compatible; and, if $\{a\}\leftrightarrow\{b\}$ we write $a\leftrightarrow b$.

A *measurement* (or *operation*) on P is a maximal orthogonal set in $P\setminus\{0\}$. We denote the set of all measurements on P by $\mathscr{M}=\mathscr{M}(P)$. Note that $\mathscr{M}(P)$ is a covering of $P\setminus\{0\}$. For a general treatment of such structures and their relation to orthomodular posets see Ref. 3. For $A,B\in\mathscr{M}$ we say that B is a *refinement* of A and write $A\leqslant B$ if for every $a\in A$ there exists a subset $B_1\subseteq B$ such that $a=VB_1$. We call $A\in\mathscr{M}$ *atomic* if every $a\in A$ is an atom of P. The following two lemmas summarize some useful properties of measurements. The proof of the first lemma is a routine verification which we leave to the reader.

Lemma 1: (1) An orthogonal set $A\subseteq P\setminus\{0\}$ is in $\mathscr{M}$ if and only if $VA=1$.

(2) For each $a\in P\setminus\{0\}$ there exists an $A\in\mathscr{M}$ such that $a\in A$.

(3) If $A\in\mathscr{M}$, then A is compatible.

(4) If $A\leqslant B$, then $a\leftrightarrow b$ for every $a\in A$, $b\in B$.

(5) $a\perp b$ if and only if there is an $A\in\mathscr{M}$ with $a,b\in A$.

(6) $a\leftrightarrow b$ if and only if there is an $A\in\mathscr{M}$ with $a,b\in\mathscr{B}(A)$.

Lemma 2: (1) $(\mathscr{M},\leqslant)$ is an atomistic poset with least element $\{1\}$ and atoms $\{a,a'\}$, $a\neq 0,1$.

(2) A is a maximal element of $(\mathscr{M},\leqslant)$ if and only if A is atomic.

(3) For $A,B\in\mathscr{M}$, $A\leftrightarrow B$ if and only if there exists a $C\in\mathscr{M}$ such that $A,B\leqslant C$.

(4) P is an atomic Boolean σ-algebra if and only if $(\mathscr{M},\leqslant)$ contains a largest element.

Proof: (1) It is clear that $\leqslant$ is reflexive and transitive on $\mathscr{M}$. To show antisymmetry assume that $A,B\in\mathscr{M}$ with $A\leqslant B$

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and $B \leqslant A$. Let $a \in A$. Then there exists an element $b \in B$ and an $a_1 \in A$ with $a_1 \leqslant b \leqslant a$. If $a \neq a_1$, then $a \perp a_1$, hence $a_1 = 0$ which is a contradiction. Thus $A \subseteq B$ and by symmetry $B \subseteq A$ so $A = B$. The other statements are straightforward.

(2) Assume $A \in \mathscr{M}$ is maximal. If $a \in A$ is not an atom then there exists $a, b \in P$ such that $0 < b < a$. Since $a = b \vee (a \wedge b')$, $(A \setminus \{a\}) \cup \{b, a \wedge b'\}$ is a proper refinement of A contradicting the maximality of A. Thus A is atomic. The converse is clear.

(3) If $A, B \leqslant C$ then $A, B \subseteq \mathscr{B}(C)$ so $A \leftrightarrow B$. Conversely, if $A \leftrightarrow B$, then $C = \{a \wedge b : a \in A, b \in B\} \setminus \{0\} \in \mathscr{M}$ and $A, B \leqslant C$.

(4) If P is an atomic Boolean σ-algebra, then the set of atoms of P is the largest measurement in P. Conversely, assume $\mathscr{M}$ has a largest element A. Then by (2) A is atomic. For $a \in P \setminus \{0,1\}$, $\{a, a'\} \leqslant A$ so P is atomic. Moreover if, $a, b \in P \setminus \{0,1\}$ then $\{a, a'\}, \{b, b'\} \leqslant A$ so, by (3), $a \leftrightarrow b$. Hence P is a Boolean σ-algebra. □

For $a \in P$ and S a set of states (or σ-additive probability measures) on P we define $a^S = \{\alpha \in S \mid \alpha(a) = 1\}$. Throughout this section we assume that P admits a strong set of states S, that is, for $a, b \in P$, $a \leqslant b$ whenever $a^S \subseteq b^S$. We then call the pair (P, S) a *strong quantum logic*. For $A \in \mathscr{M}$, define the Hilbert space

$$\mathscr{H}_A = \left\{ f : A \to \mathbb{C} \;\middle|\; \sum_{a \in A} |f(a)|^2 < \infty \right\}$$

with inner product $\langle f, g \rangle = \Sigma_{a \in A} f(a) \overline{g}(a)$. For $\alpha \in S$, let $\alpha_A \in \mathscr{H}_A$ be the function $\alpha_A(a) = \alpha(a)^{1/2}$, $a \in A$. Notice that α_A is a unit vector in $\mathscr{H}_A$ since $\|\alpha_A\|^2 = \Sigma_{a \in A} \alpha(a) = 1$. We call α_A *the state α conditioned by the measurement A*. Let $P(\mathscr{H}_A)$ be the lattice of all orthogonal projections of $\mathscr{H}_A$. We frequently identify an orthogonal projection with the closed subspace it projects onto. For $a \in P$, define $a_A \in P(\mathscr{H}_A)$ to be the closed span $\overline{\text{sp}}\{\alpha_A \mid \alpha \in a^S\}$. We call a_A *the proposition a conditioned by the measurement A*. Define the maps $J(A) : S \to \mathscr{H}_A$ and $K(A) : P \to P(\mathscr{H}_A)$ by $J(A)\alpha = \alpha_A$ and $K(A)a = a_A$. The next lemma states that the range of $J(A)$ generates $\mathscr{H}_A$ and that a state $\alpha \in S$, respectively a proposition $a \in P$, is uniquely determined by the maps $J(A)\alpha$, $A \in \mathscr{M}$, respectively, $K(A)a$, $A \in \mathscr{M}$.

Lemma 3: (1) $\mathscr{H}_A = \overline{\text{sp}}\{\alpha_A \mid \alpha \in S\}$.

(2) For $\alpha, \beta \in S$, $\alpha = \beta$ if and only if $\alpha_A = \beta_A$ for all $A \in \mathscr{M}$.

(3) For $a, b \in P$, $a = b$ if and only if $a_A = b_A$ for all $A \in \mathscr{M}$.

Proof: (1) Fix $A \in \mathscr{M}$. For $a \in A$, define $e_a \in \mathscr{H}_A$ by $e_a(b) = \delta_{ab}$ (the Kronecker delta). It is clear that $\{e_a \mid a \in A\}$ is an orthonormal basis for $\mathscr{H}_A$. Moreover, since S is strong, for each $a \in A$ there exists an $\alpha^* \in S$ such that $\alpha^*(a) = 1$. Hence $\alpha^*_A = e_a$ so that $\{e_a : a \in A\} \subseteq \{\alpha_A : A \in \mathscr{M}\}$. The result follows.

(2) Suppose $\alpha_A = \beta_A$ for every $A \in \mathscr{M}$. Let $b \in P \setminus \{0,1\}$ and let $B = \{b, b'\} \in \mathscr{M}$. Then $\alpha(b)^{1/2} = \alpha_B(b) = \beta_B(b) = \beta(b)^{1/2}$, so $\alpha(b) = \beta(b)$; hence $\alpha = \beta$.

(3) Suppose $a_C = b_C$ for every $C \in \mathscr{M}$. Let $A_0 = \{a, a'\} \in \mathscr{M}$. Then

$$\text{sp}\{e_a\} = \overline{\text{sp}}\{\alpha_{A_0} \mid \alpha \in a^S\} = a_{A_0} = b_{A_0} = \overline{\text{sp}}\{\alpha_{A_0} \mid \alpha \in b^S\}.$$

Hence, $\alpha \in b^S$ implies $\alpha_{A_0} \in \text{sp}\{e_a\}$ which implies $\alpha_{A_0} = e_a$ so $\alpha \in a^S$. Thus $b^S \subseteq a^S$ and therefore $b \leqslant a$. By symmetry $a \leqslant b$, so $a = b$. □

For $a \in P$, $\alpha \in S$, $A \in \mathscr{M}$ we define the *probability of a in the state α conditioned by the measurement A* to be $\alpha_A(a_A) = \langle a_A \alpha_A, \alpha_A \rangle = \langle K(A)aJ(A)\alpha, J(A)\alpha \rangle$. In general, $\alpha_A(a_A) \neq \alpha(a)$ (see Sec. 4). This is to be expected since a single measurement on a physical system would not in general determine the statistics of the entire system. Also, in general, $K(A)$ does not preserve all the algebraic properties of P. Again, one would not expect a single measurement to determine the complete internal structure of P. The following result shows that $K(A)$ preserves the order on P and that both $J(A)$ and $K(A)$ preserve the structure and statistics of $\mathscr{B}(A)$.

Theorem 4: (1) For $a, b \in P$ and $A \in \mathscr{M}$, $a \leqslant b$ implies $a_A \leqslant b_A$.

(2) $K(A)$ is an isomorphism on $\mathscr{B}(A)$ and $\alpha_A(a_A) = \alpha(a)$ for every $\alpha \in S$ and $a \in \mathscr{B}(A)$.

Proof: (1) If $a \leqslant b$ then $a^S \subseteq b^S$ so that $\{\alpha_A \mid \alpha \in a^S\} \subseteq \{\alpha_A \mid \alpha \in b^S\}$ and $a_A \leqslant b_A$.

(2) For each $a \in A$, $K(A)a = \text{sp}\{e_a\}$ since $\alpha(a) = 1$ implies $\alpha_A = e_a$. Let $b \in \mathscr{B}(A)$. Then there exists a set $B \subseteq A$ such that $b = VB$. Since $K(A)$ preserves order and $a \leqslant b$ for all $a \in B$ we have $K(A)a \leqslant K(A)b$ and hence $V_{a \in B} K(A)a \leqslant K(A)b$. Let $\psi \in K(A)b = \overline{\text{sp}}\{\alpha_A \mid \alpha \in b^S\}$. If $\alpha(b) = 1$ then $\alpha(a) = 0$ for each $a \in A \setminus B$ so $\alpha_A \in \overline{\text{sp}}\{e_a \mid a \in B\}$ and $\psi \in V_{a \in B} K(A)a$. Hence $K(A)b = V_{a \in B} K(A)a$. It follows that $K(A)$ is an isomorphism from $\mathscr{B}(A)$ to the Boolean σ-algebra generated by $\{\text{sp}\{e_a\} \mid a \in A\}$. To show that $\alpha_A(a_A) = \alpha(a)$ for $a \in S$, $a \in \mathscr{B}(A)$ let $b \in \mathscr{B}(A)$ with $b = VB$, $B \subseteq A$. For $a \in A$ and $\alpha \in S$ we have

$$\alpha_A(a_A) = \langle \text{sp}\ e_a (\alpha(b)^{1/2})_{b \in A}, (\alpha(b)^{1/2})_{b \in A} \rangle = \alpha(a).$$

Hence

$$\alpha_A(b_A) = \alpha_A(V_{a \in B} K(A)a) = \sum_{a \in B} \alpha_A(K(A)a) = \sum_{a \in B} \alpha(a) = \alpha(VB) = a(b).$$ □

Corollary 5: (1) If $A, B \in \mathscr{M}$ and $A \leftrightarrow B$, then there exists a refinement $C \geqslant A, B$ such that $\alpha_C(a_C) = \alpha(a)$ for all $\alpha \in S$ and $a \in \mathscr{B}(A \cup B)$.

(2) If A is atomic and $a \leftrightarrow A$, then $\alpha_A(a_A) = \alpha(a)$ for all $\alpha \in S$.

Proof: (1) Let C be the refinement in the proof of Lemma (2), part (3). Then $\mathscr{B}(C) = \mathscr{B}(A \cup B)$ and the result follows from Theorem 4.

(2) Let $B = \{a, a'\}$. The result follows from (1) since A has no proper refinement. □

Let $f : \mathscr{M} \to \mathbb{C}$. We say that f has a *limit* $\lambda \in \mathbb{C}$ and write $\lim f(A) = \lambda$ if for any $\epsilon > 0$ there exists an $A(\epsilon) \in \mathscr{M}$ such that $|f(B) - \lambda| < \epsilon$ whenever $B \geqslant A(\epsilon)$. The next corollary shows that statistics is preserved in the limit.

Corollary 6: For every $a \in P$, $\alpha \in S$ we have $\alpha(a) = \lim \alpha_A(a_A)$.

For $\alpha, \beta \in S$, *the transition probability* $T_A(\alpha, \beta)$ of α and β given A is defined by

$$T_A(\alpha, \beta)^{1/2} = \sum_{a \in A} \alpha(a)^{1/2} \beta(a)^{1/2} = \langle \alpha_A, \beta_A \rangle.$$

The *transition probability* $T(\alpha, \beta)$ is defined[4] as $T(\alpha, \beta) = \inf_{A \in \mathscr{M}} T_A(\alpha, \beta)$. It is shown in Ref. 5 that $T(\alpha, \beta)$ possesses the usual properties of a transition probability and reduces to the standard form if P is a Hilbert space logic.

Corollary 7: For any $\alpha, \beta \in S$, $T(\alpha,\beta) = \lim T_A(\alpha,\beta)$.

Proof: Given $\epsilon > 0$, by definition there exists an $A \in \mathcal{M}$ such that $|T_A(\alpha,\beta) - T(\alpha,\beta)| < \epsilon$. Now let $B \in \mathcal{M}$ with $B \geqslant A$. If $a \in A$, then there exists $a_i \in B$, $i = 1,2,\cdots$, such that $a = \forall a_i$. By Schwarz's inequality we have

$$\sum \alpha(a_i)^{1/2}\beta(a_i)^{1/2} \leqslant \left[\sum \alpha(a_i)\right]^{1/2}\left[\sum \beta(a_i)\right]^{1/2} = \alpha(a)^{1/2}\beta(a)^{1/2}.$$

Hence $T(\alpha,\beta) \leqslant T_B(\alpha,\beta) \leqslant T_A(\alpha,\beta)$ and $|T_B(\alpha,\beta) - T(\alpha,\beta)| < \epsilon$. □

There is a close relationship between measurements and observables.[6] Let x be an observable with countable spectrum $\sigma(x) = \{\lambda_i \mid i = 1,2,\cdots\}$. Then corresponding to x we have a measurement $x(\{\lambda_i\})i = 1,2,\cdots$. Conversely, if $\{a_i \mid i = 1,2,\cdots\} \in \mathcal{M}$ and $\{\lambda_i \mid i = 1,2,\cdots\} \subseteq \mathbb{R}$, then there exists an observable x with $\sigma(x) = \{\lambda_i \mid i = 1,2,\cdots\}$ and $x(\{\lambda_i\}) = a_i, i = 1,2,\cdots$. In general, if x is an arbitrary observable, then there exists a sequence of observables x_i with finite spectra such that for any state α for which the expectation $E_\alpha(x)$ exists, we have $\lim E_\alpha(x_i) = E_\alpha(x)$.[7] Moreover, if $m \leqslant n$ then the measurements corresponding to x_n is a refinement of the measurement corresponding to x_m. In this way an arbitrary observable can be associated with a sequence of measurements each being a refinement of the previous ones.

We close this section with a brief consideration of multiple measurements. There are three important types of multiple measurements: sequential measurements, simultaneous measurements and independent measurements. If $A_1,\ldots,A_n \in \mathcal{M}(P)$, then a sequential measurement given by $K(A_n)K(A_{n-1})\cdots K(A_1)$ would first apply $K(A_1)$, then on the resulting system $K(A_2)$ would be applied and so forth. In general, there appears to be no reasonable mathematical way to define this if $A_1,\ldots,A_n$ are measurements on the original quantum logic (P,S). Physically, this is because the first measurement may drastically change the original system so that A_2 no longer applies. We can define a sequential measurement if $A_1 \in \mathcal{M}(P)$, $A_2 \in \mathcal{M}[P(H_{A_1})],\cdots$ by the expression $K(A_n)\cdots K(A_1)$.

In case P is a lattice, if $A_1,\ldots,A_n$ are compatible, then there exists a common refinement $B \geqslant A_i$, $i = 1,2,\ldots,n$. One can then consider the measurement B as a simultaneous measurement of $A_1,\ldots,A_n$. If the A_i's are not compatible, there appears to be no mathematical or physical sense for their simultaneous measurement. The next result shows that if $A \leqslant B$, then in a certain sense $J(A)J(B) = J(A)$ and $K(A)K(B) = K(A)$. If $A \leqslant B$ then, by Theorem 4, $\hat{A} = K(B)A$ is a measurement on $P(H_B)$ which is isomorphic to A.

Lemma 8: If $A \leqslant B$ then $J(\hat{A})J(B)\alpha = J(A)\alpha$ and $K(\hat{A})K(B)a = K(A)a$ for every $\alpha \in S$ and $a \in P$.

Proof: Since $A \leqslant B$, we have $A \subseteq \mathcal{B}(B)$ and by Theorem 4 $\alpha_B(a_B) = \alpha(a)$ for all $a \in A$. Hence

$$J(\hat{A})J(B)\alpha = (\alpha_B(a_B)^{1/2})_{a\in A} = (\alpha(a)^{1/2})_{a\in A} = J(A)\alpha.$$

Also, for any $a \in P$,

$$\begin{aligned} K(\hat{A})K(B)a &= \overline{\text{sp}}\{J(\hat{A})J(B)\alpha : \alpha \in a^S\} \\ &= \overline{\text{sp}}\{J(A)\alpha : \alpha \in a^S\} \\ &= K(A)a. \end{aligned}$$ □

We now consider independent multiple measurements. Let $A_1,\ldots,A_n \in \mathcal{M}$. An independent measurement of $A_1,\ldots,A_n$ may be physically thought of as follows: Prepare a state α, make the measurement A_1, reprepare the state α, make the measurement $A_2,\ldots$, reprepare the state α, make the measurement A_n. The result would be an n-tuple of vectors $(\alpha_{A_1},\alpha_{A_2},\ldots,\alpha_{A_n})$. Motivated by this, we define the map $J(A_1,\ldots,A_n): S \to H_{A_1} \otimes \cdots \otimes H_{A_n}$ by

$$J(A_1,\ldots,A_n)\alpha = J(A_1)\alpha \otimes \cdots \otimes J(A_n)\alpha = \alpha_{A_1} \otimes \cdots \otimes \alpha_{A_n}$$

and the map $K(A_1,\ldots,A_n): P \to P(H_{A_1} \otimes \cdots \otimes H_{A_n})$ by

$$\begin{aligned} K(A_1,\ldots,A_n)a &= \overline{\text{sp}}\{J(A_1,\ldots,A_n)\alpha : \alpha \in a^S\} \\ &= \overline{\text{sp}}\{\alpha_{A_1} \otimes \cdots \otimes \alpha_{A_n} : \alpha \in a^S\}. \end{aligned}$$

The maps $J(A_1,\ldots,A_n)$, $K(A_1,\ldots,A_n)$ correspond to a conditioning by the independent measurements $A_1,\ldots,A_n$. Notice that

$$[J(A_1,\ldots,A_n)\alpha][K(A_1,\ldots,A_n)a] = \alpha_{A_1}(a_{A_1})\alpha_{A_2}(a_{A_2})\cdots\alpha_{A_n}(a_{A_n})$$

which is the correct statistics for independent measurements. The proof of the next lemma follows easily from Theorem 4.

Lemma 9: Let $K = K(A_1,\ldots,A_n)$.

(1) $K0 = 0$, $K1 = 1$ and $a \leqslant b$ implies $Ka \leqslant Kb$.

(2) If $a \neq b$ and $a,b \in A_j$ for some $j \in \{1,2,\ldots,n\}$ then $Ka \perp Kb$.

3. HILBERT SPACE EMBEDDINGS

We say that P is *embeddable* in Hilbert space if P is isomorphic to a sub-ortho-modular poset of $P(H)$ for some Hilbert space H. An example is given in Ref. 8 of a finite strong quantum logic (P,S) for which P is not embeddable in Hilbert space. One might ask if there are stronger conditions that can be placed on S which forces P to be embeddable in Hilbert space. One possible such condition is the Jauch–Piron condition.[9] A state α on P is a Jauch–Piron state if $\alpha(a) = \alpha(b) = 1$ implies $\alpha(c) = 1$ for some $c \leqslant a,b$; note that this reduces to the usual definition[10] when P is a lattice. It has been conjectured that if (P,S) is a quantum logic in which S is a strong set of Jauch–Piron states, then P is embeddable in Hilbert space. That this conjecture is false can be seen by combining the example cited above and the following Corollary 12. Another possible such condition is the following.

Call two states α and β of P *mutually singular* and write $\alpha \# \beta$ if $\alpha(c) = \beta(c') = 1$ for some $c \in P$. This relation of mutual singularity has been studied in Ref. 11 in the context of the Jordan–Hahn decomposition of signed states. Now let S be any set of states on P. Write $a \perp_S b$ in case $a^S \times b^S \subseteq \#$, i.e., $\alpha \# \beta$ whenever $\alpha \in a^S$ and $\beta \in b^S$. Clearly, $\perp \subseteq \perp_S$. Call S ultrastrong in case $\perp_S \subseteq \perp$.

Remark 10: (1) If S is ultrastrong then S is strong.

(2) Ultrastrong (like strong) is "ascendingly hereditary," i.e., if $S_1 \subseteq S_2$ and S_1 is ultrastrong then so is S_2.

Proof: (1) Assume S is ultrastrong and $a^S \subseteq b^S$. If $\alpha \in a^S$ and $\beta \in (b')^S$ then $\alpha(b) = \beta(b') = 1$. Hence $a \perp_S b'$ so $a \perp b'$ and $a \leqslant b$. Hence S is strong.

(2) This follows immediately from the fact $S_1 \subseteq S_2$ implies $\perp_{S_2} \subseteq \perp_{S_1}$.

We give an example in the next section which shows

that strong need not imply ultrastrong. An order determining set of dispersion-free states S on P is ultrastrong. Indeed, suppose $a\perp_S b$. If $\alpha\in a^S$ then $a(b)=0$ since otherwise $\alpha\in a^S\cap b^S$ implying $\alpha\#\alpha$ which is impossible. Hence $\alpha(b')=1$ which implies $\alpha\leqslant b'$ or $a\perp b$. In particular any σ-class[12] or σ-algebra of subsets of a set admits an ultrastrong set of states. Also, for any Hilbert space logic $P(H)$, the set $S(H)$ of all pure states is ultrastrong. To see this, let $a,b\in P(H)$ with $a\perp_S b$. If a or b equals 0 we are finished. Otherwise, let ϕ and ψ be unit vectors with $\phi\in a$ and $\psi\in b$. Then the corresponding pure states α_ϕ, α_ψ satisfy $\alpha_\phi\in a^S$ and $\alpha_\psi\in b^S$. Hence there exists $c\in P(H)$ such that $\alpha_\phi(c)=\alpha_\psi(c')=1$. This implies that $\phi\in c$ and $\psi\in c'$ so $\phi\perp\psi$. Hence $a\perp b$. □

Theorem 11: If P is atomic and every atom $a\in P$ admits a Jauch–Piron state μ_a with $\mu_a(a)=1$, then P admits an ultrastrong set S of Jauch–Piron states.

Proof: Let A be the atoms of P and let $S_0=\{\mu_a\,|a\in A\}$ be a set of Jauch–Piron states indexed by A and satisfying $\mu_a(a)=1$. For each $b\in P\setminus\{0\}$ let A_b be a maximal orthogonal set of atoms under b. Since P is separable A_b is countable so we may write $A_b=\{a_1,a_2,\cdots\}$ and, since P is σ-orthocomplete, $b=VA_b$. For $c\in P$ define

$$\mu_{A_b}(c)=\begin{cases}\dfrac{1}{n}\displaystyle\sum_{a_i\in A_b}\mu_{a_i}(c) & \text{if } A \text{ is finite with } n \text{ elements,}\\[2ex] \displaystyle\sum_{i=1}^{\infty}\frac{1}{2^i}\mu_{a_i}(c) & \text{if } A \text{ is infinite.}\end{cases}$$

Then μ_{A_b} is a state on P.

We claim that, for any $b\in P\setminus\{0\}$, $\mu_{A_b}(c)=1$ if and only if $b\leqslant c$. For, if $\mu_{A_b}(c)=1$ then, for each $a_i\in A_b$, $\mu_{a_i}(c)=1$ and hence there exists $d_i\in P$ with $d_i\leqslant a_i$ and $d_i\leqslant c$ and $\mu_{a_i}(d_i)=1$. Now $d_i\neq 0$ and $a_i\in A$ imply $d_i=a_i$ so that $a_i\leqslant c$ for each i. Hence $b=VA_b\leqslant c$. The converse is clear.

Let $S=\{\mu_{A_b}\,|b\in P\setminus\{0\}\}$. If $\mu_{A_{b_1}}(c_1)=\mu_{A_{b_2}}(c_2)=1$ then $b\leqslant c_1$, $b\leqslant c_2$ and $\mu_{A_b}(b)=1$ so each μ_{A_b} is a Jauch–Piron state. To see that S is ultrastrong on P assume that $a\perp_S b$. We may assume that $a,b\neq 0$. Then, in particular, $\mu_{A_a}\#\mu_{A_b}$ so there exists $c\in P$ with $\mu_{A_a}(c)=\mu_{A_b}(c')=1$. Hence $a\leqslant c$ and $b\leqslant c'$ so that $a\perp b$. □

Corollary 12: Every finite P which admits a strong set of states also admits an ultrastrong set of Jauch–Piron states.

Proof: Let $S(P)$ denote the set of all countably additive states on P and let S be any strong set of states on P. For each atom a of P $a^{S(P)}$ is a nonempty polytope and therefore has finitely many extreme points $\mu_1,\mu_2,\ldots,\mu_n$. The state $\mu_a:=(1/n)\Sigma_{i=1}^n\mu_i$ satisfies the following:

$$\mu_a(b)=1 \quad \text{if and only if } a\leqslant b.$$

For, if $\mu_a(b)=1$ then $\mu_i(b)=1$ for each i. Hence $\text{ext}(a^{S(P)})\subseteq b^{S(P)}$ and, since $a^{S(P)}$ is the convex hull of $\text{ext}(a^{S(P)})$ and $b^{S(P)}$ is convex, if follows that $a^{S(P)}\subseteq b^{S(P)}$ so that $a^S=a^{S(P)}\cap S\subseteq b^{S(P)}\cap S=b^S$. Since S is strong, $a\leqslant b$. The converse is easy. As in the proof of the preceding theorem μ_a is a Jauch–Piron state so that the hypotheses of that theorem are satisfied and the assertion follows. □

Corollary 13: If (P,S) is a strong quantum logic in which P is a finite lattice, then P admits a convex and ultrastrong set of Jauch–Piron states.

Proof: Review of the foregoing result and Remark 10, if P is a lattice then the set of Jauch–Piron states is a convex subset of $S(P)$. □

We note in passing that this result fails for finite orthomodular posets. The smallest orthomodular poset which is not a lattice, J_{18} the 18-element orthomodular poset due to M. F. Janowitz,[13] provides a counterexample. In this poset the convex combination of Jauch–Piron states may not be Jauch–Piron.

We now use our previous work to prove a weak embedding theorem for a certain type of quantum logic. We say that P is *measurement finite* if there exists a finite collection of measurements $A_1,\ldots,A_n$ such that $a\perp b$ implies $a,b\in\mathscr{B}(A_j)$ for some $j\in\{1,\ldots,n\}$. Orthomodular lattices L which are block-finite in the sense that there are only finitely many maximal Boolean sub-algebras were studied in Ref. 14. An immediate corollary of the main result of Ref. 15 is that an orthomodular lattice L is block finite if and only if it is measurement finite. The corresponding result for posets is still open.

We say that (P,S) is *weakly embeddable* in a Hilbert space H if there exist injective maps $J:S\to H$ and $K:P\to P(H)$ such that

(1) $K0=0$, $K1=1$, and $a\leqslant b$ if and only if $Ka\leqslant Kb$.
(2) $a\perp b$ if and only if $Ka\perp Kb$.
(3) $\alpha\#\beta$ if and only if $J_\alpha\perp J_\beta$.
(4) $Ka=\overline{\text{sp}}J(a^S)$.

Theorem 14: A separable, measurement finite strong quantum logic (P,S) is weakly embeddable in a Hilbert space if and only if S is ultrastrong.

Proof: Since P is measurement finite, there exists $A_1,\ldots,A_n\in\mathscr{M}$ such that $a\perp b$ implies, $a,b\in\mathscr{B}(A_j)$ for some $j\in\{1,\ldots,n\}$. Let $J=J(A_1,\ldots,A_n)$ and $K=K(A_1,\ldots,A_n)$. It follows from Lemma 9 that $K0=0$, $K1=1$, and $a\leqslant b$ implies $Ka\leqslant Kb$. If $a\perp b$ then $a,b\in\mathscr{B}(A_j)$ for some j so $K(A_j)a\perp K(A_j)b$ by Theorem 4. It follows that $Ka\perp Kb$. Suppose that $Ka\perp Kb$. Now there exists an A_j such that $b\in B(A_j)$. Then $b=VB$ for some $B\subseteq A_j$. If $\alpha\in a^S$, then

$$\alpha_{A_1}\otimes\cdots\otimes\alpha_{A_n}\in Ka\subseteq Kb\subseteq K(A_1)b\otimes\cdots\otimes K(a_n)b.$$

It follows that

$$\alpha_{A_j}\in K(A_j)b=\overline{\text{sp}}\{e_a:a\in B\}.$$

Hence $\alpha(a)=0$ for $a\in A_j\setminus B$. Therefore $\alpha(b)=\Sigma_{a\in B}\alpha(a)=1$. Thus $a^S\subseteq b^S$ and, since S is strong, $a\leqslant b$. It follows that K is injective and (1) holds. To complete the proof of (2) assume $Ka\perp Kb$. If $\alpha\in a^S$ and $\beta\in b^S$ then there exists an A_j such that $J(A_j)\alpha\perp J(A_j)\beta$. Hence

$$0=\langle J(A_j)\alpha,J(A_j)\beta\rangle=\sum_{a\in A_j}\alpha(a)^{1/2}\beta(a)^{1/2}.$$

Let $B=\{a\in A_j:\beta(a)=0\}$ and let $b=VB$. Since $\alpha(a)\beta(a)=0$ for all $a\in A_j$ we have $\alpha(b)=\beta(b')=1$. Hence $\alpha\#\beta$ and $a\perp_S b$. Assuming that S is ultrastrong, we conclude that $a\perp b$.

To show that J is injective, assume $\alpha,\beta\in S$ with $\alpha\neq\beta$. Then there exist $b\in P$ such that $\alpha(b)\neq\beta(b)$. Now $b\in\mathscr{B}(A_j)$ for some $j\in\{1,\ldots,m\}$ so $\alpha(a)\neq\beta(a)$ for some $a\in A_j$. Hence $J(A_j)\alpha\neq J(A_j)\beta$ and $J\alpha\neq J\beta$. To prove (3) assume $\alpha\#\beta$. Then $\alpha(c)=\beta(c')=1$ for some $c\in P$. Again $c\in\mathscr{B}(A_j)$ for some A_j and $c=VB$ for some $B\subseteq A_j$. Hence $\beta(a)=0$ for all $a\in B$ and $\alpha(a)=0$ for all $a\in A_j\setminus B$. Thus $\alpha(a)\beta(a)=0$ for all $a\in A_j$ and

$J(A_j)\alpha \perp J(A_j)\beta$. It follows that $J\alpha \perp J\beta$. Conversely assume $J\alpha \perp J\beta$. Then $J(A_j)\alpha \perp J(A_j)\beta$ for some A_j. As in the previous paragraph $\alpha \# \beta$. Condition (4) follows by definition.

Conversely, assume (P,S) is weakly embeddable in a Hilbert space and assume $a \perp_S b$. Let $\alpha \in a^S$ and $\beta \in b^S$. Then $\alpha \# \beta$, so $J\alpha \perp J\beta$. Hence,

$$Ka = \overline{\text{sp}} J(a^S) \perp \overline{\text{sp}} J(b^S) = Kb.$$

It follows that $a \perp b$ and S is ultrastrong. □

Corollary 15: If (P,S) is a finite strong quantum logic, then $(P,S(P))$ is weakly embeddable in a Hilbert space.

Proof: Since S is strong, P admits an ultrastrong set of states by Corollary 12. Hence, by Remark 10 part (2) $S(P)$ is ultrastrong. □

The example (P_0,S_0) [16] cited earlier of a strong quantum logic not embeddable in Hilbert space yields an example, namely $(P_0,S(P_0))$, of a strong quantum logic weakly embeddable in a Hilbert space but not embeddable in a Hilbert space.

4. EXAMPLES

We first give an example of a quantum logic (P,S) in which P, given in Fig. 1, is a finite orthomodular lattice and S is a strong set of pure (extremal) states which is not ultrastrong. Simpler examples can be constructed in which the states are not pure. In our notations (see Ref. 17), the vertices represent atoms of P and the straight line segments group these atoms into (3 element) maximal orthogonal sets. Table I lists a set S of 22 states and the values that these states attain on each atom. One can check [18] that each state in S is pure and that S is strong on P. However S is not ultrastrong since $a \perp_S k$ while $a \not\perp k$.

We now present some examples of measurement conditioning maps on quantum logics. Let P be a separable Boolean σ-algebra of subsets of a set X and let S be the set of Dirac measures on P. That is, every state in S has the form α_x, $x \in X$, where $\alpha_x(a) = 1$ if $x \in a$ and $\alpha_x(a) = 0$ if $x \notin a$ for each a in P. Let $A \in \mathcal{M}(P)$. Then $J(A)\alpha_x = e_a$, where a is the unique element of A containing x. It follows that

$$K(A)b = \overline{\text{sp}}\{e_a : a \cap b \neq \phi, a \in A\}.$$

Hence, $[J(A)\alpha_x][K(A)b] = \alpha_x(b)$ for all $x \in X$, $b \in P$.

Let $(P(H),S(H))$ be the Hilbertian logic in which $P(H)$ is the lattice of all closed subspaces of a separable Hilbert space H and $S(H)$ is the set of all pure states on $P(H)$. Let $\{e_i : i = 1,2,\cdots\}$ be an orthonormal basis for H. Then $A = \{\text{sp}\, e_i : i = 1,2,\cdots\}$ is a measurement. If α_ϕ is a pure state corresponding to the unit vector $\phi \in H$, then

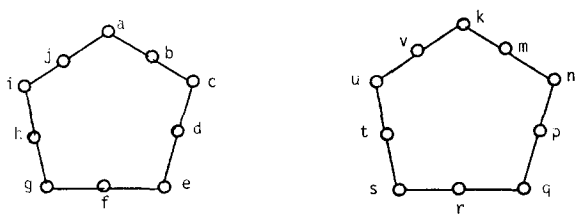

FIG. 1. An orthomodular lattice.

TABLE I. Strong but not ultrastrong states.

	a	b	c	d	e	f	g	h	i	j	k	m	n	p	q	r	s	t	u	v
1	1	0	0	1	0	1	0	1	0	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0
2	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	1	0	0	1	0	1	0	1	0	0
3	1	0	0	1	0	1	0	1	0	0	0	1	0	1	0	1	0	1	0	1
4	0	1	0	1	0	1	0	1	0	1	1	0	0	1	0	1	0	1	0	0
5	1	0	0	0	1	0	0	1	0	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0
6	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	1	0	0	0	1	0	0	1	0	0
7	1	0	0	1	0	0	1	0	0	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0
8	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	1	0	0	1	0	0	1	0	0	0
9	0	1	0	1	0	0	1	0	0	1	0	1	0	0	1	0	0	1	0	1
10	0	1	0	0	1	0	0	1	0	1	0	0	1	0	0	0	1	0	0	1
11	0	0	1	0	0	1	0	1	0	1	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0
12	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	0	1	0	0	1	0	1	0	1
13	0	0	1	0	0	0	1	0	0	1	0	1	0	1	0	1	0	1	0	1
14	0	1	0	1	0	1	0	1	0	1	0	0	1	0	0	0	1	0	0	1
15	0	1	0	1	0	1	0	0	1	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0
16	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	1	0	1	0	1	0	0	1	0
17	0	0	1	0	0	1	0	0	1	0	0	1	0	1	0	1	0	1	0	1
18	0	1	0	1	0	1	0	1	0	1	0	0	1	0	0	1	0	0	1	0
19	0	1	0	0	1	0	0	0	1	0	0	1	0	1	0	1	0	1	0	1
20	0	1	0	1	0	1	0	1	0	1	0	1	0	0	1	0	0	0	1	0
21	0	0	1	0	0	1	0	1	0	1	0	1	0	1	0	0	1	0	0	1
22	0	0	1	0	0	1	0	0	1	0	0	0	1	0	0	1	0	0	1	0

$$J(A)\alpha_\phi = (|\langle \phi, e_i \rangle| : i = 1,2,\cdots) \in l_2.$$

For $a \in P(H)$ we have

$$K(A)a = \overline{\text{sp}}\{(|\langle \phi, e_i \rangle| : i = 1,2,\cdots) : \phi \in a\}.$$

In particular, $K(A)(\text{sp}\, e_i) = \text{sp}\, \delta_i$, where $\delta_i(j) = \delta_{ij}$, $i,j = 1,2,\cdots$. If a is one-dimensional and $\psi \in a$ with $\|\psi\| = 1$, then

$$[J(A)\alpha_\phi][K(A)a] = \left[\sum |\langle \psi, e_i \rangle \langle e_i, \phi \rangle|\right]^2.$$

In particular, if $\langle \psi, e_i \rangle$, $\langle e_i, \phi \rangle \geqslant 0$ for each $i = 1,2,\cdots$, then

$$[J(A)\alpha_\phi][K(A)a] = |\langle \psi, \phi \rangle|^2 = \alpha_\phi(a).$$

Finally, let P be the six element orthomodular lattice, i.e., $P = \{0,1,a,a',b,b'\}$ is the horizontal sum of two copies of 2^2, and let S be the set of all states on P. Then $\mathcal{M}(P)$ contains two nontrivial measurements, $A = \{a,a'\}$ and $B = \{b,b'\}$. The Hilbert spaces H_A and H_B both are $\mathbb{C}^2$. Let $e_1 = (1,0)$ $e_2 = (0,1)$ be the natural orthonormal basis for $\mathbb{C}^2$. Then for every $\alpha \in S$ we have

$$J(A)\alpha = \alpha(a)^{1/2} e_1 + (1 - \alpha(a))^{1/2} e_2$$

and

$$J(B)\alpha = \alpha(b)^{1/2} e_1 + (1 - \alpha(b))^{1/2} e_2.$$

Now $K(A)a = \text{sp}\, e_1, K(A)a' = \text{sp}(e_2), K(A)b = K(A)b' = \mathbb{C}^2$ and $K(B)b = \text{sp}\, e_1, K(B)b' = \text{sp}\, e_2, K(B)a = K(B)a' = \mathbb{C}^2$. Hence $\alpha_A(a_A) = \alpha(a), \alpha_A(a'_A) = \alpha(a'), \alpha_A(b_A) = \alpha_A(b'_A) = 1$ for every $\alpha \in S$ with similar equations holding for α_B. Also $H_A \otimes H_B = \mathbb{C}^2 \otimes \mathbb{C}^2$,

$$\begin{aligned} J(A,B)\alpha &= J(A)\alpha \otimes J(B)\alpha \\ &= \alpha(a)^{1/2}\alpha(b)^{1/2} e_1 \otimes e_1 + \alpha(a)^{1/2}[1 - \alpha(b)]^{1/2} e_1 \otimes e_2 \\ &\quad + [1 - \alpha(a)]^{1/2}\alpha(b)^{1/2} e_2 \otimes e_1 \\ &\quad + [1 - \alpha(a)]^{1/2}[1 - \alpha(b)]^{1/2} e_2 \otimes e_2, \end{aligned}$$

$$K(A,B)a = \mathrm{sp}\{J(A,B)\alpha : \alpha(a) = 1\}$$
$$= \mathrm{sp}\{e_1 \otimes [\alpha(b)^{1/2}e_1 + (1 - a(b))^{1/2}e_2] : \alpha(a) = 1\}$$
$$= \mathrm{sp}\, e_1 \otimes \mathbb{C}^2$$
$$= K(A)a \otimes K(B)a.$$

Similarly $K(A,B)a' = \mathrm{sp}\, e_2 \otimes \mathbb{C}^2$, $K(A,B)b = \mathbb{C}^2 \otimes \mathrm{sp}\, e_1$, and $K(A,B)b' = \mathbb{C}^2 \otimes \mathrm{sp}\, e_2$. Moreover, if P_{e_1} denotes the projection onto $\mathrm{sp}\, e_1$, we have

$$[J(A,B)\alpha][K(A,B)a]$$
$$= \langle P_{e_1} \otimes IJ(A)\alpha \otimes J(B)\alpha, J(A)\alpha \otimes J(B)\alpha \rangle$$
$$= \langle \alpha(a)^{1/2}e_1 \otimes J(B)\alpha, J(A)\alpha \otimes J(B)\alpha \rangle$$
$$= \alpha(a)^{1/2}\langle e_1, J(A)\alpha \rangle \langle J(B)\alpha, J(B)\alpha \rangle = \alpha(a).$$

In a similar way, the statistics is preserved for $a', b, b', 0$, and 1. This example can be generalized to any finite horizontal sum of separable Boolean σ-algebras.

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Observables measured simultaneously with the potential

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(Received 21 July 1981; accepted for publication 11 December 1981)

The general form of the observables measured simultaneously with some class of potentials is given.

PACS numbers: 03.65.Bz

1. INTRODUCTION AND NOTATIONS

In quantum mechanics, two observables a and q can be measured simultaneously in an experiment if and only if their corresponding operators A and Q commute, i.e., $AQ - QA = 0$.[1] Let q be a potential field in the interval $[a,b]$. Its corresponding operator Q is a multiplication operator acting in the space $L_2[a,b]$ by the formula (see Ref. 1)

$$(Qf)(x) = q(x)f(x) \quad \forall f \in L_2[a,b].$$

Let $q(x)$ be a continuous function defined on $[a,b]$. We say that q is an n-piecewise strictly monotonic function if there exists a subdivision of the interval $[a,b]$ by the points

$$a = x_0 < x_1 < x_2 < \cdots < x_n = b,$$

such that $q(x)$ is strictly monotonic in each of the intervals (x_i, x_{i+1}), $i \in \{0,1,2,\ldots,n-1\}$.

In the present paper we study the general form of linear bounded operators corresponding to observables which can be simultaneously measured with some special types of the potential q.

2. STRICTLY MONOTONIC POTENTIALS

We first begin by considering the simple case when the potential $q(x)$ is a strictly monotonic continuous function in the interval $[a,b]$, that is to say q is a 1-piecewise strictly monotonic function.[2]

Since A commutes with Q, it commutes with all powers Q^k, $k = 1,2,\ldots$, i.e.,

$$Aq^k f = q^k A f \quad \text{for all } k.$$

Taking $f(x) = 1$ and putting $A\,1 = \varphi(x)$, we get

$$(Aq^k)(x) = \varphi(x) q^k(x) \quad \text{for all } k,$$

i.e., the operator A is a multiplication operator by the function $\varphi(x)$ on the set

$$S = \{1, q, q^2, \ldots, q^k, \ldots\}.$$

From the linearity of A, it follows that A is a multiplication operator on the set of all linear combinations of elements of S. This last set coincides with the algebra $\mathfrak{a}$ generated by $\{1,q\}$. The strict monotonicity of $q(x)$ guarantees that $\mathfrak{a}$ separates the points of $[a,b]$ which means, by the Stone–Weierstrass theorem,[3] that the uniform closure of $\mathfrak{a}$ coincides with the set of all continuous functions $C[a,b]$ defined on $[a,b]$. The set $C[a,b]$, in turn, is dense in $L_2[a,b]$. Hence the closure of $\mathfrak{a}$ (with respect to the convergence in the mean) coincides with $L_2[a,b]$. Since A is bounded, it is a multiplication operator on the whole space $L_2[a,b]$, i.e., we have proved the following.

Theorem 1: If $q(x)$ is a strictly monotonic continuous potential, then the only observables a that can be measured simultaneously with q are those with corresponding operators having the form

$$(Af)(x) = \varphi(x) f(x)$$

[i.e., a is a potential defined by the functions $\varphi(x)$].

3. TWO-PIECEWISE STRICTLY MONOTONIC POTENTIALS

Assume that $q(x)$ is a two-piecewise strictly monotonic continuous function. For definiteness, we shall assume that there exists $x_1 \in (a,b)$ such that q is strictly monotonic decreasing in (a,x_1) and strictly monotonic increasing in (x_1,b). Assume also that $q(x_1) = 0$. To satisfy these conditions we may, if necessary, multiply by (-1) or add a suitable constant. Moreover, we assume that $q(a) < q(b)$ (see Fig. 1). Now, it is clear that there exists $c \in (a,b]$ such that $q(a) = q(c)$ and for each $x \in [a,c]$ there exists $\bar{x} \in [a,c]$ such that $q(x) = q(\bar{x})$. For $x \in (c,b]$, we take $\bar{x} = x$.

Definition: We say that $f \in L_2[a,b]$ is a q-wise function if

$$f(x) = f(\bar{x}) \quad \forall x \in [a,b],$$

and anti-q-wise if

$$f(x) = -f(\bar{x}) \quad \forall x \in [a,b]$$

(we see that anti-q-wise functions are equal to zero for all $x \in (c,b]$).

It is clear that each function $f \in L_2[a,b]$ can be represented in a unique manner as a sum of two functions; one of these is q-wise and the other is anti-q-wise. In fact, put

$$g(x) = \tfrac{1}{2}(f(x) + f(\bar{x})), \quad h(x) = \tfrac{1}{2}(f(x) - f(\bar{x})).$$

We see that $g(x)$ is q-wise, $h(x)$ is anti-q-wise, and $f(x) = g(x) + h(x)$.

The uniqueness of this representation follows from: If $g(x) + h(x) = 0$ then, substituting $\bar{x}$ in place of x, we get $g(x) - h(x) = 0$. Adding the last two equalities and subtracting them, we get $g(x) = 0$ and $h(x) = 0$.

This means that the space $L_2[a,b]$ can be represented as the direct sum of the two subspaces M and N,[4]

$$L_2[a,b] = M \oplus N,$$

where M is the subspace of all q-wise functions and N the subspace of all anti-q-wise functions.

Now, consider the continuous function

$$r(x) = \begin{cases} -(q(x))^{1/2}, & x \in [a,x_1) \\ (q(x))^{1/2}, & x \in [x_1,b]. \end{cases}$$

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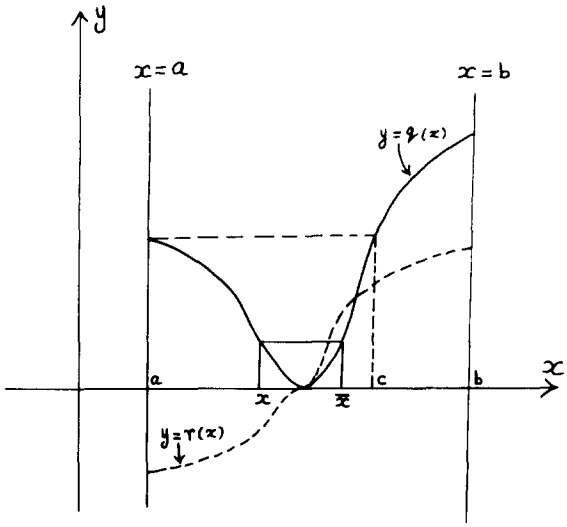

FIG. 1.

The function $r(x)$ is strictly monotonic increasing in the interval $[a,b]$. Consequently, the linear manifold $\mathfrak{a}$ generated by the sequence

$$S = \{1, r(x), r^2(x), \ldots, r^k(x), \ldots\}$$

is dense in $L_2[a,b]$.

$\mathfrak{a}$ can be written in the form

$$\mathfrak{a} = \mathfrak{M} \oplus \mathfrak{N},$$

where $\mathfrak{M}$ is the linear manifold generated by the sequence S_e of all elements with even powers in S (i.e., q-wise functions);

$$S_e = \{1, r^2, r^4, \ldots\} = \{1, q, q^2, \ldots\},$$

and $\mathfrak{N}$ the linear manifold generated by the subsequence S_o of all elements with odd powers in S (i.e., anti-q-wise functions);

$$S_o = \{r, r^3, r^5, \ldots\} = \{r, rq, rq^2, \ldots\}.$$

It is easy to verify that $\mathfrak{M}$ and $\mathfrak{N}$ are dense in M and N, respectively.

On the linear manifold $\mathfrak{M}$ and hence on the subspace M, the operator A acts as a multiplication operator by the function $q_1(x) = (A\,1)(x)$. This follows from the fact that A is a multiplication operator on the generating set S_e.

On the other hand, we have

$$Ar^{2k+1} = Aq^k r = q^k Ar = (Ar/r)\cdot r^{2k+1}.$$

Let

$$q_2(x) = \frac{(Ar)(x)}{r(x)}.$$

We see that A acts on S_o and hence on $\mathfrak{N}$ and N as a multiplication operator by the function $q_2(x)$.

Finally, if $f \in L_2[a,b]$ and we put

$$f = g + h, \quad g \in M \quad \text{and } h \in N,$$

then

$$\begin{aligned}(Af)(x) &= (Ag)(x) + (Ah)(x) \\ &= q_1(x)g(x) + q_2(x)h(x) \\ &= q_1 \frac{f(x) + f(\bar{x})}{2} + q_2 \frac{f(x) - f(\bar{x})}{2} \\ &= \tfrac{1}{2}(q_1(x) + q_2(x))f(x) + \tfrac{1}{2}(q_1(x) - q_2(x))f(\bar{x}).\end{aligned}$$

Putting

$$\lambda(x) = \tfrac{1}{2}(q_1(x) + q_2(x)),$$

$$\mu(x) = \tfrac{1}{2}(q_1(x) - q_2(x)),$$

we get the following.

Theorem 2: If the observable a can be measured simultaneously with a potential defined by a 2-piecewise strictly monotonic continuous function, then its corresponding operator acts by the formula

$$(Af)(x) = \lambda(x)f(x) + \mu(x)f(\bar{x}).$$

Open question: Related to the above problem, it would be interesting to consider the case when the potential $q(x)$ is an n-piecewise strictly monotonic function for $n > 2$.

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Joint distribution indicated by the wave equations of quantum mechanics

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(Received 27 March 1981; accepted for publication 7 August 1981)

By using the notion of conditional mean values and assuming that the classical relationship between momentum and energy remains valid, it is shown that both the Schrödinger and Klein–Gordon equations suggest a particular joint distribution expression for quantum mechanics, namely the Margenau and Hill distribution.

PACS numbers: 03.65.Bz

I. INTRODUCTION

A number of people have considered the question of a joint distribution for position and momentum in quantum mechanics.[1–11] For an ensemble of particles, such a distribution would provide the probability $P(x,p;t)\,dx\,dp$ that any particular particle in the ensemble lies within the position range x to $x+dx$ and the momentum range p to $p+dp$ at time t.[12] If the ensemble is described by the wave function $\psi(x;t)$, the joint distribution is required to satisfy the equations

$$\int_{-\infty}^{+\infty} P(x,p;t)\,dp = |\psi(x;t)|^2,$$
$$\int_{-\infty}^{+\infty} P(x,p;t)\,dx = |\phi(p;t)|^2, \tag{1}$$

where $\phi(p;t)$ is the momentum wave function obtained by taking the Fourier transform of $\psi(x;t)$.

The quantities x and p are the position value and the momentum value that an individual particle would display if a position measurement or a momentum measurement, respectively, were performed on it. We are remaining noncommittal on whether these are the actual position and momentum the particle has before measurement and, in fact, on whether a particle has any position or momentum before measurement. Thus, the joint distribution refers to the values for x and p that would be found upon measurement, not necessarily to the values (if any) existing before measurement (and definitely not to the values found by a position measurement followed by a momentum measurement, or by a momentum measurement followed by a position measurement).

Various possible expressions satisfying Eqs. (1) have been found.[1,3–5] The simplest of these are listed below.

Wigner:

$$P(x,p;t) = (1/2\pi)\int_{-\infty}^{+\infty} e^{-i\tau p}\psi^*(x-\tfrac{1}{2}\hbar\tau;t)\psi(x+\tfrac{1}{2}\hbar\tau;t)\,d\tau$$
$$= \frac{1}{(2\pi\hbar)^{1/2}}\exp\left[\frac{\hbar}{2i}\frac{\partial^2}{\partial x\partial p}\right][\psi^*(x;t)\phi(p;t)e^{ipx/\hbar}],$$

Margenau and Hill:

$$P(x,p;t) = (1/2\pi)\mathrm{Re}\left[\psi(x;t)\int_{-\infty}^{+\infty} e^{-i\tau p}\psi^*(x-\hbar\tau;t)\,d\tau\right]$$
$$= \frac{1}{(2\pi\hbar)^{1/2}}\mathrm{Re}[\psi^*(x;t)\phi(p;t)e^{ipx/\hbar}],$$

Mehta (normal ordering):

$$P(x,p;t) = \frac{1}{2\pi}\exp\left[-\frac{\hbar}{4}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial p^2}\right)\right]$$
$$\times\int_{-\infty}^{+\infty} e^{-i\tau p}\psi^*(x-\tfrac{1}{2}\hbar\tau;t)\psi(x+\tfrac{1}{2}\hbar\tau;t)\,d\tau$$
$$= \frac{1}{(2\pi\hbar)^{1/2}}\exp\left[-\frac{\hbar}{4}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial p^2}\right)\right]$$
$$\times\exp\left[\frac{\hbar}{2i}\frac{\partial^2}{\partial x\partial p}\right][\psi^*(x;t)\phi(p;t)e^{ipx/\hbar}].$$

In addition, Eqs. (1) are satisfied by the following simple expression:

$$P(x,p;t) = |\psi(x;t)\phi(p;t)|^2.$$

The first three of these possibilities suffer from the defect that they are not positive definite and hence cannot be true probability distributions.[13]

In the following sections we will investigate whether the mathematical formalism of quantum mechanics points us towards any particular joint distribution expression.

II. CONDITIONAL MEAN VALUES SUGGESTED BY THE SCHRÖDINGER EQUATION

In nonrelativistic classical mechanics, the momentum $\mathbf{p}$ and energy E of a particle are related by[14]

$$\frac{p^2}{2m} = E,$$

where m is the mass of the particle. If the particle comes under the influence of an electromagnetic field, described by a scalar potential $V(\mathbf{r},t)$ and a vector potential $\mathbf{A}(\mathbf{r},t)$, the relationship becomes

$$\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2 = E - eV, \tag{2}$$

where e is the electric charge of the particle and c is the speed of light. [In the case of Eq. (2), $\mathbf{p}$ and E represent the generalized momentum and energy of the particle.] Expanding the bracket in (2) we obtain

$$\frac{1}{2m}\left(p^2+\frac{e^2}{c^2}A^2-2\frac{e}{c}\mathbf{A}\cdot\mathbf{p}\right) = E - eV. \tag{3}$$

In considering joint distributions for quantum mechanics, we assume that there is a momentum value and an energy value associated with each particle, these being what would be found by a measurement of momentum or energy, respectively. It is reasonable to propose that the classical relation-

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ship (3) will remain valid also for these quantum-mechanical momentum and energy values.

Let us consider an ensemble of particles with a range of different momenta and energies. If we take an average over the momentum and energy values for a particular position $\mathbf{r}$ at time t, the mean values of the quantities in (3) will satisfy the equation

$$\frac{1}{2m}\left(\langle p^2\rangle_{\mathbf{r},t} + \frac{e^2}{c^2}A^2 - 2\frac{e}{c}\mathbf{A}\cdot\langle\mathbf{p}\rangle_{\mathbf{r},t}\right) = \langle E\rangle_{\mathbf{r},t} - eV, \tag{4}$$

where $\langle\ \rangle_{\mathbf{r},t}$ denotes the conditional mean value for a given position $\mathbf{r}$ at time t.

Now, the probability density $P(\mathbf{r};t)$ for our ensemble will satisfy the equation of continuity

$$\nabla\cdot\{P(\mathbf{r};t)\langle\mathbf{v}\rangle_{\mathbf{r},t}\} + \frac{\partial}{\partial t}P(\mathbf{r};t) = 0. \tag{5}$$

Using the relationship

$$\mathbf{v} = \frac{1}{m}(\mathbf{p} - \frac{e}{c}\mathbf{A}),$$

Eq. (5) may be expressed as

$$\nabla\cdot\left\{P(\mathbf{r};t)\frac{1}{m}\left(\langle\mathbf{p}\rangle_{\mathbf{r},t} - \frac{e}{c}\mathbf{A}\right)\right\} + \frac{\partial}{\partial t}P(\mathbf{r};t) = 0. \tag{6}$$

We now wish to find equations in conventional quantum mechanics which are similar in form to (4) and (6), with the aim of discovering possible expressions in terms of $\psi(\mathbf{r};t)$ for the various conditional mean values. The quantum-mechanical equation analogous to (2) is the Schrödinger equation:

$$\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)^2\psi = \left(i\hbar\frac{\partial}{\partial t} - eV\right)\psi. \tag{7}$$

By dividing (7) through by ψ and separating it into real and imaginary parts one obtains the following two equations:

$$\frac{1}{2m}\left(\mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)^2\psi\right] + \frac{e^2}{c^2}A^2 - 2\frac{e}{c}\mathbf{A}\cdot\mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right]\right) = \mathrm{Re}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)\psi\right] - eV, \tag{8}$$

$$\frac{1}{2m}\left(\mathrm{Im}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)^2\psi\right] + \hbar\nabla\cdot\frac{e}{c}\mathbf{A} - 2\frac{e}{c}\mathbf{A}\cdot\mathrm{Im}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right]\right) = \mathrm{Im}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)\psi\right]. \tag{9}$$

Multiplying (9) by $-2|\psi|^2/\hbar$ one then obtains (after some manipulation)

$$\nabla\cdot\left\{|\psi|^2\frac{1}{m}\left(\mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right] - \frac{e}{c}\mathbf{A}\right)\right\} + \frac{\partial}{\partial t}|\psi|^2 = 0. \tag{10}$$

We now wish to postulate that Eqs. (8) and (10) are equivalent to Eqs. (4) and (6), respectively.[15] Under this assumption, comparison of (4) and (8) suggests the following relationships:

$$\begin{aligned}\langle\mathbf{p}\rangle_{\mathbf{r},t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right],\\ \langle p^2\rangle_{\mathbf{r},t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)^2\psi\right],\\ \langle E\rangle_{\mathbf{r},t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)\psi\right].\end{aligned} \tag{11}$$

Similarly, comparing (6) and (10) we obtain

$$\begin{aligned}P(\mathbf{r};t) &= |\psi|^2,\\ \langle\mathbf{p}\rangle_{\mathbf{r},t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right].\end{aligned} \tag{12}$$

Thus, examining (11) and (12), we see that the Schrödinger equation suggests the general form

$$\langle A^n\rangle_{\mathbf{r},t} = \mathrm{Re}\left[\frac{1}{\psi(\mathbf{r},t)}\hat{A}^n\psi(\mathbf{r};t)\right], \tag{13}$$

where A is any observable and $\hat{A}$ is its corresponding operator. In Sec. III we show that the relativistic counterparts of (2) and (7) also lead us to (13).

III. CONDITIONAL MEAN VALUES SUGGESTED BY THE KLEIN–GORDON EQUATION

In Sec. II we have seen that the Schrödinger equation suggests a general expression for the conditional mean value at a given position of any observable quantity. It will now be shown that the Klein–Gordon equation also points to the same expression.

In classical relativistic mechanics, the relationship between the generalized momentum $\mathbf{p}$ and energy E of a particle under the influence of a scalar potential $V(\mathbf{r},t)$ and a vector potential $\mathbf{A}(\mathbf{r},t)$ is

$$(\mathbf{p} - (e/c)\mathbf{A})^2 + m_0^2c^2 = \frac{1}{c^2}(E - eV)^2,$$

i.e.,

$$p^2 + \frac{e^2}{c^2}A^2 - 2\frac{e}{c}\mathbf{A}\cdot\mathbf{p} + m_0^2c^2 = \frac{1}{c^2}(E^2 + e^2V^2 - 2eVE), \tag{14}$$

where m_0 is the rest mass of the particle. Hence, for an ensemble of particles, the mean values of momentum and energy for a particular position $\mathbf{r}$ at time t will satisfy

$$\langle p^2\rangle_{\mathbf{r},t} + \frac{e^2}{c^2}A^2 - 2\frac{e}{c}\mathbf{A}\cdot\langle\mathbf{p}\rangle_{\mathbf{r},t} + m_0^2c^2 = \frac{1}{c^2}(\langle E^2\rangle_{\mathbf{r},t} + e^2V^2 - 2eV\langle E\rangle_{\mathbf{r},t}). \tag{15}$$

The probability density $P(\mathbf{r};t)$ for our ensemble will satisfy the relativistic equation of continuity, which may be written in the form[16]

$$\partial_\mu\{P(\mathbf{r},t)\langle v^\mu\rangle_{\mathbf{r},t}\} = 0, \tag{16}$$

where a summation over $\mu = 0, 1, 2, 3$ is assumed and where the vector operator ∂_μ and the four-velocity v^μ are given by

$$\partial_\mu \equiv \left(\frac{1}{c}\frac{\partial}{\partial t}, \nabla\right)$$

and

$$v^\mu \equiv \left(c\frac{dt}{d\tau}, \frac{d\mathbf{r}}{d\tau}\right)$$

(τ being proper time). Using the relationship

$$v^{\mu} = \frac{1}{m_0}\left[\frac{1}{c}(E - eV)\ ,\ \mathbf{p} - \frac{e}{c}\mathbf{A}\right],$$

Eq. (16) may be expressed as

$$\nabla\cdot\left\{P(\mathbf{r},t)\frac{1}{m_0}\left(\langle p\rangle_{\mathbf{r},t} - \frac{e}{c}\mathbf{A}\right)\right\} + \frac{1}{c}\frac{\partial}{\partial t}\left\{P(\mathbf{r},t)\frac{1}{m_0 c}\left(\langle E\rangle_{\mathbf{r},t} - eV\right)\right\} = 0. \tag{17}$$

Now, the Klein–Gordon equation for a particle in an electromagnetic field, obtainable from (14) by the usual operator substitutions, has the form

$$\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)^2\psi + m_0^2c^2\psi = \frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t} - eV\right)^2\psi.$$

By dividing through by ψ and separating into real and imaginary parts, we obtain

$$\mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)^2\psi\right] + \frac{e^2}{c^2}A^2 - 2\frac{e}{c}\mathbf{A}\cdot\mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right] + m_0^2c^2 = \frac{1}{c^2}\left(\mathrm{Re}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)^2\psi\right] + e^2V^2 - 2eV\,\mathrm{Re}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)\psi\right]\right) \tag{18}$$

and

$$\mathrm{Im}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)^2\psi\right] + \hbar\nabla\cdot\frac{e}{c}\mathbf{A} - 2\frac{e}{c}\mathbf{A}\cdot\mathrm{Im}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right] = \frac{1}{c^2}\left(\mathrm{Im}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)^2\psi\right] - \hbar\frac{\partial}{\partial t}eV - 2eV\,\mathrm{Im}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\psi\right)\right]\right). \tag{19}$$

Multiplying (19) by $-|\psi|^2/\hbar m_0$ then gives (after some manipulation)

$$\nabla\cdot\left\{|\psi|^2\frac{1}{m_0}\left(\mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right] - \frac{e}{c}\mathbf{A}\right)\right\} + \frac{1}{c}\frac{\partial}{\partial t}\left\{|\psi|^2\frac{1}{m_0c}\left(\mathrm{Re}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)\psi\right] - eV\right)\right\} = 0. \tag{20}$$

We now postulate that Eqs. (18) and (20) are equivalent to Eqs. (15) and (17), respectively. Under this assumption, comparison of (15) and (18) suggests the following relationships:

$$\begin{aligned}
\langle\mathbf{p}\rangle_{\mathbf{r},t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right],\\
\langle p^2\rangle_{\mathbf{r},t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)^2\psi\right],\\
\langle E\rangle_{r,t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)\psi\right],\\
\langle E^2\rangle_{r,t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)^2\psi\right].
\end{aligned} \tag{21}$$

Similarly, comparing (17) and (20) we obtain

$$\begin{aligned}
P(\mathbf{r},t) &= |\psi|^2,\\
\langle\mathbf{p}\rangle_{\mathbf{r},t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(\frac{\hbar}{i}\nabla\right)\psi\right],\\
\langle E\rangle_{\mathbf{r},t} &= \mathrm{Re}\left[\frac{1}{\psi}\left(i\hbar\frac{\partial}{\partial t}\right)\psi\right].
\end{aligned} \tag{22}$$

The equations in (21) and (22) are in agreement with the general expression (13), found in Sec. II, for conditional mean values.

IV. THE JOINT DISTRIBUTION

Relationship (13) will now be used to derive a joint distribution expression for position and momentum. For the one-dimensional case of position x and momentum p, (13) yields

$$\langle p^n\rangle_{x,t} = \mathrm{Re}\left[\frac{1}{\psi(x;t)}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n\psi(x;t)\right] = \frac{1}{2}\left[\frac{1}{\psi(x;t)}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n\psi(x;t) + \frac{1}{\psi^*(x;t)}\left(i\hbar\frac{\partial}{\partial x}\right)^n\psi^*(x;t)\right]. \tag{23}$$

This expression is sufficient to determine uniquely the form of $P(x,p;t)$. We proceed by considering the mean value of the quantity $e^{i\tau p}$ for a given position x:

$$\langle e^{i\tau p}\rangle_{x,t} \equiv \int_{-\infty}^{+\infty} e^{i\tau p}P(p|x;t)\,dp.$$

This expression shows that $\langle e^{i\tau p}\rangle_{x,t}$ is the Fourier transform of $P(p|x;t)$ and so we may write

$$P(p|x;t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i\tau p}\langle e^{i\tau p}\rangle_{x,t}\,d\tau.$$

Using the general relationship

$$\begin{aligned}
P(x,p;t) &= P(p|x;t)P(x;t)\\
&= P(p|x;t)|\psi(x;t)|^2,
\end{aligned}$$

we have, therefore,

$$P(x,p;t) = \frac{1}{2\pi}|\psi(x;t)|^2\int_{-\infty}^{+\infty} e^{-i\tau p}\langle e^{i\tau p}\rangle_{x,t}\,d\tau. \tag{24}$$

Now, the conditional mean value of $e^{i\tau p}$ can be expressed also in the form

$$\langle e^{i\tau p}\rangle_{x,t} = \left\langle\sum_n\frac{(i\tau p)^n}{n!}\right\rangle_{x,t} = \sum_n\frac{(i\tau)^n}{n!}\langle p^n\rangle_{x,t}. \tag{25}$$

Hence, on combining (23) and (25), we have

$$\begin{aligned}
\langle e^{i\tau p}\rangle_{x,t} &= \sum_n\frac{(i\tau)^n}{n!}\frac{1}{2}\left[\frac{1}{\psi(x;t)}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^n\psi(x;t) + \frac{1}{\psi^*(x;t)}\left(i\hbar\frac{\partial}{\partial x}\right)^n\psi^*(x;t)\right]\\
&= \frac{1}{2\psi(x;t)}\sum_n\frac{(\hbar\tau)^n}{n!}\frac{\partial^n}{\partial x^n}\psi(x;t) + \frac{1}{2\psi^*(x;t)}\sum_n\frac{(-\hbar\tau)^n}{n!}\frac{\partial^n}{\partial x^n}\psi^*(x;t).
\end{aligned}$$

Recognizing the two summations as Taylor expansions, we obtain

$$\langle e^{i\tau p}\rangle_{x,t} = \frac{1}{2\psi(x;t)}\psi(x+\hbar\tau;t) + \frac{1}{2\psi^*(x;t)}\psi^*(x-\hbar\tau;t),$$

and inserting this into (24) yields

$$P(x,p;t) = \frac{1}{4\pi}\psi^*(x;t)\int_{-\infty}^{+\infty} e^{-i\tau p}\psi(x+\hbar\tau;t)\,d\tau + \frac{1}{4\pi}\psi(x;t)\int_{-\infty}^{+\infty} e^{-i\tau p}\psi^*(x-\hbar\tau;t)\,d\tau.$$

By replacing the integration variable τ by $-\tau$, the first integral may be rewritten as

$$\int_{-\infty}^{+\infty} e^{-i\tau p}\psi(x+\hbar\tau;t)\,d\tau = \int_{-\infty}^{+\infty} e^{i\tau p}\psi(x-\hbar\tau;t)\,d\tau.$$

Hence we have

$$P(x,p;t) = \frac{1}{2\pi}\,\mathrm{Re}\left[\psi(x;t)\int_{-\infty}^{+\infty} e^{-i\tau p}\psi^*(x-\hbar\tau;t)\,d\tau\right].$$

This may be recognized as the Margenau and Hill joint distribution (see Sec. I).

The above reasoning constitutes an independent derivation of the Margenau and Hill distribution, which was proposed by Margenau and Hill on the basis of other considerations.

V. DISCUSSION

We have found that the Schrödinger and Klein–Gordon equations suggest a particular joint distribution for quantum mechanics. However, this distribution function is not positive definite and there is no physical interpretation for negative probabilities. We are therefore led to doubt the assumptions which have been made in the derivation, such as that the observable momentum and energy values in quantum mechanics continue (as the forms of the Schrödinger and Klein–Gordon equations suggest) to satisfy the relationships of classical mechanics, or even that the joint distribution at any time is completely determined by the prevailing form of the wavefunction.

ACKNOWLEDGMENT

The author would like most sincerely to thank John R. Shepanski for many helpful discussions.

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[12] Joint distributions for quantum mechanics are usually discussed in one dimension. They can be readily generalized to three dimensions.
[13] They can, however, be useful as calculational tools. For example, the Wigner distribution has been employed in quantum thermodynamics and quantum optics. In this regard, it should be stressed that, since it is impossible to measure x and p together, only the integrals of $P(x,p)$ over x and p have experimental significance and so, from a *practical* point of view, only these integrals [rather than $P(x,p)$ itself] need be positive definite.
[14] In this section and the next we will turn to a three-dimensional treatment.
[15] Such an identification is mathematically plausible because the $\mathbf{p}$ and E terms in Eqs. (4) and (6), like their counterparts in (8) and (10), are functions of $\mathbf{r}$ and t. This explains why we have introduced the notion of conditional mean values.
[16] In this equation, $P(\mathbf{r},t)$ represents the invariant probability density at the point $\mathbf{r}$ (i.e., the probability density relative to the rest frame of the probability flow at that point).

Impact parameter representation for scattering involving arbitrary spins

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(Received 15 June 1981; accepted for publication 18 September 1981)

An impact-parameter representation that is valid at all angles and all energy has been obtained for systems with arbitrary spins. In contrast to the spinless case, this representation gives rise to generalized profile functions that are distributions even in the physical region. This proves kinematical equivalence between partial wave representation and impact parameter representation for the case of arbitrary spin systems.

PACS numbers: 03.65.Nk

I. INTRODUCTION

Generally two-particle scattering processes are analyzed in terms of phase-shifts using a partial wave representation for the amplitude. This procedure is quite satisfactory whenever the number of partial waves involved is small, which is the case for low energy scattering processes. At higher energies, however, the number of partial waves needed for such an analysis becomes so large that no reasonable estimate of the phase-shifts can be made. Therefore, approximation schemes must be used. One of the popular schemes is an eikonal approximation[1] where the scattering amplitude is written[2]

$$f(s,t) = \int_0^\infty dB\, BJ_0(B\sqrt{-t})\Gamma(s,B). \tag{1.1}$$

The usual derivation of Eq. (1.1)[1,3] is based on restrictions of small angles and high energies where the summation over partial waves is replaced by an integration over an impact parameter "B" that is related to the orbital angular momentum by the relation $2kB = 2l + 1$. These restrictions on the validity of expression (1.1) are the source of two important defects.

First, there is a limit on the spin effects that may be considered in the formalism because there is no relationship between the classical parameter B and the spin similar to $2kB = 2l + 1$. Therefore, only very limited forms[1,4] of the interactions involving spins have been considered within the formalism. For instance, the spin effect so far considered in the scattering of two spin $\frac{1}{2}$ particles (say nucleon–nucleon scattering) in the eikonal approximation are $\mathbf{L}\cdot\mathbf{S}$ and $\boldsymbol{\sigma}^1\cdot\boldsymbol{\sigma}^2$ types only, whereas the effects of the tensor force involving space–spin coupling of the form $(\boldsymbol{\sigma}^1\cdot\hat{r})(\boldsymbol{\sigma}^2\cdot\hat{r})$ and Majorana exchange forces have been arbitrarily ignored. The second defect is related to writing the inverse transform of Eq. (1.1) which is not allowed because of the restricted validity of the right hand side. This becomes a serious drawback in the analysis of the scattering data where the interaction is not known. As an example, the inverse of Eq. (1.1) is needed for expressing the scattering of two composite objects in terms of their constituents.

This paper is mainly concerned with the removal of both these drawbacks and the writing of a generalized formalism that is valid at all angles, all energies, and incorporates the general spin. Many attempts have been made to generalize the validity of the expression (1.1).[5] Most of these partially successful attempts were based on the exact relationship

$$P_l(\cos\Theta) = \int_0^\infty d\beta\, J_0(\beta y)J_{2l+1}(\beta), \tag{1.2}$$

between Legendre functions and Bessel functions for physical values of scattering angle $\cos\Theta = 1 - 2y^2$. The impact parameter representation obtained by replacing the $P_l(\cos\Theta)$ in the partial wave representation by (1.2), however, was not unique.[6] Recently, Islam[7] has obtained an exact and unique impact parameter representation or Fourier–Bessel (FB) representation using the Watson–Sommerfeld transform of the elastic scattering amplitude for two spinless particles. This representation is valid for all physical energies and scattering angles, thus removing the second defect.

Generalizing expression (1.2) to incorporate spin into the formalism is not a trivial matter. A first attempt to generalize (1.2) has been made by Kamal[8] for the pion–nucleon scattering by differentiating expression (1.2) with respect to y to obtain an expression for $P_l^1(\cos\Theta)$. But the analogous integral for $P_l^m(\cos\Theta)$ thus obtained does not exist because it blows up at infinity. In other words, differentiation of expression (1.2) is not allowed beyond the first order, yet that is precisely what one needs for scattering involving general spin. However, Kamal's[8] impact parameter representation suffers from nonuniqueness. Another attempt to incorporate spins has been made by Luming and Predazzi.[9] They have obtained an FB representation for the helicity amplitude which is valid at all angles and energies. But again it is nonunique.

The author[10] has obtained a unique impact parameter representation for the nucleon–nucleon scattering following the arguments of the Refs. 7 and 9. The scattering representation takes account of spin, isospin, and the Pauli exclusion principle in a most general fashion allowed by symmetries [see Ref. 10, Eqs. (37)–(42)]. Although the representation obtained in Ref. 10 is valid at all angles, all energies and is unique, it still has a restriction on the sum of helicities in the initial and final states. To illustrate the restriction, consider the double helicity flip amplitude for isospin I given in terms of the partial wave expansion

$$E\phi_4^I(k,z) = \frac{1}{2}\sum_j (2j+1)\{[h_{22}^+(j_+,s)\delta_{I,1} - h_1^+(j_+,s)\delta_{I,0}]P_j^+ + [h_{22}^-(j_-,s)\delta_{I,0} - h_1^-(j,s)\delta_{I,1}]P_j^-\}d^j_{-1,1}(\Theta).$$

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The impact parameter representation for the amplitude $\phi_4^I(k,z)$ is then obtained by replacing the rotation function of the first kind $d^j_{-1,1}$ by

$$d^j_{-1,1}(\Theta) = \frac{1}{2}\int_0^\infty d\beta \left[J_2(\beta \sin\Theta/2) \mp \frac{\beta^2 \sin\Theta/2}{2j(j+1)} J_0(\beta\cos\Theta/2)\right] J_{2j+1}(\beta)$$

in the above expression. But the integral expression for $d^j_{-1,1}$ is not a convergent one. To overcome this difficulty, a demand was made on the partial wave amplitudes to supply corresponding convergent factors. This restriction persists even though the uniqueness was achieved by defining the FB transform of $d^j_{-1,1}$ in the unphysical region. This difficulty is discussed in detail for a general case in Sec. II and ultimately removed by defining the Fourier–Bessel transform as a distribution in Sec. III. Then the resulting unique FB representation has its inverse transform defined. Finally, Sec. IV summarizes some of the important implications of this improved representation.

II. FOURIER–BESSEL AMPLITUDE FOR PHYSICAL ANGLES

A. Preliminaries

When spin is to be incorporated explicitly in expression (1.1), it is advantageous to work with a helicity representation of the scattering amplitude because the helicity amplitudes have well-known kinematical singularities.[11–13] This characteristic allows one to define reduced amplitudes that are free of kinematical singularities and at the same time satisfy the Mandelstam representation. Furthermore, as will become clear in the present and the following sections, the kinematical singularities also help one to write the impact parameter. Therefore, the present discussion begins with the helicity representation for the scattering amplitude with the partial wave expansion

$$f_{\lambda,\mu}(s,t) = \sum_{j=\lambda_{\max}}^{\infty} (2j+1) f_{\lambda,\mu}(j,s) d^j_{\lambda,\mu}(z), \tag{2.1}$$

which converges in the Lehman ellipse in the complex z plane. Here, λ and μ are the differences of helicities of particles in the initial and final states, and the notation followed is the same as that given in Ref. 11. The functions $d^j_{\lambda,\mu}(z)$ are the reduced rotation functions of the first kind[11,12] and are defined for z within the circle $|z-1|<2$ by

$$d^j_{\lambda,\mu}(z) = \mathrm{sign}(\lambda,\mu)\phi_{\lambda,\mu}(j,a)\left(\frac{1-z}{2}\right)^{a/2}\left(\frac{1+z}{2}\right)^{b/2} \times \frac{{}_2F_1(\lambda_{\max}-j, j+\lambda_{\max}+1; 1+a; (1-z)/2)}{\Gamma(1+a)}, \tag{2.2}$$

where

$$a = |\lambda-\mu|, \quad b = |\lambda+\mu|,$$
$$\lambda_{\max} = \mathrm{Max.}(|\lambda|,|\mu|) = \tfrac{1}{2}(a+b),$$
$$\lambda_{\min} = \mathrm{Min.}(|\lambda|,|\mu|) = \tfrac{1}{2}|b-a|,$$
$$\phi_{\lambda,\mu}(j,a) = \left[\frac{\Gamma(j+\lambda_{\max}+1)\Gamma(j+1-\lambda_{\max}+a)}{\Gamma(j-\lambda_{\max}+1)\Gamma(j+1+\lambda_{\max}-a)}\right]^{1/2},$$

and

$$\mathrm{sign}(\lambda,\mu) = \begin{cases} 1 & \text{for } \lambda+\mu \geqslant 0 \\ (-)^{\lambda-\mu} & \text{for } \lambda-\mu \leqslant 0. \end{cases}$$

For convenience $(\lambda \pm \mu) \geqslant 0$ is assumed throughout the paper. The results obtained below are quite general and the "sign" factor takes care of the other domain of λ and μ values.[11,12] The function ${}_2F_1$ appearing in the expression (2.2) is a hypergeometric function. The properties of $d^j_{\lambda,\mu}(z)$, e.g., analyticity, etc., are discussed in great detail in Refs. 11 and 12 and I will assume all of these properties here without further discussion.

To derive the impact parameter representation, one can directly start from expression (2.1) and follow the procedure of Ref. 9, but the FB amplitude derived in this fashion is quite arbitrary because the behavior of the scattering amplitude in the whole unphysical momentum transfer region is not specified. This arbitrariness can be removed by applying the Watson–Sommerfeld transform to continue analytically the amplitude in the unphysical region.[11,14] To write the Watson–Sommerfeld transform, one must rewrite expression (2.1) in terms of signatured amplitudes[12,14] so that conditions of Carlson's theorem are satisfied. Thus rewriting (2.1) in terms of signatured amplitudes yields

$$f_{\lambda,\mu}(s,t) = \sum_{j=\lambda_{\max}}^{\infty} (2j+1)\left[f^+_{\lambda,\mu}(j,s) d^+_{\lambda,\mu}(j,z) + f^-_{\lambda,\mu}(j,s) d^-_{\lambda,-\mu}(j,z)\right], \tag{2.3}$$

where

$$d^\sigma_{\lambda,\mu}(j,z) = \tfrac{1}{2}\left[d^j_{\lambda,\mu}(z) + \sigma(-)^{\lambda_{\max}-\upsilon} d^j_{\lambda,-\mu}(-z)\right]. \tag{2.4}$$

In Eqs. (2.3) and (2.4) the parameter σ takes the values ± 1, and parameter υ is equal to 0 or $\frac{1}{2}$ depending on whether the value of j is an integer or half-odd integer, respectively. Note also that the rotation function $d^\pm_{\lambda,\mu}(j,z)$ vanishes for $j-\upsilon =$ odd/even because of the symmetry properties of $d^j_{\lambda,\mu}(z)$. Thus, the scattering amplitudes of definite signature are defined by

$$f^\sigma_{\lambda,\mu}(s,t) = \sum_{j=\lambda_{\max}}^{\infty} (2j+1) f^\sigma_{\lambda,\mu}(j,s) d^\sigma_{\lambda,\mu}(j,z). \tag{2.5}$$

At this point the partial wave series (2.5) can be cast as a contour integral in the complex j plane[12,14]

$$f^\sigma_{\lambda,\mu}(s,t) = \frac{-1}{2i}\oint_c dj\,(2j+1) f^\sigma_{\lambda,\mu}(j,s) \frac{d^\sigma_{\lambda,-\mu}(j,-z)}{\sin[\pi(j-\lambda_{\max})]}, \tag{2.6}$$

where contour c encloses the positive real j axis in the clockwise direction beyond $j \geqslant \lambda_{\max}$. Here the function $f^\sigma_{\lambda,\mu}(j,s)$ is the analytically continued partial wave amplitude, and the uniqueness of the continuation follows from Carlson's theorem.[12,14]

B. Impact parameter amplitude

The impact parameter amplitude in the physical region $|z-1|<2$ (or $0<y<1$) is derived by collapsing the contour c on the real axis. In this situation (2.6) reduces to

$$f^{\sigma}_{\lambda,\mu}(s,t) = \frac{-1}{2\pi i}\int_{j=\lambda_{\max}}^{\infty} dj f^{\sigma}_{\lambda,\mu}(j,s)(2j+1)d^{\sigma}_{\lambda,-\mu}(j,-z) \times\left[\frac{\pi}{\sin[\pi(j-\lambda_{\max})_+]} - \frac{\pi}{\sin[\pi(j-\lambda_{\max})_-]}\right], \tag{2.7}$$

where

$$(j-\lambda_{\max})_{\pm} = j-\lambda_{\max} \pm i\epsilon.$$

For the physical region ($|z-1|<2$), the distribution

$$D(j,z) = -(2j+1)d^{\sigma}_{\lambda,-\mu}(j,-z) \times\left[\frac{\pi}{\sin[\pi(j-\lambda_{\max})_+]} - \frac{\pi}{\sin[\pi(j-\lambda_{\max})_-]}\right] \tag{2.8}$$

reduces to the form

$$D(j,z) = 2\pi i\sum_{n=0}^{\infty}(2n+1)d^{\sigma}_{\lambda,\mu}(j,z)\delta([j-\lambda_{\max}]-n). \tag{2.9}$$

Now to express (2.9) as an FB transform, the rotation functions $d^{j}_{\lambda,\mu}(z)$ need to be written in terms of Bessel's function in exactly the same way as is done for Legendre function [see expression (1.2)]. This result can be achieved by starting with expression (2.2) for the rotation function and using the Weber–Schafheitlin integral

$$\int_0^{\infty} t^{-\lambda'}J_{\mu'}(ct)J_{\nu}(pt) = \frac{c^{\mu'}\Gamma((\mu'+\nu'-\lambda'+1)/2)}{2^{\lambda'}p^{\mu'-\lambda'+1}\Gamma((\nu'-\mu'+\lambda'+1)/2)}\frac{{}_2F_1((\mu'+\nu'-\lambda'+1)/2,(\mu'-\lambda'-\nu'+1)/2;1+\mu';c^2/p^2)}{\Gamma(1+\mu')} \tag{2.10}$$

given by equation (29) in Sec. 7.74 of HTF 2[15] page 51. The expression (2.10) is valid for $\mathrm{Re}(\mu'+\nu'-\lambda'+1)>0$, $\mathrm{Re}\,\lambda'>1$ and $0>c>p$.

These restrictions are satisfied by replacing the hypergeometric function in (2.2) using

$${}_2F_1\left(\lambda_{\max}-j;j+\lambda_{\max}+1;1+a;\frac{1-z}{2}\right) = \left(\frac{1+z}{2}\right)^{-b}{}_2F_1\left(j-\mu+1,-j-\mu;1+a,\frac{1-z}{2}\right)$$

and then making the following identifications:

$$\lambda' = \lambda+\mu, \quad \nu' = 2j+1, \quad c = \left(\frac{1-z}{2}\right)^{1/2} = y,$$
$$p = 1, \quad \text{and} \quad \mu' = \lambda-\mu.$$

Thus expression (2.2) becomes

$$d^{j}_{\lambda,\mu}(z) = \mathrm{sign}(\lambda,\mu)\phi_{\lambda,\mu}(j,a)2^{b}\left(\frac{1+z}{2}\right)^{-b/2}\frac{\Gamma(-\lambda_{\max}+j+1)}{\Gamma(\lambda_{\max}+j+1)} \times\int_0^{\infty} d\beta\,\beta^{-b}J_a(\beta y)J_{2j+1}(\beta). \tag{2.11}$$

But notice the kinematical singularities $[(1+z)/2]^{-b/2}[(1-z)/2]^{a/2}$ appearing in expression (2.11) are contrary to the kinematical singularities appearing in the starting expression (2.2), viz. $[(1+z)/2]^{b/2}[(1-z)/2]^{a/2}$. Thus, the expression (2.11) is not yet suitable for deriving the impact parameter representation. The remedy for this defect is to identify

$$\lambda' = -b, \quad \nu' = 2j+1, \quad c = y,$$
$$p = 1, \quad \text{and} \quad \mu' = \lambda-\mu$$

in Eq. (2.10). Substituting this result into expression (2.2) yields

$$d^{j}_{\lambda,\mu}(z) = \mathrm{sign}(\lambda,\mu)\phi_{\lambda,\mu}(j,a)2^{-b}\left(\frac{1+z}{2}\right)^{b/2}\frac{\Gamma(j-\lambda_{\max}+1)}{\Gamma(j+\lambda_{\max}+1)} \times\int_0^{\infty} d\beta\,\beta^{b}J_a(\beta y)J_{2j+1}(\beta). \tag{2.12}$$

Now expression (2.12) has the right kinematical factors, viz. $[(1+z)/2]^{b/2}[(1-z)/2]^{a/2}$, but it is valid for $\mathrm{Re}\,b<1$. This restriction ($\mathrm{Re}\,b<1$) is the one that causes the problem when one writes the impact parameter representation for double helicity flip amplitude $\phi^{I}_{4}(k,z)$ in the nucleon–nucleon scattering, as mentioned in the last paragraph of Sec. I. This restriction will be removed later on.

Expression (2.12) has also been used by Luming and Predazzi[9] to derive the impact parameter; in this instance the restriction $\mathrm{Re}\,b<1$ was relaxed by requiring the profile functions $\Gamma(\beta,s)$ to supply the appropriate convergence factors. Luming and Predazzi, however, obtained two equivalent forms of the FB representation for the same helicity amplitude because they did not use the signatured amplitudes. In contrast, the formulation worked out below yields only one FB representation for the helicity amplitude $f_{\lambda,\mu}(s,t)$ in the physical region.

If the restriction $\mathrm{Re}\,b<1$ in the expression (2.12) is relaxed, the integrand blows up as $\beta\to\infty$ and representation (2.12) does not exist. However, if the singularity of $\beta=\infty$ is treated as a distribution (generalized function),[16] the integral in (2.12) which reproduces the rotation function $d^{j}_{\lambda,\mu}(z)$ of the first kind can be defined. This result is achieved by replacing β^{b} in the integral by the distribution

$$\beta^{b}_{+} = \frac{\Gamma(-j-\lambda_{\max})}{-2\pi i}\lim_{\delta\to 0}\int_{\infty}^{0+}\frac{d\Lambda}{\Lambda^{2}}(-\Lambda)^{-j-\lambda_{\max}} \times e^{-\beta^{2}/(\Lambda+\delta)}\beta^{2j+2\lambda_{\max}+b+2}, \tag{2.13}$$

where Hankel's expression for $\Gamma(z)$[17] is used in obtaining the result.

That β^{b}_{+} is an appropriate distribution for this purpose can be shown by evaluating the integral

$$I=\int_0^\infty d\beta\,\beta^b_+\,J_a(\beta y)J_{2j+1}(\beta). \tag{2.14a}$$

The steps in the evaluation of (2.14) are presented in Appendix A. The final result is

$$I=\frac{\Gamma(j+\lambda_{\max}+1)}{\Gamma(j-\lambda_{\max}+1)}2^b\left(\frac{1-z}{2}\right)^{a/2}\times\frac{{}_2F_1(\lambda_{\max}-j,j+\lambda_{\max}+1;1+a;(1-z)/2)}{\Gamma(1+a)}. \tag{2.14b}$$

At this point if expression (2.14b) is substituted for the integral in expression (2.12), the latter expression readily reduces to (2.2). This proves that (2.13) is an appropriate distribution.

Next substituting (2.13) in the expression (2.12) yields

$$d^j_{\lambda,\mu}(z)=\mathrm{sign}(\lambda,\mu)\phi_{\lambda,\mu}(j,a)2^{-b}\left(\frac{1+z}{2}\right)^{b/2}\frac{\Gamma(j-\lambda_{\max}+1)}{\Gamma(j+\lambda_{\max}+1)}\times\int_0^\infty d\beta\,\beta^b_+\,J_a(\beta y)J_{2j+1}(\beta). \tag{2.15}$$

The limit $\delta\to 0$ in (2.15) must be taken after evaluating the FB integration. Now expression (2.15) is valid for all values of b, and the integral converges because of the Gaussian factor in the distribution.

At this point the rotation function $d^j_{\lambda,\mu}(z)$ of first kind has been expressed in terms of Bessel's function $J_a(\beta y)$ for the purpose of deriving the impact parameter representation. But one needs the signatured combination of the rotation functions to derive the required result from expressions (2.7) and (2.9). This combination may be written down from (2.4) using expression (2.15) as

$$d^\sigma_{\lambda,\mu}(z)=\frac{1}{2}\int_0^\infty d\beta\left[\left(\frac{1+z}{2}\right)^{b/2}J_a(\beta y)\mathscr{D}_{\lambda,\mu}(j;a,b;\beta)+\sigma(-)^{\lambda_{\max}-v}\left(\frac{1-z}{2}\right)^{a/2}J_b(\beta x)\mathscr{D}_{\lambda,-\mu}(j;b,a;\beta)\right], \tag{2.16}$$

where

$$\mathscr{D}_{\lambda,\mu}(j;a,b;\beta)=\mathrm{sign}(\lambda,\mu)\phi_{\lambda,\mu}(j,a)2^{-b}\times\frac{\Gamma(j-\lambda_{\max}+1)}{\Gamma(j+\lambda_{\max}+1)}\beta^b_+\,J_{2j+1}(\beta). \tag{2.17}$$

Now substituting expression (2.16) into expression (2.9) and interchanging summation and integration yields

$$D(j,z)=2\pi i\int_0^\infty d\beta\left\{\frac{1}{2}\left[\left(\frac{1+z}{2}\right)^{b/2}J_a(\beta y)G_{\lambda,\mu}(j;a,b;\beta)+\sigma(-)^{\lambda_{\max}-v}\left(\frac{1-z}{2}\right)^{a/2}J_b(\beta\alpha)G_{\lambda,-\mu}(j;b,a;\beta)\right]\right\} \tag{2.18}$$

and

$$G_{\lambda,\mu}(j;a,b;\beta)=\sum_{n=0}^\infty(2n+1)\mathscr{D}_{\lambda,\mu}(j;a,b,\beta)\delta([j-\lambda_{\max}]-n). \tag{2.19}$$

Finally, expressions (2.18) and (2.19), when used in (2.7), yield the impact parameter representation for the signatured helicity amplitude

$$f^\sigma_{\lambda,\mu}(s,t)=\frac{1}{2}\int_0^\infty d\beta\left[\left(\frac{1+z}{2}\right)^{b/2}J_a(\beta y)\,{}^1\Gamma^\sigma_{\lambda,\mu}(a,b;s,\beta)+\sigma(-)^{\lambda_{\max}-v}\left(\frac{1-z}{2}\right)^{a/2}J_b(\beta x)\,{}^1\Gamma^\sigma_{\lambda,-\mu}(b,a;s,\beta)\right], \tag{2.20}$$

where the profile function is given by

$${}^1\Gamma^\sigma_{\lambda,\mu}(a,b;s,\beta)=\sum_{j=\lambda_{\max}}^\infty(2j+1)f^\sigma_{\lambda,\mu}(j,s)\mathscr{D}_{\lambda,\mu}(j;a,b,\beta). \tag{2.21}$$

The identification of variable $\beta=2kB$, where B is a usual classical impact parameter, provides the required representation.

Expression (2.20) shows the explicit symmetry for forward and backward scattering; this last feature was missed by Luming and Predazzi[9] and caused them to arrive at two different FB representations. Note also that unlike the spinless situation, the representation for the physical angles in the present case is a distribution that cannot be avoided if the extra restriction on the profile function as mentioned above is to be relaxed.

Finally, expression (2.20) with the profile function (2.21) is nonunique. The source of this nonuniqueness is the interchange of integration over j appearing in (2.7) and the infinite summation in (2.18), performed while obtaining expressions (2.20) and (2.21). This nonuniqueness is now discussed and removed.

III. UNIQUENESS OF THE REPRESENTATION

The representation of the profile function given by expression (2.21) is not unique. This nonuniqueness arises from not specifying the amplitude for the unphysical regions of angles. This cause can be seen by adding to expression (2.21), a term $H^\sigma_{\lambda,\mu}(a,s,\beta)$, defined below

$$H^\sigma_{\lambda,\mu}(a,s,\beta)=\beta\int_1^\infty dy'\,y'J_a(\beta y')F^\sigma_{\lambda,\mu}(s,y'), \tag{3.1}$$

where $F^\sigma_{\lambda,\mu}(s,y')$ is completely arbitrary. Then the equations

$$f^\sigma_{\lambda,\mu}(s,t)=\frac{1}{2}\int_0^\infty d\beta\left[\left(\frac{1+z}{2}\right)^{b/2}J_a(\beta y)\Gamma^\sigma_{\lambda,\mu}(a,b;s,\beta)+\sigma(-)^{\lambda_{\max}-v}\left(\frac{1-z}{2}\right)^{a/2}J_b(\beta x)\Gamma^\sigma_{\lambda,-\mu}(b,a;s,\beta)\right], \tag{3.2}$$

with

$$\Gamma^\sigma_{\lambda,\mu}(a,b;s,\beta)={}^1\Gamma^\sigma_{\lambda,\mu}(a,b;s,\beta)+H^\sigma_{\lambda,\mu}(a,s,\beta), \tag{3.3}$$

will still reproduce the same scattering amplitude in the physical region, since by construction for $y<1$

$$\int_0^\infty d\beta\,\beta J_a(\beta y)\int_1^\infty dy'\,y'J_a(\beta y')F^\sigma_{\lambda,\mu}(s,y')=\int_1^\infty dy'\,\delta(y-y')F^\sigma_{\lambda,\mu}(s,y')=0. \tag{3.4}$$

Thus, the origin of the nonuniqueness lies in not specifying the scattering amplitude $f^\sigma_{\lambda,\mu}(s,t)$ as a function of angle in the unphysical region $|z-1|>2$. In other words, similar argu-

ments hold here as in the spinless case.[7] Therefore, the same procedure as was followed in the spinless case by Islam[7] is justified here; namely the Watson–Sommerfeld transformation can be applied to continue analytically the $f^{\sigma}_{\lambda,\mu}(s,t)$ in the unphysical region by specifying $H^{\sigma}_{\lambda,\mu}(a,s,\beta)$.

In following this procedure, note that in expression (2.6) the scattering angle appears only in the rotation function $d^{j}_{\lambda,\mu}(-z)$. This rotation function can be analytically defined for $|z-1|>2$ using[11,12]

$$d^{j}_{\lambda,\mu}(z)=\frac{\tan\pi(j-\lambda_{\max})}{\pi}\left[e^{j}_{\lambda,\mu}(z)-e^{-j-1}_{-\lambda,-\mu}(z)\right], \tag{3.5}$$

where the rotation function of the second kind are defined by

$$e^{j}_{\lambda,\mu}(z)=\frac{1}{2}\,\mathrm{sign}(\lambda,\mu)\psi_{\lambda,\mu}(j)\left(\frac{1-z}{2}\right)^{-a/2}\left(\frac{1+z}{2}\right)^{-b/2}\left(\frac{z-1}{2}\right)^{-j-1+\lambda_{\max}} \times\frac{{}_2F_1(j-\lambda_{\max}+1,j-\lambda_{\max}+a+1;2j+2;2/(1-z))}{\Gamma(2j+2)}, \tag{3.6}$$

and

$$\psi_{\lambda,\mu}(j)=[\Gamma(j+\lambda_{\max}+1)\Gamma(j-\lambda_{\max}+1)\Gamma(j+\lambda_{\min}+1)\Gamma(j-\lambda_{\min}+1)]^{1/2}. \tag{3.7}$$

The rotation function of the second kind can again be expressed in terms of Bessel's function using the Weber–Schafheitlin integral (2.10) and identifying $\mu'=2j+1, p=y, c=1, \lambda'=-b, \nu'=-a$. The result is

$$e^{j}_{\lambda,\mu}(z)=\mathrm{sign}(\lambda,\mu)2^{-1-b}\phi_{\lambda,\mu}(j,a)\left(\frac{1+z}{2}\right)^{b/2}\frac{(-)^{j-\lambda_{\max}}\pi}{\sin\pi(j-\lambda_{\max})}\frac{\Gamma(j-\lambda_{\max}+1)}{\Gamma(j+\lambda_{\max}+1)}\int_0^{\infty}d\beta\,\beta^{b}J_a(\beta y)J_{2j+1}(\beta). \tag{3.8}$$

A similar expression could also have been derived by using the parameters $\mu'=2j+1, p=y, c=1, \lambda'=b, \nu'=a$ in (2.10). The representation thus obtained would have been valid for all j and b, but the kinematical factors appearing in $d^{j}_{\lambda,\mu}(z)$ would not be $2^{-b/2}(1+z)^{b/2}(1-z)^{a/2}$. Given this situation, I have preferred the choice as represented by expression (3.8), even though the validity domain is restricted to $\mathrm{Re}\,b<1$ and $\mathrm{Re}(2j+2\lambda_{\max}+2)>0$.

If the restriction $\mathrm{Re}\,b<1$ is to be removed, steps similar to those used in deriving expression (2.15) must be followed. This result can be achieved by smoothing the singularity at $\beta=\infty$, i.e., β^{b} is replaced by the distribution β^{b}_{+} as defined in expression (2.13). The result obtained is

$$e^{j}_{\lambda,\mu}(z)=\mathrm{sign}(\lambda,\mu)2^{-1-b}\phi_{\lambda,\mu}(j,a)\left(\frac{1+z}{2}\right)^{b/2}\frac{(-)^{j-\lambda_{\max}}\pi}{\sin[\pi(j-\lambda_{\max})]} \times\frac{\Gamma(j-\lambda_{\max}+1)}{\Gamma(j+\lambda_{\max}+1)}\int_0^{\infty}d\beta\,\beta^{b}_{+}J_a(\beta y)J_{aj+1}(\beta). \tag{3.9}$$

The correctness of this procedure is proved in later part of Appendix A.

The restriction $\mathrm{Re}(2j+2\lambda_{\max}+2)>0$ is always satisfied in the case of $e^{j}_{\lambda,\mu}(z)$. If expression (3.9) is used to define FB representation for $e^{-j-1}_{-\lambda,\mu}(z)$, one restriction on the validity still remains, viz. $\mathrm{Re}(2\lambda_{\max}-2j)>0$. This final restriction can be relaxed again by replacing $\beta^{b}_{+}J_{-2j-1}(\beta)$ by the distribution

$$\Delta(j,b,\beta)=\lim_{\delta\to0}\beta^{b}J_{-2j-1}(\beta)\left[\frac{\Gamma(\lambda_{\max}-j)}{-2\pi i}\int_{\infty}^{0+}\frac{d\Lambda}{\Lambda^{2}} \times(-\Lambda)^{\lambda_{\max}-j}e^{-\beta^{2}/(\Lambda+\delta)}\beta^{2j+2-2\lambda_{\max}}\right]. \tag{3.10}$$

The proof that (3.10) is the right distribution to give the function $e^{-j-1}_{-\lambda,-\mu}(z)$ is presented in Appendix B. Finally, one should note that the distribution defined by expression (3.10) "smooths" the power singularity both at the origin and at infinity.

At this stage the procedure for writing down the analogous expressions for the signatured combinations $d^{\sigma}_{\lambda,\mu}(j,z)$, and $e^{\sigma}_{\lambda,\mu}(j,z)$ is straightforward. The expressions are

$$e^{\sigma}_{\lambda,\mu}(j,z)=\frac{1}{2}\left[e^{j}_{\lambda,\mu}(z)+\sigma(-)^{\lambda_{\max}-\nu}e^{j}_{\lambda,-\mu}(-z)\right] \tag{3.11}$$

$$=\frac{1}{2}\int_0^{\infty}d\beta\left[\sigma(-)^{\lambda_{\max}-\nu}\left(\frac{1+z}{2}\right)^{b/2} \times J_a(\beta y)g_{\lambda,\mu}(j;a,b;\beta)\right] +\left(\frac{1-z}{2}\right)^{a/2}J_b(\beta x)\bar{g}_{\lambda,\mu}(j;a,b;\beta), \tag{3.12}$$

where

$$g_{\lambda,\mu}(j;a,b;\beta)=\frac{\pi}{2\sin\pi(j-\lambda_{\max})}\mathscr{D}_{\lambda,\mu}(j;a,b;\beta). \tag{3.13}$$

For $e^{\sigma}_{-\lambda,-\mu}(-j-1,z)$, the $\beta^{b}_{+}J_{-2j-1}(\beta)$ factor in $g_{-\lambda,-\mu}(-j-1;a,b,\beta)$ must be replaced by the distribution $\Delta(j,b,\beta)$ as defined in the Eq. (3.10). This result then for $|z-1|>2$[12]

$$d^{\sigma}_{\lambda,\mu}=\frac{\tan\pi(j-\lambda_{\max})}{\pi}\left[e^{\sigma}_{\lambda,\mu}(j,z)-e^{\epsilon_{\sigma}}_{-\lambda,-\mu}(-j-1,z)\right] \tag{3.14}$$

$$d^{\sigma}_{\lambda,\mu}=\frac{1}{2}\int_0^{\infty}d\beta\left[\sigma(-)^{\lambda_{\max}-\nu}\left(\frac{1+z}{2}\right)^{b/2}J_a(\beta y)W_{\lambda,\mu}(j;a,b;\beta) +\left(\frac{1-z}{2}\right)^{a/2}J_b(\beta x)W_{\lambda,-\mu}(j;b,a;\beta)\right], \tag{3.15}$$

where

$$W_{\lambda,\mu}(j;a,b;\beta)$$
$$= \text{sign}(\lambda,\mu)\phi_{\lambda,\mu}(j,a)2^{-b}\frac{\Gamma(-2j)\Gamma(2j+1)}{\Gamma(\lambda_{\max}-j)\Gamma(j+\lambda_{\max}+1)}$$
$$\times[(-)^{2\lambda_{\max}}\beta_+^b J_{2j+1}(\beta)+\Delta(j,b,\beta)]. \quad (3.16)$$

Substituting expression (3.15) into (2.6), the impact parameter representation for the scattering amplitude in the unphysical region $|z-1|>2$ becomes

$$f^{\sigma}_{\lambda,\mu}(s,t)$$
$$= \frac{1}{2}\int_0^\infty d\beta\left[\sigma(-)^{\lambda_{\max}-v}\left(\frac{1+z}{2}\right)^{b/2}J_a(\beta y)H^{\sigma}_{\lambda,\mu}(a,b;s,\beta)\right.$$
$$\left.+\left(\frac{1-z}{2}\right)^{a/2}J_b(\beta x)H^{\sigma}_{\lambda,-\mu}(b,a;s,\beta)\right], \quad (3.17)$$

where the profile function is given by

$$H^{\sigma}_{\lambda,\mu}(a,b;s,\beta)$$
$$= \frac{-1}{2i}\oint_c dj\,(2j+1)f^{\sigma}_{\lambda,\mu}(j,s)\frac{W_{\lambda,\mu}(j;a,b,\beta)}{\sin[\pi(j-\lambda_{\max})]}. \quad (3.18)$$

In other words, the profile function for the unphysical region appears as a contour integral instead of a summation.

Thus specifying the impact parameter in the whole z region leads to a unique impact parameter representation given by expression (3.2), where (3.3) is replaced by

$$\Gamma^{\sigma}_{\lambda,\mu}(a,b;s,\beta) = {}^1\Gamma^{\sigma}_{\lambda,\mu}(a,b;s,\beta)+H^{\sigma}_{\lambda,\mu}(a,b;s,\beta). \quad (3.19)$$

It should be noted here that the two terms appearing on the right-hand side of expression (3.19) produce zero and nonzero contribution to the integral appearing in (3.2) for different domains of the angles. That is, the function $H^{\sigma}_{\lambda,\mu}$ yields zero while ${}^1\Gamma^{\sigma}_{\lambda,\mu}$ yields the scattering amplitude $f^{\sigma}_{\lambda,\mu}$ for $y<1$; however, the opposite happens for $y>1$: $H^{\sigma}_{\lambda,\mu}$ gives the scattering amplitude and ${}^1\Gamma^{\sigma}_{\lambda,\mu}$ produces a null result. These results can be checked by substituting the expressions (A6) and (B3) for $e^{j}_{\lambda,\mu}(z)$ and $e^{-j-1}_{-\lambda,-\mu}$, respectively, in the expression (3.5). Thus the profile function given by (3.19) is unique. This uniqueness then automatically guarantees the inverse transform of expression (3.2) because amplitude (3.2) is now defined in the unphysical region with the help of analytic continuation via the Watson–Sommerfeld transform.

IV. CONCLUDING REMARKS

The new result in this paper is that, in contrast to the spinless case, the profile function (2.21) in general has to be a distribution even in the physical region, since it is of the form

$${}^1\Gamma^{\sigma}_{\lambda,\mu}(a,b;s,\beta)\propto\beta_+^b\sum_{j=\lambda_{\max}}^{\infty}(2j+1)f^{\sigma}_{\lambda,\mu}(j,s)J_{2j+1}(\beta).$$

However, if the partial wave amplitude $f^{\sigma}_{\lambda,\mu}(j,s)$ is such that the infinite sum falls off rapidly, then the distribution character of ${}^1\Gamma^{\sigma}_{\lambda,\mu}$ can be ignored. Physically, the high energy experiments do show that the profile functions generally behaves as $\exp(-\text{constant}\,\beta^2)$, consequently providing the required convergent factors.

Further, there has been no approximation made in the derivation. Therefore, this impact parameter representation is valid at all angles (physical as well as unphysical) and at all energies involving arbitrary spins. Further, the derivation shows a close relationship to the Regge formalism because here the Watson–Sommerfeld transform of signatured amplitudes has been used as is done in the discussion of Reggeization. Thus, the profile functions can be calculated from the knowledge of Regge poles, which will be presented in the case of $\pi-N$ system in a future paper.

Finally, this impact parameter formalism being a kinematical description of the scattering process in the same sense as partial wave analysis is, it may be used to analyze the experimental data with simpler parametrization of the few profile functions instead of a large number of parameters required in the phase-shift analysis at high energies. As an example, consider nucleon–nucleon scattering where five helicity amplitudes (for notation see Ref. 10)

$$E(\phi_1^I-\phi_2^I)=\sum_j(2j+1)[h_0^+(j_+,s)P_j^+\delta_{I,1}$$
$$+h_0^-(j_-,s)P_j^-\delta_{I,0}]d^j_{00}(\Theta),$$
$$E(\phi_1^I+\phi_2^I)=\sum_j(2j+1)[h_{11}^+(j_+,s)P_j^+\delta_{I,1}$$
$$+h_{11}^-(j_-,s)P_j^-\delta_{I,0}]d^j_{00}(\Theta),$$
$$E(\phi_3^I)$$
$$=\frac{1}{2}\sum_j(2j+1)\{[h_{22}^+(j_+,s)\delta_{I,1}+h_1^+(j_+,s)\delta_{I,0}]P_j^+$$
$$+[h_1^-(j_-,s)\delta_{I,1}+h_{22}^-(j_-,s)\delta_{I,0}]P_j^-\}d^j_{11}(\Theta), \quad (4.1)$$
$$E(\phi_4^I)$$
$$=\frac{1}{2}\sum_j(2j+1)\{[h_{22}^+(j_+,s)\delta_{I,1}-h_1^+(j_+,s)\delta_{I,0}]P_j^+$$
$$+[h_{22}^-(j,s)\delta_{I,0}-h_1^-(j_-,s)\delta_{I,1}]P_j^-\}d^j_{-1,1}(\Theta),$$

and

$$m(\phi_5^I)=\frac{1}{2}\sum_j(2j+1)[h_{12}^-(j_-,s)\delta_{I,1}P_j^-$$
$$+h_{12}^+(j_+,s)\delta_{I,0}P_j^+]d^j_{1,0}(\Theta),$$

for an isotopic spin I require $h_0(j,s)$, $h_1(j,s)$, $h_{22}(j,s)$, and $h_{12}(j,s)$ complex partial wave functions for each value of j. The number of values of j required to represent the scattering data faithfully then increases with energy. This makes the job of phenomenological analysis of the data quite formidable. However, if the same helicity amplitudes are expressed in impact parameter representation (see Ref. 10)

$$E[\phi_1^I(k,z)-\phi_2^I(k,z)]=-ik\int_0^\infty BdB\,[J_0(B\sqrt{-t})+(-)^{I+1}J_0(B\sqrt{-u})]\Gamma_0^I(B,s),$$
$$E[\phi_1^I(k,z)+\phi_2^I(k,z)]=-ik\int_0^\infty BdB\,[J_0(B\sqrt{-t})+(-)^{I+1}J_0(B\sqrt{-u})]\Gamma_{11}^I(B,s),$$

$$E\phi^I_3(k,z) = \frac{-ik}{2}\int_0^\infty BdB\{[(\cos^2\Theta/2)J_0(B\sqrt{-t})\delta_{\lambda,0} + (-)^M J_2(B\sqrt{-u})\delta_{\lambda,2}][{}_\lambda\Gamma^I_{22}\delta_{M,I} + {}_\lambda\Gamma^I_1\delta_{M,I+1}]\},$$

$$E\phi^I_4(k,z) = \frac{-ik}{2}\int_0^\infty BdB\{[J_2(B\sqrt{-t})\delta_{\lambda,2} + (-)^M(\sin^2\Theta/2)J_0(B\sqrt{-u})\delta_{\lambda,0}][{}_\lambda\Gamma^I_{22}\delta_{M,I} - {}_\lambda\Gamma^I_1\delta_{M,I+1}]\},$$

$$m\phi^I_5(k,z) = \frac{-ik}{2}\int_0^\infty BdB\{[(\cos\Theta/2)J_1(B\sqrt{-t}) - (-)^I(\sin\Theta/2)J_1(B\sqrt{-u})]\Gamma^I_{12}(B,s)\}, \tag{4.2}$$

with corresponding profile functions given by

$$\begin{aligned}
&\Gamma^I_N = \Gamma^I_{1,N} + \Gamma^I_{2,N}, \quad \text{for } N = 0,11,12,\\
&{}_\lambda\Gamma^I_N = {}_\lambda\Gamma^I_{1,N} + {}_\lambda\Gamma^I_{2,N}, \quad \text{for } N = 1,22,\\
&\Gamma^I_{i,N} = \Gamma^+_{i,N}\delta_{I,1} + \Gamma^-_{i,N}\delta_{I,0}, \quad \text{for } N = 0,11,\\
&\Gamma^I_{i,N} = \Gamma^-_{i,N}\delta_{I,1} + \Gamma^+_{i,N}\delta_{I,0}, \quad \text{for } N = 12,\\
&{}_\lambda\Gamma^I_{i,N} = {}_\lambda\Gamma^+_{i,N}(\delta_{N,22}\delta_{I,1} + \delta_{N,1}\delta_{I,0}) + {}_\lambda\Gamma^-_{i,N}(\delta_{N,22}\delta_{I,0} + \delta_{N,1}\delta_{I,1})
\end{aligned} \tag{4.3a}$$

and for $|z| < 1$,

$$\begin{aligned}
&\Gamma^\pm_{1,N}(k,B) = 2ik\sum_j (2j+1)h^\pm_N(j,s)\frac{J_{2j+1}(\beta)}{\beta}, \quad \text{for } N = 0,11,\\
&\Gamma^\pm_{1,N}(k,B) = -2ik\sum_j (2j+1)[j(j+1)]^{-1/2}h^\pm_N(j,s)J_{2j+1}(\beta), \quad \text{for } N = 12,\\
&{}_\lambda\Gamma^\pm_{1,N}(k,B) = \frac{ik}{2}\sum_j (2j+1)h^\pm_N(j,s)\left(\frac{\beta_+}{[j(j+1)]^{1/2}}\delta_{\lambda,0} + \frac{4}{\beta}\delta_{\lambda,2}\right)J_{2j+1}(\beta), \quad \text{for } n = 22,1,
\end{aligned} \tag{4.3b}$$

for $|z| > 1$,

$$\begin{aligned}
&\Gamma^\pm_{2,N}(k,B) = \frac{k}{2}\oint d\nu\frac{(2\nu+1)h^\pm_N(\nu,s)\mathscr{D}(\nu,\beta)}{(\sin\pi\nu)(\cos\pi\nu)}, \quad \text{for } N = 0,11,\\
&\Gamma^\pm_{2,N}(k,B) = \frac{-k\beta}{2}\oint d\nu\frac{(2\nu+1)}{[\nu(\nu+1)]^{1/2}}\frac{h^\pm_N(\nu,s)\mathscr{D}(\nu,\beta)}{(\sin\pi\nu)[\cos\pi(\nu-1)]}, \quad \text{for } N = 12,\\
&{}_\lambda\Gamma^\pm_{2,N}(k,B) = \frac{1}{8k}\oint d\nu\frac{(2\nu+1)h^\pm_N(\nu,s)\mathscr{D}(\nu\beta)}{[\sin\pi(\nu-1)][\cos\pi(\nu-1)]}\left[\frac{\beta^2}{\nu(\nu+1)}\delta_{\lambda,0} + 4\delta_{\lambda,2}\right],\\
&\mathscr{D}(\nu,\beta) = \Delta(\nu,\beta) - \beta^{-1}J_{2\nu+1}(\beta),
\end{aligned}$$

the number of profile functions remain the same throughout the energy region. Consequently, the number of parameter required for phenomenological analysis remain comparatively small.

APPENDIX A

The integral I defined in the expression (2.14) is evaluated for $y < 1$ here.

1. $y < 1$:

$$I = \lim_{\delta\to 0}\frac{\Gamma(-j-\lambda_{\max})}{-2\pi i}\int_\infty^{0+}\frac{d\Lambda}{\Lambda^2}(-\Lambda)^{-j-\lambda_{\max}}\int_0^\infty d\beta\, e^{-\beta^2/(\Lambda+\delta)}\beta^{2+b+2j+2\lambda_{\max}}J_a(\beta y)J_{2j+1}(\beta). \tag{A1}$$

Using expression (2) in Sec. 7.2.1 of HTF2,[15] (A1) becomes

$$I = \lim_{\delta\to 0}\sum_{n=0}^\infty\frac{(-)^n(y/2)^{a+2n}}{\Gamma(1+n)\Gamma(1+n+a)}\frac{\Gamma(-j-\lambda_{\max})}{-2\pi i}\int_\infty^{0+}\frac{d\Lambda}{\Lambda^2}(-\Lambda)^{-j-\lambda_{\max}}\int_0^\infty d\beta\, e^{-\beta^2/(\Lambda+\delta)}\beta^{2+2n+2j+4\lambda_{\max}}J_{2j+1}(\beta). \tag{A2}$$

The integral over the β variable can be evaluated by applying Eq. (14) in Sec. 8.6 of TIT2.[18] This process reduces expression (A2) to

$$\begin{aligned}
I = (-)&\sum_{n=0}^\infty\frac{(-)^n(y/2)^{a+2n}}{\Gamma(1+n)\Gamma(1+n+a)}\frac{\Gamma(2j+2+2\lambda_{\max}+n)}{\Gamma(2j+2)}2^{-2j-2}\frac{\Gamma(-j-\lambda_{\max})}{2\pi i}\\
&\times\int_\infty^{0+}\frac{d\Lambda}{\Lambda^2}(-\Lambda)^{-j-\lambda_{\max}}(-\Lambda)^{2+2j+2\lambda_{\max}+n}e^{-1/4\Lambda}{}_1F_1(-n-2\lambda_{\max};2j+2;\tfrac{1}{4}\Lambda),
\end{aligned} \tag{A3}$$

where the lim $\delta\to 0$ has been also taken. Now writing the confluent hypergeometric function in terms of Kummer's series and substituting $t = \frac{1}{4}\Lambda$, the expression (A3) yields

$$I = 2^b y^a \sum_{n=0}^{\infty} \frac{(-)^n y^{2n}}{\Gamma(1+n)\Gamma(1+n+a)} \frac{\Gamma(2j+2\lambda_{\max}+2+n)}{\Gamma(2j+2)}$$
$$\times \sum_{m=0}^{\infty} \frac{\Gamma(m-2\lambda_{\max}-n)}{\Gamma(-2\lambda_{\max}-n)} \frac{\Gamma(2j+2)}{\Gamma(m+2j+2)} \frac{1}{\Gamma(1+m)} \frac{(-)^{m+n}\Gamma(-j-\lambda_{\max})}{(-)2\pi i} \int_{\infty}^{0+} dt\,(-t)^{j+\lambda_{\max}+m+n} e^{-t}. \tag{A4}$$

The integral over t variable can be evaluated using Hankel's representation for $\Gamma(z)$[17] and the result is

$$I = 2^b y^a \sum_{n=0}^{\infty} \frac{y^{2n}}{\Gamma(1+n)\Gamma(1+n+a)} \frac{\Gamma(2j+2\lambda_{\max}+2+n)}{\Gamma(2j+2)}$$
$$\times \frac{\Gamma(-j-\lambda_{\max})}{\Gamma(-j-\lambda_{\max}-n)} {}_2F_1(-n-2\lambda_{\max}, j+\lambda_{\max}+n+1; 2j+2; 1), \tag{A5}$$

where the summation over m gives the hypergeometric function. Now using expression (46) in Sec. 2.8 of HTF1,[15] (A5) reduces to

$$I = 2^b y^a \frac{\Gamma(j+\lambda_{\max}+1)}{\Gamma(j-\lambda_{\max}+1)} \frac{{}_2F_1(\lambda_{\max}-j, j+\lambda_{\max}+1; 1+a; (1-z/2))}{\Gamma(1+a)}. \tag{A6}$$

In deriving expressions (A6), Eqs. (3) and (4) in Sec. 1.2 of HTF1[15] has also been used. This is the desired result quoted earlier in equation (2.15).

2. $y > 1$:

In the present case (A1.1) is rewritten substituting $\beta y = x'$ as

$$I = \lim_{\delta \to 0} \frac{\Gamma(-j-\lambda_{\max})}{(-)2\pi i} \int_{\infty}^{0+} \frac{d\Lambda}{\Lambda^2} (-\Lambda)^{-j-\lambda_{\max}} y^{-3-2j-2\lambda_{\max}-b}$$
$$\times \int_0^{\infty} dx'\, e^{-x'^2/(\Lambda y^2+\delta)} x'^{(2j+2\lambda_{\max}+b+2)} J_a(x') J_{2j+1}(x'/y). \tag{A7}$$

Again integration over x' is performed using Eq. (14) in Sec. 8.6 of TIT2,[16] which yields

$$I = \sum_{n=0}^{\infty} \frac{(-)^n y^{2\lambda_{\max}-b} 2^{-2j-2-a-2n}}{\Gamma(1+n)\Gamma(n+2j+2)}$$
$$\times \frac{\Gamma(-j-\lambda_{\max})}{2\pi i} \int_{\infty}^{0+} \frac{d\Lambda}{\Lambda^2} (-\Lambda)^{-j-\lambda_{\max}} (\Lambda)^{2j+2\lambda_{\max}+2+n}$$
$$\times e^{-1/4\Lambda y^2} {}_1F_1(-2j-\lambda_{\max}-1-(b-a)/2-n; 1+a; \Lambda y^2/4), \tag{A8}$$

where $\lim \delta \to 0$ has also been taken after evaluating the integral. Following the similar procedure as followed in going from (A3) to (A5), expression (A8) becomes

$$I = 2^b y^{-2-2j-b} \sum_{n=0}^{\infty} \frac{y^{-2n}}{\Gamma(1+n)\Gamma(n+2j+2)} \frac{\Gamma(2j+2\lambda_{\max}+2+n)}{\Gamma(1+a)}$$
$$\times \Gamma(-j-\lambda_{\max}) \frac{{}_2F_1(-2j-2\lambda_{\max}-1+a-n, j+\lambda_{\max}+n+1; 1+a; 1)}{\Gamma(-j-\lambda_{\max}-n)}. \tag{A9}$$

Finally, following similar steps as used in going from (A5) to (A6), yields

$$I = 2^b y^{-2-2j-b} \frac{\Gamma(j+\lambda_{\max}+1)}{\Gamma(-j-\lambda_{\max}+a)} \frac{{}_2F_1(j+\lambda_{\max}+1; j+\lambda_{\max}-a+1; 2j+2; 2/(1-z))}{\Gamma(2j+2)}. \tag{A10}$$

Now substituting the expression (A10) for the integral in expression (3.9) reduces the latter to the expression (3.6), which shows that the distribution defined in the expression (2.13) is the proper one for both $y \gtrless 1$.

APPENDIX B

Here the proof that the distribution (3.10) is appropriate in writing the FB representation for the rotation function $e^{-j-1}_{-\lambda,-\mu}(z)$ of the second kind will be presented. Again here the integral

$$I_1 = \int_0^{\infty} d\beta\, \beta^b J_a(\beta y) J_{-2j-1}(\beta), \tag{B1}$$

is replaced by

$$I_1 = \int_0^{\infty} d\beta\, J_a(\beta y) \Delta(j, b, \beta). \tag{B2}$$

The steps in evaluating the integral in Eq. (B2) are the same as discussed in Appendix A. Therefore, the details are not presented. The final results are

1. $y<1$:

$$I_1 = \frac{\Gamma(\lambda_{\max}-j)}{\Gamma(-\lambda_{\max}-j)}\,2^b y^a\,\frac{{}_2F_1(\lambda_{\max}-j, j+\lambda_{\max}+1; 1+a; (1-z)/2)}{\Gamma(1+a)}. \tag{B3}$$

2. $y>1$:

$$I_1 = \frac{\Gamma(\lambda_{\max}-j)}{\Gamma(j-\lambda_{\max}+a+1)}\,2^b y^{2j-b}\,\frac{{}_2F_1(\lambda_{\max}-j, -j+\lambda_{\max}-a; -2j; 2/(1-z))}{\Gamma(-2j)}. \tag{B4}$$

Substituting (B4) into the expression

$$e^{-j-1}_{-\lambda,-\mu}(z) = \mathrm{sign}(-\lambda,-\mu)2^{-1-b}\phi_{-\lambda,-\mu}(-j-1,a)\,\frac{\Gamma(-j-\lambda_{\max})}{\Gamma(\lambda_{\max}-j)}\,\frac{\pi(-)^{j-\lambda_{\max}}}{\sin[\pi(j-\lambda_{\max})]}\int_0^\infty d\beta\, J_a(\beta y)\Delta(y,b,\beta),$$

yields

$$e^{-j-1}_{-\lambda,-\mu}(z) = \mathrm{sign}(-\lambda,-\mu)\,\frac{1}{2}\,\psi_{-\lambda,-\mu}(-j-1)\left(\frac{1-z}{2}\right)^{-a/2}\left(\frac{1+z}{2}\right)^{-b/2} \times\left(\frac{z-1}{2}\right)^{j+\lambda_{\max}}\frac{{}_2F_1(-j-\lambda_{\max}, -j-\lambda_{\max}+a; -2j, 2/(1-z))}{\Gamma(-2j)} \tag{B5}$$

as required.

Further, the $y<1$ result is used in proving the uniqueness of the representation in the end of Sec. 3.

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[2] The notation used throughout the paper is a standard one. f denotes the amplitude. $J_n(z)$, $F(a,b;c;z)$, $F(a,c,z)$ and $\Gamma(z)$ are, respectively, Bessel, hypergeometric, confluence hypergeometric, and Gamma functions. Variables s,t,u,k,B,j are the square of total center of mass energy, the negative square of momentum transfer, the negative square of exchange momentum transfer, the center of mass momentum, the impact parameter, and the total angular momentum, respectively. Angle here is always the center of mass scattering angle; and $z=\cos\Theta$, $y=\sin\Theta/2$, $x=\cos\Theta/2$.

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Semiclassical calculation of a radial path integral

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(Received 24 February 1981; accepted for publication 28 August 1981)

A semiclassical method of evaluating a path integral for the central potential problem is presented. The Langer transformation $r = e^x$, when applied properly to a radial path integral, brings about an appropriate range of integration and the desired angular momentum modification $(l(l+1))^{1/2}\hbar \to (l+1/2)\hbar$. The resultant path integral becomes assessable by semiclassical calculations. The method is seen to work for obtaining the exact energy spectra of the isotropic harmonic oscillator and the hydrogen atom bound states.

PACS numbers: 03.65.Sq

I. INTRODUCTION

It is a curious fact that the Coulomb problem which in a sense symbolizes the success of quantum mechanics has generally been resistant to an exact treatment with the Feynman path integral technique. Some progress has been made, nonetheless. Gutzwiller[1] is the first who has obtained the correct energy levels of the hydrogen atom by evaluating semiclassically the path integral for the Coulomb potential. Goovaerts and Devreese,[2] on the other hand, have performed an exact summation of a modified perturbation expansion to determine the s-like energy spectrum for the hydrogen atom. A recent paper by Duru and Kleinert[3] attempts to reduce the Coulomb path integral into a Gaussian form by means of a nonlinear canonical transformation without assuring the canonical invariance of the integral.

Finding a path integral solution for the Coulomb problem is certainly important, but facilitating a general procedure for the path integral treatment of any spherically symmetric potential would be more desirable. At the present stage of development, the path integral technique is impractical not only for the Coulomb problem but also for the central potential problem in general. The only central potential for which the path integration has been carried out without approximation is of the form[4,5] $V(r) = ar^2 + br^{-2}$. In this regard, in the present paper, we focus our attention on the semiclassical approximation of the path integral for a spherically symmetric potential. The bound-state energy calculation of the hydrogen atom will be an application.

In the central potential problem, the range of the radial coordinate variable r is semi-infinite, whereas the usual WKB method is applied under the condition that the wave function vanishes at $\pm\infty$. Furthermore, in the WKB treatment of the radial Schrödinger equation, correct expressions for the energy spectra such as the Bohr formula for the hydrogen atom can be obtained only after making the angular momentum replacement $[l(l+1)]^{1/2}\hbar \to (l+\frac{1}{2})\hbar$. Langer[6] has shown that the angular momentum modification comes about when the change of variables $r = e^x$ is made which maps the semi-infinite range $(0,\infty)$ of r to the infinite range $(-\infty,\infty)$ of x. Presumably it is the difficulty in implementing this modification in a path integral that led Gutzwiller[1] to state that the separation of variables has an adverse effect on the phase integral approximation. Thus he carries out the calculation in momentum space where the orbits in the Coulomb potential are simply circles.

As we shall see, the separation of the propagator into radial and angular parts need not be deterimental to the semi-classical treatment of potentials with spherical symmetry. Indeed, the propagator for a spherically symmetric potential can be expressed in spherical polar coordinates as [4,7]

$$K(\mathbf{r}'',\mathbf{r};\tau) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} K_l(r'',r';\tau) \times Y_l^{m*}(\theta'',\varphi'')Y_l^m(\theta',\varphi'), \tag{1.1}$$

where the l-wave propagator is given as a path integral

$$K_l(r'',r';\tau) = \frac{1}{r'r''}\int_0^{\infty}\mathscr{D}r(t)\exp\left\{\frac{i}{\hbar}\int_0^{\tau}L_l(r,\dot{r})\,dt\right\} \tag{1.2}$$

with

$$L_l(r,\dot{r}) = \tfrac{1}{2}m\dot{r}^2 - l(l+1)\hbar^2/2mr^2 - V(r). \tag{1.3}$$

To find a semiclassical approximation of the radial propagator (1.2), the standard procedure[8] may be applied. However, if we apply it directly to (1.2), we immediately encounter serious difficulties.

Suppose we expand the action $S = \int L_l\,dt$ in (1.2) about the stationary solution $r^c(t)$ by setting $r(t) = r^c(t) + \rho(t)$ where $\rho(0) = \rho(\tau) = 0$. Then we get

$$K_l(r'',r';\tau) = (r'r'')^{-1}\exp\left\{\frac{i}{\hbar}S^c\right\}\int\mathscr{D}\rho(t)\exp\left\{\frac{i}{\hbar}\delta^2 S\right\}. \tag{1.4}$$

The major contribution is expected to come from the classical action S^c defined along the classical trajectory $r = r^c(t)$. The first shortcoming we can foresee is that the classical action having the Lagrangian (1.3) in its integrand will yield only an incorrect $l(l+1)$-dependent expression of the energy spectrum. The second problem is the range of integration over ρ in (1.4) which is neither infinite nor semi-infinite. Since the range of r is semi-infinite, the variable ρ describing the deviation from the classical trajectory varies from $-r^c$ to infinity. Therefore, the path integration in (1.4) cannot be completed even though the measure is Gaussian. If either infinite or semi-infinite range is chosen for approximating

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 0022-2488/82/122402-06$02.50

the real integration range, then important quantum corrections would be lost. In fact, in order to use the shifting formulas of Gel'fand and Yaglom[9] properly, the range of the integration variable has to be infinite.

For these reasons, we propose to apply the Langer transformation $r = ae^x$ ($a = 1$: a unit of length) to the radial path integral (1.2) before making the semiclassical approximation. However, it is important that the transformation is applied in each short time integral. The Langer transformation, if used formally in the Lagrangian (1.3) and the finite time path integral (1.2), will alter the physical content of the propagator, and will not serve for our purpose. After transforming the variable in a short time integral, we make the midpoint expansion[10] and retain terms up to order $(\Delta x)^4$. The fourth-order term gives rise to an angular momentum correction which results in the Langer modification. Section II demonstrates this path integral formulation of the Langer modification. In Sec. III, Langer's wave equation is derived from the Hamiltonian path integral in the Langer variables. To show how the semiclassical method may be implemented for the Langer-modified propagator, in Sec. IV, we evaluate the bound-state energy spectrum for a central potential. In particular, for the isotropic harmonic oscillator and the hydrogen atom, we obtain the exact energy spectra.

II. DERIVATION OF THE LANGER MODIFICATION

The radial propagator (1.2) may be written more explicitly as

$$K_l(r'',r';\tau) = \lim_{N\to\infty} \frac{1}{r'r''}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2N} \times \int_0^\infty \prod_{j=1}^{N-1}(dr_j)\exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N} S(r_j,r_{j-1};\epsilon)\right\}, \quad (2.1)$$

when $S(r_j,r_{j-1};\epsilon)$ is the radial action for a short time $\epsilon = \tau/N$ given by

$$S(r_j,r_{j-1};\epsilon) = (m/2\epsilon)(r_j - r_{j-1})^2 - \epsilon U(r_j) \quad (2.2)$$

with

$$U(r_j) = l(l+1)\hbar^2/(2mr_jr_{j-1}) + V(r_j). \quad (2.3)$$

Now we make the change of variable by the Langer transformation

$$r_j = e^{xj}$$

for all j. As has been pointed out by McLaughlin and Schulman,[10] $(\Delta q)^2$ of any generalized coordinate variable q behaves like ϵ in a short time integral. Thus, expanding r_j and r_{j-1} about the midpoint $\bar{x}_j = \frac{1}{2}(x_j + x_{j-1})$ retaining terms up to order ϵ, i.e.,

$$r_j = e^{\bar{x}_j}(1 + \tfrac{1}{2}\Delta x_j + \tfrac{1}{8}(\Delta x_j)^2 + \tfrac{1}{48}(\Delta x_j)^3 + \cdots),$$
$$r_{j-1} = e^{\bar{x}_j}(1 - \tfrac{1}{2}\Delta x_j + \tfrac{1}{8}(\Delta x_j)^2 - \tfrac{1}{48}(\Delta x_j)^3 + \cdots), \quad (2.4)$$

we express (2.2) in terms of x as

$$S(x_j,x_{j-1}:\epsilon) = (m/2\epsilon)e^{2\bar{x}_j}\left[(\Delta x_j)^2 + \tfrac{1}{12}(\Delta x_j)^4\right] - \epsilon U(e^{\bar{x}_j}). \quad (2.5)$$

Correspondingly, the measure in (2.1) transforms into

$$\sum_{j=1}^{N-1}(dr_j) = \exp\{-\tfrac{1}{2}(x' + x'')\}\sum_{j=1}^{N-1}(dx_j)\sum_{j=1}^{N}(e^{\bar{x}_j}), \quad (2.6)$$

where $x' = x_0$ and $x'' = x_N$. The radial path integral (2.1) then becomes

$$K_l(e^{x''},e^{x';\tau}) = \lim_{N\to\infty}\exp\{-\tfrac{1}{2}(x' + x'')\}\int_{-\infty}^{\infty}\prod_{j=1}^{N-1}(dx_j)\prod_{j=1}^{N}(me^{2\bar{x}_j}/2\pi i\hbar\epsilon)^{1/2} \times\exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N}S(x_j,x_{j-1};\epsilon)\right\}. \quad (2.7)$$

Thus the Langer transformation of the radial path integral (2.1) has been completed. Evidently, the semi-infinite range of integration in (2.1) is converted into the infinite range of (2.7). However, the propagator given in the form (2.7) is not yet very useful because it contains the $(\Delta x_j)^4$ term in the action (2.5). The presence of the non-Gaussian factor makes it difficult to implement semiclassical calculations on (2.7). If we completely discard the undesirable term, then there will be no Langer modification on the angular momentum. In fact, we have no justification for discarding the term. If we expect that $(\Delta x_j)^2 \sim \epsilon$, we have to consider the $(\Delta x_j)^4$ term as the same in the order of magnitude as the potential term. Its effect cannot simply be ignored. Assuming $(\Delta x_j)^2 \sim \epsilon$, therefore, we attempt to replace the $(\Delta x_j)^4$ term by an equivalent potential term.[10,11]

First we notice that for $\epsilon^{1/2}$ small the jth integral in (2.7) can be approximated by

$$\int dx_j e^{\bar{x}_j}\exp\left\{\frac{i}{\hbar}S(x_j,x_{j-1};\epsilon)\right\} = \int dx_j e^{\bar{x}_j}\exp\left\{\frac{im}{2\hbar\epsilon}e^{2\bar{x}_j - 1}(\Delta x_j)^2\right\} \times\left\{1 + \frac{im}{24\hbar\epsilon}e^{2\bar{x}_j}(\Delta x_j)^4 + Q(\Delta x_j)\right\}, \quad (2.8)$$

where

$$Q(\Delta x_j) = (im/2\hbar\epsilon)e^{2x_j - 1}(e^{\Delta x_j} - 1)(\Delta x_j)^2 - \epsilon U(e^{\bar{x}_j}). \quad (2.9)$$

which is assumed to be at most of order $\epsilon^{1/2}$. If $\Delta x_j = 2\bar{x}_j - 2x_{j-1}$ is of order $\epsilon^{1/2}$, we may use in (2.8)

$$e^{3\bar{x}_j}(\Delta x_j)^4/\epsilon \approx e^{3x_j - 1}(\Delta x_j)^4/\epsilon \quad (2.10)$$

since the contributions from terms higher than ϵ can be neglected in the path integral calculation. Now utilizing the identity,

$$\int_{-\infty}^{\infty} e^{-ax^2}x^4\,dx = \tfrac{3}{4}a^{-2}\int_{-\infty}^{\infty}e^{-ax^2}\,dx, \quad (2.11)$$

we transform the $(\Delta x_j)^4$ term in (2.8) into a potential correction,

$$\Delta U(e^{\bar{x}_j}) = (\hbar^2/8m)e^{-2\bar{x}_j}. \quad (2.12)$$

Here again we have ignored the terms of order higher than ϵ which stem from the factor $\exp(-3\Delta x_j/2)$. As a result, we obtain

$$\int dx_j e^{\bar{x}_j}\exp\left\{\frac{i}{\hbar}S(x_j,x_{j-1};\epsilon)\right\} = \int dx_j e^{\bar{x}_j}\exp\left\{\frac{im}{2\hbar\epsilon}e^{2\bar{x}_j - 1}(\Delta x_j)^2\right\} \times\{1 - \epsilon\Delta U_j + Q_j\}. \quad (2.13)$$

Exponentiating the last factor in (2.13), we observe that the short time action (2.5) is equivalent for small ϵ to a new

action,

$$\tilde{S}(x_j,x_{j-1};\epsilon) = (m/2\epsilon)e^{2\bar{x}_j}(\Delta x_j)^2 - \epsilon\tilde{U}(e^{\bar{x}_j}), \tag{2.14}$$

where

$$\tilde{U}(e^{\bar{x}_j}) = U(e^{\bar{x}_j}) + \Delta U(e^{\bar{x}_j}). \tag{2.15}$$

With the help of (2.3), (2.4), and (2.12), the modified effective potential becomes

$$\tilde{U}(\bar{r}_j) = (l+\tfrac{1}{2})^2\hbar^2/2mr_jr_{j-1} + V(\bar{r}_j), \tag{2.16}$$

where $\bar{r}_j = (r_jr_{j-1})^{1/2}$. As is expected, the $(\Delta x_j)^4$ term has turned out to be of order ϵ and has brought precisely the Langer modification $l(l+1)\hbar^2 \to (l+\frac{1}{2})^2\hbar^2$. Thus, replacing the action S by the equivalent action $\tilde{S}$, we can rewrite the propagator (2.7) as

$$K_l(e^{x''},e^{x'};\tau) = \tilde{K}_l(x'',x';\tau)\exp\{-3(x'+x'')/2\}, \tag{2.17}$$

where

$$\tilde{K}_l(x'',x';\tau) = \int_{-\infty}^{\infty}\mathscr{D}x\exp\left\{\frac{i}{\hbar}\int_0^{\tau}\tilde{L}_l(x,\dot{x})\,dt\right\} \tag{2.18}$$

with

$$\mathscr{D}x = \prod_{j=1}^{N-1}(dx_j)\prod_{j=1}^{N}(me^{2\bar{x}_j}/2\pi i\hbar)^{1/2} \tag{2.19}$$

and

$$\tilde{L}_l(x,\dot{x}) = \tfrac{1}{2}me^{2x}\dot{x}^2 - [(l+\tfrac{1}{2})^2\hbar^2/2m]e^{-2x} - V(e^x). \tag{2.20}$$

In this way, we have achieved the change in the range of integration and the Langer modification, both of which are desirable for semiclassical calculations. It must be remarked that the formal application of the Langer transformation to the effective radial Lagrangian (1.3) does not yield the modified Lagrangian (2.20). The Langer modification in (2.20) results only from the conversion of the $(\Delta x_j)^4$ term appearing in the short time integral into a correction term in the effective potential.

III. DERIVATION OF LANGER'S EQUATION

In establishing the path integral formulation of the Langer modification, it may be worthwhile to show that the integral equation having the modified propagator (2.18) as the kernel,

$$\tilde{\psi}_l(x,t+\epsilon) = \int\tilde{K}_l(x,x';\epsilon)\tilde{\psi}_l(x',t)dx', \tag{3.1}$$

leads to Langer's equation.[6]

$$i\hbar e^{2x}\frac{\partial}{\partial t}\tilde{\psi}_l(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{(l+\frac{1}{2})^2\hbar^2}{2m} + e^{2x}V(e^x)\right]\tilde{\psi}_l(x,t). \tag{3.2}$$

To this end, we make use of the Fourier transformation formula

$$\int_{-\infty}^{\infty}dk\exp\{ixk - ak^2\} = (\pi/a)^{1/2}\exp(-x^2/2a) \tag{3.3}$$

to express (2.18) in the Hamiltonian form

$$K_l(x'',x';\tau) = \lim_{N\to\infty}\int\int\prod_{j=1}^{N}(dp_j/2\pi\hbar)\prod_{j=1}^{N-1}(dx_j) \times\exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N}(p_j\Delta x_j - \epsilon\tilde{H}_j)\right\}, \tag{3.4}$$

where

$$\tilde{H}_j = (1/2m)e^{-2\bar{x}_j}p_j^2 + [(l+\tfrac{1}{2})^2\hbar^2/2m]e^{-2\bar{x}_j} + V(e^{\bar{x}_j}). \tag{3.5}$$

In the short time limit, the propagator (3.4) takes the form,

$$\begin{aligned}K_l(x'',x';\epsilon) &= \frac{1}{2\pi\hbar}\int dp\,e^{(i/\hbar)p(x''-x')} \\ &\quad\times\left\{1 - \frac{i\epsilon}{2m\hbar}e^{-x''-x'}p^2 - \frac{i\epsilon\hbar}{2m}(l+\tfrac{1}{2})^2\right. \\ &\quad\left.\times e^{-x''-x'}\frac{i\epsilon}{\hbar}V(e^{(1/2)(x''+x')})\right\} \\ &= \delta(x''-x')\left\{1 - \frac{i\epsilon}{\hbar}e^{-2x'}\right. \\ &\quad\times\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2}\right. \\ &\quad\left.\left.+\frac{(l+\frac{1}{2})^2\hbar^2}{2m} + e^{2x'}V(e^{x'})\right]\right\}.\end{aligned} \tag{3.6}$$

Substitution of (3.8) into (3.1) straightforwardly yields Langer's equation (3.2).

The radial Schrödinger wave function

$$\psi_l(r,t) = R_l(r)\exp\{iEt/\hbar\}$$

satisfies

$$\psi_l(r'',t+\epsilon) = \int K_l(r'',r';\epsilon)\psi_l(r',t)r'^2\,dr', \tag{3.7}$$

where $K_l(r'',r';\epsilon)$ is the radial propagator given by (1.2). We can easily show via (2.4) and (2.17) that

$$\psi_l(x,t) = \psi_l(e^x,t)\exp(3x/2). \tag{3.8}$$

It is also interesting to note that $\tilde{H}$ playing a role of the effective Hamiltonian in (3.4) is indeed related to the effective radial Lagrangian (2.20) as

$$\tilde{H} = \dot{x}p - L_l \tag{3.9}$$

with

$$p = \frac{\partial\tilde{L}_l}{\partial\dot{x}} = me^{2x}\dot{x}. \tag{3.10}$$

IV. SEMICLASSICAL DETERMINATION OF ENERGY SPECTRUM

The very reason why we have formulated the Langer modification in the path integral is to prepare the radial path integral (2.1) for evaluation by semiclassical methods. In the following, we wish to show how the semiclassical method will work on the radial propagator after the Langer transformation, particularly, in determining the bound-state energy spectrum for a central potential.

To find the semiclassical approximation for the propagator $\tilde{K}_l(x'',x';\tau)$ expressed in terms of the Langer variable, we first expand the effective action

$$\tilde{S}(x'',x';\tau)=\int_0^\tau \tilde{L}_l(x,\dot{x})\,dt \tag{4.1}$$

with the effective Lagrangian (2.20) about the stationary solution $q(t)$ by setting

$$x(t)=q(t)+\hbar^{1/2}\eta(t), \tag{4.2}$$

where $\eta(0)=\eta(\tau)=0$. Retaining terms up to first order in $\hbar$, we approximate the action (4.1) as

$$\tilde{S}=\tilde{S}^0+\tfrac{1}{2}\hbar\int_0^\tau [L_{\dot{q}\dot{q}}\dot{\eta}^2+2L_{q\dot{q}}\eta\dot{\eta}+L_{qq}\eta^2]\,dt. \tag{4.3}$$

Here $\tilde{S}^0$ is the "classical" action $\tilde{S}(x=q)$ for which $\delta\tilde{S}=0$. The coefficients, $L_{q\dot{q}}$, etc., in the integrand are the values of the second-order derivatives, $L_{x\dot{x}}=(\partial^2\tilde{L}_l/\partial x\partial\dot{x})$, etc., evaluated at $x=q$, and explicitly given by

$$L_{\dot{q}\dot{q}}=me^{2q}, \tag{4.4}$$

$$L_{q\dot{q}}=2me^{2q}\dot{q}, \tag{4.5}$$

$$L_{qq}=2me^{2q}\dot{q}^2-2(l+\tfrac{1}{2})^2\hbar^2e^{-2q}/m-V_{qq}, \tag{4.6}$$

where $V_{qq}=(\partial^2V/\partial x^2)_{x=q}$.

Rigorously speaking, we are not keeping only terms up to first order in $\hbar$. The centrifugal potential term with the Langer modification in $\tilde{S}^0$ and L_{qq} contains $\hbar^2$. As is in the usual WKB treatment for the central potential problem,[12] we need to retain the centrifugal term in order to characterize the resultant approximate propagator properly as a partial wave propagator. Therefore, we are in a way dealing in $\tilde{S}^0$ and L_{qq} with a classical object in a semiclassical effective potential,

$$\tilde{U}(r)=V(r)+(l+\tfrac{1}{2})^2\hbar^2/2mr^2. \tag{4.7}$$

In this context, the stationary action $\tilde{S}^0$ and the trajectory described by the stationary solution $x=q(t)$ are not exactly classical but may be treated as classical without any ambiguity.

In the present approximation, the partial propagator (2.18) is given by

$$\tilde{K}_l(x'',x';\tau)=\hbar^{-1/2}\exp\left\{\frac{i}{\hbar}\tilde{S}^0(\tau)\right\}\times\int\mathscr{D}\eta\exp\left\{\tfrac{1}{2}i\int_0^\tau[L_{\dot{q}\dot{q}}\dot{\eta}^2+2L_{q\dot{q}}\eta\dot{\eta}+L_{qq}\eta^2]\,dt\right\}, \tag{4.8}$$

where

$$\mathscr{D}\eta=\prod_{j=1}^{N-1}(d\eta_j)\prod_{j=1}^{N}(me^{2q_j}/2\pi i\epsilon)^{1/2}, \tag{4.9}$$

the factor $\exp\{\hbar^{1/2}\eta_j\}$ being ignored. The remaining path integral in (4.7) can be calculated by using the shifting methods of Gal'fand and Yaglom.[9] Since the cross term $2L_{q\dot{q}}\eta\eta'$ is present in the integrand, the calculation is rather complicated. Fortunately, a general prescription has been provided by Balachandram *et al.*[13] to treat path integrals of this type. Their work is an extension of the methods of Gel'fand and Yaglom to arbitrary time-independent Hamiltonian systems. Essentially, a double shifting of variables is performed in order to remove cross terms like that mentioned above. Hence, if we follow their prescription, we can reduce (4.8) into the form

$$K_l(x'',x';\tau)=(2\pi i\hbar)^{-1/2}|L_{q\dot{q}}(\tau)/L_{\dot{q}\dot{q}}(0)|^{1/4}|\partial^2S^0/\partial x'\partial x''|^{1/2}\times\exp\{(i/\hbar)S^0\} \tag{4.10}$$

which we have now to evaluate.

From (4.4), it is evident that

$$|L_{\dot{q}\dot{q}}(\tau)/L_{\dot{q}\dot{q}}(0)|^{1/4}=\exp\{\tfrac{1}{2}(x''-x')\}, \tag{4.11}$$

where $x'=q(0)$ and $x''=q(\tau)$. As for the last preexponential factor of (4.10), we observe that for a classical action S^c in general the following relation holds:

$$\frac{\partial^2S^c}{\partial q(0)\partial q(\tau)}=-\frac{\partial^2W}{\partial E\partial q(0)}\frac{\partial^2W}{\partial E\partial q(\tau)}\frac{dE}{d\tau}, \tag{4.12}$$

where $W=S^c+Et$. As has been mentioned earlier, S_0 is not quite a classical action. Nevertheless we can easily justify the use of (4.12) for our semiclassical system. The characteristic function defined by $W_l=\tilde{S}^0+E^0t$ satisfies the Hamilton–Jacobi equation for the Hamiltonian (3.9),

$$\frac{1}{2m}e^{-2q}\left(\frac{\partial W_l}{\partial q}\right)^2+\tilde{U}(e^q)-E^0=0, \tag{4.13}$$

from which follows

$$W_l=\int_{q(0)}^{q(t)}p(q)\,dq \tag{4.14}$$

with

$$p=\{2me^{2q}[E^0-U(e^q)]\}^{1/2}. \tag{4.15}$$

Therefore, via (3.10) and (4.12), we get

$$\frac{\partial^2W}{\partial E^0\partial q}=\frac{\partial p}{\partial E^0}=\frac{me^{2q}}{p}=\frac{1}{\dot{q}}, \tag{4.16}$$

and

$$\frac{\partial^2S^0}{\partial q(0)\partial q(\tau)}=-\frac{1}{\dot{q}(0)}\frac{1}{\dot{q}(\tau)}\frac{dE^0}{d\tau}. \tag{4.17}$$

Substitution of (4.11) and (4.17) into (4.10) yields the semiclassical expression for the partial propagator,

$$\tilde{K}_l(x'',x';\tau)=(2\pi i\hbar)^{-1/2}\exp\{\tfrac{1}{2}(x''-x')\}\times|(\dot{q}(0)\dot{q}(\tau))^{-1}\frac{dE^0}{d\tau}|^{1/2}\exp\{(i/\hbar)\tilde{S}^0(\tau)\}. \tag{4.18}$$

In particular, for a periodic case where $q(0)=q(\tau)=x$, we have

$$K_l(x,x;\tau)=(2\pi i\hbar)^{-1/2}|\dot{x}(\tau)|^{-1}|dE^0/d\tau|^{1/2}\exp\{i\tilde{S}^0(\tau)/\hbar\}. \tag{4.19}$$

The energy levels for the bound states can be found as the poles of the resolvent[8]

$$G_l(E)=\frac{i}{\hbar}\int_0^\infty d\tau\,e^{(i/\hbar)E\tau}\int dx\,\tilde{K}_l(x,x;\tau). \tag{4.20}$$

Assuming that the basic period of motion is $T=\tau/n$ where n is the number of traverses of the orbit, we insert (4.19) into (4.20) to obtain

$$G_l(E)=\frac{i}{\hbar}(2\pi i\hbar)^{-1/2}\sum_{n=1}^{\infty}\int_0^\infty dT\int dx|\dot{x}(T)|^{-1}|n\frac{dE^0}{dT}|^{1/2}e^{-in\pi}\times\exp\{(i/\hbar)n[S^0(T)+ET]\}. \tag{4.21}$$

Here we have used $|\dot{x}(nT)| = |\dot{x}(T)|$ and $\tilde{S}^0(nT) = n\tilde{S}^0(T)$. We have also added the phase factor $e^{-in\pi}$ for every complete orbit. Following the standard procedure,[8,14] we can now straightforwardly calculate (4.21). To perform the T integration, we adopt the stationary phase approximation once again. Practically, we approximate the exponential factor in (4.21) as

$$\exp\left\{\frac{i}{\hbar}n\left[\tilde{S}^0(T_E) + ET_E + \frac{1}{2}\left(\frac{\partial^2 S^0}{\partial T^2}\right)_E (T - T_E)^2\right]\right\} \tag{4.22}$$

by setting $E = -(\partial\tilde{S}^0/\partial T)_E = E^0(T_E)$ where T_E is the value of T for E. Noticing that $(\partial^2 S^0/\partial T^2)_E = |(dE^0/dT)_E|$, and utilizing the relation $\exp(iat^2) \sim (i\pi/a)^{1/2}\delta(t)$, we can further rewrite (4.22) in the form

$$(2\pi i\hbar)^{1/2}|(dE^0/dT)|^{-1/2}\delta(T - T_E)\exp\{inW_l(E)/\hbar\}, \tag{4.23}$$

where $W_l(E) = S^0(T_E) + ET_E$. Replacement of the exponential factor in (4.21) by (4.23) certainly simplifies the T integration, resulting in

$$G_l(E) = \frac{i}{\hbar}\sum_{n=1}^{\infty}(-1)^n\int dx\,|\dot{x}(T_E)|^{-1}\exp\left\{\frac{i}{\hbar}nW_l(E)\right\}. \tag{4.24}$$

For $x(0) = x(T_E)$, $W_l(E)$ is independent of x. Therefore, the x integration in (4.24) is trivial,

$$\int dx\,|\dot{x}|^{-1} = \oint_E dT = T_E. \tag{4.25}$$

After summing over n, the resolvent (4.24) takes the usual from

$$G_l(E) = -(i/\hbar)T_E e^{(i/\hbar)W_l(E)}\left[1 + e^{(i/\hbar)W_l(E)}\right]^{-1}, \tag{4.26}$$

which has poles for

$$W_l(E) = (2n_r + 1)\pi\hbar, \tag{4.27}$$

where $n_r = 0, 1, 2, \cdots$.

The energy spectrum $E = E(n_r, l)$ readily follows from (4.27) if the integral (4.14) can be evaluated for $t = T_E$. In evaluating (4.14) for $W_l(E)$, it is more convenient to reexpress the integral in terms of the radial variable $r = e^q$. Namely,

$$W_l(E) = 2\int_{r_1}^{r_2} dr\left\{2m\left[E - \frac{(l+\frac{1}{2})^2\hbar^2}{2mr2} - V(r)\right]\right\}^{1/2}, \tag{4.28}$$

where r_1 and r_2 are turning points. Apparently the condition (4.27) for the poles coincides with the WKB quantization rule applied to the radial motion. The integral number n_r corresponds to the radial quantum number. For instance, an isotropic oscillator with $V(r) = \frac{1}{2}m\omega^2 r^2$ has

$$W_l(E) = -\pi\{(l + \tfrac{1}{2})\hbar - E/\omega\}. \tag{4.29}$$

Combining (4.27) and (4.29) immediately yields the exact spectrum,

$$E = (n + \tfrac{1}{2})\hbar\omega \tag{4.30}$$

with $n = 2n_r + l + 1 = 1,2,3,\cdots$. Similarly, for the Coulomb potential $V(r) = -Ze^2/r^2$,

$$W_l(E) = -2\pi\{(l + \tfrac{1}{2})\hbar - \tfrac{1}{2}Ze^2(2m/-E)^{1/2}\}. \tag{4.31}$$

The formula (4.27) leads to the exact expression for the hydrogen energy levels,

$$E = -mZ^2e^2/2\hbar^2n^2, \tag{4.32}$$

where $n = n_r + l + 1 = 1,2,3,\cdots$.

V. CONCLUDING REMARKS

In this paper, establishing the Langer modification for radial path integrals, we have demonstrated the utility of polar coordinate path integrals in the semiclassical approximation for spherically symmetric potentials. First we have performed the Langer transformation in the path integral so as to map the semi-infinite range of the radial variable to one of infinite range. This mapping is vital in calculating the Gaussian type integrals which appear after the semiclassical expansion. Furthermore, the transformation, applied in each short time integral with the aid of the midpoint method, gives rise to a correction to the centrifugal potential which is necessary for the Langer modification $(l(l+1))^{1/2} \to (l + \frac{1}{2})$. This is in contrast to the considerations of McLaughlin[15] where the same transformation is carried out in the radial wave equation prior to writing down its path integral solutions. There is a good deal of ambiguity with respect to canonical invariance of path integrals.[16,17] Thus our calculation of the Langer transformation may in turn be considered as a direct check on the midpoint method[10,11] in implementing canonical contact transformations in path integrals.

The semiclassical calculation of the radial path integral with the Langer modification has enabled us to obtain, for instance, the exact energy spectra for the three-dimensional harmonic oscillator and the hydrogen atom. The present semiclassical formulation of the radial path integral should be applicable to other central potentials. The same scheme can also be incorporated to the S-matrix calcuation.[18] This will be discussed elsewhere.

In closing we would like to remark that there is room for improvement in the determination of the propagator. This concerns the introduction of the sum over all traverses of the trajectory in (4.21). The number of traverses n is closely related to the winding number which delineates the various inequivalent classes of paths when the configuration space is multiply connected. In the study of problems involving periodic constraints, such as the entanglement of polymers[5] and the Aharonov–Bohm effect,[19,20] considerations of the winding number are important. The sum over n arises from the imposition of a periodic constraint so as to include paths from all possible equivalence classes. The sum in (4.12) may indeed be seen as arising from the topology of paths in configuration spaces.

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Convergence of the T-matrix approach in the potential scattering

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(Received 6 October 1981; accepted for publication 29 April 1982)

Convergence of the T-matrix scheme is established for the potential scattering.

PACS numbers: 03.80. + r, 11.20. − e

1. INTRODUCTION

Consider the potential scattering problem

$$(-\nabla^2 + q(x) - k^2)u = 0,$$

$$u = u_0 + v,\ k > 0,\ \mathrm{Im}\, q(x) = 0, \tag{1}$$

where $u_0 = \exp[ik(n,x)]$, n is the unit vector, $x \in \mathbb{R}^3$, and v is the outgoing wave. For v the following integral equation is well known:

$$(I + T)v = f, \quad Tv = \int g(x,y)q(y)v\, dy, \tag{2}$$

$$g(x,y) = \exp(ik|x-y|)/4\pi|x-y|, \quad f = -Tu_0. \tag{3}$$

Let us assume first that

$$q(x) = 0 \quad \text{if} \quad |x| \leqslant R. \tag{4}$$

This assumption will be removed: only a power fall-off of $q(x)$ is actually needed. The T-matrix scheme, which is very popular in diffraction theory,[1] can be described for Eq. (2) as follows. Let $\{f_j\}$, $1 \leqslant j < \infty$, be an orthonormal basis of $H = L^2(B_R)$,

$$B_R = \{x : |x| \leqslant R\}, \quad f_R = \begin{cases} f, & |x| \leqslant R \\ 0, & |x| > R \end{cases}, \quad v_N = \sum_{j=1}^{N} c_j f_j,$$

L_N be the linear span of $\{f_1, \ldots, f_N\}$, and P_N be the orthoprojection in H onto L_N. Consider the equation

$$v_N + P_N T v_N = P_N f_R. \tag{5}$$

The problem is to prove that (5) is solvable for sufficiently large N and $v_N \to v$, where v solves (2).

2. STATEMENT OF THE RESULT

It is clear that

$$\|P_N T - T\| \to 0 \quad \text{as} \quad N \to \infty \tag{6}$$

because T is compact in H and $P_N \to I$ strongly in H; I is the identity, $\|\cdot\|$ denotes the operator norm on H. Suppose for a moment that the operator $I + T : H \to H$ is invertible. Then (6) implies that $I + P_N T$ is invertible for sufficiently large N and $\|v_N - w\| \to 0$ as $N \to \infty$, where w is the solution of the equation

$$w + Tw = f_R. \tag{7}$$

Note that if the solution of (7) is known then the solution of (2) is known:

$$v = w \text{ if } |x| \leqslant R,\ v = f - Tw \text{ if } |x| > R. \tag{8}$$

Let us formulate the result. We prove that $I + T : H \to H$ is invertible afterwards.

Theorem 1: If $q(x)$ satisfies assumptions (1) and (4) then the T-matrix scheme (5) converges as $N \to \infty$ to the solution of the scattering problem (1).

Proof: In order to complete the proof we need the following lemma.

Lemma 1: If $(I + T)w = 0$ then $w = 0$.

Indeed, from Lemma 1 and the compactness of T it follows that $I + T$ is invertible in H.

Proof of Lemma 1: If $w = -Tw$ then w is an outgoing wave and

$$[\nabla^2 + k^2 - q(x)]w = 0 \text{ in } \mathbb{R}^3. \tag{9}$$

Since $\mathrm{Im}\, q(x) = 0$ one concludes that $w \equiv 0$.

Indeed, from the radiation condition for w,

$$\lim_{r \to \infty} \int_{|x| = r} \left| \frac{\partial w}{\partial |x|} - ikw \right|^2 dx$$

$$= \lim_{r \to \infty} \int_{|x| = r} ds \left[\left| \frac{\partial w}{\partial |w|} \right|^2 + k^2 |w|^2 + ik\left(\bar{w} \frac{\partial w}{\partial |x|} - w \frac{\partial \bar{w}}{\partial |x|} \right) \right] = 0, \tag{10}$$

and the equality (the bar denotes the complex conjugation)

$$\lim_{r \to \infty} \int_{|x| = r} \left(\bar{w} \frac{\partial w}{\partial |x|} - w \frac{\partial \bar{w}}{\partial |x|} \right) ds = 0, \tag{11}$$

it follows that

$$\lim_{r \to \infty} \int_{|x| = r} \left(\left| \frac{\partial w}{\partial |x|} \right|^2 + k^2 |w|^2 \right) ds = 0. \tag{12}$$

It is a well-known result[2] that (9) and (12) imply $w \equiv 0$. The only point which needs clarification is (11). It is at this point one uses the real-valuedness of q. To derive (11) consider (9) and

$$(\nabla^2 + k^2 - q(x))\bar{w} = 0 \quad (\bar{q} = q). \tag{9'}$$

Multiply (9) by $\bar{w}$ and (9') by w and subtract. Then apply Green's formula and obtain (11). Lemma 1 is proved.

Remark 1: If $\mathrm{Im}\, q \neq 0$ then Lemma 1 is not valid: there exists $q \in C_0^\infty$ such that Eq. (9) has a nontrivial outgoing solution. Example: take $w = \exp(ikr)/r$ if $r \geqslant 1$, $r = |x|$. Since $|w|_{r=1} = 1 > 0$ one can define w for $r \leqslant 1$ so that $|w| > 0$ if $r \leqslant 1$ and $w \in C^\infty$. For this w one has $(\nabla^2 + k^2)w = f \in C^\infty$. It is clear that w satisfies Eq. (9) with

$$q(x) = \begin{cases} 0, & |x| = r \geqslant 1, \\ \dfrac{f(x)}{w(x)}, & r \leqslant 1, \end{cases} \tag{13}$$

and $q(x) \in C^\infty$.

The argument which was used in the proof of Lemma 1

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is borrowed from Ref. 3, p. 328, the example given in Remark 1 was used in Ref. 4, p. 170.

Remark 2: The assumption that $q(x)$ vanishes outside of a ball is not important. If $|q(x)| \leqslant c(1 + |x|)^{-a}$, $a > 2$, then the operator T is compact on $C(\mathbb{R}^3)$ and the above arguments are valid. One can use instead of $C(\mathbb{R}^3)$ the weighted space $L^2(\mathbb{R}^3,p(x))$ with an appropriate $p(x)$. The basis $\{f_j\}$ is now a basis of $L^2(\mathbb{R}^3,p(x))$. One can also consider the sequence q_m of the truncated potentials,

$$q_m = \begin{cases} q(x), & |x| \leqslant m, \\ 0, & |x| > m, \end{cases}$$

solve the scattering problem by the T-matrix scheme for the truncated potential, and prove that the solution v_m of the truncated problem goes to the solution $v(x)$ of the original problem as $m \to \infty$.

3. BIBLIOGRAPHICAL REMARKS

The T-matrix scheme in diffraction theory is described in Ref. 1. There was no proof of convergence of this scheme and the problem of the mathematical justification of the scheme was pointed out by many speakers at the symposium.[1] This problem was solved in Ref. 5, where some information on the rate of convergence of the scheme and on the choice of the basis functions was given. The problem of the choice of the basis functions is closely related to the Rayleigh hypothesis (conjecture) about the convergence of the series in outgoing solutions of Helmholtz's equation on the surface of the obstacle. This conjecture is known to be false in general, and in Ref. 5 a choice of the basis functions is given which does not use the Rayleigh conjecture. For these functions the corresponding series converges on the boundary and in the exterior domain. In this paper the same ideas as in Ref. 5 are used for potential scattering. In Ref. 6 the results of Ref. 5 are strengthened and some numerical results are given.

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Linkages and Hamiltonians at null infinity

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(Received 21 June 1982; accepted for publication 23 July 1982)

The relation between the linkage and the symplectic approaches to conserved quantities associated with the Bondi–Metzner–Sachs groups in general relativity is examined.

PACS numbers: 04.20. – q

I. INTRODUCTION

In the framework of general relativity, there are two regimes in which one can investigate the properties of isolated gravitating systems: *at large space-like distances from sources* and *at large null separations*. The spatial regime is well-suited for investigating the Coulombic properties of the gravitational field, while the null regime is geared to the study of radiation. At spatial infinity, it is possible to impose physically reasonable boundary conditions which yield the Poincaré group as the group of asymptotic symmetries. Associated with these symmetries, there are ten conserved quantities, which represent the *total* energy–momentum and angular momentum of the isolated system under consideration.[1] Thus, as far as symmetries and conserved quantities are concerned, the overall situation at spatial infinity is rather simple; nothing unexpected occurs. At null infinity, on the other hand, the presence of gravitational radiation complicates matters considerably. First of all, since gravitational waves can carry away energy–momentum and angular momentum, one cannot hope to obtain absolutely conserved quantities of the type that exist at spatial infinity. Rather, one must associate these quantities with cross sections of null infinity, $\mathscr{I}$, and allow for leakage of fluxes between any two cross sections. Secondly, in presence of radiation, one cannot introduce sufficiently strong boundary conditions which can yield the Poincaré group as the group of asymptotic symmetries; one has, instead, the infinite dimensional Bondi–Metzner–Sachs[2] (BMS) group. Consequently, one is led to introduce infinitely many quantities, rather than just ten. Since the BMS group has a preferred four-dimensional translation subgroup, one can select from these quantities the four which represent the energy–momentum of the system (which is left over after allowing for leakage due to radiation prior to the retarded time represented by the given cross section). However, since the BMS group admits neither a preferred Lorentz subgroup nor a preferred Poincaré subgroup, the notion of angular momentum becomes qualitatively different from that at spatial infinity, acquiring the so-called supertranslational ambiguities.

Thus, at null infinity, the problem is to obtain the expression for the conserved quantity $Q_\xi[C]$ associated with BMS vector field ξ^a, evaluated at the cross section C of $\mathscr{I}$. $Q_\xi[C]$ is to depend only on the given gravitational field, the BMS generator ξ^a and the cross section C. If, in addition, there exists a function F_ξ on $\mathscr{I}$ which depends only on the gravitational field and and ξ^a, such that $Q_\xi[C] - Q_\xi[C'] = \int_\Delta F_\xi d^3\mathscr{I}$, where Δ is the three-dimensional region of $\mathscr{I}$ bounded by C and C', we shall say that $Q_\xi[C]$ *admits a local flux*. Clearly, from a physical viewpoint, it is desirable that such a local flux exists.

There exist, in the literature, several approaches to the problem of obtaining these conserved quantities.[3–8] Each approach focuses on a feature of conserved quantities of simple systems and generalizes it to the gravitational field at null infinity. Unfortunately, different methods lead to distinct expressions and none of these is completely satisfactory. Thus, even if one adopts the attitude that the BMS group must be faced squarely and the so-called supertranslational ambiguities must be accepted, one is still left with the problem of obtaining the most useful *expression* of these BMS conserved quantities. Among the known approaches, so far only two have been shown to lead to local fluxes.[7,8] The purpose of the paper is to examine the relation between them.

The first of these two approaches is based on linkage integrals[3] which are generalizations of the Komar[9] integrals, available in presence of Killing vectors. The generalization consists of using a (suitable extension within space–time of a) BMS vector field—, i.e., an asymptotic Killing field—in the Komar integral, in place of the Killing field. The resulting conserved quantities, ${}^L Q_\xi[C]$, have several interesting properties. First, if ξ^a is a BMS translation, ${}^L Q_\xi[C]$ is the corresponding component of the Bondi four-momentum evaluated on C; ${}^L Q_\xi[C]$ yields the correct expression in the case of translations. Second, ${}^L Q_\xi[C]$ admits a local flux ${}^L F_\xi$.[7] Furthermore, if the BMS vector field ξ^a is the extension to $\mathscr{I}$ of a Killing field in the physical space–time and if the space–time satisfies the vacuum equations near $\mathscr{I}$, ${}^L F_\xi$ vanishes identically. Finally, if we allow matter near infinity, but retain the Killing condition on ξ^a, we have ${}^L F_\xi = T_{ab}\xi^a n^b$ at $\mathscr{I}$, with n^b the null normal to $\mathscr{I}$. In this case, ${}^L F_\xi$ yields the flux of the conserved quantity, carried away by matter. There is, however, what appears to be an important drawback: already in Minkowski space, ${}^L F_\xi$ fails to vanish if ξ^a is a BMS vector field which does not arise from an exact Killing field. (In particular if ξ^a is a supertranslation but not a translation, ${}^L F_\xi$ fails to vanish.) Consequently, even in Minkowski space, the conserved quantities ${}^L Q_\xi[C]$

[a)] Alfred P. Sloan Research Fellow. Supported in part by the NSF contract PHY 80-08155 and by the Research and Equipment Fund of Syracuse University.
[b)] Supported in part by the NSF contract PHY 800823.

 0022-2488/82/122410-08$02.50

associated with such BMS vector fields fail to vanish if C is a shearing cross section. This failure obscures the physical interpretation of ${}^{L}Q_{\xi}[C]$ and of ${}^{L}F_{\xi}$.

The second approach[8] is based on symplectic, or, Hamiltonian methods. Here, one first constructs the phase space of radiative modes of the gravitational fields, shows that the induced action of the BMS group on this space preserves the symplectic structure thereon and computes the Hamiltonians generating these canonical transformations. Analogous analysis of Maxwell and scalar fields in Minkowski space suggests the physical interpretation of these Hamiltonians: the Hamiltonian densities, ${}^{H}F_{\xi}$, represent fluxes. Thus, in the symplectic approach, fluxes arise as primary quantities and one has to "integrate" them to obtain the two-sphere integrals ${}^{H}Q_{\xi}[C]$. Such an integration has been carried out in the case when ξ^a is a BMS supertranslation. The general case, however, remains unresolved. In the case of BMS translations, ${}^{H}Q_{\xi}[C] = {}^{L}Q_{\xi}[C]$; the Hamiltonian framework also yields the Bondi four-momentum. The flux ${}^{H}F_{\xi}$ has all the interesting properties of the linkage flux ${}^{L}F_{\xi}$, listed above. Furthermore, unlike ${}^{L}F_{\xi}$, the Hamiltonian flux ${}^{H}F_{\xi}$ vanishes identically when the Bondi news vanishes. (Thus, if ξ is not a BMS translation, ${}^{H}F_{\xi} \neq {}^{L}F_{\xi}$ and ${}^{H}Q_{\xi}[C] \neq {}^{L}Q_{\xi}[C]$, in general.) In particular, in Minkowski space, ${}^{H}F_{\xi} = 0$ for all BMS vector fields ξ^a and ${}^{H}Q_{\xi}[C] = 0$ for all supertranslations ξ^a and for all cross sections C. The drawback here is that one has not been able to obtain the expression for ${}^{H}Q_{\xi}[C]$ for BMS fields ξ^a which are not supertranslations.

In Sec. II we show that, although ${}^{L}F_{\xi}$ and ${}^{H}F_{\xi}$ are not related to each other in a simple manner in general, in a large number of physically interesting cases, the integrals of these fluxes over suitably chosen regions do have a simple relation. It turns out that, for BMS translations, αn^a, ${}^{L}F_{\alpha n} = {}^{H}F_{\alpha n}$, while for BMS rotations, ξ^a, $\int_C ({}^{H}F_{\xi} - \frac{1}{2}{}^{L}F_{\xi}) d^2S = 0$, where C is any cross section of $\mathscr{I}$ to which ξ^a is tangential. This relative factor of 2 between translations and rotations is important and complicates the relation between ${}^{L}F_{\xi}$ and ${}^{H}F_{\xi}$ for a general BMS generator ξ^a. In Sec. III, we show that, in spite of these complications, ${}^{L}F_{\xi}$ and ${}^{H}F_{\xi}$ both define one-forms (on a suitably constructed space of asymptotic gravitational fields) whose curls are proportional. Furthermore, the curl is precisely the symplectic structure on the radiative phase space. This analysis sheds light on the structural differences between ${}^{L}F_{\xi}$ and ${}^{H}F_{\xi}$. The Appendix summarizes the conventions used in this paper.

II. RELATION BETWEEN FLUX EXPRESSIONS ${}^{L}F_{\xi}$ AND ${}^{H}F_{\xi}$

Consider an asymptotically flat space–time $(\hat{M}, \hat{g}_{ab})$ and let (M, g_{ab}) denote one of its Penrose completions. Thus, $M = \hat{M} \cup \mathscr{I}$ is a manifold with boundary, $\mathscr{I}$, such that the following conditions are satisfied: i) On $\hat{M}$, $g_{ab} = \Omega^2 \hat{g}_{ab}$, and, on $\mathscr{I}$, $\Omega = 0$, $\nabla_a \Omega \neq 0$ and $\nabla_a \nabla_b \Omega = 0$; ii) The restriction to $\mathscr{I}$ of the vector field $n^a = \nabla^a \Omega$ is complete and the manifold of its orbit is diffeomorphic to S^2; and iii) $\hat{g}_{ab}$ satisfies the vacuum equations $\hat{R}_{ab} = 0$ in a neighborhood of $\mathscr{I}$. (In Sec. IV, we shall briefly discuss the issue of weakening the last assumption.)

Fix any vector field ξ^a on $\hat{M}$ such that $\Omega^2 \mathscr{L}_{\xi} \hat{g}_{ab}$ vanishes on $\mathscr{I}$. Then, the restriction to $\mathscr{I}$ of ξ^a yields a BMS vector field. Furthermore, on M, ξ^a satisfies

$$\mathscr{L}_{\xi} g_{ab} = 2k g_{ab} + 2\Omega X_{ab} \tag{1}$$

for some symmetric tensor field X_{ab}, where k is given by $k = \Omega^{-1} \xi^m n_m \equiv \Omega^{-1} \xi^m \nabla_m \Omega$. The linkage flux, ${}^{L}F_{\xi}$, associated with the BMS vector field ξ^a on $\mathscr{I}$ is constructed from X_{ab}:

$$ {}^{L}F_{\xi} \hat{=} \frac{1}{4\pi} \Big\{ - \nabla_a \nabla_b X^{ab} + 3 \nabla_a X^a + \frac{3}{4} \nabla^2 X + \frac{1}{24} R X \Big\} \tag{2}$$

where, $X^a = \Omega^{-1} X^{ab} n_b$, $X = X^{ab} g_{ab}$, R is the scalar curvature of g_{ab}, and $\hat{=}$ stands for "equal, at points of $\mathscr{I}$, to". (Here, we have modified the definition in Ref. 7 by a factor of $(4\pi)^{-1}$ to ensure that ${}^{L}F_{\xi}$ yields *precisely* the Bondi[2] flux in the case when ξ^a is a *unit* BMS translation. For conventions, see Appendix.) It has been shown that ${}^{L}F_{\xi}$ depends only on the BMS generator ξ^a on $\mathscr{I}$ and is insensitive to the choice of extension of ξ in $\hat{M}$ satisfying Eq. (1).

The Hamiltonian flux, ${}^{H}F_{\xi}$ is constructed from quantities defined intrinsically on $\mathscr{I}$. Let q_{ab} denote the pull-back to $\mathscr{I}$ of g_{ab}. Let q^{ab} be any symmetric tensor field within $\mathscr{I}$, satisfying $q_{am} q^{mn} q_{bn} = q_{ab}$. Let N_{ab} denote the news tensor field[10] on $\mathscr{I}$, (pull-back to $\mathscr{I}$ of $S_{ab} \equiv R_{ab} - \frac{1}{6} R g_{ab}$ in a Bondi conformal frame[11]). Finally, let D denote the torsion-free connection on $\mathscr{I}$, induced by ∇.[12] Then, the Hamiltonian flux ${}^{H}F_{\xi}$ associated with the BMS generator ξ^a is given by[13]

$$ {}^{H}F_{\xi} = -(1/16\pi)(N_{ab}[\mathscr{L}_{\xi} D_c - D_c \mathscr{L}_{\xi}] l_d + 2 N_{ab} l_c D_d k) q^{ac} q^{bd}, \tag{3}$$

where l_a is any covector field on $\mathscr{I}$ satisfying $l_a n^a = 1$, k (as before) is defined on $\mathscr{I}$ by $\mathscr{L}_{\xi} q_{ab} = 2k q_{ab}$, and where a factor of $(1/8\pi)$ has been introduced in the definition of Ref. 8 to ensure the correct normalization for the flux of the four-momentum.

To compare the two expressions, it is convenient to take their Lie derivatives wrt n^a. Using Eq. (32) of Ref. 7, we obtain, in the case of the linkage flux,

$$ n^a D_a {}^{L}F_{\xi} \hat{=} (1/16\pi) K^{ab} X_{ab} \hat{=} (1/16\pi) K^{ab} \times ([\mathscr{L}_{\xi} D_a - D_a \mathscr{L}_{\xi}] l_b + 2 l_a D_b k), \tag{4}$$

where we have set, following Geroch's[12] conventions from the Cincinnati lecture notes, $K^{ac} \hat{=} -4\Omega^{-1} C^{abcd} n_b n_d$. We now compute $\mathscr{L}_n {}^{H}F_{\xi}$. It is easy to verify that

$$\mathscr{L}_n N_{ab} = -(1/2) K_{ab},$$

$$\mathscr{L}_n (\mathscr{L}_{\xi} D_a - D_a \mathscr{L}_{\xi}) l_b = -(1/2) \mathscr{L}_{\xi} (S_{ab} + n^m l_p S_m{}^p q_{ab}) - D_a D_b k + (\mathscr{L}_n l_c) q^{cd} D_d k q_{ab} - 2 (\mathscr{L}_n l_{(a}) D_{b)} k,$$

and

$$\mathscr{L}_n l_c D_d k = (\mathscr{L}_n l_c) D_d k,$$

where, S_{ab} is the pull-back to $\mathscr{I}$ of $(R_{ab} - \frac{1}{6} R g_{ab})$.[14] Hence,

using Eq. (3), we obtain:

$$\mathscr{L}_n {}^H F_\xi = (1/32\pi)[K^{ab}(\mathscr{L}_\xi D_a - D_a \mathscr{L}_\xi) l_b + N^{ab} \mathscr{L}_\xi S_{ab}] + (1/16\pi)[K^{ab} l_a D_b k + N^{ab} D_a D_b k]. \quad (5)$$

Since the right sides of Eqs. (4) and (5) involve only those quantities which can be defined intrinsically on $\mathscr{I}$, it is now easy to compare the two expressions. It is clear that the two expressions are quite different for arbitrary BMS generators ξ^a.[15] We shall therefore divide the analysis into various cases.

A. BMS translations

Let us begin with the simplest BMS fields. Let $\xi^a = \alpha n^a$ be a BMS translation. Then, $k = 0$. Furthermore,

$$\begin{aligned} q^{ac}q^{bd}N_{ab}\mathscr{L}_{\alpha n}S_{cd} &= -(\alpha/2)q^{ac}q^{bd}N_{ab}K_{cd} \\ &= -(\alpha/2)K^{ab}N_{ab} \\ &= K^{ab}(\mathscr{L}_{\alpha n}D_a - D_a\mathscr{L}_{\alpha n})l_b \\ &\quad + (1/2)K^{ab}(\alpha\rho_{ab} + 2D_aD_b\alpha), \end{aligned} \quad (6)$$

where ρ_{ab} is the unique symmetric tensor field on $\mathscr{I}$ satisfying $D_{[a}\rho_{b]c} \hat{=} 0$, $n^a\rho_{ab} \hat{=} 0$, and $q^{ab}\rho_{ab} \hat{=} \mathscr{R}$, (the "scalar curvature" of q_{ab}). Now, αn^a is a BMS translation if and only if $2D_aD_b\alpha + \alpha\rho_{ab} \hat{=} 0$. Hence, we have

$$\mathscr{L}_n {}^H F_{\alpha n} = (1/16\pi)K^{ab}(\mathscr{L}_{\alpha n}D_a - D_a\mathscr{L}_{\alpha n})l_b,$$

whence,

$$\mathscr{L}_n({}^L F_{\alpha n} - {}^H F_{\alpha n}) = 0. \quad (7)$$

Thus, we conclude that, for BMS translations, ${}^L F_{\alpha n} = {}^H F_{\alpha n} + f_{\alpha n}$ where $\mathscr{L}_n f_{\alpha n} = 0$. Since ${}^L F_\xi$ and ${}^H F_\xi$ are both functions on $\mathscr{I}$ which involve only the gravitational field and the BMS generator ξ^a under consideration and since the dependence on the gravitational field is local, $\mathscr{L}_n f_{\alpha n} = 0$ implies that $f_{\alpha n}$ is a function on $\mathscr{I}$ which depends only on the BMS generator[16]; it is purely "kinematical". Hence, we can evaluate it in any geometry. Let us evaluate it in Minkowski space. Since ${}^L F_{\alpha n}$ and ${}^H F_{\alpha n}$ both vanish in Minkowski space, it follows that $f_{\alpha n} = 0$. *Thus, ${}^L F_{\alpha n} = {}^H F_{\alpha n}$ for all BMS translations αn^a and for all gravitational fields.*

Remark: Since the flux ${}^L F_{\alpha n}$ has been explicitly given in Ref. 7 in terms of quantities intrinsic to $\mathscr{I}$, one already knew that ${}^L F_{\alpha n} = {}^H F_{\alpha n}$ ($\hat{=} (\alpha/32\pi)N_{ab}N_{cd}q^{ac}q^{bd}$). One also knows that the two-sphere integrals ${}^L Q_{\alpha n}[C]$ and ${}^H Q_{\alpha n}[C]$ agree on any cross section C, being equal to the Bondi–Sachs four-momentum integrals. The main reason behind the preceding analysis was to illustrate the method which, as we show below, is applicable to supertranslations and rotations for which expressions involving only those fields which are defined intrinsically on $\mathscr{I}$ are not available.

B. BMS supertranslations

Set $\xi^a = \alpha n^a$, with α on arbitrary function on $\mathscr{I}$ satisfying $\mathscr{L}_n\alpha \hat{=} 0$. Since $\mathscr{L}_{\alpha n}q_{ab} \hat{=} 0$, k continues to be zero. Hence, from Eqs. (5) and (6), it follows that

$$\mathscr{L}_n {}^H F_{\alpha n} = (1/16\pi)K^{ab}(\mathscr{L}_\xi D_a - D_a\mathscr{L}_\xi)l_b + (1/64\pi)K^{ab}(\alpha\rho_{ab} + 2D_aD_b\alpha). \quad (8)$$

Thus, we obtain

$$\begin{aligned} \mathscr{L}_n({}^H F_{\alpha n} - {}^L F_{\alpha n}) &= (1/64\pi)K^{ab}(\alpha\rho_{ab} + 2D_aD_b\alpha) \\ &= -(1/32\pi)\mathscr{L}_n N^{ab}(\alpha\rho_{ab} + 2D_aD_b\alpha) \end{aligned} \quad (9)$$

which, in general, fails to vanish. As in the case of BMS translations, we can integrate this equation and obtain

$${}^H F_{\alpha n} - {}^L F_{\alpha n} = -(1/32\pi)N_{cd}(\alpha\rho_{ab} + 2D_aD_b\alpha) \times q^{ac}q^{bd} + f_{\alpha n}$$

for some "kinematical" field $f_{\alpha n}$ (satisfying $\mathscr{L}_n f_{\alpha n} = 0$) which can depend on the choice of the supertranslation αn^a, but not on the specific gravitational field under consideration.[16] To evaluate it, we recall the situation in *Minkowski space–time*, where ${}^H F_{\alpha n}$ vanishes and, in a Bondi conformal frame,[11]

$${}^L F_{\alpha n} = (1/16\pi)(q^{ab}q^{cd}D_aD_bD_cD_d\alpha + 2q^{ab}D_aD_b\alpha). \quad (10)$$

Thus, in the general context, in a Bondi conformal frame, the difference between the Hamiltonian and the linkage flux is given by

$${}^H F_{\alpha n} - {}^L F_{\alpha n} = -(1/16\pi)N_{cd}(D_aD_b\alpha)q^{ac}q^{bd} - (1/16\pi)(D^4\alpha + 2D^2\alpha), \quad (11)$$

where we have used the fact that, in a Bondi frame, ρ_{ab} is proportional to q_{ab}. The difference arises from two factors: there is a contribution from the fact that ${}^L F_{\alpha n}$ fails to vanish in Minkowski space, and, in addition, there is a contribution due to the presence of radiation. It turns out that, for a large class of space–times, the two contributions can cancel each other provided the fluxes are *integrated over suitable regions of $\mathscr{I}$*. Let us suppose that $(\hat{M}, \hat{g}_{ab})$ is such that the radiation is confined to a compact region of $\mathscr{I}$. Let C denote a shear-free cross section in the past of this region, and C', a shear-free cross section in the future. Let Δ be the part of $\mathscr{I}$ bounded by C and C'. *Then, it turns out that the linkage flux of supermomentum through Δ equals the Hamiltonian flux.* To see this, we first reexpress the news tensor in a convenient way. Denote by D^0 the restriction of D to the past of C and by D'^0, the restriction of D to the future of C'. Since the support of radiation is contained within Δ, D^0 and D'^0 are "classical vacua" in the sense of Ref. 17. Fix a one-form l_a on $\mathscr{I}$ such that $D^0_a l_b = 0$, $D_{[a}l_{b]} = 0$ and $l_a n^a = 1$. Then, $\gamma_{ab} \doteq D_a l_b$ is the shear of the connection D (wrt D^0), where $\doteq$ denotes "equal to the trace-free part of". It is easy to check that $-2\mathscr{L}_n\gamma_{ab} = N_{ab}$. Furthermore, it follows from the analysis in Ref. 17 that, *on C'*, γ_{ab} is given by $\gamma_{ab} \doteq D_aD_b\beta$ where β is the BMS supertranslation relating C to C'. We are now ready to prove the result stated above. We have

$$\int_\Delta ({}^H F_{\alpha n} - {}^L F_{\alpha n}) d^3\mathscr{I} = +(1/16\pi)\int_\Delta (\mathscr{L}_n \gamma_{cd})$$
$$\times (2D_a D_b \alpha) q^{ac} q^{bd}\, d^3\mathscr{I}$$
$$-(1/16\pi)\int_\Delta (D^4\alpha + 2D^2\alpha)\, d^3\mathscr{I}$$
$$= (1/16\pi)\int_{C'} [2\gamma_{cd} D_a D_b \alpha q^{ac} q^{bd}$$
$$-\beta(D^4\alpha + 2D^2\alpha)]\, d^2S$$
$$= (1/16\pi)\int_{C'} [2(D_c D_d \beta - (1/2) q^{mn} D_m D_n \beta q_{cd})$$
$$\times D_a D_b \alpha q^{ac} q^{bd} - \beta(D^4\alpha + 2D^2\alpha)]\, d^2S = 0,$$

where, in the second step, we have used the facts that $\mathscr{L}_n (q^{ac} q^{bd} D_a D_b \alpha) = 0$, $\gamma_{ab} = 0$ on C, and that β, satisfying $\mathscr{L}_n \beta = 0$, is the supertranslation joining C and C', and where, in the last step, we have carried out integrations by part. (Here $d^3\mathscr{I}$ and d^2S are, respectively, the intrinsic volume elements on $\mathscr{I}$ and C', in the given conformal Bondi frame. Incidently, note that β is defined only up to an addition of a BMS translation since there is a translational freedom in the definition of C and C'. However, the ambiguity does not affect the above calculation at all.) To understand the result intuitively, let us introduce a third cross-section $\overline{C}$, obtained by time-translating C into the future of the support of radiation. Let us divide Δ into two regions: $\overline{\Delta}$ bounded by C and $\overline{C}$, and, Δ' bounded by $\overline{C}$ and C'. Then, the integral over $\overline{\Delta}$ has contribution only from the news part (i.e., first term) of Eq. (11), while the integral over Δ' has only the Minkowskian contribution [second term in Eq. (11)], and the two contributions exactly cancel one another.

To summarize, although ${}^L F_{\alpha n} \neq {}^H F_{\alpha n}$, the integral over a region of $\mathscr{I}$ bounded by, shear-free cross sections of the difference ${}^L F_{\alpha n} - {}^H F_{\alpha n}$ does vanish, (even when the cross sections are related to each other by a supertranslation.)[18]

Remarks: i) In physically reasonable space–times, one expects the radiation to die off at suitable rates as one approaches i^+ as well as i^0 along $\mathscr{I}^+$. In such space–times, the *total* flux of ${}^H F_{\alpha n}$ through all of $\mathscr{I}$ exists and is finite.[8] What is the situation wrt the linkage flux? In Minkowski space, the linkage flux is given by Eq. (10) and satisfies $\mathscr{L}_n {}^L F_{\alpha n} = 0$. Hence the total flux across all of $\mathscr{I}$ is not well-defined: If one performs the u-integration first, the result is infinite, while, if one performs the (θ,ϕ)-integration first, the result is zero. Equation (11) shows that this state of affairs would continue to hold in any physically reasonable space–time. However, one can use the result of this subsection to give a prescription to define the total linkage flux: to compute this flux, one can simply demand that the integration be performed only over regions bounded by shear-free cross sections in the distant past and distant future. This "regularized" total linkage flux vanishes in Minkowski space, and, more generally, equals the total Hamiltonian flux.

ii) Let (M, g_{ab}) be radiation free. Then, $N_{ab} = 0$, whence ${}^H F_{\alpha n} = 0$. Equation (11) now implies that the integrated linkage flux, $\int_C {}^L F_{\alpha n} d^2S$ over any cross section vanishes identically. Now consider the case when $(\hat{M}, \hat{g}_{ab})$ is radiation free in a neighborhood within $\mathscr{I}$ of a cross section $\overline{C}$. Since Eq. (9) implies that

$$\int_C - \int_{\overline{C}} [({}^H F_{\alpha n} - {}^L F_{\alpha n}) + (1/32\pi)(N_{cd} q^{ac} q^{bd}$$
$$\times (\alpha \rho_{ab} + 2D_a D_b \alpha))] n^p \epsilon_{pmn} dS^{mn} = 0,$$

and since the integral over $\overline{C}$ vanishes, it follows that, for any cross section C of $\mathscr{I}$,

$$\int_C {}^L F_{\alpha n} d^2S = \int_C [{}^H F_{\alpha n} + (1/32\pi) N^{ab} (\alpha \rho_{ab}$$
$$+ 2D_a D_b \alpha)]\, d^2S. \tag{12}$$

C. BMS rotations

Fix a Bondi conformal frame on $\mathscr{I}$ and consider any BMS vector field ξ^a whose projection to the space of generators of $\mathscr{I}$ yields a nonzero killing field of the two-sphere metric induced by q_{ab}. Such a BMS generator, ξ^a, will be called a *rotation* and it satisfies, on $\mathscr{I}$, $\mathscr{L}_\xi q_{ab} = 0$. Hence, we have, from Eqs. (4) and (5),

$$\mathscr{L}_n ({}^H F_\xi - {}^L F_{\frac{1}{2}\xi}) = (1/32\pi) N^{ab} \mathscr{L}_\xi S_{ab}$$
$$= (1/64\pi) \mathscr{L}_\xi (N^{ab} N_{ab}) \tag{13}$$

since $\mathscr{L}_\xi q_{ab} = 0$, and, since $S_{ab} - N_{ab}$ is proportional to q_{ab} in a Bondi frame. It is straightforward to verify that[12]

$$N^{ab} N_{ab} = -4 D_a P^a$$

with

$$P^a = (1/4) K^{am} l_m + (D_m l_p) N^{p[m} n^{a]}.$$

It follows that

$$D_a \{ n^a ({}^H F_\xi - {}^L F_{\frac{1}{2}\xi}) \} = -(1/16\pi) \mathscr{L}_\xi D_a P^a$$
$$= -(1/16\pi) D_a \mathscr{L}_\xi P^a, \tag{14}$$

where, in the last step, we have used the fact that $D_a \xi^a = 3k = 0$. Integrating Eq. (14) over a region of $\mathscr{I}$ bounded by any two cross sections C_1 and C_2, one obtains

$$\int_{C_1} - \int_{C_2} [n^a ({}^H F_\xi - {}^L F_{\frac{1}{2}\xi})$$
$$+ (1/16\pi) \mathscr{L}_\xi P^a] \epsilon_{abc}\, dS^{bc} = 0.$$

If ξ is tangential to a cross section C of $\mathscr{I}$, $\int_C (\mathscr{L}_\xi P^a) \epsilon_{abc}\, dS^{bc} = 0$. Let us therefore choose C_1 and C_2 such that ξ^a is tangential to them. Then,

$$\int_{C_1} - \int_{C_2} n^a ({}^H F_\xi - {}^L F_{\frac{1}{2}\xi}) \epsilon_{abc}\, dS^{bc} = 0. \tag{15}$$

Now, let us suppose that there is a cross section $\overline{C}$ of $\mathscr{I}$, to which ξ^a, is tangential and in the neighborhood of which the radiation vanishes. Then, ${}^H F_\xi = 0$ on $\overline{C}$, and, using Eq. (5.6) of the second paper in Ref. 3 and Eq. (15), it follows[19] that $\int_{\overline{C}} n^a ({}^L F_{\frac{1}{2}\xi}) \epsilon_{abc} dS^{bc} = 0$. Using $\overline{C}$ in place of C_2 in Eq. (15), we now obtain

$$\int_{C_1} n^a ({}^H F_\xi - {}^L F_{\frac{1}{2}\xi}) \epsilon_{abc} dS^{bc} = 0. \tag{16}$$

To summarize, if $\mathscr{I}$ admits a cross section $\overline{C}$ to which ξ^a is tangential and a neighborhood (within $\mathscr{I}$) of $\overline{C}$ which is radiation free, then the Hamiltonian flux associated with ξ^a

through any cross section of $\mathscr{I}$ to which ξ^a is tangential equals the linkage flux associated with $\frac{1}{2}\xi^a$ through that cross section.

Remarks: i) The condition that $\overline{C}$ should exist is not a very stringent one: It is satisfied, in particular, if a neighborhood of i^0 or i^+ is radiation free.

ii) Note that for translations, the Hamiltonian and the linkage fluxes agree, whereas for rotations they differ by a factor of 2: $\int_C({}^H F_\xi - \frac{1}{2}{}^L F_\xi) d^2S = 0$. Suppose then that ${}^H F_\xi$ yields some standard units of energy and angular momentum for the choice of translational and rotational generators $\xi^a = t^a$ and $\xi^a = \phi^a$, respectively. Then ${}^L F_\xi$ would yield these standard units for $\xi^a = t^a$ and $\xi^a = \frac{1}{2}\phi^a$ (in terms of the present definitions). The usual conventions, derived from special relativity, are that energy is associated with a *unit* vector t^a and that angular momentum is associated with a rotational generator ϕ^a whose orbit parameter has period 2π. Reference to the linkage (or Komar) integrals for the energy momentum of Kerr space-time, given in the Appendix, shows that it is ${}^H F_\xi$ which is consistent with the usual special relativistic conventions.

III. SYMPLETIC POTENTIALS FROM ${}^L F$ AND ${}^H F$

In this section, we construct an infinite dimensional space of asymptotic gravitational fields and show that ${}^L F$ and ${}^H F$ naturally define one-forms on this space which can serve as potentials for the gravitational symplectic structure. Since the main purpose of the discussion is only to bring out the structural differences between ${}^L F$ and ${}^H F$, we shall not be rigorous wrt functional analysis; a rigorous treatment would require substantially more space than is warranted for our purpose.

Fix a four-manifold M with boundary $\mathscr{I}$ which is topologically $S^2 \times R$. Fix a function Ω on M such that $\Omega \doteq 0$ and $\nabla_a \Omega$ is nowhere zero, where, as before $\doteq$ denotes "equals, at points of $\mathscr{I}$, to". Fix a metric g_{ab} at points of $\mathscr{I}$, such that $g^{ab}\nabla_a\Omega\nabla_b\Omega \doteq 0$ and $n^a \doteq g^{ab}\nabla_b\Omega$ is a complete vector field on $\mathscr{I}$ whose manifold of orbits is diffeomorphic to S^2. We shall use the notation of Sec. II to denote various tensor fields defined intrinsically on $\mathscr{I}$. M is to be regarded as a "small thickening of $\mathscr{I}$" and $\hat{M} = M - \mathscr{I}$ will represent the "asymptotic region" of a class of space-times.

Denote by $\hat{S}$ the set of vacuum metrics $\hat{g}_{ab}$, defined on $\hat{M}$, such that $(M, g_{ab} = \Omega^2 \hat{g}_{ab})$ is a Penrose completion of $(\hat{M}, \hat{g}_{ab})$ in the sense of Sec. II. Note that g_{ab} is required to equal the pre-specified metric at points of $\mathscr{I}$. It is easy to check (e.g., using Bondi coordinates) that, given *any* asymptotically flat space-time $(\hat{M}', \hat{g}'_{ab})$, one can find its Penrose completion, $(M', g'_{ab} = \Omega'^2 \hat{g}'_{ab})$, such that there is a diffeomorphism from a neighborhood of $\mathscr{I}'$ in M' to a neighborhood of $\mathscr{I}$ in M, which maps Ω' to Ω and g'_{ab} to g_{ab} for *some* $\hat{g}_{ab}$ in $\hat{S}$. Thus, even though we have fixed Ω on M and g_{ab} on $\mathscr{I}$ in constructing $\hat{S}$, $\hat{S}$ does contain all asymptotically flat *physical* metrics $\hat{g}_{ab}$. We shall denote the space of metrics $g_{ab} = \Omega^2 \hat{g}_{ab}$, with $\hat{g}_{ab}$ in $\hat{S}$, by S. We assume that S is endowed with the structure of an infinite dimensional manifold.

Fix an element g_{ab} of S and consider a curve $g_{ab}(\lambda)$ passing through this g_{ab}; $g_{ab}(0) = g_{ab}$. Since all elements of $g_{ab}(\lambda)$ agree on $\mathscr{I}$, $d/d\lambda\ (g_{ab}(\lambda)) \doteq 0$. Hence, there exists a tensor field X_{ab} on M such that

$$\frac{d}{d\lambda} g_{ab}(\lambda)\Big|_{\lambda=0} = \Omega X_{ab}.$$

By construction, $\Omega^{-1} X_{ab}$ satisfies the linearized Einstein's equation on $(\hat{M}, \hat{g}_{ab} = \Omega^{-2} g_{ab})$. As a consequence, on $\mathscr{I}$, X_{ab} satisfies

$$\begin{aligned} &2n^a X_a + n^a \nabla_a X \doteq 0, \\ &\nabla^a X_{ab} - 3X_a - \nabla_b X \doteq 0, \end{aligned} \tag{17}$$

where $X_a = \Omega^{-1} X_{ab} n^b$. Here X_{ab} is to be regarded as a tangent vector at the point g_{ab} of S. A particular class of tangent vectors arises from the BMS generators ξ^a. Let ξ^a be a vector field in M satisfying Eq. (1). Then,

$$\begin{aligned} X_{ab} &\equiv \Omega^{-1}(\tfrac{1}{2}\mathscr{L}_\xi g_{ab} - k g_{ab}) \\ &= (\Omega/2)\mathscr{L}_\xi \hat{g}_{ab} \end{aligned}$$

defines a tangent vector to S at g_{ab}. On (M, g_{ab}), the linkage flux, ${}^L_v F_\xi = \int_v {}^L F_\xi d^3\mathscr{I}$, through a region v of $\mathscr{I}$ is a linear mapping from the tangent vectors X_{ab}, at a point of S, (arising from BMS generators) to the real numbers. Clearly, the mapping admits an obvious extension to all tangent vectors X_{ab},

$$\begin{aligned} {}^L_v F(x) := \frac{1}{4\pi}\int_v \Big(&- \nabla_a \nabla_b X^{ab} + 3\nabla_a X^a \\ &+ \frac{3}{4}\nabla^2 X + \frac{R}{24} X \Big) d^3\mathscr{I}. \end{aligned} \tag{18}$$

This ${}^L_v F$ is thus a one-form on S. It will be called the *linkage one-form*. In a similar fashion, we can define the *Hamiltonian one-form* ${}^H_v F$:

$${}^H_v F(X) = -(1/16\pi)\int_v N_{ab} X_{cd} q^{ac} q^{bd} d^3\mathscr{I}. \tag{19}$$

Again, if X_{ab} arises via Eq. (1) from a BMS generator ξ^a then ${}^H_v F(X)$ gives the integral over v of the Hamiltonian flux ${}^H F_\xi$. We now show that these two one-forms have the same curl except for a factor of two.

We shall use the identity

$$\begin{aligned} &\mathscr{L}_Y F_\mu Z^\mu - \mathscr{L}_Z F_\mu Y^\mu \\ &\quad = 2Y^\mu Z^\nu \nabla_{[\mu} F_{\nu]} + F_\mu (\mathscr{L}_Y Z)^\mu, \end{aligned}$$

which holds for arbitrary vector fields Y^μ and Z^ν and arbitary one-forms F_μ. Fix a point g_{ab} of S and consider a two-parameter family of curves $g_{ab}(y,z)$ in S such that $g_{ab}(0,0) = g_{ab}$. The tangent vectors $\partial/\partial y$ and $\partial/\partial z$ are to play the role of Y^μ and Z^μ. Thus, $\mathscr{L}_Y Z = 0$. Let $\partial g_{ab}/\partial y\,|_{(0,0)} = \Omega Y_{ab}$ and $\partial g_{ab}/\partial z\,|_{(0,0)} = \Omega Z_{ab}$. Then we have

$$[d({}^L_v F)]\cdot(Y,Z) = \frac{\partial}{\partial y}{}^L_v F(Z) - \frac{\partial}{\partial z}{}^L_v F(Y).$$

Using the equations

$$\frac{\partial}{\partial y}\nabla_a\nabla_b Z^{ab} \hat{=} YZ_a n^a - (1/2)\mathcal{L}_n(Y_{ab}Z^{ab}) - (1/2)Z^{ab}\mathcal{L}_n Y_{ab} + \nabla_a\nabla_b\frac{\partial}{\partial y}Z^{ab},$$

$$\frac{\partial}{\partial y}\nabla_a Z^a \hat{=} (1/2)YZ_a n^a + \nabla_a\frac{\partial}{\partial y}Z^a,$$

$$\frac{\partial}{\partial y}\nabla^2 Z \hat{=} (1/2)Y\mathcal{L}_n Z + \nabla^2\frac{\partial Z}{\partial y}, \text{ and}$$

$$\frac{\partial}{\partial y}R \hat{=} 2Y_a n^a - 2\mathcal{L}_n Y,$$

which hold at $\mathscr{I}$, the field equations (17) at $\mathscr{I}$, and the fact that $\mathcal{L}_Y Z = 0$, we obtain

$$\begin{aligned}[d({}^L_v F)]\cdot(Y,Z) &= -(1/8\pi)\int_v [\,Y^{ab}\mathcal{L}_n(Z_{ab} - (1/2)Zq_{ab}) \\ &\quad - Z^{ab}\mathcal{L}_n(Y_{ab} - (1/2)Yq_{ab})]\,d^3\mathscr{I} \qquad (20)\\ &=: -{}_v\omega(Y,Z).\end{aligned}$$

Next, we consider the Hamiltonian one-form. Using the fact that $(\partial/\partial y)N_{ab}$ equals the pull-back to $\mathscr{I}$ of $-\mathcal{L}_n(Y_{ab} - (1/2)Yg_{ab})$, one obtains

$$\begin{aligned}[d({}^H_v F)]\cdot(Y,Z) &= -(1/16\pi)\int_v Y^{ab}\mathcal{L}_n(Z_{ab} - (1/2)Zq_{ab}) \\ &\quad - Z^{ab}\mathcal{L}_n(Y_{ab} - (1/2)Yq_{ab})d^3\mathscr{I} \\ &= -(1/2){}_v\omega(Y,Z). \qquad (21)\end{aligned}$$

Note that ${}_v\omega(Y,Z)$ is precisely the symplectic structure associated with the region v of $\mathscr{I}$, used in Ref. 8 (expressed in terms of normalizations used here).

Remarks: (i) The radiative phase space Γ is constructed from connections D on $\mathscr{I}$ induced by ∇.[8] Hence, there is a natural projection ψ from S on to Γ; whereas Γ has information only about the radiative modes associated with g_{ab}, S has all the information about g_{ab}. The two-form ${}_v\omega$ introduced above is the pull-back to S of the natural symplectic structure on Γ_v, the subspace of Γ obtained by restricting connections D on $\mathscr{I}$ to the region v. Hence, on S, ${}_v\omega$ is degenerate, although the natural symplectic tensor on Γ_v *is* weakly nondegenerate.[8] The one-form ${}^H_v F$ is also the pull-back to S of a one-form on Γ_v; ${}^H_v F$ refers only to the radiative phase space. Hence, the result that ${}^H_v F$ is a symplectic potential could have been obtained directly on Γ_v, without any reference to S. Note, incidentally, that ${}^H_v F$ is a *natural* symplectic potential on Γ_v: it vanishes identically at all classical vacua D^0. The reason why we had to construct S is that the linkage one-form is *not* a pull-back to S of any one-form on Γ_v; ${}^L_v F$ cannot be projected down to Γ_v unambiguously. This is because ${}^L_v F$ has information also about longitudinal modes. To see this, let $\hat{g}_{ab}$ be the Minkowski metric and $\hat{g}_{ab}(y)$, the one-parameter family of Schwarzschild perturbations:

$$\hat{g}_{ab}(y)dx^a dx^b = -(1 - (2my/r))du^2 - 2dudr + r^2(d\theta^2 + \sin^2\theta d\phi^2).$$

Then, with $\Omega = 1/r$, we obtain $Y_{ab} = 2m\Omega^2(\nabla_a u)(\nabla_b u)$ and ${}^L_v F(Y) = (1/2\pi)m\int_v d^3\mathscr{I} \neq 0$. (The action of the Hamiltonian one-form on this Y_{ab} is of course zero since N_{ab} vanishes identically in Minkowski space.) Thus, the linkage one-form probes the asymptotic geometry to a higher order than the Hamiltonian one-form; although both are symplectic potentials, they contain different information.

(ii) Since ${}^L_v F$ and ${}^H_v F$ have the same curl, their difference is a closed one-form ${}_v\alpha$. It would be interesting to know if ${}_v\alpha$ is exact, and, if so, find the function ${}_v f$ on S whose gradient gives ${}_v\alpha$. Results of Sec. II show that, already for linearized Y_{ab} associated with BMS generators, ${}_v\alpha(Y)$ has nontrivial properties; for example, ${}_v\alpha(Y)$ vanishes if Y is associated with Poincaré generators (in which case Y itself vanishes) but not for supertranslations or for a general BMS rotation. Therefore ${}_v f$ would have a rich structure if it exists.

(iii) Note that the fact that a one-form ${}_v F$ has the property that its curl gives the symplectic structure does not, by itself, imply that ${}_v F(Y)$ is the Hamiltonian for some canonical transformation associated with Y. But ${}^H_v F_\xi$ does have the interpretation of the Hamiltonian generating the canonical transformation on Γ_v induced by the BMS generator ξ^a because it satisfies $\mathcal{L}_Y({}^H_v F_\xi) = \omega_v(X_\xi, Y)$ for all vector fields Y on Γ_v induced by the BMS generator ξ^a.

IV. DISCUSSION

From general considerations, one desires that a definition of the BMS conserved quantities, $Q_\xi[C]$, should have the following properties:[20]

1. $Q_\xi[C]$ should be linear in the BMS vector field ξ^a.
2. The expression of $Q_\xi[C]$ should involve only those fields which can be constructed from the knowledge of ξ^a, Ω and g_{ab} in an arbitrarily small neighborhood of C.
3. For the case when ξ^a is a BMS translation, $Q_\xi[C]$ should be the corresponding component of the Bondi four-momentum evaluated at C.
4. If ξ^a is the restriction to $\mathscr{I}$ of a Killing field of the physical space-time, $Q_\xi[C]$ should be (independent of C and) proportional to the Komar integral, $K_\xi := (1/8\pi)\int_C \epsilon_{ab}{}^{cd}(\nabla_c \Omega^{-2}\xi_d)dS^{ab}$, associated with ξ^a.
5. In Minkowski space, $Q_\xi[C]$ should vanish for all BMS vector fields ξ^a and cross sections C.
6. There should exist a local flux F_ξ, linear in ξ, such that, for all C and C', $Q_\xi[C] - Q_\xi[C'] = \int_\Delta (F_\xi + \lambda T_{ab}\xi^a n^b)d^3\mathscr{I}$ for some constant λ, independent of ξ^a, where Δ is the volume within $\mathscr{I}$ bounded by C and C', and $T_{ab} = \Omega^{-2}\hat{T}_{ab}$, with $\hat{T}_{ab}$ the physical stress energy tensor.[21]
7. F_ξ should vanish in absence of gravitational radiation, i.e., when the Bondi news vanishes.

How do the linkage and Hamiltonian expressions fare with respect to these criteria? The linkages satisfy all properties except 5 and 7. Furthermore, a stronger version of property 4 is satisfied: If ξ^a is a Killing field, ${}^L Q_\xi[C] = K_\xi$; the proportionality factor is just unity, irrespective of ξ^a. The failure to satisfy 7 is closely related to this fact. Indeed, from arguments given in Ref. 7 it follows that *there exists no expression whatsoever for* $Q_\xi[C]$ *which can satisfy properties* 1,6,7 *and the stronger version,* $Q_\xi[C] = K_\xi$, *of* 4. Thus, the

failure of ${}^{L}Q_{\xi}[C]$ to conform to requirement 7 is a direct consequence of the fact that the linkage integral is a generalization of the Komar integral.

In the Hamiltonian approach, so far, one has the expression of ${}^{H}Q_{\xi}[C]$ only for supertranslations ξ^{a}. This expression satisfies all the seven conditions.[22] Furthermore, for the class of space-times in which matter and gravitational radiation, (i.e., Bondi news N_{ab} and ${}^{*}K^{abcd}n_{b}n_{d}$, or, in the Newman–Penrose notation, $\dot{\sigma}^{0}$, $\psi_{4}{}^{0}$, $\psi_{3}{}^{0}$ and Im $\psi_{2}{}^{0}$) has support only in the future of some cross section C_{0} of $\mathscr{I}^{+}$, one can trivially extend the definition of ${}^{H}Q_{\xi}[C]$ to all BMS generators ξ: assign values ${}^{H}Q_{\xi}[\bar{C}]$ for some cross section $\bar{C}$ in the past of C_{0} (with independence of $\bar{C}$ following from 6)[23] and define ${}^{H}Q_{\xi}[C]$ for an arbitrary cross section C using condition 6 and the known flux expressions ${}^{H}F_{\xi}$. In the case when ξ^{a} is a supertranslation, this procedure yields precisely the known expression. In the general case, by construction, this ${}^{H}Q_{\xi}[C]$ satisfies all properties except 2: it is not clear if the expression of ${}^{H}Q_{\xi}[C]$ obtained here by a simple u-integration of the flux ${}^{H}F_{\xi}$ can be reexpressed in terms of fields defined *locally* in a neighborhood of C. It is of considerable interest to resolve this issue. If one succeeds in obtaining a local expression, one would have a satisfactory notion of BMS conserved quantities. If, on the other hand, one can demonstrate that a local expression cannot exist in general, one would have a strong indication that it may be impossible to satisfy all the desired conditions.

ACKNOWLEDGMENTS

One of us (AA) thanks Gary Horowitz for discussions.

APPENDIX: CONVENTIONS

Since the relation between linkage and Hamiltonian fluxes involve factors of 2 in a delicate way, we collect our conventions here, for the convenience of the reader.

1. Space-time fields:

a) g_{ab} has signature $-+++$

b) Curvature tensors are defined via: $(1/2R_{abc}{}^{d}k_{d} = \nabla_{[a}\nabla_{b]}k_{c}$, $R_{ab} = R_{amb}{}^{m}$ and $R = R_{a}{}^{a}$.

c) The alternating tensor satisfies $\epsilon_{abcd}\epsilon_{mnpq}g^{am}g^{bn}g^{cp}g^{dq} = -4!$

2. Fields on $\mathscr{I}$:

Our definitions of fields q_{ab}, D_{a}, $S_{a}{}^{b}$, ρ_{ab}, N_{ab}, K^{ab}, ${}^{*}K^{ab}$, ϵ_{abc}, ϵ^{abc} are the same as those of Ref. 12 (and Ref. 8). We therefore only recall the relation between these quantities defined intrinsically on $\mathscr{I}$ and space-time fields.

a) K^{ab} is the pull-back to $\mathscr{I}$ of $-4\Omega^{-1}C^{ambn}n_{m}n_{n}$.

b) ϵ^{abc} is the restriction to $\mathscr{I}$ of $\epsilon^{abcd}n_{d}$.

The symplectic structure Ω on the radiative phase space is

$$\Omega|_{\{D\}}(\gamma,\tilde{\gamma}) = (1/8\pi)\int_{\mathscr{I}}(\gamma_{ab}\mathscr{L}_{n}\tilde{\gamma}_{cd} - \tilde{\gamma}_{ab}\mathscr{L}_{n}\gamma_{cd})q^{ac}q^{bd}\epsilon_{mnp}\,ds^{mnp}.$$

3. Integrals:

a) On a metric manifold C, our convention is

$$\int_{C}\epsilon_{ab}\,dS^{ab} = \int_{C}d^{2}S = 4\pi, \text{ if } C \text{ is a unit two-sphere.}$$

On a region v of $\mathscr{I}$, the convention is

$$\int_{v}f\epsilon_{abc}\,ds^{abc} = \int_{v}f d^{3}\mathscr{I}.$$

It is because of these conventions that the factors involving π had to be introduced in the definitions of fluxes. Note that, if t^{a} denotes the standard stationary Killing field, and, ϕ^{a}, the standard rotational Killing field in Kerr space-time, with the present conventions,

$$m = -(1/8\pi)\oint\epsilon_{ab}{}^{cd}\nabla_{c}t_{d}\,dS^{ab},$$

$$ma = (1/16\pi)\oint\epsilon_{ab}{}^{cd}\nabla_{c}\phi_{d}\,dS^{ab}.$$

4. Corrections to relevant formulas in Refs. 7 and 8:

a) In Ref. 7, Eq. (23) should read (in the notation used in that reference):

$$F = (1/4)\tau^{-1}(\nabla^{2} - 2\Omega^{-1}n^{a}\nabla_{a})H + (1/2)\tau^{-1}X^{ab}X_{ab} - (1/4)\tau^{-1}X^{2}$$

and, Eq. (25) should read

$$F = (1/2)\tau N^{ab}N_{ab}.$$

Note, however, that N_{ab} used in the present paper (and in Refs. 12 and 8) is -2 times N_{ab} used in Ref. 7.

b) In Ref. 8, Eq. (4.12) should read

$$H_{(\alpha n)} = \frac{1}{2}\int_{\mathscr{I}}N_{ab}(\alpha S_{cd} + D_{c}D_{d}\alpha)q^{ac}q^{bd}\epsilon_{mnp}\,dS^{mnp}$$

and, expression (4.13) should read

$$\frac{1}{4}\int\alpha N_{ab}N_{cd}q^{ac}q^{bd}\epsilon_{mnp}\,dS^{mnp}.$$

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[10] Note that N_{ab}, defined here is (-2) times that used in Ref. 7. With the exception of Ref. 7, our present convention is the one which is used in the literature.

[11] A Bondi conformal frame is the one in which (the projection to the space of generators of $\mathscr{I}$ of) q_{ab} is unit two-sphere metric.

[12] For details, see R. Geroch, in *Asymptotic Structure of Space-Time*, edited by P. Esposito and L. Witten (Plenum, New York, 1977).

[13] Since various quantities which enter in ${}^{H}F_{\xi}$ are defined intrinsically on $\mathscr{I}$ the symbol $\hat{=}$ is unnecessary; equality holds only at points of $\mathscr{I}$ simply because both sides are defined *only* at points of $\mathscr{I}$.

[14] One can also define S_{ab} intrinsically on $\mathscr{I}$ from the curvature tensor of D. See, e.g., Ref. 12. Note, however, that there is an error of a factor of 2 in

that reference. The correct result is $2D_{[a}D_{b]}K_c = (9_{c[a}S_{b]}{}^{d} + S_{c[a}\delta_{b]}{}^{d})K_d$.

[15]Note, however, that in Minkowski space, $\mathcal{L}_n {}^{H}F_\xi = \mathcal{L}_n {}^{L}F_\xi = 0$ for all BMS vector fields ξ^a.

[16]Here we are using the fact that the gravitational field under consideration is arbitrary; functions of f on $\mathcal{I}$ constructed locally (from derivatives of the metric g_{ab}), which satisfy $\mathcal{L}_n f \hat{=} 0$ for all permissible g_{ab}, can depend only on those fields on $\mathcal{I}$ which are common to all asymptotically flat gravitational fields. Alternatively, the kinematic nature of f_{an} can be directly established, using the methods of Sec. II, by showing that f_{an} is invariant under perturbations of the metric.

[17]A. Ashtekar, J. Math. Phys. **22**, 2885 (1981).

[18]Although we have worked in a Bondi frame, the final result holds in any conformal frame since the linkage as well as the Hamiltonian fluxes are conformally invariant.

[19]Let $\bar{C}_1$ be a cross section in this region to which ξ^a is tangential and $\bar{C}_2$, a nearby cross section in the same region, related, to $\bar{C}_1$ by a BMS time translation which commutes with ξ^a. Let Δ be the region enclosed by $\bar{C}_1$ and $\bar{C}_2$. Then, $\int_\Delta {}^{L}F_\xi d^3\mathcal{I} = a\int_{\bar{C}_1} {}^{L}F_\xi \, d^2S$ by Eq. (15), where the constant a denotes the translation relating $\bar{C}_1$ and $\bar{C}_2$. But by Eq. (5.6) of the second paper in Ref. 3, $\int_\Delta {}^{L}F_\xi \, d^3\mathcal{I} = 0$. Hence $\int_{\bar{C}_1} {}^{L}F_\xi \, d^2S = 0$.

[20]Note that property 4 implies that, if ξ^a is the restriction to $\mathcal{I}$ of a Killing field in the physical space-time, $F_\xi = 0$.

[21]Here, we weaken condition (iii) from the definition of asymptotic flatness given at the beginning of Sec. II and allow for matter near $\mathcal{I}$ such that the stress energy goes to zero to order 4 in the terminology of Ref. 12.

[22]From the phase space description of, e.g., Einstein–Maxwell systems (Appendix B, Ref. 17) it follows that, in the Hamiltonian method, fluxes ${}^{H}F_\xi$ due to gravitational radiation and $T_{ab}\xi^a n^b$ due to matter, just add to give the total flux.

[23]For instance, set $Q_\xi(\bar{C}) = (1/32\pi)\int_{\bar{C}} {}^*K_{abcd} l^a \xi^b dS^{cd}$ where ${}^*K_{abcd} = \Omega^{-1}\epsilon_{ab}{}^{mn}C_{mncd}$, where l^a is any vector field satisfying $l^a n_a \hat{=} 1$, and where $\bar{C}$ is a shear-free cut in the stationary region. This then gives the correct values for energy and angular momentum in stationary space-times.

Functional integration treatment of one-dimensional ionic mixtures

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(Received 2 March 1982; accepted for publication 28 May 1982)

The classical one-dimensional jellium with several ionic components is treated exactly by the method of functional integration. It is found that ionic demixion does not occur and that the state is crystalline at all temperatures. The period is determined by the greatest common divisor of the ionic charges. The structure of low temperature states of some binary mixtures is investigated in detail by means of the conditional particle distribution densities.

PACS numbers: 05.20. – y

I. INTRODUCTION

We present in this paper an exact treatment of the statistical mechanics of a multicomponent one-dimensional jellium by the method of functional integration. The multicomponent jellium model consists of a collection of ions of various charges, multiples of a basic charge immersed in a background of uniform charge density $-\rho_B$.

It has been known for a long time that the one-dimensional Coulomb gas of positive and negative point charges (without background) can be explicitly solved by the sine-Gordon transformation.[1] The one-dimensional jellium with a single type of ion was also rigorously treated in the canonical formalism in Ref. 2, establishing the crystalline nature of the state in the thermodynamic limit. Moreover, a transformation analogous to sine-Gordon adapted to the jellium (corresponding to a grand-canonical formulation of this system) has been proposed in various papers[3–5] but, in this formalism, it is only recently that the mechanism by which the breaking of translation invariance occurs has been made mathematically completely precise.[6,7]

One interest of the functional integration formulation of the jellium is that it applies without modification to the case where several ionic components are present, allowing, thus, the discussion of the possible existence of the phenomenon of phase separation which may occur in such ionic mixtures.

A characteristic feature of the jellium is that, because of the neutrality condition, the total charge density of the ions must be identical to that of the background. Therefore, in a N-component jellium with given background density $-\rho_B$, only $N-1$ ion densities (or $N-1$ activities) can be considered as independent quantities. In particular the ionic density of a one-component jellium is fixed: In this case, our grand-canonical treatment and the canonical formalism of Ref. 2 lead simply to two different mathematical representations of the same state.

However, the binary ionic jellium presents a richer structure since it has one additional parameter, the relative proportion of ions, and it serves as a model to study the miscibility of ions in a pressure-ionized mixture (Ref. 8, and references quoted there). In this system at sufficiently high density and low temperature, the electron gas is degenerate and forms a uniform neutralizing background for the ions. Since the ions are much heavier than the electrons, they can be treated classically and the ionic fluid is thus modelled by the two component classical jellium. If ion–electron collisions are neglected, the free energy of the whole system consists of the sum of the ionic and of the electronic contribution, the latter being taken as the ground-state energy of the weakly interacting electron gas. Therefore, in these approximations, the discussion of the miscibility problem requires essentially the knowledge of the free energy of a classical ionic mixture. We obtain here that this ionic contribution to the total free energy is an analytic function of the thermodynamic parameter, indicating that in one dimension, ions are miscible at all temperatures and densities. Although such a result may be expected, it deserves a proof because of the long range of the Coulomb force.

Concerning the structure of the state, we show that it is always nontrivially periodic in space with period $a = e\rho_B^{-1}$, e being the greatest common divisor of the ionic charges. Furthermore, the state is unique in the sense that thermodynamic limits with different boundary charges (or boundary electric fields) give the same physical state up to translations in the fundamental period. This follows from the fact that boundary charges can always be exactly screened by means of a global transport of the ionic lattice in the background, with no additional polarization in the bulk. Thus from a static viewpoint, the jellium behaves as a perfect crystalline ionic conductor and could be considered as an elementary prototype of a solid electrolyte. We remark that the situation is very different for the two component Coulomb gas, which is known to be an insulator and to have several dielectric phases characterized by their internal degree of polarization.[7,9]

These features can be understood on the basis of the following simple electrostatic arguments. The electric field $E(x)$ corresponding to a configuration of ions of charge $e_1 = e$ and $e_2 = 2e$, say, has discontinuities $2e_i$ at points where charges are located and a slope $-2\rho_B$ otherwise, ($\rho_B > 0$) (Fig. 1). Since the energy is proportional to $\int E^2(x)\,dx$, typical configurations in the Gibbs state at low temperature are those for which the electric field has the smallest possible fluctuations around zero. In particular, in the ground state, each ion occupies the center of a segment of background of length $e_i\rho_B^{-1}$ proportional to its charge e_i. By Newton's theorem, these neutral entities (i.e., the ions with their neutralizing portion of background) do not interact anymore and, therefore, the ground-state energy is invariant

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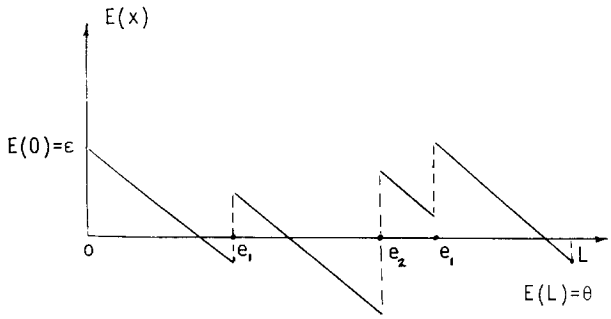

FIG. 1. The electric field $E(x)$ corresponding to a configuration of ions of charge $e_1 = e$ and $e_2 = 2e$, which has discontinuities $2e_i$ at points where charges are located.

under their permutations. Because of this degeneracy, ions of large charges have no tendency to segregate from those of smaller charges.

Moreover, this degeneracy implies that in ground state configurations a given type of ion can occupy any site of a lattice of period $a = e\rho_B^{-1}$. In fact, charges which are even multiples of e will be found on the lattice $\{x = ke\rho_B^{-1}, k\in\mathbb{Z}\}$, whereas charges which are odd multiples of e will sit on points of the shifted lattice $\{x = (k+\frac{1}{2})e\rho_B^{-1}, k\in\mathbb{Z}\}$. The expected periodicity of the state is thus $a = e\rho_B^{-1}$. As a result of the noncoincident distributions of odd and even ions, the neutralization of the background in thermal states occurs on the scale a, which could be smaller than the neutralizing intervals $e_r\rho_B^{-1}$ corresponding to individual ions.

The absence of ionic separation in one dimension shows that the phenomenon has to be attributed to multipolar forces which exist in higher dimensions. For instance, we can consider in two dimensions the interaction potential between neutral squares consisting of ions in the center of square shaped portions of background. By a multipolar expansion, one finds that the potential between two such squares behaves asymptotically as gr^{-8}, where r is the distance between the centers of the squares and g depends on the relative orientation of the squares. One finds also that g has not a constant sign, and hence the interaction can be repulsive as well as attractive at large distances.[10] This indicates that ionic demixion (if it occurs in a purely classical jellium) has to do with a delicate balance between repulsive and attractive parts of the multipolar forces.

The definition of the system and the statements of results are given in Sec. II. In Sec. III, we express the statistical mechanical quantities of the general system (with boundary charges) in terms of functional integrals in the sine-Gordon language, and establish various properties of the state in the thermodynamic limit. It should be noted that one could use as well the equivalent electric field ensemble formalism developed in Refs. 1 and 7, but the sine-Gordon formalism is more directly adapted to the calculation of particle correlations and distribution functions. Technically, the main difference with the two component Coulomb gas[1] is that the transfer matrix of the jellium is never self-adjoint, and we study it as a contractive positivity preserving semigroup.

Section VI is devoted to the analysis of the state at low temperature by means of the conditional distribution functions. These quantities, which enter in the DLR equilibrium conditions,[11] give the probability distribution of particles in a local region of the infinite system, given the external configuration. In a one-dimensional Coulomb system, they take a particularly simple form due to the fact that the charge configuration external to a local region determines the electric field acting at the boundary of this region.[7] Therefore, the conditional probabilities are of the form of finite Gibbs distribution with prescribed electric field at the boundaries, and thus explicitly known. The usual distribution functions are then recovered by averaging the conditional probabilities on the equilibrium electric field distributions. In this way, it is possible to exhibit the structure of the low temperature state and to see that it is close to the ground state. In particular, in the grand-canonical formalism where densities are not fixed and particles can flow in and out of the system, the state of an ionic mixture converges as the temperature tends to zero to the state of a jellium with a single species of ions, those having the smallest charge. In other words, ionic densities vanish at low temperatures except that corresponding to the smallest charge. This follows from the fact that local neutralization of the background is best achieved by small charges. We illustrate this behavior in two simple examples of binary mixtures.

Some elements of proofs are given in Appendices A and B. A complete and detailed account of all proofs can be found in Ref. 10.

II. GRAND-CANONICAL ENSEMBLES AND STATEMENT OF THE RESULTS

The system consists of N types of point charges $e_1, e_2, \ldots, e_N$ in the interval $[0, L]$ with a background charge density $-\rho_B, \rho_B > 0$. The charges e_r, $r = 1,\ldots,N$, are assumed to be distinct multiples of a common charge which is taken equal to 1, i.e., $e_r\in\mathbb{Z}\setminus\{0\}$. Without further specification, charges can have both signs with the single restriction that at least, one of the species is positively charged (say $e_1 > 0$). Denoting by e the greatest common divisor of the e_r, $r = 1,\ldots,N$, we will have $e_r = s_r e$ $(s_1 > 0)$, where s_r, $r = 1,\ldots,N$, is a set of distinct integers with greatest common divisor equal to 1.

The system is submitted to a constant external field D [which may be due to boundary charges $(q, -q)$ located in 0 and L with $D = 2q$]. The charge density, electric field, and energy corresponding to a configuration of n particles, $Q^n = \{x_1\sigma_1,\ldots,x_n\sigma_n\}$, $x_j\in[0,L]$, $\sigma_j\in\{e_1\cdots e_N\}$, are thus

$$c(x; Q^n) = \sum_{j=1}^{N} \sigma_j\, \delta(x - x_j) - \rho_B$$

with total charge

$$C(Q^n) = \sum_{j=1}^{n} \sigma_j - \rho_B L\,,$$

$$E(x; Q^n) = \sum_{j=1}^{N} \sigma_j\, \mathrm{sgn}(x - x_j) - 2\rho_B\, x + \rho_B L + D\,, \tag{1}$$

$$\mathrm{sgn}\, x = \frac{x}{|x|} = \begin{cases} 1, & x > 0, \\ -1, & x < 0, \end{cases}$$

and

$$H(Q^n) = \frac{1}{4}\int_0^L [E(x; Q^n)]^2\, dx$$
$$= -\frac{1}{2}\int_0^L dx \int_0^L dy\, c(x; Q^n)|x-y|\, c(y; Q^n)$$
$$- D\int_0^L x\, c(x; Q^n)\, dx + \frac{[C(Q^n)+D]^2}{4} L\,. \quad (2)$$

To each species we associate an activity parameter $z_r \equiv z_{e_r} = (2\pi m_r/\beta\hbar^2)^2 \exp(\beta\mu_r)$, where m_r and μ_r are the masses and chemical potentials of the particles. With $H(Q^n)$ we construct finite volume grand canonical ensembles for which the total charge has a fixed value $C \in \mathbb{R}$. Since for any configuration Q^n, $\Sigma_{i=1}^n \sigma_i$ belongs to $e\mathbb{Z}$, the condition $C(Q^n) = C$ implies that such ensembles can only be realized in intervals of length of the form

$$L = (le - C)\rho_B^{-1} = la - \frac{Ca}{e}, \quad a = e\rho_B^{-1}, \quad (3)$$

where l is a positive integer.

The ensemble is characterized by its total charge C and the external field D, or equivalently by the two numbers ϵ, $\theta \in \mathbb{R}$ which are the boundary values of the electric fields in 0 and L,

$$\epsilon = E(0; Q^n) = D - C,$$
$$\theta = E(L; Q^n) = D + C. \quad (4)$$

We shall speak of the (θ, ϵ)-ensembles when the boundary values (4) are specified and the condition (3) fulfilled. Writing $H(Q^n|\,\theta, \epsilon)$ for the energy (2), the partition function of the (θ, ϵ)-ensemble is

$$Z_L(\theta, \epsilon) = \sum_{n=0}^{\infty} \sum_{\sigma_1 \cdots \sigma_n} \frac{z_{\sigma_1} \cdots z_{\sigma_n}}{n!}$$
$$\times \int_0^L dx_1 \cdots \int_0^L dx_n \exp[-\beta H(Q^n|\theta, \epsilon)] \quad (5)$$

with the summation restricted by the constraint $\Sigma_{j=1}^n \sigma_j - L\rho_B = C$.

The one particle density is

$$\rho_L^{(\theta,\epsilon)}(x\sigma) = \frac{z_\sigma}{Z_L(\theta, \epsilon)} \sum_{n=0}^{\infty} \sum_{\sigma_1 \cdots \sigma_n} \frac{z_{\sigma_1} \cdots z_{\sigma_n}}{n!}$$
$$\times \int_0^L dx_1 \cdots \int_0^L dx_n \exp[-\beta H(x\sigma Q^n|\theta, \epsilon)] \quad (6)$$

with the summation restricted to the configurations such that $\sigma + \Sigma_{j=1}^n \sigma_j - \rho_B L = C$. The higher order correlation functions $\rho_L^{(\theta,\epsilon)}(x_1\sigma_1, \ldots, x_n\sigma_n)$ are given by similar expressions.

We remark that if there is only one type of ion, the (θ, ϵ)-ensemble is canonical since the sum (5) has only one nonvanishing term compatible with the constraint $ne_1 - L\rho_B = C$. In this case, the $\theta = \epsilon = 0$ state coincides with that treated in Ref. 2.

We establish the following facts concerning states obtained as thermodynamic limits of (θ, ϵ)-ensembles.

Proposition 1:

(i) $\beta p = \lim_{L\to\infty} (1/L) \ln Z_L(\theta, \epsilon)$ exists and is independent of ϵ and θ.

(ii) $p = p(z_1, \ldots, z_r, \beta)$ is analytic in each activity z_r and in the temperature β^{-1} in a neighborhood of the positive real axis.

The physical interpretation of (i) is the following. The macroscopic average polarization $\mathscr{P}$ in a neutral state $(C = 0, \theta = D)$ is found to be from (2)

$$\mathscr{P} = \lim_{L\to\infty} \left\langle \frac{1}{L}\int_0^L x\, c(x)\, dx \right\rangle$$
$$= \beta^{-1} \lim_{L\to\infty} \frac{1}{L}\frac{\partial}{\partial D} \ln Z_L + \frac{D}{2}$$
$$= \frac{\partial p}{\partial D} + \frac{D}{2} = \frac{D}{2}.$$

Therefore (i) shows that $\mathscr{P}$ equals the boundary charge $q = D/2$. Thus no polarization is created in the bulk and the average internal electric field $\langle E \rangle = D - 2\mathscr{P}$ vanishes. The point (ii) means that phase segregation does not occur. For instance, in a binary mixture, p will essentially depend on a single activity parameter w fixing the relative proportion of ions (see Remark 2, end of Sec. III). Analyticity in w implies that one cannot have two coexisting phases at the same temperature with different ionic densities.

Proposition 2:

(i) The thermodynamic limit $\rho^{(\theta,\epsilon)}$ of the (θ, ϵ)-ensemble exists and is spatially periodic of period $a = e\rho_B^{-1}$. Precisely, fixing the origin in $L/2$ and according to the parity of L [i.e., l even or odd in (3)], one has

$$\lim_{L\to\infty} \rho_L^{(\theta,\epsilon)}\left(x + \frac{L}{2}, \sigma\right) = \begin{cases} \rho\left(x - \dfrac{Da}{2e}, \sigma\right), & l \text{ even}, \\ \rho\left(x - \dfrac{Da}{2e} - \dfrac{a}{2}, \sigma\right), & l \text{ odd}, \end{cases}$$

where ρ is the state with $\theta = \epsilon = 0$ boundary conditions. Moreover $\rho(x + a, \sigma) = \rho(x, \sigma)$. The same relations hold for the higher order correlation functions.

(ii) The correlations are analytic in $z_1, \ldots, z_N$, β in a neighborhood of the positive real axis.

(iii) The correlations have an exponential clustering.

(iv) Neutrality holds in the period a,

$$\sum_{r=1}^{N} e_r \frac{1}{a}\int_0^a \rho(x, e_r)\, dx = \rho_B\,. \quad (7)$$

Finally, we have

Proposition 3: Let all charges be positive. For any open set of values of β, the density $\rho(x, \sigma)$ of ions with charge σ being an odd multiple of e is not a constant.

Proposition 3 asserts that the state is never translation invariant in the whole temperature range. More informations on the periodic structure of the state will be given in Sec. III.

The global shift of the state by the quantity $Da/2e$, due to the external field, results again from the perfect screening of the boundary charge q. This is discussed in more detail in Sec. III C.

III. FUNCTIONAL INTEGRATION

A. Representation of the state

Since the functional integration formalism for a Coulomb system is well known (see references in the Introduction), we have only to adapt it to our situation, and we shall therefore give briefly the main steps. The treatment generalizes that found in Ref. 6 by allowing several types of charges and incorporating the general boundary conditions (θ, ϵ).

Using $-|x-y| = \min(x,y) + (x+y)/2$, the energy (2) can be written in the form

$$H(Q^n) = \int_0^L dx \int_0^L dy\, c(x; Q^n) \min(x,y)\, c(y; Q^n) - \theta \int_0^L x\, c(x; Q^n)\, dx + \frac{\theta^2}{4} L . \tag{8}$$

One then introduces the Gaussian measure $\langle - \rangle_{\theta, \varphi_0}$ on the real random field $\varphi(x)$ defined by its finite dimensional distributions

$$R_{\theta,\varphi_0}(\varphi_1 x_1,\ldots,\varphi_n x_n) = R_\theta(\varphi_n - \varphi_{n-1}, x_n - x_{n-1}) \cdots R_\theta(\varphi_2 - \varphi_1, x_2 - x_1)\, R_\theta(\varphi_1 - \varphi_0, x_1),$$

where

$$R_\theta(\varphi,x) = \frac{1}{(4\pi\beta x)^{1/2}} \exp\left(-i\varphi \frac{\theta}{2} - \frac{\varphi^2}{4\beta x} \right)$$

is the fundamental solution of the equation

$$\left[\frac{\partial}{\partial x} + \beta \left(-i \frac{\partial}{\partial \varphi} + \frac{\theta}{2} \right)^2 \right] R_\theta(\varphi, x) = 0 \tag{9}$$

[one should note that when $\theta = 0$, $\langle - \rangle_{0,\varphi_0}$ is the Wiener measure for trajectories $\varphi(x)$ with initial condition $\varphi(0) = \varphi_0$, $H(Q^n)$ is the corresponding covariance]. For general θ, a Gaussian integration gives

$$\left\langle \exp i \int_0^L c(x; Q^n)\, \varphi(x)\, dx \right\rangle_{\theta, \varphi_0} = \exp[-\beta H(Q^n)] \exp[i\varphi_0 C(Q^n)] . \tag{10}$$

Since from (3) $C(Q^n) - Ce \in e\mathbb{Z}$, the fixed total charge condition is easily implemented by defining the measure

$$\langle - \rangle_{\theta,\epsilon} = \frac{e}{2\pi} \int_{-\pi/e}^{\pi/e} d\varphi_0 \langle - \rangle_{\theta,\varphi_0} \exp(-i\varphi_0 C),$$

so

$$\left\langle \exp i \int_0^L c(x; Q^n)\, \varphi(x)\, dx \right\rangle_{\theta,\epsilon} = \begin{cases} \exp[-\beta H(Q^n|\theta,\epsilon)], & C(Q^n) = C \\ 0, & C(Q^n) \neq C. \end{cases} \tag{11}$$

With (10), all statistical mechanical quantities can be expressed as functional integrals with respect to the measure $\langle - \rangle_{\theta,\epsilon}$ and then be computed by means of the Feynman–Kac formula.[12] One gets from (5) and (6)

$$Z_L(\theta,\epsilon) = \left\langle \exp\left[\int_0^L dx \left(\sum_{r=1}^n z_r \exp[ie_r \varphi(x)] - i\rho_B \varphi(x) \right) \right] \right\rangle_{\theta,\epsilon} = \int_{-\infty}^{\infty} d\varphi \frac{e}{2\pi} \int_{-\pi/e}^{\pi/e} d\varphi_0\, U_L^\theta(\varphi,\varphi_0) \exp(-i\varphi_0 C) \tag{12}$$

and

$$\rho_L^{(\theta,\epsilon)}(x,\sigma) = \frac{z_\sigma}{Z_L(\theta,\epsilon)} \left\langle \exp[i\sigma\varphi(x)] \times \exp\left[\int_0^L dy \left(\sum_{r=1}^n z_r \exp[ie_r \varphi(y)] - i\rho_B \varphi(y) \right) \right] \right\rangle_{\theta,\epsilon} = \frac{z_\sigma}{Z_L(\theta,\epsilon)} \int_{-\infty}^{\infty} d\varphi \frac{e}{2\pi} \int_{-\pi/e}^{\pi/e} d\varphi_0 \,(U_{L-x}^\theta \times \exp(i\sigma\Phi)\, U_x^\theta)(\varphi,\varphi_0) \exp(-i\varphi_0 C) . \tag{13}$$

$U_x^\theta(\varphi,\varphi_0) = (\exp \Gamma^\theta x)(\varphi,\varphi_0)$ is the kernel on $\mathscr{L}^2(\mathbb{R}, d\varphi)$ of the contractive semigroup generated by

$$\Gamma^\theta = -\beta(p + \theta/2)^2 + \sum_{r=1}^N z_r \exp(ie_r\Phi) - i\rho_B \Phi . \tag{14}$$

Here $p = -id/d\varphi$ and Φ is the operator of multiplication by φ in $\mathscr{L}^2(\mathbb{R}, d\varphi)$.

One should note two important properties of U_x^θ: U_x^0 and U_x^θ are unitarily equivalent,

$$U_x^\theta = \exp\left(-i\Phi \frac{\theta}{2} \right) U_x^0 \exp\left(i\Phi \frac{\theta}{2} \right) . \tag{15}$$

Under a translation α in the φ variable U_x^θ transforms as

$$\exp(-i\alpha p)\, U_x^\theta(z_1,\ldots,z_N,\rho_B) \exp(i\alpha p) = U_x^\theta(z_1 \exp(-i\alpha e_1),\ldots,z_N \exp(-i\alpha e_N)) \exp(i\alpha\rho_B x) . \tag{16}$$

Other properties of U_x^θ are given in Appendix A.

B. The transfer matrix

The thermodynamic limit of the grand-canonical ensemble (12) and (13) can be taken by the usual mechanism of the transfer matrix. The proper definition of the transfer matrix for the jellium is a consequence of the following fundamental observation: Equation (16) shows that U_x^θ is invariant under the discrete subgroup of translations $\tau = \{\varphi \to \varphi + 2\pi n/e, n \in \mathbb{Z}\}$ whenever x is an integer multiple of $a = e\rho_B^{-1}$. Therefore U_a^θ is decomposed by the direct integral $\mathscr{L}^2(\mathbb{R}) = \int^\oplus \mathscr{L}^2([-\pi/e, \pi/e])$ (Ref. 13) and we can define its component $\bar{U}_a^\theta$ on $\mathscr{L}^2([-\pi/e, \pi/e], d\varphi)$ by the periodized kernel

$$\bar{U}_a^\theta(\varphi,\varphi') = \sum_{n=-\infty}^{\infty} U_a^\theta\left(\varphi + \frac{2\pi n}{e}, \varphi' \right) . \tag{17}$$

More generally, if A is a τ-invariant operator on $\mathscr{L}^2(\mathbb{R}, d\varphi)$ we define $\bar{A}$ to be the corresponding periodized operator on $\mathscr{L}^2([-\pi/e, \pi/e], d\varphi)$. One has in particular[13]

Lemma 1a: $\exp(ie\Phi)$ and p are τ invariant and $\bar{p}$ is the

operator $-i(d/d\varphi)$ on $\mathscr{L}^2([-\pi/e,\ \pi/e],\ d\varphi)$ with periodic boundary conditions.

In the case where a τ invariant A has a kernel on $\mathscr{L}^2(\mathbb{R},\ d\varphi)$,

$$\bar{A}(\varphi,\varphi') = \sum_{n=-\infty}^{\infty} A\left(\varphi + \frac{2\pi n}{e}, \varphi'\right), \tag{18}$$

periodic in both arguments. We introduce then the Fourier representation of $\mathscr{L}^2([-\pi/e,\ \pi/e],\ d\varphi)$ by the vectors $(\varphi|u) = (e/2\pi)^{1/2}\exp(ieu\varphi)$, $u\in\mathbb{Z}$, and

$$(u|A|v) = \frac{e}{2\pi}\int_{-\pi/e}^{\pi/e} d\varphi \int_{-\pi/e}^{\pi/e} d\varphi' \times\exp(-ieu\varphi + iev\varphi')A(\varphi,\varphi'). \tag{19}$$

Finally, we extend the definition (18) (when it is well defined) to operators which are not necessarily τ invariant by considering the right-hand side of (18) as a kernel acting on $\mathscr{L}^2([-\pi/e,\ \pi/e],\ d\varphi)$. We have

Lemma 1b: If A is τ invariant and B is an operator with kernel $B(\varphi,\varphi')$ on $\mathscr{L}^2(\mathbb{R}, d\varphi)$ (not necessarily τ invariant), then one has $\overline{AB} = \bar{A}\bar{B}$, $\overline{A^*} = (\bar{A})^*$, and $\overline{A^{-1}} = (\bar{A})^{-1}$.

Lemma 2 shows that $\bar{U}_a^\theta$ has all the usual properties of a transfer matrix. We shall write simply $\bar{U}^\theta = \bar{U}_a^\theta$ and when $\theta = 0$, $\bar{U}_a^0 = \bar{U}$.

Lemma 2:

(i) $\bar{U}^\theta$ is compact and has a unique eigenvector Ω^θ with positive Fourier coefficients $(u|\Omega^\theta)$. The corresponding eigenvalue $\exp(\gamma^\theta)$ is positive and has the largest modulus of the characteristic numbers of $\bar{U}^\theta$. $(\bar{U}^\theta)^*$ has a unique positive eigenvector Ω_c^θ with the same eigenvalue.

We have

$$(\bar{U}^\theta)^l = \exp(l\gamma^\theta)P + R^l, \quad l\in\mathbb{N},$$

where $P = |\Omega^\theta)(\Omega_c^\theta|/(\Omega^\theta|\Omega_c^\theta)$ is the eigenprojection on $\exp(\gamma^\theta)$ and the spectral radius $\exp(\gamma_1^\theta)$ of R is strictly smaller than $\exp(\gamma^\theta)$.

(ii) $\bar{U}^\theta(z_1,\ldots,z_N,\beta)$ is analytic in $z_1,\ldots,z_N$ and β for $\mathrm{Re}\,\beta > 0$.

(iii) $\bar{U}^\theta$ and $\bar{U}$ are similar with $\bar{U}^\theta = \bar{A}^{-1}\bar{U}\bar{A}$, with $\bar{A} = U_{\theta a/2e}\exp(i\Phi(\theta/2))$. In particular, for $\theta = 2e$, $\bar{U}^{2e}$ and $\bar{U}$ are unitarily equivalent with $\bar{U}^{2e} = \exp(-ie\Phi)\bar{U}\times\exp(ie\Phi)$.

(iv) $\bar{U}^\theta(z_1,\ldots,z_N)$ and $\bar{U}^\theta(z_1\exp(-ie_1\alpha),\ldots,z_N\times\exp(-ie_N\alpha))\times\exp(i\alpha e)$ are unitarily equivalent for any $\alpha\in\mathbb{R}$.

(v) The charge conjugation $e_r\to -e_r$, $\rho_B\to-\rho_B$, $\theta\to-\theta$ is represented by $C\bar{U}^\theta C = (\bar{U}^{-\theta})^*$ and $C\Omega^\theta = \Omega_c^{-\theta}$.

Before proving the lemma, let us note that the matrix elements of $\bar{U} = \bar{U}_a^{\theta=0}$ have a simple interpretation. If $L = la$, l integer, it follows from (12) and (15) that

$$Z_{la}(\theta,\epsilon) = \frac{e}{2\pi}\int_{-\infty}^{\infty} d\varphi \int_{-\pi/e}^{\pi/e} d\varphi_0 \times\exp\left(-i\frac{\theta}{2}\varphi + i\frac{\epsilon}{2}\varphi_0\right)(U_a)^l(\varphi,\varphi_0).$$

For the particular boundary condition $\theta = 2eu$, $\epsilon = 2ev$, $u,v\in\mathbb{Z}$, we get with the definitions (17) and (19)

$$Z_{la}(2eu,2ev) = (u|(\bar{U})^l|v). \tag{20}$$

The matrix elements of $(\bar{U})^l$ are thus partition functions of finite system in $[0,la]$ with integer boundary conditions.

Proof of lemma 2: To prove part (i) of the lemma, it suffices to show by theorem β'' [14] that (a) $\bar{U}^\theta$ is compact, (b) $(u|\bar{U}^\theta|v)\geqslant 0$, (c) for any pair (u,v) there exists an integer M such that $(u|(\bar{U}^\theta)^l|v) > 0$ for $l\geqslant M$.

All these properties are displayed by expanding the transfer matrix as a power series in the activities (see Appendix A).

$$\bar{U}^\theta = \exp(-ie\Phi)\left[\sum_{n=0}^{\infty}\int_0^a dx_n \int_0^{x_n} dx_{n-1} \cdots \int_0^{x_2} dx_1\, G(a,x_n)\left(\sum_{r=1}^N z_r\exp(ie_r\Phi)\right)\cdots G(x_2,x_1)\left(\sum_{r=1}^N z_r\exp(ie_r\Phi)\,G(x,0)\right)\right], \tag{21}$$

with

$$G(x,y) = \exp\left[-\beta\rho_B^2\frac{(x-y)^3}{12}\right]\times\exp\left[-\beta\left(\bar{p} + \frac{\theta}{2} - \rho_B\left(\frac{x+y}{2}\right)\right)^2(x-y)\right]. \tag{22}$$

Since $G(x,y)$ is norm continuous and $\|G(x,y)\|\leqslant 1$ for $x\geqslant y$ the integrals are defined in the norm Riemann sense and the series are norm convergent with

$$\|\bar{U}^\theta\| \leqslant \exp(a\,\Sigma_{r=1}^N |z_r|).$$

This implies that $\bar{U}^\theta$ is compact since $G(x,y)$ is compact on $\mathscr{L}^2([-\pi/e,\pi/e],\ d\varphi)$ for $x > y$. Moreover $\exp(ie_r\Phi)|u) = |u + s_r)$ and $G(x,y)$ acts as a multiplication by a positive function in Fourier's representation showing that $\bar{U}^\theta$ preserves positivity. Point (c) is easy to check from the following property of the matrix $(u|\bar{U}^\theta|v)$:

$$(u-1|\bar{U}^\theta|u) > 0 \text{ for all } u\in\mathbb{Z}; \tag{23a}$$

there exists $w > 0$ such that

$$(u+v|\bar{U}^\theta|u) > 0 \text{ for all } v\geqslant w; \tag{23b}$$

Eq. (23a) arises from the zero order term in (21).

The contribution of order $\Pi_{j=1}^n z_{\sigma_j}$ in (21) to $\bar{U}^\theta|u)$ is proportional to

$$\left|u + \sum_{j=1}^n \sigma_j/e - 1\right) = \left|u + \sum_{r=1}^N m_r s_r - 1\right),$$

where $m_r\geqslant 0$ is the number of values of the σ_j equal to $e_r = s_r e$. Equation (23b) follows then from the fact that given a set of integers $s_1, s_2,\ldots,s_N$ with $s_1 > 0$ and greatest common divisor equal to 1, any positive number v, except of finite number of them, can be written as $v = \Sigma_{r=1}^N m_r s_r - 1$, $m_r\in\mathbb{N}^+$. By the theorem of Bezout,[15] there exists integers $t_1,\ldots,t_N$ such that $\Sigma_{r=1}^N t_r s_r = 1$. Choose $v\geqslant w = \Sigma_{r=1}^N (t_r)^2 s_r$, then $v + 1 = s_1\,\Sigma_{r=1}^N (t_r)^2 s_r + ps_1 + q$ with $p\geqslant 0$ and $0\leqslant q < s_1$ by the algorithm of Euclid; and thus

$$v = s_1 \sum_{r=1}^{N} (t_r)^2 s_r + p s_1 + q\left(\sum_{r=1}^{N} t_r s_r\right) - 1$$

$$= (t_1^2 s_1 + p + t_1 q) s_1 + \sum_{r=2}^{N} ((t_r)^2 s_1 + t_r q) s_r - 1 ,$$

which is clearly of the desired form since $(t_r)^2 \geqslant |t_r|$.

(ii) follows from the fact that $G(x, y)$ is analytic and bounded with $\mathrm{Re}\,\beta > 0$ and the uniform convergence of the series (21).

For (iii), one has from (15) and the semigroup property of U_x,

$$U_a^\theta = \exp\left(-i\Phi\frac{\theta}{2}\right) U_{-\theta a/2e}\, U_a\, U_{\theta a/2e} \exp\left(i\Phi\frac{\theta}{2}\right).$$

Equation (16) implies that $A = U_{\theta a/2e} \exp(i\Phi(\theta/2))$ is τ invariant and thus (ii) follows from Lemma 1b.

Since $\exp(ie\Phi)$ is itself τ-invariant, $\bar{U}^{2e}$ and $\bar{U}$ are unitarily equivalent.

(iv) is a consequence of (16) and the fact that $\exp(i\alpha p)$ is τ-invariant, $\alpha \in \mathbb{R}$.

(v) follows immediately from the definitions. ■

We turn now to the proof of Propositions 1 and 2.

With the definition (18) the partition function (12) and the density (13) read for general values of θ and ϵ,

$$Z_L(\theta, \epsilon) = \frac{e}{2\pi} \int_{-\pi/e}^{\pi/e} d\varphi \int_{-\pi/e}^{\pi/e} d\varphi_0\, \bar{U}_L^\theta(\varphi_1 \varphi_0) \exp(-i\varphi_0 C), \tag{24}$$

$$\rho_L^{(\theta,\epsilon)}(x,\sigma) = \frac{z_\sigma}{Z_L(\theta,\epsilon)} \frac{e}{2\pi} \int_{-\pi/e}^{\pi/e} d\varphi \int_{-\pi/e}^{\pi/e} d\varphi_0 \times \overline{(U_{L/2-x}^\theta \exp(i\sigma\Phi)\, U_{L/2+x}^\theta)}(\varphi,\varphi_0) \exp(-i\varphi_0 C). \tag{25}$$

In (25), we have shifted the origin from 0 to $L/2$.

We choose L of the form (4), setting $L = 2la - Ca/e$, l integer. [The thermodynamic limit obtained from an odd sequence $L = (2l+1)a - Ca/e$, l integer, can be treated in the same way.] The operators involved in (24) and (25) are not τ-invariant for general ϵ and θ. But, using the semigroup property of U_x and Lemma 1b, we can write

$$\bar{U}_L^\theta = \overline{U_{2la}^\theta\, U_{-Ca/e}^\theta} = (\bar{U}^\theta)^{2l} \bar{B}, \tag{26}$$

with $B = U_{-Ca/e}^\theta$ (B is not τ-invariant).

In the same way, one gets

$$\overline{U_{L/2-x}^\theta \exp(i\sigma\Phi)\, U_{L/2+x}^\theta} = (\bar{U}^\theta)^l\, \overline{U_{-(x+Ca/2e)}^\theta \exp(i\sigma\Phi)\, U_{x+Ca/2e}^\theta}\, (\bar{U}^\theta)^l \bar{B}. \tag{27}$$

When (26) and (27) are inserted in (24) and (25), one obtains in view of the asymptotic behavior (i) of the transfer matrix

$$\lim_{L\to\infty} \frac{1}{L} Z_L(\theta,\epsilon) = \frac{1}{a}\gamma^{(\theta)} = \beta p, \tag{28}$$

$$\lim_{L\to\infty} \rho_L^{(\theta,\epsilon)}(x,\sigma) = z_\sigma (\Omega_c^\theta | \Omega^\theta)^{-1} (\Omega_c^\theta| \times \overline{U_{-(x+Ca/2e)}^\theta \exp(i\sigma\Phi)\, U_{x+Ca/2e}^\theta}\, |\Omega^\theta). \tag{29}$$

The similarity of $\bar{U}^\theta$ and $\bar{U}$ implies that $\gamma^{(\theta)} = \gamma$ is independent of θ. Moreover, inserting $\Omega^\theta = \bar{A}^{-1}\Omega$ and $\Omega_c^\theta = \bar{A} * \Omega_c$ in (29) one has with the definition of A, the relation (15), and $D = \theta - C$,

$$\bar{A}\, \overline{U_{-(x+Ca/2e)}^\theta \exp(i\sigma\Phi)\, U_{x+Ca/2e}^\theta}\, \bar{A}^{-1} = \overline{U_{-(x-Da/2e)} \exp(i\sigma\Phi)\, U_{x-Da/2e}}.$$

This shows that

$$\lim_{L\to\infty} \rho_L^{(\theta,\epsilon)}(x,\sigma) = z_\sigma (\Omega_c|\Omega)^{-1}(\Omega_c| \times \overline{U_{-(x-Da/2e)} \exp(i\sigma\Phi)\, U_{x-Da/2e}}\, |\Omega) = \rho\left(x - \frac{Da}{2e}, \sigma\right) \tag{30}$$

is independent of θ and ϵ except for the shift $-Da/2e$.

Finally, the unitary equivalence of U^{2e} and U implies $\lim_{L\to\infty} \rho_L^{(2e,2e)}(x,\sigma) = \lim_{L\to\infty} \rho_L^{(0,0)}(x,\sigma)$ and therefore with (30), one has $\rho(x,\sigma) = \rho(x-a,\sigma)$.

The arguments can be generalized to the higher order correlation functions establishing thus the first parts of Propositions 1 and 2.

Since $\bar{U}$ is analytic in $z_1,\ldots,z_N$ and β ($\mathrm{Re}\,\beta > 0$), and that its maximal eigenvalue $\exp(\gamma)$ is simple and positive when $z_1,\ldots,z_N$ and β are real and positive, we can conclude by the Kato–Rellich theorem[16] that $\exp(\gamma)$ is analytic in each argument in a neighborhood of the positive real axis. A similar consideration will give the analyticity of the correlation functions. As usual, the exponential clustering comes from the gap in the spectrum of the transfer matrix. The neutrality relation is a consequence of the unitary equivalence given in part (iv) of Lemma 2. This unitary equivalence implies that

$$\exp(\gamma(z_1,\ldots,z_N)) = \exp[i\alpha e + \gamma(z_1 \exp(-i\alpha e_1),\ldots,z_N \exp(-i\alpha e_N))]$$

and hence

$$\sum_{r=1}^{N} e_r z_r \frac{\partial}{\partial z_r} \gamma(z_1,\ldots,z_N) = e. \tag{31}$$

By definition of the grand-canonical potential and the periodicity of $\rho(x,\sigma)$ one has

$$\frac{z_\sigma}{a}\frac{\partial}{\partial z_\sigma}\gamma = \lim_{L\to\infty} z_\sigma \frac{\partial p_L}{\partial z_\sigma} = \lim_{L\to\infty} \frac{1}{L}\int_0^L \rho_L(x,\sigma)\,dx = \frac{1}{a}\int_0^a \rho(x,\sigma)\,dx. \tag{32}$$

Thus (31) gives (iii) of Proposition 2.

Proof of Proposition 3: To have the result of Proposition 3, we show by an explicit calculation that $(d^2/dx^2)\rho(x,\sigma)|_{x=0} > 0$ when all charges are positive and σ is an odd multiple of e [$(d/dx)\rho(x,\sigma)|_{x=0} = 0$ since the state with $\theta = \epsilon = 0$ is invariant under space inversion]. One

gets from (30) and by working out the action of the double commutator

$$\frac{d^2}{dx^2}\rho(x,\sigma)\Big|_{x=0} = z_\sigma(\Omega_c|\Omega)^{-1}(\Omega_c|\overline{[[\exp(i\sigma\Phi),\Gamma],\Gamma]}|\Omega)$$

$$= \frac{\beta z_\sigma}{(\Omega_c|\Omega)}\left\{2\sum_{r=1}^{N} z_r e_r\left(\sum_{u\in\mathbb{Z}}(u|\Omega)(\Omega_c|u+\sigma/e+s_r)\right)\right.$$

$$\left.+\sum_{u\in\mathbb{Z}}(\beta\sigma e^2(2u+\sigma/e)^2-2\rho_B)(u|\Omega)(\Omega_c|u+\sigma/e)\right\}. \tag{33}$$

The first term in (33) is obviously positive. The second term is also positive for β large enough since $(2u+\sigma/e)^2\geqslant 1$ when σ/e is odd, $u\in\mathbb{Z}$. We conclude that $\rho_\beta(x,\sigma)$ is not constant for $\beta\geqslant\beta_0$. Choose x_0 such that $\rho_{\beta_0}(x_0,\sigma)-\rho_{\beta_0}(0,\sigma)\neq 0$, then, by Proposition 2 (ii) the holomorphic function $\rho_\beta(x_0,\sigma)-\rho_\beta(0,\sigma)$ of β cannot vanish on an open set of the real positive axis.

Remarks:

(1) In the proof of Lemma 2, the point (c) is trivial if one of the species has its charge equal to e. The given argument is needed when all ionic charges differ from e.

(2) Because of the neutrality (7), the grand canonical potential depends on only $N-1$ activities in a nontrivial way. For instance, if we introduce in a binary mixture e_1,e_2 the two new parameters w_1 and w_2 defined by $z_1=w_1^{e_1}$ $z_2=w_2(z_1)^{e_2/e_1}$, (31) implies that the grand-canonical potential is necessarily of the form

$$\beta p=\rho_B\ln w_1-f(w_2);$$

$f(w_2)$ depends only on w_2 and is the Legendre transform of βp with respect to the background charge density; w_2 determines the relative ionic proportions. In a one component jellium $\beta p=\rho_B\ln z-f$ and f is the canonical free energy defined in Ref. 2.

(3) The proof of Proposition 3 uses in an essential way the positivity of all ionic charges. One sees that $\rho(x,\sigma)$ has a local minimum in $x=0$ for odd charges: Odd charges will not occupy the lattice $\{ka,k\in\mathbb{Z}\}$ but the shifted lattice $\{(k+\frac{1}{2})a,k\in\mathbb{Z}\}$. This point will be discussed in more detail in the next section.

The proof of Proposition 3 cannot be extended in a straightforward way to the case where some particles have negative charges. At low temperature, one expects that a jellium with charges of both signs will consist of an ionic crystal with an additional gas of neutral molecules, showing therefore a more complicated structure. For instance, low energy configurations of a binary jellium with charges e and $-e$ will have $+e$ ions neutralizing the background on the lattice $\{(k+\frac{1}{2})a,k\in\mathbb{Z}\}$, and the other charges will form neutral dipoles $(e,-e)$. This class of systems will not be discussed in more detail in the present paper.

C. The semi-infinite system

We show here that in the jellium system, boundary charges are perfectly screened. For this, we compute the ionic densities for the semi-infinite system, fixing now the origin at the position of the left wall. We treat the case where there is no excess charge, $C=0$, $\theta=\epsilon=D$ is the applied external field, and $L=la$, l integer. Equation (13) gives

$$\rho_L^{(\theta,\theta)}(x,\sigma)=\frac{z_\sigma}{Z_L(\epsilon,\theta)}$$

$$\times(0|(\bar{U}^\theta)^l\,\overline{U^\theta_{-x}\exp(i\sigma\Phi)\,U^\theta_x}|0). \tag{34}$$

With Lemma 2(i), the limiting density $\rho^\theta(x,\sigma)$ is simply

$$\rho^\theta(x,\sigma)=\lim_{L\to\infty}\rho_L^{(\theta,\theta)}(x,\sigma)$$

$$=z_\sigma(\Omega_c^\theta|0)^{-1}(\Omega_c^\theta|\,\overline{U^\theta_{-x}\exp(i\sigma\Phi)\,U^\theta_x}|0). \tag{35}$$

We remark that, using again the transfer matrix, $\rho^\theta(x,\sigma)$ converges exponentially fast to its bulk value (30) as $x\to\infty$.

Let us now compute the total charge in the interval $[0,y]$. From the identity

$$\frac{d}{dx}(U_{-x}pU_x)=U_{-x}\left(\sum_{r=1}^{N}z_r e_r\exp(ie_r\Phi)-\rho_B\right)U_x, \tag{36}$$

one gets

$$c(x)=\sum_{r=1}^{N}e_r\rho^\theta(x,e_r)-\rho_B$$

$$=(\Omega_c^\theta|0)^{-1}\frac{d}{dx}(\Omega_c^\theta|\,\overline{U^\theta_{-x}\,p\,U^\theta_x}|0) \tag{37}$$

and, since $\bar{p}|0)=0$.

$$\int_0^y c(x)\,dx=(\Omega_c^\theta|0)^{-1}(\Omega_c^\theta|\,\overline{U^\theta_{-y}\,pU^\theta_y}|0). \tag{38}$$

Setting $y_l=la+\theta a/2e$, l integer, and letting $l\to\infty$, we obtain the total charge in the neighborhood of the wall,

$$\lim_{l\to\infty}\int_0^{y_l}c(x)\,dx$$

$$=(\Omega_c^\theta|\Omega^\theta)^{-1}(\Omega_c^\theta|\,\overline{U^\theta_{-Da/2e}\,p\,U^\theta_{Da/2e}}\,|\,\Omega^\theta)$$

$$=(\Omega_c|\Omega)^{-1}(\Omega_c|\exp\left(i\Phi\frac{\theta}{2}\right)p\exp\left(-i\Phi\frac{\theta}{2}\right)|\Omega)$$

$$=\frac{(\Omega_c|\bar{p}|\Omega)}{(\Omega_c|\Omega)}-\frac{\theta}{2}=-\frac{D}{2}. \tag{39}$$

The second equality results of the relation between $\bar{U}^\theta$ and $\bar{U}$ given in Lemma 2 (iii), $(\Omega_c|\bar{p}|\Omega)=0$ follows from (iv) in Lemma 2 and the fact that $\bar{p}$ is odd under charge conjugation. Equation (39) is the statement of perfect screening of the boundary charge $q=D/2$. One can see by similar considerations that when $C\neq 0$, the fraction $C/2$ of the excess charge will be located near each boundary, and the state in the bulk remains unchanged.

IV. LOW TEMPERATURE STATES

In this section, we shall only consider pure ionic systems with all charges $e_1,\ldots,e_N$ positive and as before

$a = e\rho_B^{-1}$. The state of the infinite system will always correspond to the $\epsilon = \theta = 0$ boundary conditions.

A. Ground state of the finite system

For an ordered configuration $0 \leqslant x_1 \leqslant x_2 \leqslant \cdots \leqslant x_n \leqslant L$ the finite volume energy (2) (with $\epsilon = \theta = 0$) can also be written as a quadratic form:

$$H(Q^n|00) = \rho_B \sum_{j=1}^{n} \sigma_j (x_j - x_j^0)^2 - \rho_B \sum_{j=1}^{n} \sigma_j (x_j^0)^2 + \left[\left(\sum_{j=1}^{n} \sigma_j\right)^3 \Big/ 3\right] \rho_B^{-1}, \tag{40}$$

with

$$x_j^0 = \left(\sum_{i=1}^{j-1} \sigma_i + \frac{\sigma_j}{2}\right) \frac{a}{e}.$$

Thus the static equilibrium positions of the ions are of the form $k_1 a$ or $(k_2 + \frac{1}{2})\, a$, when the charges are, respectively, even or odd multiples of e, k_1, k_2 being some integers.

By permutations of the ions, there are $(m_1 + \cdots + m_N)!/m_1! \cdots m_N!$ different ground state configurations, where m_r is the number of charges e_r.

B. Conditional probabilities and distribution of the electric field

The structure of the state is best understood by means of its conditional probabilities, which take a very simple form in one-dimensional Coulomb systems. The point is that a particle configuration external to an interval $[y_1, y_2]$ determines the electric field $E(y_1)$ and $E(y_2)$ at y_1 and y_2.[7] Thus conditional probabilities for an ionic distribution Q^n in $[y_1, y_2]$ are specified by the possible boundary values of the electric field at y_1 and y_2.

$$\mu_{[y_1, y_2]}(Q^n | E(y_2), E(y_1)) = \left[\left(\prod_{j=1}^{n} z_{\sigma_j}\right) \Big/ Z(E(y_2), E(y_1))\right] \times \exp[-\beta H(Q^n | E(y_2), E(y_1))] \tag{41}$$

if

$$\sum_{j=1}^{n} \sigma_j - \rho_B (y_2 - y_1) = \frac{E(y_2) - E(y_1)}{2}$$

and zero otherwise.

We note from (2) that in a jellium state with $\epsilon = \theta = 0$ conditions, $E(x)$ belongs to $2e\mathbb{Z}$ whenever $x \in a\mathbb{Z}$. When the interval $[y_1, y_2]$ is a multiple of the period, i.e., $y_1 = 0$, $y_2 = la$, l integer, we will have $E(0) = 2ev$, $E(la) = 2eu$ with $u, v \in \mathbb{Z}$ and by (20), $Z(E(la), E(0)) = (u|(\bar{U})^l|v)$. In this case, we shall simply write $\mu_l(Q^n|u,v)$ for the conditional probability (41),

$$\mu_l(Q^n|u,v) = 0 \quad \text{if} \quad \sum_{j=1}^{n} \sigma_j/e - l \neq u - v \tag{42}$$

and we have the normalization relation

$$\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\sigma_1 \cdots \sigma_n} \int_0^{la} dx_1 \cdots \int_0^{la} dx_n\, \mu_l(x_1 \sigma_1 \cdots \sigma_n x_n | u,v) = 1. \tag{43}$$

In particular $\mu_l(\varnothing|u,v) = 1$ if $u = l + v$ and $\mu(\varnothing|u,v) = 0$ otherwise.

Moreover, it is known[1,7] that the electric field $E(x)$, $x \in a\mathbb{Z}$, is itself a Markov process with stationary distribution $(\Omega_c|u)(u|\Omega)/(\Omega_c|\Omega)$ and joint distribution given by

$$P_l(u,v) = P(E(la) = 2eu,\, E(0) = 2ev) = \exp(-\gamma la)\, \frac{(\Omega_c|u)(u|(\bar{U})^l|v)(v|\Omega)}{(\Omega_c|\Omega)}, \tag{44}$$

$$0 \leqslant P_l(u,v) \leqslant 1, \quad \sum_{u,v \in \mathbb{Z}} P_l(u,v) = 1. \tag{45}$$

The probability densities $\mu_l(Q^n)$ for an ionic configuration Q^n in $[0, la]$ can then be constructed by averaging the conditional probabilities (41) over the electric field distribution

$$\mu_l(Q^n) = \sum_{u,v \in \mathbb{Z}} P_l(u,v)\, \mu_l(Q^n|u,v). \tag{46}$$

In the low temperature limit, probabilities of electric field configurations will be small except those corresponding to particle configurations with minimal energy. One expects therefore that all $P_l(u,v)$ will vanish as $\beta \to \infty$ except for boundary fields $E(0) = 2ev$, $E(la) = 2eu$ corresponding to ground state configurations. Then, the particle distributions $\mu_l(Q^n)$ will essentially be determined by one (or a few) conditional probabilities which are explicitly given by (41). One has therefore to estimate the joint electric field distribution at low temperature: This will be done for the two binary ionic jellium with charges $e_1 = e$, $e_2 = 2e$ and $e_1 = 2e$, $e_2 = 3e$.

C. The binary ionic mixture $e_1 = e$, $e_2 = 2e$

The lowest energy configurations of particles of charges $e_1 = e$ and $e_2 = 2e$ in the interval $[0,a]$ is [see (40)]

$$H(x_1, e_1|00) = \rho_B \left(x - \frac{a}{2}\right)^2 + \frac{e^2 a}{12}. \tag{47}$$

It consists of a single charge e_1 in $[0,a]$ with boundary fields $(E(a), E(0)) = (0,0)$. Because of the constraint (42), the corresponding partition function is simply

$$Z_a(0,0) = z_1 \int_0^a \exp[-\beta H(x, e_1|0,0)]\, dx. \tag{48}$$

Any ionic configuration compatible with boundary fields $(E(a), E(0)) = (2eu, 2ev) \neq (0,0)$ will have higher energy because neutralization of the background will be less effective. We therefore expect that the ratio of the partitions functions for the interval $[0,a]$

$$\frac{Z_a(2eu, 2ev)}{Z_a(0,0)} = \frac{(u|\bar{U}|v)}{(0|\bar{U}|0)},$$

will vanish as $\beta \to \infty$ if $(u,v) \neq (0,0)$.

This fact is the content of the next proposition which is proved in Appendix B.

Proposition 4:

(i) Define $\hat{U} = \bar{U}/(0|\bar{U}|0)$ and let P_0 be the projector on $(\varphi|0) = (e/2\pi)^{1/2}$ in $\mathscr{L}^2([-\pi/e, \pi/e], d\varphi)$. Then $\|\hat{U}\|_2 < \infty$ where $\|\cdot\|_2$ is the Hilbert–Schmidt norm in $\mathscr{L}^2([-\pi/e, \pi/e], d\varphi)$ and

$$\|\hat{U} - P_0\|_2 = O\left(\frac{1}{\beta^{1-\epsilon}}\right),\ \beta\to\infty,\ \epsilon>0.$$

(ii) $\|\Omega - |0)(0|\Omega)\| = O\left(\frac{1}{\beta^{1-\epsilon}}\right)$.

(iii) Let $\lambda = \exp(\gamma)/(0|\bar{U}|0)$ be the maximal eigenvalue of $\bar{U}$. Then $1\leqslant\lambda = 1 + O(1/\beta^{2-\epsilon}), \beta\to\infty$.

The same results hold for $\hat{U}^*$ and its eigenvector Ω_c.

One can then immediately find the low temperature behavior of the joint distribution of the electric field:

$$P_l(0,0) = 1 + O\left(\frac{1}{\beta^{2-\epsilon}}\right),\quad \beta\to\infty\ . \tag{49}$$

Indeed since $\lambda\geqslant 1$ and $(0|(\hat{U})^l|0)\geqslant 1$, one gets

$$\begin{aligned}
0\leqslant 1 - P_l(0,0)
&= 1 - \frac{(0|\Omega)(\Omega_c|0)}{(\Omega_c|\Omega_c)}\frac{(0|(\hat{U})^l|0)}{\lambda^l}\\
&= \lambda^l - \frac{(0|\Omega)(\Omega|0)}{(\Omega_c|\Omega)}\\
&= \lambda^l - 1 + \frac{(\Omega_c|\Omega) - (0|\Omega)(\Omega_c|0)}{(\Omega_c|0)}\\
&\leqslant \lambda^l - 1 + \frac{1}{(\Omega_c|\Omega)}\|\Omega_c - |0)(0|\Omega_c)\|\,\|\Omega - |0)(0|\Omega)\|\\
&= O\left(\frac{1}{\beta^{2-\epsilon}}\right)
\end{aligned}$$

by (ii) and (iii) of Proposition 4.

Proposition 5: Let $f(Q^n)$ be a continuous function on $[0,la]$, then

$$\int dQ^n f(Q^n)(\mu_l(Q^n) - \mu_l(Q^n|0,0)) = O\left(\frac{1}{\beta^{2-\epsilon}}\right). \tag{50}$$

Proof: It follows from the normalization (43) of the conditional probabilities that

$$\left|\int dQ^n f(Q^n)\mu_l(Q^n|u,v)\right| \leqslant \|f\|_\infty n!. \tag{51}$$

Hence, we obtain with (46), (51), and (49)

$$\begin{aligned}
&\int dQ^n f(Q^n)(\mu_l(Q^n) - \mu_l(Q^n|0,0))\\
&\leqslant (1 - P_l(0,0))\left|\int dQ^n f(Q^n)\mu_l(Q^n|0,0)\right|\\
&\quad + \sum_{(u,v)\neq(0,0)} P_l(u,v)\left|\int dQ^n f(Q^n)\mu_l(Q^n|u,v)\right|\\
&\leqslant 2(1 - P_l(0,0))\,\|f\|_\infty\, n! = O\left(\frac{1}{\beta^{2-\epsilon}}\right).
\end{aligned}$$

We see that, at low temperature, the particle distribution $\mu_l(Q^n)$ is approximated by the conditional distribution $\mu_l(Q^n|0,0)$ with vanishing boundary fields. By (40) and (41), we have $\mu_l(Q^n)$ proportional to $\exp[-\beta H(Q^n|0,0)]$, showing that ions are found with highest probability on ground state configurations with essentially Gaussian fluctuations. Because of the symmetry under permutations of $\mu_l(x_1\sigma_1,\ldots,x_n\sigma_n)$, each lattice site $(k+\frac{1}{2})a$ and ka, $k\in\mathbb{Z}$, is occupied with equiprobability by ions e_1 and e_2, respectively.

However, the density of ions of the largest charge vanishes at low temperature since the background is best screened by small charges. (This only occurs in a grand-canonical state where densities are not fixed.)

The neutrality and the normalization imply

$$\int_0^a \rho(x,e_1)\,dx + 2\int_0^a \rho(x,e_2)\,dx = 1$$

and with (42), (43)

$$\mu_1(Q^n|0,0) = 0 \quad \text{if} \quad Q^n\neq(x,e_1)$$

and

$$\int_0^a \mu_1(x,e_1|0,0)\,dx = 1.$$

One has therefore by the positivity of μ_l and P_l

$$\begin{aligned}
1&\geqslant\int_0^a \rho(x,\epsilon_1)\,dx\\
&\geqslant\int_0^a \mu_1(x,e_1)\,dx\\
&\geqslant P_1(0,0)\int_0^a \mu_1(x,e_1|0,0) = P_1(0,0)
\end{aligned}$$

showing with (49) that the average densities of ions e_1 (and e_2) are ρ_B (and zero) to order $O(1/\beta^{2-\epsilon})$.

The asymptotic form of the pressure can be found from part (iii) of Proposition 5,

$$\beta p = \frac{1}{a}\gamma = \frac{1}{a}(\ln(0|\bar{U}|0) + \ln\lambda).$$

From (47) and (48) one finds as $\beta\to\infty$

$$\begin{aligned}
(0|\bar{U}|0) = &\frac{z_1(\pi)^{1/2}\rho_B^{-1}}{(\beta a)^{1/2}}\\
&\times\exp\left(-\frac{\beta e^2 a}{12}\right)[1 + O(\exp(-\tfrac{1}{2}(\beta e^2 a)^{1/2}))]
\end{aligned} \tag{52}$$

and thus

$$\beta p = \frac{1}{2a}\ln\left(\frac{\pi}{\beta e\,\rho_B}\right) - \frac{\beta e^2}{12} + \frac{1}{a}\ln z_1 + O\left(\frac{1}{\beta^{2-\epsilon}}\right). \tag{53}$$

The first two terms in (53) represent exactly the canonical free energy of a one component jellium of charges $e_1 = e$,[2] and there is no contribution to p from the charges e_2 to order $O(1/\beta^{2-\epsilon})$.

More generally, it is not hard to show by explicit estimations of the $\mu_l(Q^n|0,0)$ that $\mu_l(Q^n)$ converges to the (symmetrized) distribution corresponding to the ground state of a one component jellium of charge e_1,

$$\lim_{\beta\to\infty}\mu_l(x_1\sigma_1,\ldots,x_n\sigma_n) = \begin{cases}\operatorname{Sym}\prod_{j=1}^n \delta\left(x_j - ja + \frac{a}{2}\right) & \text{if } n=l \text{ and}\\ & \sigma_j = e_1, j = 1\cdots n\\ 0 & \text{otherwise}\end{cases}$$

and for the densities

$$\lim_{\beta\to\infty}\rho(x,\sigma)$$

$$=\begin{cases}\sum_{k\in\mathbb{Z}}\delta\left(x-ka+\frac{a}{2}\right), & \sigma=e_1\\ 0, & \sigma=e_2.\end{cases}$$

D. The binary ionic mixture $e_1=2e$, $e_2=3e$

This system presents the new feature that the greatest common divisor e of the charges is strictly smaller than both of them. Ground state configurations of the mixture e_1, e_2 differ then from those of a single component with charge e_1 in the following respect. In the mixture ions e_1 can occupy any lattice site ka, $k\in\mathbb{Z}$ (see Sec. A) whereas in the single component system, charges e_1 are necessarily found on a lattice of double period $2a$. As in the preceding case, the density $\rho(x,e_2)$ of the largest ions will vanish at low temperature and as a result, the state will converge to the convex superposition of ground state of e_1 ions on the lattices $2ka$ and $(2k+1)a$, $k\in\mathbb{Z}$.

As before, we compare partition functions for finite systems in $[0,a]$ and arbitrary boundary fields $(E(a),E(0))$ with those corresponding to the lowest possible energy configurations.

The latter consists of having no particles in $[0,a]$ and corresponds to the two possible boundary values $(E(a),E(0))=(-2e,0)$ or $(0,2e)$. The energy $e^2a/3$ and the associate partition functions are simply

$$(-1|\bar U|0)=(0|\bar U|1)=\exp\left(-\beta\frac{e^2a}{3}\right). \tag{54}$$

We now set $\hat U=\bar U/(0|\bar U|1)$.

Notice that the configurations of one e_1 ion in $[0,a]$ have boundary fields $(2e,0)$ or $(0,-2e)$ and energy

$$H(x,e_1|0,-1)=H(a-x,e_1|1,0)=2e\rho_B x^2+e^2a/3.$$

The associated partition functions are $(1|\bar U|0)=(0|\bar U|-1)$ and we define

$$g(\beta)=(0|\hat U|-1)$$

$$=\frac{z_1}{2}\left(\frac{\pi}{2e\rho_B}\right)^{1/2}\left[\frac{1}{\sqrt{\beta}}+O(\exp(-(2\beta e^2a)^{1/2}))\right]. \tag{55}$$

One can now formulate the equivalent of Proposition 4. Proofs and details can be found in Ref. 10.

Proposition 6:

(i) Let N be the operator defined by $(u|N|v)=\delta_{-1,u}\,\delta_{0,v}+\delta_{0,u}\,\delta_{1,v}$ Then

$$\sqrt{2}\,g(\beta)\leqslant\|\hat U-N\|_2=O\left(\frac{1}{\sqrt{\beta}}\right).$$

(ii)

$$\|\Omega-|-1)(-1|\Omega)\|=\|\Omega_c-|1)(1|\Omega)\|=O\left(\frac{1}{\beta^{1/6}}\right).$$

(iii) Let $\lambda=\exp(\gamma)/(0|\bar U|1)$ be the maximal eigenvalue of $\hat U$. Then

$$(2g(\beta))^{1/2}\leqslant\lambda=(2g(\beta))^{1/2}+O(\exp(-\tfrac{5}{4}\beta e^2a)).$$

(iv) One has moreover the more detailed estimates

$$2\frac{(\Omega_c|0)(0|\Omega)}{(\Omega_c|\Omega)}$$

$$\simeq 4\frac{(\Omega_c|1)(1|\Omega)}{(\Omega_c|\Omega)}\simeq 2\lambda^2\frac{(\Omega_c|1)(-1|\Omega)}{(\Omega_c|\Omega)}$$

$$\simeq\frac{8}{\lambda^2}\frac{(\Omega_c|-1)(1|\Omega)}{(\Omega_c|\Omega)}\simeq 1, \tag{56}$$

where the above equalities hold up to terms $O(\exp(-\frac{5}{4}\beta e^2a))$ as $\beta\to\infty$. One should note here that, contrary to the previous case, the eigenprojection $P=|\Omega)(\Omega_c|/(\Omega_c|\Omega)$ has no limit as $\beta\to\infty$ [in fact, by (ii) $(\Omega_c|\Omega)\to 0$, $\beta\to\infty$]. $\hat U$ itself converges in the Hilbert–Schmidt norm to the nilpotent operator N.

As a consequence of (iii) one finds that the grand-canonical potential $\beta p=(1/a)\gamma$ is asymptotically that of a single component jellium with ions $e_1=2e$. Indeed, using (54) and (55) βp is of the form (53) as $\beta\to\infty$ with e replaced by $2e$. Hence, the density of ions $e_2=3e$ vanishes as $\beta\to\infty$.

To investigate the structure of the low temperature state, we compute from (iv) the joint distribution $P_2(u,v)$ of the electric field for the interval $[0,2a]$. One finds five types of boundary conditions relevant as $\beta\to\infty$. They are $(0,0)$ and $\mathscr{A}=\{(1,1),(-1,-1),(-1,1),(1,-1)\}$ with

$$P_2(0,0)=\tfrac{1}{2}+O(\exp(-\tfrac{5}{4}\beta e^2a)), \tag{57}$$

$$P_2(u,v)=\tfrac{1}{8}+O(\exp(-\tfrac{5}{4}\beta e^2a)). \tag{58}$$

For instance, Proposition 6 (iv) and (44) give

$$P_2(0,0)=\frac{(0|\Omega)(\Omega_c|0)}{(\Omega_c|\Omega)}\frac{(0|(\hat U)^2|0)}{\lambda^2}$$

$$=\frac{1}{2}\frac{(0|(\hat U)^2|0)}{\lambda^2}+O(\exp(-\tfrac{5}{4}\beta e^2a));$$

since $(0|(\hat U)^2|0)=2(0|\hat U|-1)=2g(\beta)$, (57) follows from Proposition 6 (iii); (58) is proved in a similar way.

As a result of (57), (58), and (46), there are five conditional probabilities which determine the particle distribution in $[0,2a]$ as $\beta\to\infty$,

$$\mu_2(Q^n)=\tfrac{1}{2}\mu(Q^n|0,0)+\tfrac{1}{8}\sum_{(u,v)\in\mathscr{A}}\mu_2(Q^n|u,v)$$
$$+O(\exp(-\tfrac{5}{4}\beta e^2a)) \tag{59}$$

(the inequality holds in the weak sense, proof as in Proposition 5).

According to the constraint (42), these boundary conditions allow no particles in $[0,2a]$ for $(-1,1)$, one ion e_1 for $(0,0),(-1,-1),(1,1)$, and two ions e_1 for $(1,-1)$. The corresponding energies are

$$H(\varnothing|-1,1)=\tfrac{2}{3}e^2a,$$

$$H(x,e_1|0,0)=2e\rho_B(x-a)^2+\tfrac{2}{3}e^2a,$$

$$H(x,e_1|-1,-1)=H(2a-x|1,1)=2e\rho_B x^2+\tfrac{2}{3}e^2a,$$

$$H(x_1,e_1;x_2e_1|1,-1)$$
$$=2e\rho_B x_1^2+2e\rho_B(x_2-2a)^2+\tfrac{2}{3}e^2a. \tag{60}$$

One deduces from (60) that the conditional probabilities $\mu_2(Q^n|u,v)$ with $(u,v)\in\mathscr{A}$ locate particles at the boundaries of the interval $[0,2a]$, whereas $\mu_2(Q^n|0,0)$ locates a single ion e_1 in a.

Thus $\mu_2(Q^n)\simeq 0$ for $Q^n \neq \{\varnothing; x, e_1\}$ and $\mu_2(x, e_1)\simeq \frac{1}{2}\mu_2(x, e_1|0,0)$ when x belongs to a neighborhood $\Lambda_\epsilon = (\epsilon, 2a-\epsilon)$ of a, $\epsilon > 0$. Since $\mu_2(x, e_1|0,0)\to\delta(x-a)$, $\beta\to\infty$, there will be essentially a probability $\frac{1}{2}$ to find an ion e_1 in a at low temperature.

In fact, one can prove the following statement for the distributions $\mu_{\Lambda_\epsilon}(Q^n)$ corresponding to intervals Λ_ϵ strictly smaller than $[0,2a]$ (this is to avoid problems with particles at the boundaries).

Proposition 7:

$$\lim_{\beta\to\infty}\mu_{\Lambda_\epsilon}(Q^n) = \begin{cases} \frac{1}{2}, & n=0 \\ \frac{1}{2}\delta(x-a), & n=1, \quad Q=(x,e_1) \\ 0, & n>1 \end{cases}$$

and for the densities

$$\lim_{\beta\to\infty}\rho(x,\sigma) = \begin{cases} \frac{1}{2}\sum_{k\in\mathbb{Z}}\delta(x-ka), & \sigma = e_1 \\ 0, & \sigma = e_2 \end{cases}.$$

To demonstrate Proposition 7, one uses the compatibility relations to relate $\mu_{\Lambda_\epsilon}(Q^n)$ to the distributions $\mu_2(Q^n)$ in the larger interval $[0,2a]$. The latter are evaluated with the help of (59) and the explicit form of the conditional probabilities. The neutrality relation (7) and the normalization relation (43) give the conclusion.[10] The proposition establishes that the state converges to the convex superposition of the ground state of ions e_1 on the lattice $2ka$ and $(2k+1)a$, $k\in\mathbb{Z}$, with equal weight $\frac{1}{2}$.

APPENDIX A

The semigroup generated by Γ^θ is defined in the following way. Consider first the contractive semigroup $U^{1\theta}$ generated by $-\beta(p+\theta/2)^2 - i\rho_B\Phi$. $U_x^{1\theta}$ is explicitly given by

$$U_x^{1\theta} = \exp\left[\frac{-\beta\rho_B^2 x^3}{12}\right]\exp\left[-\beta\left(p+\frac{\theta}{2}+\frac{\rho_B x}{2}\right)^2 x\right] \times\exp[-i\rho_B\Phi x], \quad x\geqslant 0. \tag{A1}$$

Since $\Sigma_{r=1}^N z_r \exp[ie_r\Phi]$ is bounded, U_x^θ is defined as a perturbation of $U_x^{1\theta}$ by the norm convergent series

$$U_x^\theta = \sum_{n\geqslant 0}\int_0^x dx_1\cdots\int_0^{x_{n-1}} dx_n\, U_{x-x_n}^{1\theta} \times\left(\sum_{r=1}^N z_r\exp(ie_r\Phi)\right) U_{x_n-x_{n-1}}^{1\theta}\cdots U_{x_1}^{1\theta}. \tag{A2}$$

We write the series (A2) in terms of τ-invariant operators by replacing everywhere $U_{x-y}^{1\theta}$ by

$$G(x,y) = \exp(i\rho_B\Phi x)\, U_{x-y}^{1\theta}\exp(-i\rho_B\Phi y). \tag{A3}$$

$G(x,y)$ is τ-invariant and has the form (20).

The series (19) is then obtained by setting $x=a$ and considering all operators acting in $\mathscr{L}^2[[-\pi/e, \pi/e], d\varphi]$.

APPENDIX B: PROOF OF PROPOSITION 4

To show (i), we have to estimate the sum

$$\|\hat{U} - P_0\|_2^2 = \sum_{(u,v)\neq(0,0)}\left|\frac{(u|\bar{U}|v)}{(0|\bar{U}|0)}\right|^2. \tag{B1}$$

We have from (47) and (48) [see (52)]

$$(0|\bar{U}|0)\sim\frac{c_1}{\sqrt{\beta}}\exp\left(-\frac{\beta e^2 a}{12}\right), \quad \beta\to\infty. \tag{B2}$$

Notice first that the constraint (42) implies $(u|\bar{U}|v)=0$ if $u-v\leqslant -2$. We divide the other terms of the sum (B1) into four classes according to the value of the boundary fields at 0 and a. These classes are

(a) $u-v=-1$: no particles in $[0,a]$ [see (42)],

(b) $u-v\geqslant 0$, $u\leqslant -1$: configurations with nonpositive electric field,

(c) $u-v\geqslant 0$, $v\geqslant 1$: configurations with nonnegative electric field,

(d) $u-v\geqslant 0$, $u\geqslant 0\geqslant v$, $(u,v)\neq(0,0)$: configurations where the electric field changes its sign.

For Case (a), we have $(u|\bar{U}|u+1) = \exp\{-\beta e^2 a[(u+\frac{1}{2})^2+\frac{1}{12}]\}$, which gives with (B2)

$$\sum_{u\in\mathbb{Z}}|(u|\hat{U}|u+1)|^2 \leqslant c_2\beta\sum_{u\in\mathbb{Z}}\exp[-2\beta e^2 a(a+\tfrac{1}{2})^2] = O\left[\beta\exp\left(-\beta\frac{e^2 a}{2}\right)\right]. \tag{B3}$$

In Case (b), one notes that the energy is reduced by putting all particles at the left boundary.

From (1), $D = e(u+v)$, and (42) one has

$$E(x, Q^{(n)}) = \sum_{j=1}^n \sigma_j\,\mathrm{sgn}(x-x_j) - 2\rho_B x + \rho_B a + e(u+v) \leqslant E(x, \{x_j=0, \sigma_j\}) = -2[\rho_B x - e(u+1)]\leqslant 0.$$

Hence

$$H(Q^{(n)}|u,v)\geqslant\frac{1}{4}\int_0^a |E(x,\{x_j=0,\sigma_j\})|^2\,dx$$
$$=e^2a\left[(u+\tfrac{1}{2})^2+\tfrac{1}{12}\right]. \tag{B4}$$

It follows from (5) and (B4) that

$$(u|\bar{U}|v)\leqslant\exp\{-\beta e^2a\left[(u+\tfrac{1}{2})^2+\tfrac{1}{12}\right]\}$$
$$\times\sum_{n=[(u-v)/2+1]}\frac{(2az)^n}{n!} \tag{B5}$$
$$\leqslant\exp\{-\beta e^2a\left[(u+\tfrac{1}{2})^2+\tfrac{1}{12}\right]\}$$
$$\times\frac{(2az)^{[(u-v)/2+1]}}{[(u-v)/2+1]!}e^{2az}. \tag{B6}$$

In (B5), $[(u-v)/2+1]$ is the integer part of $(u-v)/2+1$ and $z=\max(z_1,z_2)$. The restriction on the summation in (B5) comes from the constraint $\Sigma_{j=1}^n\,\sigma_j/e=u-v+1$, $\sigma_j=e$ or $2e$, which implies $n\geqslant[(u-v)/2+1]$.

With the estimate (B6) and (B2), we find again

$$\sum_{v<u<-1}\left|\frac{(u|\bar{U}|v)}{(0|\bar{U}|0)}\right|^2$$
$$=O\left[\beta\exp\left(-\beta\frac{e^2a}{2}\right)\right]. \tag{B7}$$

The terms of Class (c) and (d) are estimated in a similar way, but the contribution of the terms (d) to (B1) has only bound of the form $O(1/\beta^{2-\epsilon})$, $\epsilon>0$ (see Ref. 10).

Proof of (i) and (ii). Since λ is the largest eigenvalue of the compact operator $\hat{U}$, one has $\lambda=\lim_{n\to\infty}\|\hat{U}^n\|^{1/n}$.

The fact that $(0|\hat{U}|0)=1$ and that all matrix elements of $\hat{U}$ are nonnegative implies $\|\hat{U}^n\|\geqslant1$ for all n, hence $\lambda\geqslant1$. Moreover, using the eigenvalue equation for Ω and assuming $\|\Omega\|=1$, one gets

$$\lambda^2\|\Omega-|0)(0|\Omega)\|^2$$
$$=\lambda^2\sum_{u\neq0}|(u,\Omega)|^2$$
$$=\sum_{u\neq0}\left(\sum_v(u|\hat{U}|v)(v|\Omega)\right)^2$$
$$\leqslant\sum_{u\neq0}\sum_v(u|\hat{U}|v)^2\leqslant\|\hat{U}-P_0\|_2^2.$$

Thus (ii) follows from (i) and the fact that $\lambda\geqslant1$.

One deduces again from the eigenvalue equation

$$0\leqslant(\lambda-1)(0|\Omega)$$
$$=\sum_{v\neq0}(0|\hat{U}|v)(v|\Omega)$$
$$\leqslant\left(\sum_{v\neq0}(0|\hat{U}|v)^2\sum_{u\neq0}(u|\Omega)^2\right)^{1/2}$$
$$\leqslant\|\hat{U}-P_0\|_2\,\|\Omega-|0)(0|\Omega)\|=O\left(\frac{1}{\beta^{2-\epsilon}}\right).$$

Since by (ii) $(0|\Omega)\to1$ as $\beta\to\infty$, this last inequality completes the proof of (iii).

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On the mean motion and some statistical properties of a quasiperiodic observable in a fermion–boson model

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(Received 18 February 1982; accepted for publication 28 May 1982)

We study properties of an atomic observable of a fermion–boson model in the region after a long time, compared to its initial "collapse" and "revival" times, had elapsed. We determine its mean motion which characterizes its mean oscillation. We also determine its average frequency of achieving a particular value. Its behavior in the small average boson number limit is shown to be particularly interesting.

PACS numbers: 05.30. – d

I. INTRODUCTION

A simple idealized model Hamiltonian which has been used as a prototype for studies of fermion–boson interactions is

$$\hat{H} = \tfrac{1}{2}\hbar\omega_0\hat{\sigma}_z + \hbar\omega\hat{a}^\dagger\hat{a} + \hbar\lambda\,(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^\dagger), \tag{1.1}$$

where the boson operators $\hat{a}^\dagger$ and $\hat{a}$ create and destroy photons and the fermion operators $\hat{\sigma}_z$, $\hat{\sigma}_+$, and $\hat{\sigma}_-$ (Pauli matrices) represent a two-state atom or molecule.[1] Hamiltonian (1.1) is used, besides in quantum optics,[2] in spin–phonon resonance, and in quantum field theory.[3]

Despite its apparent simplicity, the associated dynamical problem is essentially non-linear. Recent papers[4] have reported interesting periodic spontaneous collapses and revivals of certain observables in the dynamics of this model when the field is initially fully coherent.

A central role in these studies is played by infinite sums of the form

$$x(t) = \sum_{k=0}^{\infty} a_k \cos(\Omega_k t + \delta_k). \tag{1.2}$$

For example, the atomic inversion, or the expectation value of the atomic excitation energy, is given by[4]

$$w_m(t) = m\sum_{k=0}^{\infty} p_k\left\{\frac{\Delta^2}{\Omega_k^2(m)} + \left(1 - \frac{\Delta^2}{\Omega_k^2(m)}\right)\cos[\Omega_k(m)t]\right\}, \tag{1.3}$$

where

$$\Delta = \omega_0 - \omega, \tag{1.4}$$

$$\Omega_k^2(m) = \Delta^2 + 4\lambda^2[k + (m+1)/2]. \tag{1.5}$$

and where $m = -1$ or 1 specifies whether the atom is initially in the lower or upper state. p_k represents the initial photon distribution. Equation (1.3) was derived from solving the coupled Heisenberg equations of motion

$$\begin{aligned} i\dot{\sigma}_- &= \omega_0\sigma_- - \lambda\sigma_z a, \\ i\dot{a} &= \omega a + \lambda\sigma_-, \\ i\dot{\sigma}_z &= 2\lambda\,(\sigma_+ a - a^\dagger\sigma_-) \end{aligned} \tag{1.6}$$

for σ_z, assuming the initial density matrix has the form $\rho = |m\rangle\langle m| \otimes \rho_f$, where ρ_f is the field density matrix. The expectation value $w_m(t)$ of $\sigma_z(t)$ is obtained from

$$w_m(t) \equiv \langle\sigma_z(t)\rangle = \sum_{n=0}^{\infty}\langle n|\rho_f|n\rangle\langle m,n|\sigma_z|m,n\rangle. \tag{1.7}$$

The physical quantity $w_m(t)$ given by Eq. (1.3) has the form of Eq. (1.2) with $\delta_k = 0$.

For the initial state of the field represented by the initial photon distribution p_k, we shall consider coherent, thermal, and mixed (coherent and thermal) cases. In this paper, we concern ourselves with studying properties of the quasiperiodic function (1.2) or (1.3) in the region after a long time, compared to the initial collapse and revival times, had elapsed, namely in the region where the behavior of this function appears irregular. We ask what quantities should characterize these irregular behaviors. Is there a statistical distribution, and is there a meaningful mean frequency of oscillation? One of the results which we obtained, as will be seen, is that such "mean" angular frequency of oscillation can be defined in the irregular region, and when the initial state of the field is coherent and represented by a Poissonian photon distribution, it is identical to the Rabi frequency normally used for the regularly oscillatory region.

The mathematical analysis we use in this paper originated with the work of Lagrange, Wintner,[5] Weyl,[6] and others in their pioneering study of the perturbed planetary orbits. Similar analysis has since been applied to molecular physics[7] and statistical mechanics.[8] It is hoped that our present paper will stimulate further applications of these techniques for problems in quantum optics.

II. THE PROBABILITY DENSITY *P(x)*

The characteristic function $f(\alpha)$ of $x(t)$ of Eq. (1.2) is

$$f(\alpha) = \lim_{T\to\infty}(1/T)\int_0^T \exp[i\alpha x(t)]\,dt. \tag{2.1}$$

We assume that Δ^2 in Eq. (1.5) is irrational so that the frequencies Ω_k (the m dependence is often dropped for convenience) are linearly independent in the sense that no set of integers $\{m_k\}$ except $\{m_k = 0\}$ can be found to satisfy

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$$\sum_k m_k \Omega_k = 0. \tag{2.2}$$

We can thus use the Kronecker–Weyl theorem[9] to replace the time average in (2.1) by the corresponding phase average and get

$$f(\alpha) = \lim_{N\to\infty} \frac{1}{(2\pi)^N} \int_0^{2\pi} \cdots \int_0^{2\pi} \times \exp\left(i\alpha \sum_{k=0}^{N-1} a_k \cos\varphi_k\right) d\varphi_0 \ldots d\varphi_{N-1}$$

$$= \prod_{k=0}^{\infty} J_0(a_k \alpha), \tag{2.3}$$

where $J_0(x)$ is the zeroth-order Bessel function. The probability density $P(x)$ of $x(t)$ is the Fourier transform of the characteristic function $f(\alpha)$ and is therefore given by

$$P(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \prod_{k=0}^{\infty} J_0(a_k\alpha) e^{-i\alpha x}\, d\alpha. \tag{2.4}$$

To proceed in order to obtain simpler expressions for $P(x)$, we consider the following two specific cases of photon distribution for the p_k of Eq. (1.3):

(i) For the Poissonian photon distribution, p_k is given by

$$p_k = [(\bar{n})^k/k!]e^{-\bar{n}}. \tag{2.5}$$

(ii) For the thermal photon distribution, p_k is given by

$$p_k = (1 - e^{-\beta})e^{-k\beta} = \frac{1}{1+\bar{n}}\left(\frac{\bar{n}}{1+\bar{n}}\right)^k, \tag{2.6}$$

where the mean photon number $\bar{n}$ for the respective photon distribution is defined by

$$\bar{n} = \sum_{k=0}^{\infty} k\, p_k \tag{2.7}$$

and where β in Eq. (2.6) denotes $1/kT$. We shall consider a mixed Poissonian and thermal photon distribution in Appendix A.

We shall be interested in the case when the detuning Δ is very small, but in order to have the set of frequencies Ω_k completely linearly independent, we shall assume that Δ^2 is small but finite and irrational (the irrationality condition can be relaxed in practice). Putting $\Delta^2 \simeq 0$ and comparing Eqs. (1.3) with (1.2), we find that

$$a_k = p_k, \quad k = 0,1,2,\cdots \quad \text{for } m = +1, \tag{2.8}$$

but that $a_0 = 0$, $a_k = -p_k$, $k = 1,2,\cdots$ for $m = -1$. Since the statistical properties of $-x(t)$ and $x(t)$ are clearly the same, we shall, for definiteness, take

$$a_0 = 0, \quad a_k = p_k, \quad k = 1,2,\cdots \quad \text{for } m = -1. \tag{2.9}$$

We now proceed with Eq. (2.4). We know that when z is small,

$$J_0(z) = 1 - \left(\frac{z}{2}\right)^2 + \frac{1}{4}\left(\frac{z}{2}\right)^4 - \cdots$$

$$= \exp\left[-\frac{z^2}{4} - \frac{z^4}{64} - O(z^6)\right]. \tag{2.10}$$

Since $J_0(z)$ is peaked at $z = 0$, the product of N $J_0(z)$'s is even more peaked as $N \to \infty$. Then

$$\prod_{k=0}^{\infty} J_0(a_k\alpha) = \exp\left[\left(-\tfrac{1}{4}\alpha^2 \sum_{k=0}^{\infty} a_k^2\right) - \left(\tfrac{1}{64}\alpha^4 \sum_{k=0}^{\infty} a_k^4\right) + \cdots\right]. \tag{2.11}$$

It is shown in Appendix B that for large $\bar{n}$ and $l \geqslant 1$,

$$\sum_{k=0}^{\infty} a_k^{2l} = \begin{cases} (2^{-l}\pi^{-l+1/2}/l^{1/2})(\bar{n})^{-l+1/2} \\ \text{for the Poissonian distribution,} \end{cases} \tag{2.12}$$

$$\begin{cases} (1/2l)(\bar{n})^{-2l+1} \\ \text{for the thermal distribution.} \end{cases} \tag{2.13}$$

Thus, if we ignore Σa_k^4, Σa_k^6, etc. in Eq. (2.11) by taking the large $\bar{n}$ limit, and substitute (2.11) into (2.4), we obtain

$$P(x) \simeq (1/\pi^{1/2}\sigma)\exp(-x^2/\sigma^2), \tag{2.14}$$

where

$$\sigma^2 = \sum_{k=0}^{\infty} a_k^2. \tag{2.15}$$

The half-width σ defined by (2.15) of the Gaussian form (2.14) can be expressed in closed form for both the Poissonian and the thermal photon distribution (as well as for the mixed case, see Appendix A). We find, from Eqs. (2.5), (2.6), (2.8), (2.9), and (2.15), that

$$\sigma^2 = \begin{cases} e^{-2\bar{n}}[I_0(2\bar{n}) - \tfrac{1}{2}(1-m)] \\ \text{for the Poissonian distribution,} \end{cases} \tag{2.16}$$

$$\begin{cases} (1+2\bar{n})^{-1} - \tfrac{1}{2}(1-m)(1+\bar{n})^{-2} \\ \text{for the thermal distribution,} \end{cases} \tag{2.17}$$

where $I_0(x)$ in (2.16) is the modified Bessel function. For large $\bar{n}$, the σ's are given by

$$\sigma^2 \simeq \begin{cases} (1/4\pi\bar{n})^{1/2} & \text{for the Poisson distribution,} \quad (2.18) \\ 1/2\bar{n} & \text{for the thermal distribution.} \quad (2.19) \end{cases}$$

For $\bar{n}$ not too large, in the region $1 < \bar{n} < 5$, say, we can improve the Gaussian approximation (2.14) by including the quartic term and the sextic term in the exponential:

$$P(x) \simeq \frac{A}{\sigma} \exp\left[-\left(\frac{x}{\sigma}\right)^2 - c_4\left(\frac{x}{\sigma}\right)^4 - c_6\left(\frac{x}{\sigma}\right)^6 - \cdots\right], \tag{2.20}$$

where the coefficients c_4, c_6, $\cdots$ can be obtained from the expansion (2.11). The behavior of $P(x)$ in the region $0 < \bar{n} < 1$ is more complicated, and it will be briefly discussed in Sec. V.

III. AVERAGE FREQUENCY

Beside the probability density $P(x)$, where $P(x)\,dx$ is a measure of the average time spent by the variable $x(t)$ in the region $x \leqslant x(t) \leqslant x + dx$, we may also consider the average frequency with which $x(t)$ of Eq. (1.2) achieves particular value q. One defines $L(q)$, the average frequency of $x(t) = q$ by

$$L(q) = \lim_{T\to\infty} (1/T) N_T(q), \tag{3.1}$$

where $N_T(q)$ is the number of zeros of

$$F(t) = x(t) - q. \tag{3.2}$$

Analytic expression for $L(q)$ was first given by Kac[10]:

$$L(q)=\frac{1}{2\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\eta^{-2}\cos q\alpha\left[\prod_{k=0}^{\infty}J_0(a_k\alpha)-\prod_{k=0}^{\infty}J_0(a_k(\alpha^2+\eta^2\Omega_k^2)^{1/2})\right]d\alpha\,d\eta. \tag{3.3}$$

A simpler derivation of (3.3) was given by Mazur and Montroll.[8] Now

$$J_0(a_k(\alpha^2+\eta^2\Omega_k^2)^{1/2})=1-\frac{1}{(1!)^2}a_k^2\left(\frac{\alpha^2+\eta^2\Omega_k^2}{4}\right)+\frac{1}{(2!)^2}a_k^4\left(\frac{\alpha^2+\eta^2\Omega_k^2}{4}\right)^2-\cdots. \tag{3.4}$$

We note that, for large $\bar{n}$ (see Appendix B),

$$\sum_k a_k^{2l}\Omega_k^{2m}\simeq\begin{cases}(2^{2m-l}\pi^{-l+1/2}/l^{1/2})(\bar{n})^{-l+1/2}(\bar{n}^{1/2}\lambda)^{2m} & \text{for the Poissonian distribution,} \quad (3.5)\\ [2^{m-1}\Gamma(m+1)/l^{m+1}](\bar{n})^{-2l+1}(\bar{n}^{1/2}\lambda)^{2m} & \text{for the thermal distribution.} \quad (3.6)\end{cases}$$

Let us take

$$\epsilon\equiv\bar{n}^{1/2}\lambda \tag{3.7}$$

to be our "order parameter," which, as can be recognized, is the Rabi frequency commonly used in the pure oscillation case. Then in (3.4), collecting terms of orders up to ϵ^2, i.e., summing all terms $a_k^{2l}\Omega_k^2$ for $l=1,2,\cdots$, gives

$$J_0(a_k(\alpha^2+\eta^2\Omega_k^2)^{1/2})=J_0(a_k\alpha)-\frac{1}{(1!)^2}\frac{a_k^2\Omega_k^2\eta^2}{4}+\frac{1}{(2!)^2}\frac{2a_k^4\Omega_k^2\alpha^2\eta^2}{4^2}-\frac{1}{(3!)^2}\frac{3a_k^6\Omega_k^2\alpha^4\eta^2}{4^3}+\cdots$$
$$=J_0(a_k\alpha)+\frac{a_k^2\Omega_k^2\eta^2}{2(a_k\alpha)}\frac{d}{d(a_k\alpha)}J_0(a_k\alpha). \tag{3.8}$$

Thus,

$$\prod_{k=0}^{\infty}J_0(a_k(\alpha^2+\eta^2\Omega_k^2)^{1/2})$$
$$=\prod_{k=0}^{\infty}J_0(a_k\alpha)+\sum_j\left(\frac{a_j\Omega_j^2\eta^2}{2\alpha}\frac{d}{d(a_j\alpha)}J_0(a_j\alpha)\right)\times\prod_{k\neq j}J_0(a_k\alpha)+\cdots$$
$$=\prod_{k=0}^{\infty}J_0(a_k\alpha)\left(1+\frac{\eta^2}{2\alpha}\sum_{j=0}^{\infty}a_j\Omega_j^2\frac{dJ_0(a_j\alpha)/d(a_j\alpha)}{J_0(a_j\alpha)}+\cdots\right)$$
$$\simeq\prod_{k=0}^{\infty}J_0(a_k\alpha)\left(1-\frac{\eta^2}{4}\sum_{j=0}^{\infty}a_j^2\Omega_j^2+\cdots\right)$$
$$\simeq e^{-\sigma^2\alpha^2/4}e^{-\omega^2\eta^2/4}, \tag{3.9}$$

where σ^2 is defined by (2.15) and ω^2 is defined by

$$\omega^2=\sum_{j=0}^{\infty}a_j^2\Omega_j^2. \tag{3.10}$$

Substituting (3.9) into (3.3) gives

$$L(q)\simeq\frac{1}{2\pi^2}\int_{-\infty}^{\infty}\cos q\alpha\,e^{-\sigma^2\alpha^2/4}d\alpha\times\int_{-\infty}^{\infty}\eta^{-2}(1-e^{-\omega^2\eta^2/4})\,d\eta$$
$$=\frac{\tilde{\Omega}}{\pi}\exp\left(-\frac{q^2}{\sigma^2}\right), \tag{3.11}$$

where

$$\tilde{\Omega}=\omega/\sigma, \tag{3.12}$$

ω and σ being defined by Eqs. (3.10) and (2.15), respectively. We have thus shown that the average frequency with which $x(t)$ of Eq. (1.2) achieves particular value q also, to a good approximation, has a Gaussian distribution.

We have found exact closed form expressions for ω^2, and they are given by (see Appendices A and B)

$$\omega^2=\begin{cases}e^{-2\bar{n}}\{4\bar{n}\lambda^2I_1(2\bar{n})+[2(m+1)\lambda^2+\Delta^2]\times I_0(2\bar{n})-\frac{1}{2}(1-m)4\lambda^2\} & \text{for Poissonian distribution,} \quad (3.13)\\ 4\lambda^2\left(\frac{\bar{n}}{2\bar{n}+1}\right)^2+[2(m+1)\lambda^2+\Delta^2]\times\left(\frac{1}{2\bar{n}+1}\right)-\frac{1}{2}(1-m)\frac{4\lambda^2}{(\bar{n}+1)^2} & \text{for thermal distribution.} \quad (3.14)\end{cases}$$

For large $\bar{n}$, these are approximately given by

$$\omega^2\simeq\begin{cases}2\bar{n}^{1/2}\lambda^2/\pi^{1/2} & \text{for the Poisson distribution,} \quad (3.15)\\ \lambda^2 & \text{for the thermal distribution.} \quad (3.16)\end{cases}$$

It follows from the definition of $L(q)$ that the quantity $\tilde{\Omega}$ in (3.11) is the average angular frequency of $x(t)$ crossing the $x(t)=0$ axis. From Eqs. (3.13), (3.14), (2.16), (2.17), and (3.12), $\tilde{\Omega}$ can be expressed in closed forms. In particular, for large $\bar{n}$, we find, using (3.15), (3.16), (2.18), and (2.19) that

$$\tilde{\Omega}\simeq\begin{cases}2\bar{n}^{1/2}\lambda & \text{for the Poissonian distribution,} \quad (3.17)\\ (2\bar{n})^{1/2}\lambda & \text{for the thermal distribution.} \quad (3.18)\end{cases}$$

It will be noted that these are of the form of the Rabi frequency.

To improve the approximation (3.11) for $\bar{n}$ not too large, say, in the region $1<\bar{n}<5$, we may collect and sum terms up to ϵ^4 in (3.4), and express $L(q)$ in the form

$$L(q)\simeq\frac{\tilde{\tilde{\Omega}}}{\pi}\exp\left[-\left(\frac{q}{\sigma}\right)^2-d_4\left(\frac{q}{\sigma}\right)^4-\cdots\right], \tag{3.19}$$

where the coefficient d_4 is determined by the terms of order ϵ^4 in (3.4). The behavior of $L(q)$ in the small $\bar{n}$ region will be discussed in Sec. V.

If $x(0)=1$, the inverse of $L(1-\delta)$, where δ is a small number, gives the average recurrence time for $x(t)$ to assume its original value to within an uncertainty δ. Our approximate expression (3.11) for $L(q)$, however, is only accurate

within the fluctuation range $-\sigma < q < \sigma$. It is not accurate when q is close to unity, and is certainly wrong for $q = 1$ since $L(1)$ should be equal to zero. The formula given by Slater,[7] which is valid for q very close to unity, unfortunately, also cannot be used for our case where the photon distribution a_k steadily decreases as k increases. Thus we have not been able to obtain a good simple expression for the Poincaré recurrence time for our problem, although one can give numerical estimates, for given values of $\bar{n}$, λ, and δ, by evaluating the double integral in Eq. (3.3) numerically.

IV. MEAN ANGULAR FREQUENCY

As is known from the pioneering work of Lagrange, Wintner, and Weyl, a central quantity in the study of quasi-periodic functions is the so-called "mean motion" or mean angular frequency. This quantity is somewhat different from the quantity $\tilde{\Omega}$, which we found in the preceding section, as we shall see.

Let $x(t)$ of Eq. (1.2) be the real part of a complex quantity $z(t)$ given by

$$z(t) = \sum_{k=0}^{\infty} a_k e^{i(\Omega_k t + \delta_k)}. \tag{4.1}$$

Let us write Eq. (4.1) as

$$z(t) = r(t) e^{i\varphi(t)}. \tag{4.2}$$

Then

$$z'(t) = [r'(t) + ir(t)\varphi'(t)] e^{i\varphi(t)}, \tag{4.3}$$

so that

$$\varphi'(t) = \mathrm{Re}(z'/iz). \tag{4.4}$$

The "mean motion" or the mean angular frequency Ω is defined by

$$\Omega = \lim_{T\to\infty} (1/T) \int_0^T \varphi'(t)\, dt = E\{\mathrm{Re}(z'/iz)\}, \tag{4.5}$$

where E denotes the expectation value. Since the set of frequencies Ω_k are linearly independent, we can apply the Kronecker–Weyl theorem[6,9] to obtain

$$\begin{aligned}\Omega &= \lim_{N\to\infty} E\{\Phi(\theta_1,\theta_2,\ldots,\theta_N)\} \\ &= \lim_{N\to\infty} \int_0^{2\pi}\cdots\int_0^{2\pi} \Phi(\theta_1,\theta_2,\ldots,\theta_N)\, d\theta_1 d\theta_2 \cdots d\theta_N,\end{aligned} \tag{4.6}$$

where

$$\Phi(\theta_1,\ldots,\theta_N) = \mathrm{Re}\left(\frac{\Sigma_k a_k \Omega_k e^{i\theta_k}}{\Sigma_k a_k e^{i\theta_k}}\right), \tag{4.7}$$

or

$$\Omega = \sum_k W_k \Omega_k \tag{4.8}$$

with

$$W_k = \frac{1}{(2\pi)^N} \int_0^{2\pi}\cdots\int_0^{2\pi} \times \left(\mathrm{Re}\,\frac{a_k e^{i\theta_k}}{\Sigma_j a_j e^{i\theta_j}}\right) d\theta_1 \cdots d\theta_N. \tag{4.9}$$

In Eq. (4.9), consider first the integration with respect to θ_n. Let

$$z(\theta_n) = a_n e^{i\theta_n} + b, \tag{4.10}$$

with

$$b = \sum{}' a_k e^{i\theta_k}, \tag{4.11}$$

where $'$ means the exclusion of the nth term. By considering a contour integration around a circle of radius a_n whose center is located at b, it is easy to see that W_n can be written as

$$\begin{aligned}W_n = \frac{1}{(2\pi)^N} &\int_0^{2\pi}\cdots\int_0^{2\pi} F \\ &\times d\theta_0 d\theta_1 \cdots d\theta_{n-1} d\theta_{n+1} \cdots d\theta_N,\end{aligned} \tag{4.12}$$

where

$$F = \begin{cases} 1 & \text{if } |b| = |\sum{}' a_k e^{i\theta_k}| < a_n, \\ 0 & \text{if } |b| > a_n. \end{cases} \tag{4.13}$$

This, however, is exactly the probability that a random walker walking in a two-dimensional space, in a sequence of N steps of lengths $a_0, a_1, a_2, \ldots, a_{n-1}, a_{n+1}, \ldots, a_N$, spans a distance less than a_n. This probability is given by (see Appendix C)

$$P(r;a_1,a_2,\ldots,a_N) = r\int_0^{\infty} J_1(r\rho) \prod_{k=1}^{N} J_0(a_k \rho)\, d\rho \tag{4.14}$$

for $a_n = r$ and steps of lengths $a_1, a_2, \ldots, a_N$. Thus we finally find, for $x(t)$ of Eq. (1.2), that the mean motion or the mean angular frequency Ω is given by

$$\Omega = \sum_{n=0}^{\infty} W_n \Omega_n \tag{4.15}$$

with

$$W_n = a_n \int_0^{\infty} J_1(a_n \rho) \prod_{j=0}^{\infty}{}' J_0(a_j \rho)\, d\rho, \tag{4.16}$$

where the prime means that the factor $J_0(a_n \rho)$ is excluded. The formulas (4.15) and (4.16) were first given by Wintner.[5]

The integral in Eq. (4.16) can be evaluated approximately in the large $\bar{n}$ case by making the Gaussian approximation for the product of Bessel functions of zeroth order as we have done previously. We find

$$\begin{aligned}W_n &\simeq a_n \int_0^{\infty} J_1(a_n \rho) \exp\left(-\frac{1}{4}\rho^2 \sum_{k=0}^{\infty}{}' a_k^2\right) d\rho \\ &\simeq \frac{1}{2} a_n \int_0^{\infty} \rho \exp\left[-\left(\frac{1}{4}\sum_{k=0}^{\infty} a_k^2 - \frac{1}{8}a_n^2\right)\rho^2\right] d\rho \\ &= \frac{a_n}{\Sigma_{k=0}^{\infty} a_k^2 - \frac{1}{2}a_n^2},\end{aligned} \tag{4.17}$$

and hence

$$\Omega = \sum_{n=0}^{\infty} \frac{a_n^2 \Omega_n}{\Sigma_{k=0}^{\infty} a_k^2 - \frac{1}{2}a_n^2}. \tag{4.18}$$

For large $\bar{n}$, we find (see Appendix B)

$$\Omega \simeq \begin{cases} 2\bar{n}^{1/2}\lambda & \text{for the Poissonian distribution,} \quad (4.19) \\ (\pi/2)^{1/2}\bar{n}^{1/2}\lambda & \text{for the thermal distribution.} \quad (4.20) \end{cases}$$

We note that these again have the form of the Rabi frequency.

Comparing this mean angular frequency Ω of rotation of $z(t)$ of Eq. (4.1) in the complex plane with the average angular frequency $\tilde{\Omega}$ of $x(t)$ of Eq. (1.2) crossing the $x(t)=0$ axis given by Eqs. (3.17) and (3.18), we notice that, for the large $\bar{n}$ case, while $\Omega=\tilde{\Omega}$ for the Poissonian distribution, Ω is not identical to $\tilde{\Omega}$ for the thermal distribution although they are proportional to each other. Indeed we found that the constant of proportionality is

$$\tilde{\Omega}/\Omega=(4/\pi)^{1/2}=1.128 \tag{4.21}$$

for the thermal photon distribution, compared to 1 for the Poissonian photon distribution.

An important conclusion which we draw from the result of this section is that even in the region where the behavior of $x(t)$ appears irregular, the Rabi frequency still characterizes the mean angular frequency of oscillations.

V. $P(x)$, $L(x)$, and Ω in the case of small $\bar{n}$

In the very small region $0<\bar{n}<1$, the functions $P(x)$ and $L(x)$ are far from being Gaussian. We shall give a brief qualitative discussion of what they look like and on how they gradually become Gaussian-like as $\bar{n}$ increases beyond 1. A fuller quantitative account of these studies will be presented elsewhere.

To be more specific, let us consider the Poissonian photon distribution with the atom initially in the upper level $(m=+1)$.

When $\bar{n}=0$, $x(t)$ of Eq. (1.2) is given simply by a single oscillation

$$x(t)=\cos\Omega_0 t$$

where

$$\Omega_0=(4\lambda^2+\Delta^2)^{1/2}, \tag{5.1}$$

since from Eq. (2.8) and (2.5), $a_0=1$ and $a_k=0$ for $k\geqslant 1$. It is clear from the definition of $L(q)$ that the distribution $L(q)$ must look like the curve shown in Fig. 1(a), namely,

$$L(q)=\begin{cases}\Omega_0/\pi & \text{for } |q|<1,\\ 0 & \text{for } |q|>1,\end{cases} \tag{5.2}$$

where the constant value of $L(q)$ for $|q|<1$ is obtained from $2(\Omega_0/2\pi)$, the factor of 2 coming from counting the crossings of $x(t)=q$ line from above as well as from below. This result can be confirmed by using Kac's formula (3.3) as follows: We have for this case $a_0=1$, and $a_k=0$ for $k\geqslant 1$, so

$$L(q)=\frac{1}{2\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\eta^{-2}\cos q\alpha\,[J_0(\alpha)-J_0((\alpha^2+\eta^2\Omega_0^2)^{1/2})]\,d\alpha\,d\eta. \tag{5.3}$$

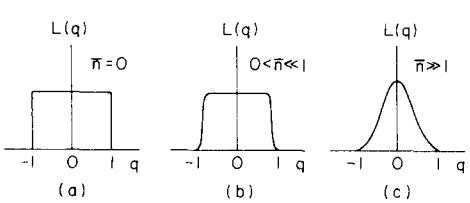

FIG. 1. $L(q)$ vs q for different values of $\bar{n}$.

Using the representations

$$J_0(\alpha)=\frac{1}{\pi}\int_0^{\pi}e^{i\alpha\cos\theta}\,d\theta, \tag{5.4}$$

$$J_0((\alpha^2+\beta^2)^{1/2})=\frac{1}{\pi}\int_0^{\pi}e^{i(\alpha\cos\theta+\beta\sin\theta)}\,d\theta, \tag{5.5}$$

we can write

$$\begin{aligned}L(q)&=\frac{1}{2\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\eta^{-2}\cos q\alpha\,\frac{1}{\pi}\int_0^{\pi}e^{i\alpha\cos\theta}\\&\quad\times(1-e^{i\Omega_0\eta\sin\theta})\,d\theta\,d\alpha\,d\eta\\&=\frac{1}{2\pi^2}\int_{-\infty}^{\infty}d\alpha\int_0^{\pi}d\theta\,\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{1-e^{i\Omega_0\eta\sin\theta}}{\eta^2}\\&\quad\times d\eta\,e^{i\alpha\cos\theta}\cos q\alpha\\&=\frac{1}{2\pi^2}\int_{-\infty}^{\infty}d\alpha\int_0^{\pi}e^{i\alpha\cos\theta}|\Omega_0\sin\theta|\,d\theta\cos q\alpha,\end{aligned} \tag{5.6}$$

where we have used the formula

$$|\mu|=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{1-\cos\eta\mu}{\eta^2}\,d\eta. \tag{5.7}$$

Since $\sin\theta$ remains positive when θ varies from 0 to π, we have,

$$\begin{aligned}L(q)&=\frac{1}{2\pi^2}\int_{-\infty}^{\infty}d\alpha\cos q\alpha\int_0^{\pi}e^{i\alpha\cos\theta}\Omega_0\sin\theta\,d\theta\\&=\frac{\Omega_0}{2\pi^2}\int_{-\infty}^{\infty}d\alpha\cos q\alpha\int_{-1}^{1}e^{i\alpha x}\,dx\\&=\frac{\Omega_0}{2\pi^2}\int_{-\infty}^{\infty}d\alpha\cos q\alpha\,\frac{2\sin\alpha}{\alpha}\\&=\begin{cases}\Omega_0/\pi & \text{if } |q|<1,\\ 0 & \text{if } |q|>1,\end{cases}\end{aligned} \tag{5.8}$$

in agreement with Eq. (5.2). We notice that the result (5.8) can be written as

$$L(q)=(\tilde{\Omega}/\pi)\exp(-|q/\sigma|^{\nu}) \tag{5.9}$$

with

$$\nu=\infty,\quad \tilde{\Omega}=\Omega_0,$$

where σ, which from Eq. (2.15) equals 1, still characterizes the "half-width" of the distribution shown in Fig. 1(a).

As $\bar{n}$ increases, slightly from the value zero, we expect $L(q)$ to "round off" slightly near $|q|=1$ to have a shape shown in Fig. 1(b). The form (5.9) may still characterize this distribution with σ given by (2.16) still characterizes the half-width and with ν assuming a large but finite positive value. As $\bar{n}$ increases beyond the value 5 say, the shape of the distribution quickly becomes Gaussian with $\nu=2$ and (5.9) coincides with (3.11) as shown in Fig. 1(c).

For $P(x)$, its shape in the region $0<\bar{n}<1$ is a little more complicated. For a single oscillation of frequency Ω_0 in the case $\bar{n}=0$, we have

$$\begin{aligned}P(x)&=\frac{1}{2\pi}\int_{-\infty}^{\infty}J_0(\alpha)e^{-i\alpha x}\,d\alpha\\&=\begin{cases}\dfrac{1}{\pi}\dfrac{1}{(1-x^2)^{1/2}} & \text{for } |x|<1,\\ 0 & \text{for } |x|>1,\end{cases}\end{aligned} \tag{5.10}$$

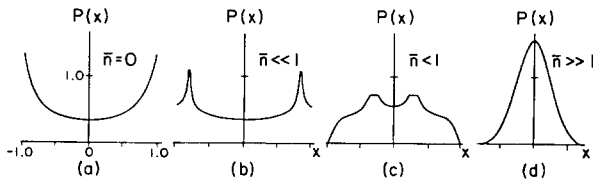

FIG. 2. $P(x)$ vs x for different values of $\bar{n}$.

namely, $P(x)$ become infinite at $|x| = 1$. This is shown in Fig. 2(a). As $\bar{n}$ increases slightly from zero, let us assume that the "effective number" of oscillators now becomes two, or

$$P(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} J_0(a_0\alpha)J_0(a_1\alpha)e^{-i\alpha x}\,d\alpha. \tag{5.11}$$

This integral can still be evaluated exactly,[11] and the result is

$$P(x) = \begin{cases} \dfrac{2}{\pi^2}\dfrac{1}{[(a_0+a_1)^2-x^2]^{1/2}}K\left(\left[\dfrac{4a_0a_1}{(a_0+a_1)^2-x^2}\right]^{1/2}\right) & \text{if } (a_0-a_1)^2 > x^2, \\ \dfrac{2}{\pi^2}\dfrac{1}{(4a_0a_1)^{1/2}}K\left(\left[\dfrac{(a_0+a_1)^2-x^2}{4a_0a_1}\right]^{1/2}\right) & \text{if } (a_0-a_1)^2 < x^2 < (a_0+a_1)^2, \end{cases} \tag{5.12}$$

where $K(k)$ is the complete elliptic integral of the first kind. This is shown in Fig. 2(b), where $P(x)$ has logarithmic infinities at $x = \pm(a_0 - a_1)$.

If $\bar{n}$ is increased further but still $\ll 1$ so that the "effective number" of oscillators now becomes three, i.e.,

$$P(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} J_0(a_0\alpha)J_0(a_1\alpha)J_0(a_2\alpha)e^{-i\alpha x}\,d\alpha, \tag{5.13}$$

then $P(x)$ can no longer be expressed in closed form. But expression such as (5.13) has been studied and numerically plotted in lattice dynamics,[11,12] and this is shown qualitatively in Fig. 2(c). It has a number of sharp corners (and hence not everywhere differentiable) but no longer has infinities, and it approaches zero continuously as $|x|$ approaches 1 from below.

As $\bar{n}$ increases further, we expect the distribution curve becoming smoother, and quickly becoming a Gaussian form as $\bar{n} > 5$, as shown in Fig. 2(d).

Finally, let us consider Ω in the case of small $\bar{n}$. If $\bar{n} = 0$, we have, of course, $\Omega = \Omega_0$. If $\bar{n}$ is increased slightly from 0 so that the effective number of oscillators becomes two or three with $a_0 \gg a_1$ and $a_0 \gg a_2$, we shall show that Ω is still precisely equal to Ω_0 with Ω_1 and Ω_2 contributing nothing to Ω. From Eq. (4.15) and (4.16), we have[13]

$$\Omega = W_0\Omega_0 + W_1\Omega_1 + W_2\Omega_2, \tag{5.14}$$

with

$$\begin{aligned} W_0 &= a_0\int_0^{\infty} J_1(a_0\rho)J_0(a_1\rho)J_0(a_2\rho)\,d\rho, \\ W_1 &= a_1\int_0^{\infty} J_0(a_0\rho)J_1(a_1\rho)J_0(a_2\rho)\,d\rho, \\ W_2 &= a_2\int_0^{\infty} J_0(a_0\rho)J_0(a_1\rho)J_1(a_2\rho)\,d\rho. \end{aligned} \tag{5.15}$$

A theorem of Bailey[14] gives

$$\begin{aligned} &\int_0^{\infty} J_\mu(ct\sin\varphi\cos\Phi)J_\nu(ct\cos\varphi\sin\Phi)J_\rho(ct)\,dt \\ &\quad = \Gamma\{\tfrac{1}{2}(1+\mu+\nu+\rho)\}\sin^\mu\varphi\cos^\mu\Phi\cos^\nu\varphi\sin^\nu\Phi \\ &\quad \times c^{\mu+\nu+1}\Gamma(\mu+1)\Gamma(\nu+1)\Gamma\{\tfrac{1}{2}(1-\mu-\nu+\rho)\} \\ &\quad \times F[\tfrac{1}{2}(1+\mu+\nu-\rho),\tfrac{1}{2}(1+\mu+\nu+\rho);\mu+1;\sin^2\varphi] \\ &\quad \times F[\tfrac{1}{2}(1+\mu+\nu-\rho),\tfrac{1}{2}(1+\mu+\nu+\rho);\nu+1;\sin^2\Phi], \end{aligned} \tag{5.16}$$

where φ and Φ are positive angles whose sum is acute and where $F(a,b;c;x)$ is the Gauss hypergeometric function. Applying (5.16) to (5.15), with $a_0 = c$, $a_1 = c\sin\varphi\cos\Phi$, and $a_2 = c\cos\varphi\sin\Phi$, we obtain

$$\begin{aligned} &W_0 = F(0,1;1;\sin^2\varphi)F(0,1;1;\sin^2\Phi) = 1, \\ &W_1 = W_2 = 0 \end{aligned}$$

because $\Gamma\{\tfrac{1}{2}(1-1-0+0)\} = \Gamma\{\tfrac{1}{2}(1-0-1+0)\}$

$$= \Gamma(0) = \infty. \tag{5.17}$$

We thus find

$$\Omega = \Omega_0. \tag{5.18}$$

This indicates that the expression for Ω, (4.19) and (4.20), which we obtained for large $\bar{n}$, may still hold approximately for small $\bar{n}$ if we replace $\bar{n}$ in (4.19) and (4.20) by $\bar{n} + \frac{1}{2}(1+m)$, where $m = -1$ or $+1$ specifies the initial state of the atom.

VI. SUMMARY

We have studied the behavior of an observable, the atomic inversion of a fermion–boson model (1.1) (the so-called Jaynes–Cummings model in quantum optics) in the region after a long time (compared to the initial collapse and revival times) had elapsed, namely in the region where the behavior of the observable appears irregular. We have considered its probability density $P(x)$, its average frequency $L(q)$ and its mean angular frequency (or mean motion) Ω. We have derived simple approximate expressions for these functions which are valid for almost all values of $\bar{n} > 1$. To a very good approximation, both $P(x)$ and $L(x)$ are found to be Gaussian with their half-widths characterized by σ defined by Eq. (2.15) and given as functions of $\bar{n}$ by Eqs. (2.16) and (2.17). We have also found that the mean angular frequency of oscillations is characterized by Ω given by (4.15) which for large $\bar{n}$ is found to be identical with the Rabi frequency of oscillation which has been commonly used previously only

in the pure oscillation region. Another quantity of interest which is contained in $L(x)$ is $\tilde{\Omega}$, the average angular frequency of crossing the $x(t)=0$ axis. A simple relationship is found to exist between $\tilde{\Omega}$ and Ω.

When times are scaled according to Ω and $\tilde{\Omega}$ and the x-coordinates are scaled by σ, the behavior of $x(t)$ of (1.2) would become remarkably regular in the sense that different plots of $x(t)$ for widely different values of $\bar{n}$ would appear remarkably similar. From this point of view, we have learned the major characteristics of the function $x(t)$.

Finally, we mention that the techniques we used in this paper can be applied to other models provided that the frequencies of oscillations are linearly independent. For example, if one considers the model considered by Buck and Sukumar[15] with a small but finite detuning[16] in which the Hamiltonian is given by

$$\hat{H}=\tfrac{1}{2}\hbar\omega_0\hat{\sigma}_z+\hbar\omega\hat{a}^\dagger\hat{a}+\hbar\lambda\,[\hat{\sigma}_+\hat{a}(\hat{a}^\dagger\hat{a})^{1/2}+\hat{\sigma}_-(\hat{a}^\dagger\hat{a})^{1/2}\hat{a}^\dagger], \tag{6.1}$$

then the condition of linear independence of frequencies is satisfied. We can find, for example, that the mean angular frequency of the atomic inversion for this model is

$$\Omega\simeq\begin{cases}2\bar{n}\lambda & \text{for the Poissonian photon distribution,} \quad (6.2)\\ \bar{n}\lambda & \text{for the thermal photon distribution.} \quad (6.3)\end{cases}$$

These can be compared with Eqs. (4.19) and (4.20), respectively, for the Jaynes–Cummings model.

Note added in proof: The plots of $P(x)$ obtained numerically from Eq. (2.4) vs x are presented in Fig. 3 for $\bar{n}=0.1$, 0.5, 1.0, 5.0 which may be compared with Fig. 2. I am grateful to Mr. David Kuebel for his assistance in producing Fig. 3.

ACKNOWLEDGMENTS

This research is partially supported by the U.S. Department of Energy.

I would like to thank Professor J. H. Eberly for first suggesting a statistical study of the Jaynes–Cummings model and for many useful discussions; Dr. J. J. Sanchez-Mondragon for giving me a copy of his Ph.D. thesis from which I learned much about the background of the problem; and Mr. H.-I. Yoo for telling me the form of the mixed Poissonian and thermal distribution given by Eq. (A1) in Appendix A and for showing me some numerical results which indicate the accuracies of some of the approximations made in this paper. I would also like to thank Professor Elliott Montroll, from whose lectures given some years ago I learned the beautiful work of A. Wintner, H. Weyl, and M. Kac, as well as his own work in the related subject.

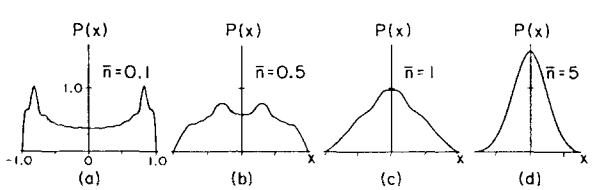

FIG. 3. Actual $P(x)$ vs x for different values of $\bar{n}$.

APPENDIX A: MIXED POISSONIAN AND THERMAL DISTRIBUTION

Instead of considering separately the Poissonian and the thermal photon distributions (2.5) and (2.6), we may consider the following mixed distribution, which contains (2.5) and (2.6) as special cases:

$$\begin{aligned}p_k&=(1-e^{-\beta})e^{-k\beta}e^{-\bar{n}_c(1-e^{-\beta})}L_k(-\bar{n}_c e^{\beta}(1-e^{-\beta})^2)\\&=\frac{1}{\bar{n}_T+1}\left(\frac{\bar{n}_T}{\bar{n}_T+1}\right)^k\exp\left(-\frac{\bar{n}_c}{\bar{n}_T+1}\right)\\&\quad\times L_k\left(-\frac{\bar{n}_c}{\bar{n}_T(\bar{n}_T+1)}\right),\end{aligned} \tag{A1}$$

where $\bar{n}_c$ and $\bar{n}_T$ are the mean photon numbers corresponding to the pure Poissonian and pure thermal distributions respectively, and where $L_n(x)$ is the nth Laguerre polynomial. The pure Poissonian distribution (2.5) and the pure thermal distribution (2.6) can be obtained from (A1) by letting $n_T=0$ and $n_c=0$, respectively.

It turns out that, for this mixed distribution (A1), both σ^2 and ω^2 defined by Eqs. (2.15) and (3.10), respectively, can still be expressed in closed forms. The principal formula used in obtaining these closed form expressions is the Mehler's formula[17]:

$$\begin{aligned}&\sum_{n=0}^{\infty}\frac{n!}{\Gamma(n+\alpha+1)}L_n^{\alpha}(x)L_n^{\alpha}(y)z^n\\&\quad=(1-z)^{-1}\exp\left(-z\frac{x+y}{1-z}\right)(xyz)^{-\alpha/2}\\&\qquad\times I_\alpha\left(\frac{2(xyz)^{1/2}}{1-z}\right),\quad |z|<1,\end{aligned} \tag{A2}$$

where $I_\nu(x)$ is the modified Bessel function. We find

$$\begin{aligned}\sigma^2&=\frac{1}{2\bar{n}_T+1}\exp\left(-\frac{2\bar{n}_c}{2\bar{n}_T+1}\right)I_0\left(\frac{2\bar{n}_c}{2\bar{n}_T+1}\right)\\&\quad-\frac{1}{2}(1-m)\frac{1}{(\bar{n}_T+1)^2}\exp\left(-\frac{2\bar{n}_c}{\bar{n}_T+1}\right),\end{aligned} \tag{A3}$$

$$\begin{aligned}\omega^2&=4\lambda^2\left(\frac{\bar{n}_T+1}{2\bar{n}_T+1}\right)^3\exp\left(-\frac{2\bar{n}_c}{2\bar{n}_T+1}\right)\\&\quad\times\left\{\left[\frac{\bar{n}_T^2(2\bar{n}_T+1)}{(\bar{n}_T+1)^3}+\frac{2\bar{n}_c\bar{n}_T}{(\bar{n}_T+1)^2}\right]I_0\left(\frac{2\bar{n}_c}{2\bar{n}_T+1}\right)\right.\\&\quad\left.+\frac{2\bar{n}_T^2+2\bar{n}_T+1}{(\bar{n}_T+1)^2}\bar{n}_c I_1\left(\frac{2\bar{n}_c}{2\bar{n}_T+1}\right)\right\}\\&\quad+[2(m+1)\lambda^2+\Delta^2]\frac{1}{2\bar{n}_T+1}\\&\quad\times\exp\left(-\frac{2\bar{n}_c}{2\bar{n}_T+1}\right)I_0\left(\frac{2\bar{n}_c}{2\bar{n}_T+1}\right)\\&\quad-\frac{1}{2}(1-m)[2(m+1)\lambda^2+\Delta^2]\frac{1}{(\bar{n}_T+1)^2}\\&\quad\times\exp\left(-\frac{2\bar{n}_c}{\bar{n}_T+1}\right).\end{aligned} \tag{A4}$$

Let

$$v \equiv \tanh\tfrac{1}{2}\beta = \frac{1}{2\bar{n}_T + 1}. \tag{A5}$$

For $\bar{n}_c \gg \bar{n}_T$, we find, from (A3) and (A4),

$$\sigma^2 \simeq (v/4\pi\bar{n}_c)^{1/2}, \tag{A6}$$

$$\omega^2 \simeq (4\pi\bar{n}_c v)^{-1/2}\{2\bar{n}_c v(1+v^2)\lambda^2 + [(1-v)^2 + 2\bar{n}_c v(1-v^2)]\lambda^2 + [2(m+1)\lambda^2 + \Delta^2]v\}. \tag{A7}$$

For $\bar{n}_c \ll \bar{n}_T$, on the other hand, we find

$$\sigma^2 \simeq v, \tag{A8}$$

$$\omega^2 \simeq \lambda^2 + [2(m+1)\lambda^2 + \Delta^2]v. \tag{A9}$$

APPENDIX B: THE SUM $\sum_{k=0}^{\infty} a_k^{2\mu}\Omega_k^{2\nu}$ IN THE CASE OF LARGE $\bar{n}$ ($\mu \geqslant 1$, $\nu \geqslant 0$)

The Poissonian distribution is known to become Gaussian in the case of large $\bar{n}$:

$$p_k = \frac{(\bar{n})^k}{k!}e^{-\bar{n}} \simeq \frac{1}{(2\pi\bar{n})^{1/2}}\exp\left[-\frac{(k-\bar{n})^2}{2\bar{n}}\right].$$

Thus for $\Delta \simeq 0$, $\bar{n}$ large, $\mu \geqslant 1$, $\nu \geqslant 0$, we find

$$\begin{aligned}\sum_{k=0}^{\infty} a_k^{2\mu}\Omega_k^{2\nu} &= (2\lambda)^{2\nu}\sum_{k=0}^{\infty} a_k^{2\mu}k^{\nu} \\ &\simeq (2\lambda)^{2\nu}(2\pi\bar{n})^{-\mu}\int_{-\infty}^{\infty} dx\, x^{\nu} \\ &\times \exp\left[-\frac{\mu}{\bar{n}}(x-\bar{n})^2\right] \\ &= 2^{2\nu-\mu}\pi^{-\mu+1/2}(\bar{n})^{-\mu+1/2}\mu^{-1/2}(\bar{n}^{1/2}\lambda)^{2\nu} \\ &\times\left[1 + \sum_{j=1}^{\infty}\frac{\nu(\nu-1)\cdots(\nu-j+1)}{j!}\Gamma\left(\frac{j+1}{2}\right)(\bar{n})^{-j/2}\right].\end{aligned} \tag{B1}$$

For the case of the thermal distribution, we find

$$\begin{aligned}\sum_{k=0}^{\infty} a_k^{2\mu}\Omega_k^{2\nu} &\simeq (2\lambda)^{2\nu}(1-e^{-\beta})^{2\mu}\int_0^{\infty} e^{-2\nu\beta x}x^{\nu}\,dx \\ &= (2\lambda)^{2\nu}(1-e^{-\beta})^{2\mu}\frac{\Gamma(\nu+1)}{(2\mu\beta)^{\nu+1}} \\ &= 2^{\nu-1}\Gamma(\nu+1)(\bar{n})^{-2\mu+1}\mu^{-\nu-1}(\bar{n}^{1/2}\lambda)^{2\nu},\end{aligned} \tag{B2}$$

where $\bar{n} = e^{-\beta}(1-e^{-\beta})^{-1}$ and where large $\bar{n}$ corresponds to high temperature since $\bar{n} \simeq \beta^{-1}$ in that case.

For μ, ν equal to integers in the case of the thermal distribution, the sum $\Sigma a_k^{2\mu}\Omega_k^{2\nu}$ can be exactly expressed in closed form which can be verified to agree with (B2) for large $\bar{n}$.

For the Poissonian distribution, only $\sigma^2 = \Sigma a_k^2$ and $\omega^2 = \Sigma a_k^2\Omega_k^2$ can be exactly expressed in closed forms in terms of the modified Bessel functions $I_0(2\bar{n})$ and $I_1(2\bar{n})$, by noting the relations

$$I_{\nu}(z) = \left(\frac{1}{2}z\right)^{\nu}\sum_{k=0}^{\infty}\frac{(\frac{1}{4}z^2)^k}{k!\,\Gamma(\nu+k+1)} \tag{B3}$$

and

$$I_0'(z) = I_1(z). \tag{B4}$$

By using the asymptotic formula

$$I_{\nu}(z) \sim \frac{e^z}{(2\pi z)^{1/2}}\left(1 - \frac{4\nu^2-1}{8z} + \cdots\right) \quad \text{as } z \to \infty, \tag{B5}$$

it can be verified that (2.16) becomes (2.18) and (3.13) becomes (3.15), in agreement with the results from putting $\mu = 1$, $\nu = 0$ and $\mu = 1$, $\nu = 1$, respectively in (B1).

APPENDIX C

In Eq. (4.14), we wrote down a result for the probability that a random walker in a two-dimensional continuum space, in a sequence of n steps of lengths $a_1, a_2, \ldots, a_n$, spans a distance less than r from the origin. This result was given by Kluyver.[18] For the three-dimensional random walk, the corresponding result was given by Chandrasekhar.[19] The more general result for a random walk on a d-dimensional continuum space ($d = 2,3,4,\ldots$) does not seem to have been given. We give, in this appendix, this general result and its derivation.

Let us use the hyperspherical coordinates of d dimensions[20] for the position vector

$$\mathbf{r} = (x_1, x_2, \ldots, x_d), \tag{C1}$$

where

$$\begin{aligned} x_1 &= r\cos\theta_1, \\ x_2 &= r\sin\theta_1\cos\theta_2, \\ &\cdots \\ x_{d-1} &= r\sin\theta_1\sin\theta_2\cdots\sin\theta_{d-2}\cos\varphi, \\ x_d &= r\sin\theta_1\sin\theta_2\cdots\sin\theta_{d-2}\sin\varphi, \end{aligned} \tag{C2}$$

where $r = |\mathbf{r}|$, $0 \leqslant \theta_j \leqslant \pi$, and $0 \leqslant \varphi \leqslant 2\pi$. The surface element of the hypersphere is known to be

$$dS = (\sin\theta_1)^{d-2}(\sin\theta_2)^{d-3}\cdots(\sin\theta_{d-2})\,d\theta_1\cdots d\theta_{d-2}\,d\varphi \tag{C3}$$

and the total surface area is

$$S = 2\pi^{d/2}/\Gamma(d/2). \tag{C4}$$

Let

$$\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \cdots, \alpha_d). \tag{C5}$$

The joint characteristic function of the joint $x_1, x_2, \ldots, x_d$ probability density is

$$f(\boldsymbol{\alpha}) = E\{\exp(i\boldsymbol{\alpha}\cdot\mathbf{r})\}. \tag{C6}$$

Without loss of generality, we may choose

$$\boldsymbol{\alpha} = (\alpha, 0, 0, \ldots, 0). \tag{C7}$$

Then

$$\begin{aligned} f(\boldsymbol{\alpha}) = \prod_{j=1}^{n}\frac{1}{S}\int_0^{\pi}\cdots\int_0^{\pi}\int_0^{2\pi} e^{ia_j\alpha\cos\theta_1} \\ \times(\sin\theta_1)^{d-2}(\sin\theta_2)^{d-3}\cdots(\sin\theta_{d-2}) \\ \times d\theta_1 d\theta_2\cdots d\theta_{d-2}\,d\varphi. \end{aligned} \tag{C8}$$

But

$$\int_0^{\pi}\cdots\int_0^{\pi}\int_0^{2\pi}(\sin\theta_2)^{d-3}(\sin\theta_3)^{d-4}\cdots(\sin\theta_{d-2})\times d\theta_2 d\theta_3\cdots d\theta_{d-2}d\varphi = \frac{S}{\int_0^{\pi}(\sin\theta_1)^{d-2}d\theta_1} = S\frac{\Gamma(d-1)}{2^{d-2}\left[\Gamma\left(\frac{d-1}{2}\right)\right]^2} \quad \text{(C9)}$$

and

$$\int_0^{\pi}e^{ia_j\alpha\cos\theta}(\sin\theta)^{d-2}d\theta = \int_{-1}^{1}e^{ia_j\alpha x}(1-x^2)^{(d-3)/2}dx = \pi^{1/2}\left(\frac{2}{a_j\alpha}\right)^{(d-2)/2}\Gamma\left(\frac{d-1}{2}\right)J_{(d-2)/2}(a_j\alpha); \quad \text{(C10)}$$

hence,

$$f(\alpha) = \left[\frac{\pi^{1/2}\Gamma(d-1)}{2^{(d-2)/2}\Gamma((d-1)/2)}\right]^n\prod_{j=1}^{n}\frac{J_{(d-2)/2}(a_j\alpha)}{(a_j\alpha)^{(d-2)/2}}. \quad \text{(C11)}$$

Thus the joint probability density function $p_n(\mathbf{r})$ is

$$p_n(\mathbf{r}) = \frac{1}{(2\pi)^d}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}f(\alpha)e^{-i\alpha\cdot\mathbf{r}}d\alpha_1\cdots d\alpha_d. \quad \text{(C12)}$$

Now

$$d\alpha_1\cdots d\alpha_d = \alpha^{d-1}(\sin\theta_1)^{d-2}(\sin\theta_2)^{d-3}\cdots(\sin\theta_{d-2})\times d\alpha\, d\theta_1\cdots d\theta_{d-2}d\varphi, \quad \text{(C13)}$$

and we choose $\mathbf{r} = (r, 0, 0, \ldots, 0)$ so that

$$\alpha\cdot\mathbf{r} = \alpha r\cos\theta_1; \quad \text{(C14)}$$

then, using (C9) and the following result,

$$\int_0^{\pi}e^{-i\alpha r\cos\theta}(\sin\theta)^{d-2}d\theta = \pi^{1/2}\left(\frac{2}{\alpha r}\right)^{(d-2)/2}\Gamma\left(\frac{d-1}{2}\right)J_{(d-2)/2}(\alpha r), \quad \text{(C15)}$$

we get, from (C12),

$$p_n(\mathbf{r}) = \frac{\Gamma(d-1)}{\pi^{(d-1)/2}2^{(3d-4)/2}\Gamma(d/2)\Gamma((d-1)/2)}\left(\frac{1}{r}\right)^{(d-2)/2}\times\int_0^{\infty}d\alpha\,\alpha^{d/2}J_{(d-2)/2}(\alpha r)f(\alpha), \quad \text{(C16)}$$

where $f(\alpha)$ is given by (C11).

The distribution function $P(r)$ which is the probability that $|r|$ after n steps is less than r has the property

$$dP(r) = \frac{2\pi^{d/2}}{\Gamma(d/2)}r^{d-1}p_n(r)dr. \quad \text{(C17)}$$

Thus, using (C16), we find

$$P(r) = \frac{\pi^{1/2}\Gamma(d-1)}{2^{(3d-6)/2}\Gamma((d-1)/2)[\Gamma(d/2)]^2}\times\left(\frac{\pi^{1/2}\Gamma(d-1)}{2^{(d-2)/2}\Gamma((d-1)/2)}\right)^n\int_0^{\infty}d\alpha\int_0^{r}d\rho\,\rho^{d/2}\times J_{(d-2)/2}(\alpha\rho)\alpha^{d/2}\prod_{j=1}^{n}\frac{J_{(d-2)/2}(a_j\alpha)}{(a_j\alpha)^{(d-2)/2}}$$
$$= \frac{1}{2^{d-2}[\Gamma(d/2)]^2}\left(\frac{\pi^{1/2}\Gamma(d-1)}{2^{(d-2)/2}\Gamma((d-1)/2)}\right)^{n+1}\times r^{d/2}\int_0^{\infty}d\alpha\,\alpha^{(d-2)/2}J_{d/2}(r\alpha)\prod_{j=1}^{n}\frac{J_{(d-2)/2}(a_j\alpha)}{(a_j\alpha)^{(d-2)/2}}, \quad \text{(C18)}$$

where we have made use of the relation

$$\int_0^{r}d\rho\,\rho^{d/2}J_{d/2-1}(\alpha\rho) = (1/\alpha)r^{d/2}J_{d/2}(\alpha r),$$

which follows from the more general relation

$$\left(\frac{1}{z}\frac{d}{dz}\right)^k[z^{\nu}J_{\nu}(z)] = z^{\nu-k}J_{\nu-k}(z).$$

Equations (C16) and (C18) are the results which we set out to derive. It can be verified that, for $d = 2$,

$$p_n(\mathbf{r}) = \frac{1}{2\pi}\int_0^{\infty}d\alpha\,\alpha J_0(r\alpha)\prod_{j=1}^{n}J_0(a_j\alpha) \quad \text{(C19)}$$

and

$$P(r) = r\int_0^{\infty}d\alpha J_1(r\alpha)\prod_{j=1}^{n}J_0(a_j\alpha). \quad \text{(C20)}$$

Equation (C20) is the result quoted in Eq.(4.14) which was first given by Kluyver.[18]

For $d = 3$, we have, from (C16),

$$p_n(\mathbf{r}) = \frac{1}{2\pi^2}\frac{1}{r}\int_0^{\infty}d\alpha\,\alpha\sin(r\alpha)\prod_{j=1}^{n}\frac{\sin(a_j\alpha)}{a_j\alpha}, \quad \text{(C21)}$$

where we have made use of the relation

$$J_{1/2}(x) = (2/\pi x)^{1/2}\sin x. \quad \text{(C22)}$$

Equation (C21) is the result given by Chandrasekhar.[19]

[1]See, e.g., L. Allen and J. H. Eberly, *Optical Resonance and Two-Level Atoms* (Wiley, New York, 1975), Sec. 7.
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Fermion clustering in a soluble one-dimensional many-body system

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(Received 26 May 1981; accepted for publication 30 July 1982)

A one-dimensional gas of N fermions with ν intrinsic degrees of freedom, such that N/ν is integer, with the particles interacting via attractive delta pair potentials is considered in its ground state. In particular, the "clustering" into N/ν entities is shown to appear and studied comparatively from both the Schrödinger and Hartree–Fock approximation viewpoints in terms of the energy and wavefunction overlap. The Schrödinger ground state energy for all nonzero densities is calculated numerically and compared to the nonzero density Hartree–Fock results for $\nu = 2$.

PACS numbers: 05.30.Fk, 03.65. – w

1. INTRODUCTION

Among the very few exactly soluble[1] ("continuous" vs "spin" or "lattice") many-body problems is the one-dimensional gas of particles interacting via an attractive delta pair potential.[2] The exact ground state properties of this system were first deduced by McGuire[2] for no specific permutation symmetry of the particles, and subsequently for fermion statistics by Yang[3] and independently Gaudin,[4] and finally for boson statistic by Calogero and Degasperis.[5]

The Hamiltonian is

$$H = T + V = -\frac{\hbar^2}{m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} - 2v_0\sum_{i<j}^{N}\delta(x_i - x_j), \quad v_0 > 0, \tag{1}$$

and, using the Bethe *ansatz*,[6] McGuire[2] finds that the only bound-state eigenfunction of (1) for "open" (i.e., no "walls" of any kind to contain the N particles) boundary conditions is the symmetric expression

$$\Psi \propto \exp\left\{-\frac{mv_0}{2\hbar^2}\sum_{i<j}^{N}|x_i - x_j|\right\}, \tag{2}$$

with energy eigenvalue

$$E_0(N) = -\frac{mv_0^2}{12\hbar^2}N(N^2 - 1). \tag{3}$$

The Hartree–Fock approximation to (2) has been studied and compared with the exact or Schrödinger solution for both bosons[5,7] and spin one-half fermions.[8] Now we consider in this paper the general case of N fermions with ν intrinsic degree of freedom such that $2 \leqslant \nu \leqslant N$ while N/ν is integer, showing the formation of N/ν clusters. This is accomplished in Sec. 2 by obtaining and comparing the energy of the system for the exact Schrödinger solution and the Hartree–Fock solution. The latter can be improved by making the center-of-mass corrections as is illustrated in Sec. 3. The comparison of the exact and approximate solutions is also made in terms of the overlap of the respective wave functions, Sec. 4. In Sec. 5 we construct rigorous *lower* bounds for both the Schrödinger and Hartree–Fock energies per particle for any density. In Sec. 6, we present *upper* bounds for the energy per particle with several nonunique solutions of the Hartree–Fock equations. Finally, we state our conclusions in Sec. 7.

2. ONE-DIMENSIONAL FERMI GAS CLUSTERS

We shall here consider the case of N fermions with ν intrinsic degrees of freedom such that $2 \leqslant \nu \leqslant N$ while N/ν is integer. If $\nu = 2$ we have the above mentioned spin-one-half case (e.g., the electron gas or neutron matter). For $\nu = 4$ one might think of nuclear matter of spin-up and spin-down neutrons and protons.

If the intrinsic wave function is denoted by $\chi(\sigma_1, \sigma_2, \ldots, \sigma_\nu)$ and is antisymmetric under permutations, the ground state of (1) will consist of an *ideal* gas of ν-component entities which are "solitons"[9] in that two such colliding clusters will at most be phase-shifted.[2] For $\nu = 2$ the clusters will be like "Cooper pairs", for $\nu = 4$ α-particles, and for ν larger one might even think of the so called "$1/N$ expansion" models[10] of high energy physics, where, as in the present model, one has strong interparticle coupling for large interparticle separations. The total wave function will be given by the totally antisymmetric expression

$$F(1,2,\ldots,\nu)F(\nu+1,\nu+2,\ldots,2\nu)\cdots F(N+1-\nu,\ldots,N-1,N) \pm \text{all permutations of indices belonging to } \textit{different } F\text{'s}, \tag{4}$$

$$F(1,2,\ldots,\nu) \equiv \prod_{i<j}^{\nu} e^{-\frac{mv_0}{2\hbar^2}|x_i - x_j|}\chi(\sigma_1,\sigma_2,\ldots,\sigma_\nu),$$

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 0022-2488/82/122439-06$02.50

while the total energy of the N particle, N/ν cluster system, will be given by (3) through the equation

$$E_0(N) = (N/\nu)E_0(\nu). \tag{5}$$

Following Ref. 8 one can see that for N/ν integer, N even, the Hartree–Fock energy of our ν-component fermion system is also of the form (5), namely

$$E_0^{\rm HF}(N) = (N/\nu)E_0^{\rm HF}(\nu), \tag{6}$$

since there exists a set of N orthonormal, single-particle functions $\psi \equiv \{\psi_i(x;\sigma_1,\sigma_2,...,\sigma_\nu) | i = 1,2,...N\}$ such that, in unrestricted HF,

$$\psi_i(x;\sigma_1,\sigma_2,...,\sigma_\nu) = \sum_{\alpha=1}^{\nu} \psi_i^{(\alpha)}(x)\chi(\sigma_\alpha), \tag{7}$$

and which minimizes the expectation value

$$\mathscr{E}(\psi) \equiv \langle D_\psi | H | D_\psi \rangle, \tag{8}$$

between the single Slater determinant

$$D_\psi \equiv (N!)^{-1/2} \det [\psi_i(x_j;\sigma_1^j,\sigma_2^j,...,\sigma_\nu^j)], \quad i,j = 1,2,...,N, \tag{9}$$

such that

$$E_0^{\rm HF}(N) \equiv \inf_\psi \mathscr{E}(\psi) \geqslant E_0(N). \tag{10}$$

The last inequality is just a result of the Rayleigh–Ritz variational principle. Furthermore, the expectation value (8) can be written as

$$\mathscr{E}(\psi) \equiv \sum_{\alpha=1}^{\nu} T_\psi^{(\alpha)} + U_\psi + K_\psi, \tag{11}$$

$$T_\psi^{(\alpha)} \equiv \frac{\hbar^2}{m} \sum_{j=1}^{N} \int dx \left| \frac{d}{dx} \psi_j^{(\alpha)}(x) \right|^2, \tag{12}$$

$$U_\psi \equiv -2v_0 \int dx \sum_{\alpha<\beta}^{\nu} \rho_\psi^{(\alpha)}(x)\rho_\psi^{(\beta)}(x), \tag{13}$$

$$\rho_\psi^{(\alpha)}(x) \equiv \sum_{j=1}^{N} |\psi_j^{(\alpha)}(x)|^2, \tag{14}$$

$$K_\psi \equiv 2v_0 \int dx \sum_{\alpha<\beta}^{\nu} \left| \sum_{j=1}^{N} \psi_j^{(\alpha)}(x)\psi_j^{(\beta)}(x) \right|^2. \tag{15}$$

Again, since N/ν is integer and N is even, it follows from Ref. 8 that *unrestricted* HF, given by (7), gives the same HF energy as *restricted* HF defined through the single-particle orbitals

$$\begin{aligned} \psi_i(x;\sigma_1,\sigma_2,...,\sigma_\nu) &= f_i(x)\chi(\sigma_1) \quad \text{for } 1 \leqslant i \leqslant n_1, \\ &= f_i(x)\chi(\sigma_2) \quad \text{for } n_1 < i \leqslant n_2, \\ &\cdots \qquad\qquad \cdots \\ &= f_i(x)\chi(\sigma_\nu) \quad \text{for } n_{\nu-1} < i \leqslant N \end{aligned} \tag{16}$$

with n_α integers, and such that

$$\langle f_i | f_j \rangle = \delta_{ij}, \tag{17}$$

if $1 \leqslant i,j \leqslant n_1$ or $n_1 < i,j \leqslant n_2$ or ... or $n_{\nu-1} < i,j \leqslant N$.

Eq. (14) then becomes ($n_0 \equiv 0$)

$$\rho_\psi^{(\alpha)}(x) = \sum_{j=n_{\alpha-1}+1}^{n_\alpha} |f_j(x)|^2. \tag{18}$$

By choosing

$$f_j(x) = f_{j+n_\alpha}(x) \text{ for } n_{\alpha-1} + 1 \leqslant j < n_\alpha, \tag{19}$$

with $n_\alpha = \alpha N/\nu$, so that $n_1 = N/\nu, n_2 = 2N/\nu,..., n_\nu = N$, then (18) becomes

$$\rho_\psi^{(\alpha)}(x) = \sum_{j=1}^{N/\nu} |f_j(x)|^2 \equiv \rho_\psi(x), \tag{20}$$

i.e., independent of $\alpha = 1, 2,...,\nu$. Consequently, from (11) to (15) one has

$$K_\psi \equiv 0, \tag{21}$$

$$\begin{aligned} U_\psi &= -2v_0 \tfrac{1}{2}\nu(\nu-1) \int dx\, \rho_\psi^2(x) \\ &= -v_0\nu(\nu-1) \int dx\, f^4(x), \end{aligned} \tag{22}$$

$$\mathscr{E}(\psi) = \nu \frac{\hbar^2}{m} \int dx |f'(x)|^2 - v_0\nu(\nu-1) \int dx\, f^4(x). \tag{23}$$

If e is a Lagrange multiplier then the functional variation

$$\frac{\delta}{\delta f} \left\{ \mathscr{E}(\psi) - e\nu \int dx\, f^2(x) \right\} = 0, \tag{24}$$

immediately gives the HF equation

$$-\frac{\hbar^2}{m} f''(x) - 2v_0(\nu-1)f^3(x) = ef(x) \tag{25}$$

with unique[11] solution

$$f(x) = \left[\frac{mv_0(\nu-1)}{4\hbar^2} \right]^{1/2} \operatorname{sech} \frac{mv_0(\nu-1)}{2\hbar^2} x, \tag{26}$$

$$e = -\frac{mv_0^2(\nu-1)^2}{4\hbar^2}, \quad \int dx\, f^2(x) = 1. \tag{27}$$

Finally since

$$E_0^{\rm HF}(\nu) = \nu e + v_0\nu(\nu-1) \int dx\, f^4(x) \tag{28}$$

$$= -\frac{mv_0^2\nu(\nu-1)^2}{12\hbar^2} \tag{29}$$

we have for the ratio of HF to Schrödinger ground state energies, using (5) and (6),

$$\frac{E_0^{\rm HF}}{E_0(N)} = \frac{E_0^{\rm HF}(\nu)}{E_0(\nu)} = \frac{\nu-1}{\nu+1}, \tag{30}$$

which approaches unity as ν increase. For $\nu = 2$ this is only 1/3, but for $\nu = 4$ the ratio improves to 3/4, etc. Moreover, for $\nu \to N$ one recovers the N-boson case[5] for which the HF energy becomes the Schrödinger energy in the thermodynamic limit $N \gg 1$.

Note that our problem here really reduces to that of N/ν independent systems and that we actually have a Hartree calculation.

3. CENTER-OF-MASS CORRECTIONS

In this section we show how the HF-to-Schrödinger energy ratio improves as one corrects for the spurious center-of-mass effect found in standard HF theory. Instead of Eqs. (8) to (10), or the equivalent ones for a ν-particle system, consider the expectation value

$$\mathscr{E}(\phi) \equiv \langle \phi | H - T_{\rm cm}(\nu) | \phi \rangle, \tag{31}$$

where the center-of-mass kinetic energy is

$$T_{\rm cm}(\nu)\equiv\frac{\hbar^2}{\nu m}\left(\sum_{\alpha=1}^{\nu}\frac{d}{dx_\alpha}\right)^2, \tag{32}$$

and ϕ is the ν-particle determinant

$$\phi\equiv(\nu!)^{-1/2}\det\,[\tilde f_\alpha(x_\beta)];\ \alpha,\beta=1,2,...,\nu. \tag{33}$$

Then the new (projection *before* variation) HF energy will be

$$\tilde E_0^{\rm HF}(\nu)=\inf_\phi \mathscr{E}(\phi)\geqslant E_0(\nu), \tag{34}$$

where the variation gives the new HF equation

$$-\left(\frac{\nu-1}{\nu}\right)\frac{\hbar^2}{m}\tilde f''(x)-2v_0(\nu-1)\tilde f^3(x)=\tilde e\tilde f(x), \tag{35}$$

which, in analogy to Eq. (25), has the unique solution

$$\tilde f(x)=\left(\frac{\nu v_0 m}{4\hbar^2}\right)^{1/2}\operatorname{sech}\,\frac{\nu v_0 m}{2\hbar^2}x, \tag{36}$$

$$\tilde e=-\nu(\nu-1)\frac{v_0^2 m}{4\hbar^2},\quad \int\tilde f(x)dx=1. \tag{37}$$

Therefore, the new HF energy is

$$\begin{aligned}\tilde E_0^{\rm HF}(\nu)&=\nu\tilde e+v_0\nu(\nu-1)\int dx\tilde f^4(x)\\&=-\frac{\nu^2(\nu-1)v_0^2 m}{12\hbar^2}\end{aligned} \tag{38}$$

so that the HF-to-Schrödinger energy ratio is

$$\frac{\tilde E_0^{\rm HF}(\nu)}{E_0(\nu)}=\frac{\nu}{\nu+1}, \tag{39}$$

a clear improvement over Eq. (30).

A less satisfactory center-of-mass subtraction procedure than the above (which is necessarily very common in may nuclear calculations) can be called "projection *after* variation" and consists in first calculating the expectation value

$$\begin{aligned}t_{\rm cm}(\nu)&\equiv\langle D_\psi|T_{\rm cm}(\nu)|D_\psi\rangle\\&=\frac{mv_0^2(\nu-1)^2}{12\hbar^2},\end{aligned} \tag{40}$$

where D_ψ now stands for a ν-particle determinant with orbitals Eq. (26). Finally, the aforementioned ratio is computed as

$$\frac{E_0^{\rm HF}(\nu)-t_{\rm cm}(\nu)}{E_0(\nu)}=\frac{\nu-1}{\nu} \tag{41}$$

which is better than Eq. (30) but worse than Eq. (39).

4. WAVE FUNCTION OVERLAPS

Besides the HF-to-Schrödinger energy ratio as a criterion of goodness, it is also instructive to consider the overlap between the corresponding wave functions. Suppressing the intrinsic wave function, which is always given as in Eq. (4), the ν-particle Schrödinger and HF ground-state wave functions are, respectively.

$$\begin{aligned}\Psi_\nu&=\left[(\nu-1)!\left(\frac{v_0 m}{\hbar^2}\right)^{\nu-1}\right]^{1/2}\prod_{\alpha<\beta}^{\nu}e^{-\frac{mv_0}{2\hbar^2}|x_\alpha-x_\beta|};\\ \tilde\Phi&=\sqrt{\nu}\prod_{\alpha=1}^{\nu}\tilde f(x_\alpha)\end{aligned} \tag{42}$$

with $\tilde f(x)$ defined as in Eq. (45). Defining the scalar product

$$\begin{aligned}\langle F|G\rangle\equiv\int dx_1\cdots\int dx_\nu\delta\left(\frac{x_1+x_2+\cdots+x_\nu}{\nu}\right)\\ \times F(x_1,...,x_\nu)G(x_1,...,x_\nu),\end{aligned} \tag{43}$$

then the required overlap will be

$$\mathscr{O}_\nu\equiv\langle\Psi_\nu|\tilde\Phi_\nu\rangle^2/\langle\tilde\Phi_\nu|\tilde\Phi_\nu\rangle\langle\Psi_\nu|\Psi_\nu\rangle. \tag{44}$$

Although the calculation of (44) for $\nu>2$ is very difficult we have been able to do numerically the case for $\nu=3$, but defer all details to the Appendix and here only quote the results:

$$\begin{aligned}\mathscr{O}_2&=0.9774\ (\text{and } 0.8953\ \textit{with}\ \text{center-of-mass})\\ \mathscr{O}_3&=0.9726.\end{aligned} \tag{45}$$

5. LOWER BOUNDS

We here construct, along the lines of Ref. 8, rigorous *lower* bounds to both the Schrödinger $\epsilon(\rho)\equiv\tilde E(N,L)/N$ as well as the $\epsilon^{\rm HF}(\rho)\equiv E^{\rm HF}(N,L)/N$ energies per particles, for *any* density $\rho\equiv N/L$, L being the size of a box wherein the system is contained. (If $L\to\infty$, N fixed, then $\rho\to0$ and we recover the "open" boundary condition cases discussed heretofore.) *Upper* bounds will be considered in the following section.

Let the Hamiltonian (1) be written, for λ real and $0\leqslant\lambda\leqslant1$, as

$$H=T+V=(\lambda T+V)+(1-\lambda)T. \tag{46}$$

Since the Hamiltonian $\lambda T+V$ is that of a gas of N fermions with ν species and mass m/λ, we have from Eq. (3), valid at $\rho=0$, Eq. (5) and from the fact[8] that the ground state energy-per-particle must be nondecreasing in ρ, that

$$N^{-1}\langle\lambda T+V\rangle\geqslant-\frac{mv_0^2}{12\hbar^2\lambda}(\nu^2-1), \tag{47}$$

where the expectation value is between the exact ground state wave function. Furthermore, the Rayleigh–Ritz principle allows the assertion

$$N^{-1}\langle T\rangle\geqslant\pi^2\hbar^2\rho^2/3m\nu^2. \tag{48}$$

Combining (47) and (48) one has, for (46), that

$$\epsilon(\rho)\geqslant-\frac{mv_0^2}{12\hbar^2\lambda}(\nu^2-1)+(1-\lambda)\frac{\pi^2\hbar^2\rho^2}{3m\nu^2}, \tag{49}$$

which on maximizing with respect to $0\leqslant\lambda\leqslant1$ gives (taking $\hbar=m=1$),

$$\begin{aligned}\frac{\epsilon(\rho)}{|\epsilon(0)|}&\geqslant\frac{4\pi^2}{\nu^2(\nu^2-1)}\left(\frac{\rho}{v_0}\right)^2-\frac{4\pi}{\nu\sqrt{\nu^2-1}}\frac{\rho}{v_0}\\ &\left(\text{for }\frac{\rho}{v_0}\geqslant\frac{\nu(\nu^2-1)^{1/2}}{2\pi}\right),\geqslant-1\left(\text{for }\frac{\rho}{v_0}\leqslant\frac{\nu(\nu^2-1)^{1/2}}{2\pi}\right),\end{aligned} \tag{50}$$

where $\epsilon(0)$ represents the exact (zero-density) energy per particle appearing on the RHS of Eq. (47) with $\lambda=1$. Since the zero-density HF value is also known from Eq. (29) and (6), we can similarly find the lower bounds

$$\frac{\epsilon^{\mathrm{HF}}(\rho)}{|\epsilon(0)|} \geqslant \frac{4\hbar^2}{\nu^2(\nu^2-1)}\left(\frac{\rho}{v_0}\right)^2 - \frac{4\pi}{\nu(\nu+1)}\frac{\rho}{v_0}$$
$$\left(\text{for } \frac{\rho}{v_0} \geqslant \frac{\nu(\nu-1)}{2\pi}\right), \geqslant -\left(\frac{\nu-1}{\nu+1}\right)\left(\text{for } \frac{\rho}{v_0} \leqslant \frac{\nu(\nu-1)}{2\pi}\right). \tag{51}$$

Both (50) and (51) follow from the nondecreasing property of the energy per-particle as function of ρ which is verified not only in the Schrödinger but also in the HF case.

In the following section we give several *upper* bounds which are also HF solutions but *not* unique–i.e., they are *not* the lowest minimum as in (10)—in order to see how near or far energetically they may lie with respect to the unique solution (10). The prime motivation in this, of course, is that these kinds of solutions, in contrast to the unique one known in one dimension, are easily constructed in higher, particularly three, dimensions.

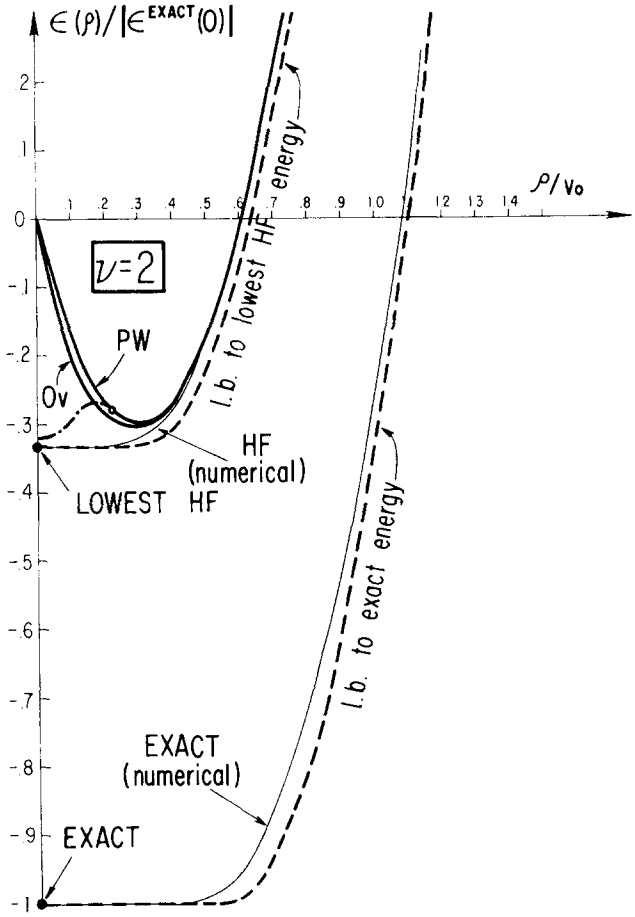

FIG. 1. Energy-per-particle, in units of the exact (Schrödinger) value at zero-density, vs. ρ/v_0 for a many-fermion (two species) system with Hamiltonian Eq. (1) with $\hbar = m = 1$. The lower dot on the ordinate axis corresponds to the exact result while the connecting dashed curve gives the lower bound Eqs. (50). The upper dot on the same axis is the lowest energy (i.e., unique solution) in the HF approximation and the connecting dashed curve the lower bound Eq. (51). The dot-dash curve is the (nonunique) exponential orbitals HF energy Eq. (54), which bifurcates from the plane wave HF energy Eq. (52) (upper full curve). The Overhauser HF energy Eq. (53) is also shown (lower full curve), and is everywhere below the plane wave curve except at $\rho/v_0 = 0$ and ∞ where they both coincide. The thin curves labelled "numerical" correspond to the HF results of Ref. 19 and to our finite density Schrödinger ground state energy calculation of Sec. 7.

6. OTHER (NONUNIQUE) SOLUTIONS

It is well-known[12] that the set of orthonormal, plane-wave single-particle orbitals satisfy (trivially) the HF equations. Two non plane wave (or nontrivial) solutions are provided by the Overhauser[13] and the so called "exponential" orbitals.[14] These have been extensively studied in Ref. 14 in both one and three dimensions, and we here simply state the results appropriately transcribed for the N fermion, ν species system under consideration. In units of the exact result $\epsilon(0)$ one has (for $\hbar = m = 1$), for the plane-wave (PW), Overhauser (Ov) and exponential (EXP) cases

$$\frac{\epsilon^{\mathrm{PW}}(\rho)}{|\epsilon(0)|} = \frac{4\pi^2}{\nu^2(\nu^2-1)}\left(\frac{\rho}{v_0}\right)^2 - \frac{12}{\nu(\nu+1)}\frac{\rho}{v_0}; \tag{52}$$

$$\frac{\epsilon^{\mathrm{Ov}}(\rho)}{|\epsilon(0)|} = \frac{12\pi^2}{\nu^2(\nu^2-1)}\left(\frac{\rho}{v_0}\right)^2 - \frac{12\pi^2}{\nu^2(\nu^2-1)}\left(\frac{\rho}{v_0}\right)^2 \times \coth\left[\frac{2\pi^2}{\nu(\nu-1)}\frac{\rho}{v_0}\right]; \tag{53}$$

$$\frac{\epsilon^{\mathrm{EXP}}(\rho)}{|\epsilon(0)|} = \min_{\alpha}\left\{\frac{4\pi^2}{\nu^2(\nu^2-1)}\left(\frac{\rho}{v_0}\right)^2\left[1+6\alpha\frac{I_1(2\alpha)}{I_0(2\alpha)}\right] - \frac{12}{\nu(\nu+1)}\frac{I_0(4\alpha)}{I_0^2(2\alpha)}\frac{\rho}{v_0}\right\}, \tag{54}$$

where in (54) one carries out the minimization in the exponential orbitals variational parameter $0 \leqslant \alpha < \infty$ numerically, and $I_1(x)$ is the modified Bessel function.[15] Note that for $\alpha = 0$, (54) becomes (52), as it should.

Figures 1 and 2 illustrate the results for two extreme cases, the 2-species system and the 32-species one, respec-

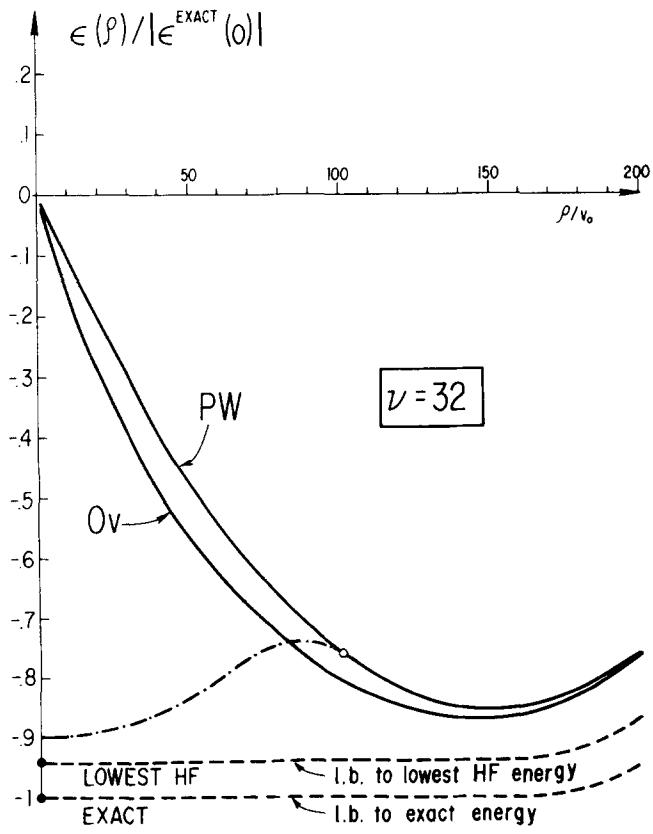

FIG. 2. Same as Fig. 1 but for a $\nu = 32$ species, N-fermion system.

TABLE I. Finite density Schrödinger ground state energy (57), for several densities.

ρ/v_0	0	0.15	0.31	0.41	0.54	0.70	0.90	0.99	1.08	1.13
$4\epsilon(\rho)/v_0^2$	-1	-1.000	-1.000	-0.995	-0.980	-0.860	-0.510	-0.275	$+0.016$	$+0.198$

tively. Note that all three nonunique solutions PW, Ov and EXP, violate the non decreasing-in-ρ property but that the EXP case is clearly the better of the three at low density, even qualitatively. For $\nu = 2$, $\epsilon^{\mathrm{EXP}}(0)/|\epsilon^{\mathrm{HF}}(0)|$ is about -0.96,[14] and for $\nu = 4$ calculations[16] employing more realistic pair interactions suggest that this value is almost -1.

We note that all expressions (52) to (54), being rigorous *upper* bounds, are greater than or equal to unity.

7. FINITE DENSITY SCHRÖDINGER GROUND STATE ENERGY

To obtain the exact ground state energy of (1) (with $m = \hbar = 1$) for $\rho/v_0 > 0$ we must solve the Gaudin[4] equations for the function $f(q)$ and the limit value Q, namely

$$\frac{1}{2}f(q) = 1 - \frac{v_0}{2\pi}\int_{-Q}^{Q} dq' \frac{f(q')}{v_0^2 + (q-q')^2}, \quad v_0 > 0, \tag{55}$$

$$\rho = \frac{1}{\pi}\int_{-Q}^{Q} dq f(q). \tag{56}$$

Knowing these one then substitutes into the energy per particle

$$\epsilon(\rho) = -\frac{v_0^2}{4} + \frac{1}{\pi\rho}\int_{-Q}^{Q} dq q^2 f(q). \tag{57}$$

These are essentially the same equations solved by Lieb and Liniger[17] for the *repulsive* delta function boson gas save, of course, for a sign change in v_0 and the absence of the binding energy term $-v_0^2/4$ in (57).

The equation to be solved initially, (55), is an inhomogeneous Fredholm integral equation of the second kind. We have used a collocation and least-squares method[18] based upon an expansion of $f(q)$ in terms of 12 Chebyschev functions. The results are shown in Table I and graphed in Fig. 1 (lower thin curve). We note the closeness of the exact result to the lower bound (lower dashed curve). For comparison, in Fig. 1 also shown are the results of Gutiérrez and Plastino[19] for the HF energy for $\rho/v_0 \geqslant 0$ (upper thin curve).

8. CONCLUSIONS

We have compared the HF with the Schrödinger ground state energies for a system of N fermions, ν species, and such that N/ν is integer, for a one-dimensional Hamiltonian with attractive pair interactions of the delta function kind capable of producing "clusters" of ν particles. Some nonunique HF solutions which are easily constructed in higher dimensions were compared. In general, we found that as ν grows the HF energy approaches (from above) the Schrödinger energy and becomes, as $\nu \to N$, the well-known boson case for which both energies coincide in the thermodynamic limit. Finally, we have calculated numerically, for nonzero density, the Schrödinger ground state energy for the case $\nu = 2$ and compared this with all our results as well as the finite-density lowest (or, unique) HF result.

ACKNOWLEDGMENTS

The authors appreciate discussions with Professor L. Döhnert, Professor E. H. Lieb and Professor M. Moshinsky.

Also, V. C. Aguilera-Navarro thanks FINEP (Brazil), E. Ley-Koo and M. de Llano ININ (Mexico), M. de Llano CONACYT (Mexico) and A. Plastino CONICET and CIC (Argentina), for partial support.

The assistance of C. Mostaccio and J. Pouchou of the Numerical Analysis Lab, La Plata National University is appreciated.

This work was also supported by the U. S. Department of Energy, contract No. W-7405-Eng-82, Division of Nuclear Theory.

APPENDIX

Here we outline how the overlaps (54) were obtained for $\nu = 2$ and 3. We use the abbreviation $c \equiv mv_0/\hbar^2$ throughout.

For $\nu = 2$ the calculation can be done analytically since, recalling the definition (52), one has

$$\langle\tilde{\Phi}_2|\tilde{\Phi}_2\rangle = c^2\int_{-\infty}^{\infty} dx\ \mathrm{sech}^4 cx = \frac{4}{3}c; \langle\Psi_2|\Psi_2\rangle = 2, \tag{A1}$$

while

$$\langle\Psi_2|\tilde{\Phi}_2\rangle = \sqrt{2}c^{3/2}\int_{-\infty}^{\infty} dx\ \mathrm{sech}^2 cx e^{-c|x|} = (8c)^{1/2}\left(\frac{\pi}{2} - 1\right), \tag{A2}$$

so that, finally, in view of (53)

$$\mathcal{O}_2 = \tfrac{3}{4}(\pi - 2)^2 = 0.9774\cdots. \tag{A3}$$

If we had used the orbital $f(x)$, instead of $\tilde{f}(x)$ as above, then

$$\langle\Phi_2|\Phi_2\rangle = \frac{2}{3}c;$$

$$\langle\Psi_2|\Phi_2\rangle = 2(2c)^{1/2}\int_0^{\infty} dy\, e^{-2y}\,\mathrm{sech}^2 y = 2(2c)^{1/2}(2\ln 2 - 1), \tag{A4}$$

so that

$$\mathcal{O}_2\,(\text{with center-of-mass}) = 6(2\ln 2 - 1)^2 = 0.8953\cdots. \tag{A5}$$

For $\nu = 3$ one has

$$\langle\tilde{\Phi}_3|\tilde{\Phi}_3\rangle = \frac{27c}{16}\int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dv\ \mathrm{sech}^2 u\ \mathrm{sech}^2 v\ \mathrm{sech}^2(u+v), \tag{A6}$$

where $u \equiv 3cx_1/2$ and $v \equiv cx_2/2$. The transformation $u \equiv \frac{1}{2}(x+y)$ and $v \equiv \frac{1}{2}(x-y)$ allows the double integral (A6) to be reduced to integrals found in Ref. 20, with the result

$$\langle \tilde{\Phi}_3 | \tilde{\Phi}_3 \rangle = \frac{27c}{16}(12 - \pi^2). \tag{A7}$$

on the other hand, to evaluate $\langle \Psi_3 | \Psi_3 \rangle$ exactly one can introduce the Jacobi coordinates

$$\begin{aligned} x_a &\equiv \frac{1}{\sqrt{2}}(x_1 - x_2), \\ x_b &\equiv \frac{1}{\sqrt{6}}(x_1 + x_2 - 2x_3), \\ x_c &\equiv \frac{1}{\sqrt{3}}(x_1 + x_2 + x_3), \end{aligned} \tag{A8}$$

which constitute an orthogonal transformation so that the Jacobian is unity. Then

$$\langle \Psi_3 | \Psi_3 \rangle = 2c^2\sqrt{3}\int_{-\infty}^{\infty} dx_a \int_{-\infty}^{\infty} dx_b \exp\left[-\sqrt{2}c(|x_a| + \left| x_a \cos\frac{\pi}{3} + x_b \sin\frac{\pi}{3} \right| + \left| x_b \sin\frac{\pi}{3} - x_a \cos\frac{\pi}{3} \right| \right], \tag{A9}$$

and if we define r and θ by

$$\begin{aligned} x_a &\equiv r\cos\theta \quad 0 \leqslant r < \infty, \\ x_b &\equiv r\sin\theta \quad 0 \leqslant \theta \leqslant 2\pi, \end{aligned} \tag{A10}$$

the integral (A9) takes on the more convenient form

$$\begin{aligned} \langle \Psi_3 | \Psi_3 \rangle &= 24\sqrt{3}c^2 \int_{-\infty}^{\infty} dr\, r \int_0^{\pi/6} d\theta \exp\left[-2\sqrt{2}cr\cos\theta \right] \\ &= 3\sqrt{3}\int_0^{\pi/6} d\theta \cos^{-2}\theta = 3. \end{aligned} \tag{A11}$$

However, the integral $\langle \Psi_3 | \tilde{\Phi}_3 \rangle$ does not seem to be do-able exactly; we thus resorted to numerical evaluation via two routes: i) by reducing it to a single integration and ii) by numerically doing the original double integration. One has

$$\langle \Psi_3 | \tilde{\Phi}_3 \rangle = \frac{1}{4}(54c)^{1/2}\int_0^{\infty} dr\, r \int_0^{2\pi} d\theta \operatorname{sech}(r\sin\theta) \operatorname{sech}\left(r\sin\left(\theta + \frac{\pi}{3}\right)\right) \times \operatorname{sech}\left(r\sin\left(\theta - \frac{\pi}{3}\right)\right) \exp\left[-\frac{1}{\sqrt{3}} r \left\{ |\cos\theta| + \left|\cos\left(\theta + \frac{\pi}{2}\right)\right| + \left|\cos\left(\theta - \frac{\pi}{2}\right)\right| \right\} \right], \tag{A12}$$

which, after some tedious analysis, can be reduced to the form

$$\frac{(54c)^{1/2}}{4}\int_0^{\infty} du\, e^{-u} f(u), \tag{A13}$$

where, as before $u \equiv 3cx_1/2$, and

$$\begin{aligned} f(u) \equiv (\sinh 3u)^{-1} \ln\left[e^{3u} \frac{\cosh u}{\cosh 2u} \right] - (\cosh 3u)^{-1} \\ \times \ln\left[2\cosh 2u\right] + (\cosh 3u)^{-1} e^{-u} \left\{ 2\tan^{-1} e^{u} \right. \\ \left. + (\sinh 3u)^{-1} \ln\left[\frac{\cosh u}{\cosh 2u} \right] - \frac{\pi}{2} \right\}. \end{aligned} \tag{A14}$$

Numerical integration gives 1.762 952 3 for the double integral (A12) and 1.762 952 5 for the single integral (A13). Thus

$$\mathcal{O}_3 = \frac{2(1.762\,952)^2}{3(12 - \pi^2)} = 0.972\,589\cdots. \tag{A15}$$

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Optimal control of the decay of nonequilibrium statistical correlations[a)]

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(Received 18 January 1982; accepted for publication 29 July 1982)

A quasithermodynamic interpretation of the stochastic control of irreversible thermodynamic diffusion processes is presented in which the drift is the control parameter. The joint entropy, considered as a function of the initial data is the negative of the optimal expected total cost, and the generalized Hamilton–Jacobi equation, which it satisfies, is the dynamic programming equation for the optimal stochastic drift control. The two cost functions, proposed by Yasue, are shown to differ by a stochastic gauge transformation and constitute equivalent variational problems. Yasue's results are shown to apply in two limiting cases: the asymptotic time limit, where the nonequilibrium statistical correlations have worn off, or the weak noise limit, where random thermal fluctuations have a negligible importance. The asymptotic expected total cost is governed by a minimum relative entropy principle and the goodness of the thermodynamic drift control in the stochastic problem is determined.

PACS numbers: 05.40. + j, 05.70.Ln

I. INTRODUCTION AND SUMMARY

The Onsager–Machlup (OM) function has recently been interpreted as a local cost function in the stochastic theory of optimal control.[1] An analogy was drawn between irreversible thermodynamic diffusion processes and a minimum principle for determining the smallest eigenvalue and corresponding eigenfunction of the Schrödinger equation in which the smallest eigenvalue was shown to be the minimun cost of a stochastic control problem.[2] The dynamics was described by a stochastic differential equation and control was exercised by choosing the drift as the control. The cost of using the control was then identified as the asymptotic time average of the expected value of the energy and the smallest eigenvalue was identified as the minimum energy of the system.

By specifying the dynamics through a stochastic differential equation, Holland[2] was able to convert the Schrödinger equation into a dynamic programming equation of optimal stochastic control theory. In order to apply the same analysis to irreversible thermodynamic diffusion processes Yasue[1] had to consider two diffusion processes: the uncontrolled irreversible thermodynamic process and a controlled diffusion process in which the drift acted as the control. Yasue's major result was that the optimal stochastic drift control is the thermodynamic drift control since it minimizes the OM function which he interpreted as a local cost function.

Yasue circumvented the dynamic programming analysis by showing that the OM function met all the prerequisites of a cost function and that the minimum expected value was obtained by setting the optimal stochastic drift control equal to the thermodynamic drift. Yet, deterministic control, at best, can only be an approximation to optimal stochastic control due to the presence of noise.

When random thermal fluctuations are taken into account in irreversible thermodynamics, statistical correlations arise between nonequilibrium states that are not well separated in time. An analysis of nonequilibrium statistical correlations was performed using the kinetic analog of Boltzmann's principle.[3] Whereas Boltzmann's principle determines the probability density in terms of the entropy, its kinetic analog determines the transition probability density in terms of the entropy difference of the endpoints of transition and the joint entropy which accounts for the statistical correlations between the nonequilibrium states. With the passage of time, all predominantly dissipative systems tend to "forget" and in the asymptotic limit, the joint entropy reduces to the sum of the entropies of the two states indicating that they are statistically independent in this limit. Asymptotically then, Boltzmann's principle is recovered for the probability of a spontaneous fluctuation from equilibrium.

A novel feature of the present analysis will be to show that the generalized Hamilton–Jacobi equation for the joint entropy is derivable from the dynamic programming equation of optimal stochastic control. The joint entropy then can be interpreted as the negative of the minimum expected total cost when considered as a function of the initial data. In contrast to Yasue's result, the optimal stochastic drift control will, in general, be shown not to coincide with the thermodynamic drift. This will be attributed to the presence of nonequilibrium statistical correlations between the terminal states. However, there are two important limiting situations in which Yasue's result applies: in the long time limit, where the statistical correlations have had ample time to have worn off, and in the "thermodynamic" limit,[4] where the random thermal fluctuations play a negligible role.

The outline and basic results of the paper are as follows. In Sec. II, the expected relative cost is defined in terms of the expected value of the logarithm of the probability measure density for the conversion of sample paths belonging to the controlled diffusion process into the irreversible thermodynamic process. An expected total cost is also defined and differs from the expected relative cost by a stochastic gauge transformation. These two cost functions are identical to those introduced by Yasue in the event that the rotational

[a)] Work supported in part by the CNR.

 0022-2488/82/122445-07$02.50

probability current vanishes. Hence, the two cost functions constitute equivalent variational problems. In Sec. III, a comparison is made between a "free" diffusion process (i.e., with zero drift) and an irreversible thermodynamic diffusion process. The joint entropy is introduced into the description of the nonequilibrium statistical correlations between states that are not well separated in time.[3] By the method of dynamic programming, it is shown that when the joint entropy is considered as a function of the initial data, it coincides with the negative of the optimal expected total cost for the transfer of the system between given states under optimal stochastic control. The long time expected value of the optimal total cost is equal to the expected entropy difference and is therefore positive semidefinite by virtue of the second law. In Sec. IV, the OM function is shown to be a cost function when the velocity is chosen as the control in the thermodynamic limit of vanishing noise intensity. This is precisely Yasue's result[1] which is shown to apply either in the limit of small noise intensities or in the long time limit. In the thermodynamic limit two classes of optimal trajectories emerge, depending on the imposed boundary conditions, and are shown to be the maximum likelihood paths for the growth and decay of fluctuations.[4] In Sec. V, the asymptotic expected total cost is shown to reduce to the terminal costs, as measured in terms of the entropy difference for the transfer of the system between nonequilibrium states under the application of the thermodynamic drift control. Furthermore, it will be shown that the long time total cost for the transfer of the system from any neighborhood of the stationary state to the most probable state on the boundary at which exit is expected to occur is governed by a minimum relative entropy principle, provided there exists a unique state on the boundary with maximum entropy.[4] Finally, in Sec. VI, we answer the question of how good is the use of the thermodynamic drift in the stochastic control problem. It is shown that to leading order in the small noise intensity parameter, the optimal relative stochastic cost differs from the relative thermodynamic cost by a term proportional to the square of the noise intensity parameter.

II. STOCHASTIC CONTROL OF IRREVERSIBLE PROCESSES UNDER THE INFLUENCE OF RANDOM THERMAL FLUCTUATIONS

The deterministic optimal control problem is converted into a stochastic optimal control problem when random thermal fluctuations are taken into account. For then, the deterministic optimal control given by the phenomenological laws of irreversible thermodynamics cannot, in general, be achieved. However, if the noise intensity is small or if a long enough time has elapsed so as to ensure statistical independence, the stochastic control problem approximates the unperturbed problem. In this section, we formulate the stochastic control problem.

The state of the system is assumed to be completely observable at each instant in time. This assumption is essential if the stochastic control problem is to reduce to a solution of a partial differential equation via dynamic programming.[5] The state process $\tilde{X}(t)$ is a vector in n-dimensional space $\mathbb{R}^n$ and evolves according to the stochastic differential equation

$$d\tilde{X}(t) = b(\tilde{X}(t))\,dt + \epsilon\sigma\,dB(t), \quad \tilde{X}(s) = x \tag{1}$$

written in vector-matrix notation. The Wiener process $B(t)$ is a mathematical idealization of Brownian motion which results from an enormous number of small displacements fluctuating at random. The increments have a Gaussian distribution with zero mean and variance $2D\,dt$ where $D = \frac{1}{2}\sigma\sigma^{\dagger}$ is the positive symmetric diffusion matrix and $\sigma^{\dagger}$ is the transpose of σ. The last term in Eq. (1) represents the effect of random thermal fluctuations upon an otherwise deterministic system of equations. The small positive parameter ϵ serves as a measure of the noise intensity.

The drift field b is specified by the phenomenological laws of irreversible thermodynamics which are compatible with the existence of an invariant probability distribution. The drift field can be decomposed into what is essentially the gradient of a scalar potential, namely the entropy S, and a vector field A, viz.,[6]

$$b = D(\nabla S + A). \tag{2}$$

From a probabilistic point of view, the entropy determines the invariant probability density p_∞ via Boltzmann's principle

$$\epsilon^2 \ln p_\infty(x) = S(x) + \text{const.} \tag{3}$$

And since p_∞ satisfies the time-independent Fokker–Planck equation $\nabla\cdot p_\infty v_\infty = 0$ which in integrated form reads

$$bp_\infty - \epsilon^2 D\nabla p_\infty = v_\infty p_\infty, \tag{4}$$

where $v_\infty p_\infty$ is the rotational probability current, the two thermodynamic fields in (2) satisfy

$$D{:}(\nabla S A^{\dagger} + \epsilon^2 \nabla A) = 0 \tag{5}$$

with $v_\infty = DA$. In the thermodynamic limit as $\epsilon \to 0^+$, a necessary condition for the existence of an invariant probability density given by Boltzmann's principle (3) is that the gradient field be orthogonal to rotational probability current velocity v_∞[4,7] [cf. (54) below].

The irreversible thermodynamic diffusion process (1) can be compared with a controlled diffusion process where the drift acts as the control.[1] The controlled diffusion process $X(t)$ is described by the stochastic differential equation

$$dX(t) = u(X(t))\,dt + \epsilon\sigma\,dB(t), \quad X(s) = x \tag{6}$$

which has the same local variance as (1) but with a different drift field u that acts as the control. The controlled diffusion process $X(t)$ is, in a certain sense, close to the irreversible thermodynamic process $\tilde{X}(t)$ and its corresponding probability measure μ is close to the measure $\tilde{\mu}$ of the irreversible thermodynamic diffusion process.

In order that the two measures be absolutely continuous with respect to one another, it is necessary and sufficient that the local variance matrices of the two measures should be equal on the entire interval $[s,T]$ while the two drift fields can be different.[8] In other words, the two diffusion processes have the same sample functions on $[s,T]$ but are considered as distinctly different stochastic processes with respect to their probability measures. Since $\tilde{\mu} \ll \mu$, the probability measure density exists and is given by the well-known Girsanov formula[9]:

$$\frac{d\tilde{\mu}}{d\mu}(X(\cdot)) = \exp\left\{(\epsilon\sigma)^{-1}\int_s^T (b-u)\,dB(t) - (4\epsilon^2)^{-1}\int_s^T ||u-b||^2_{D^{-1}}\,dt\right\}, \tag{7}$$

where $||\cdot||_M$ denotes the quadratic form associated with the symmetric matrix M. Since the drift fields are nonanticipating (which is to say that they depend upon only those $X(s)$ in the past $s \leqslant t$), the drift fields and the increments $dB(t)$ are statistically independent. From this it follows that the conditional expectation of the first integral in the exponent of (7) vanishes. This martingale property is used to define the expected relative cost for the use of the control u in the following way. Taking the conditional expectation of the logarithm of the probability measure density (7) we obtain

$$\begin{aligned} C^u(x,s) &\equiv -2\epsilon^2 \mathbb{E}_{xs}\left\{\ln\left(\frac{d\tilde{\mu}}{d\mu}\right)\right\} \\ &= \mathbb{E}_{xs}\left\{\frac{1}{2}\int_s^T ||u-b||^2_{D^{-1}}\,dt\right\} \\ &\equiv \mathbb{E}_{xs}\left\{\int_s^T L(u,X(t))\,dt\right\} \end{aligned} \tag{8}$$

which is Yasue's representation of the expected value of the QM function as a cost function.[1]

The expected total cost for the transfer of an initial state x to some target set, under the control u, can be obtained from the expected relative cost (8) via a "stochastic gauge" transformation. The integrand in (8) is expanded and the cross term is evaluated with the aid of the controlled diffusion process (6). Then introducing the drift field (2), we obtain the expected total cost as

$$\begin{aligned} C^{*u}(x,s) &\equiv C^u(x,s) + \mathbb{E}_{xs}S(X_T) - S(x) \\ &\equiv \mathbb{E}_s\left\{\int_s^T L^*(u,X(t))\,dt\right\}, \end{aligned} \tag{9}$$

where the loss function L^* is defined as[6]

$$L^*(u,x)\,dt \equiv [\tfrac{1}{2}||u||^2_{D^{-1}} + V(x)]\,dt - A\circ dX(t), \tag{10}$$

which represents the net energy dissipation. The scalar potential V is referred to as the QM potential,[1]

$$V(x) = \tfrac{1}{2}||b||^2_{D^{-1}} + \epsilon^2\nabla\cdot b, \tag{11}$$

and the small circle in the last term denotes Fisk–Stratonovich symmetric multiplication, viz.,

$$\begin{aligned} A\circ dX(t) &= (A + \tfrac{1}{2}dA)\,dX(t) \\ &= A\,dX(t) + \epsilon^2 D{:}\nabla A\,dt. \end{aligned} \tag{12}$$

The stochastic control problems (8) and (9) can be said to be equivalent in the sense that their integrands differ merely by the mean forward stochastic derivative of the entropy, viz.,

$$d_t\mathbb{E}_{xs}S(X(t)) = \mathbb{E}_{xs}G^uS(X(t)), \tag{13}$$

where

$$G^u = u\cdot\nabla + \epsilon^2 D{:}\nabla\nabla \tag{14}$$

which is the infinitesimal generator of the controlled diffusion process (6). In analogy with the corresponding concept in electrodynamics, we shall call

$$L^*(u,x) = L(u,x) + G^uS(x) \tag{15}$$

a stochastic gauge transformation. Since the Weierstrass excess function E, corresponding to the Lagrangian L, is

$$\begin{aligned} E(u,u^0,x) &= L(u,x) - L(u^0,x) - (u-u^0)\nabla_u L(u^0,x) \\ &= \tfrac{1}{2}||u-u^0||^2_{D^{-1}} \geqslant 0, \end{aligned} \tag{16}$$

where u^0 is the optimal drift control, there exists a stochastic gauge transformation (15) giving rise to equivalent stochastic control problems. Moreover, if E^* is the excess function corresponding to the Lagrangian L^* we obtain, by direct substitution, that

$$E(u,u^0,x) = E^*(u,u^0,x). \tag{17}$$

The Weierstrass condition (16) is the condition for a "strong" minimum; that is, when the extremum is not just a local minimum but rather an absolute minimum.[10]

The stochastic gauge transformation (15) provides the connecting link between the two cost functions introduced by Yasue,[1] namely, the local cost function (8) and the cost (9), without taking the asymptotic time limit. Rather we shall refer to (9) as the expected total cost since it contains the expected state costs as measured by the expected entropy difference in the transfer of the initial state x under the drift control u.

III. QUASITHERMODYNAMIC DESCRIPTION OF NONEQUILIBRIUM STATISTICAL CORRELATIONS AND DYNAMIC PROGRAMMING

In this section, we apply Girsanov's measure substitution theorem to obtain a quasithermodynamic description of the statistical correlations between nonequilibrium states that are not well separated in time. Rather than comparing the irreversible thermodynamic diffusion process (1) with a controlled diffusion process, we now compare it with a free, uncontrolled diffusion process,

$$d\hat{X}(t) = \epsilon\sigma\,dB(t), \quad \hat{X}(s) = s. \tag{18}$$

Through the application of nonequilibrium external constraints, which are subsequently partially released, the free diffusion process (18) is converted into the irreversible thermodynamic diffusion process (1).[3] Since the local variance matrices of the two diffusion processes are the same, the probability measure $\hat{\mu}$, corresponding to the process $\hat{X}(t)$, is absolutely continuous with respect to the probability measure $\tilde{\mu}$ for the process $\tilde{X}(t)$. The probability measure density on $[s,T]$ is

$$\frac{d\tilde{\mu}}{d\hat{\mu}}(\hat{X}(\cdot)) = \exp\left\{(2\epsilon^2)^{-1}\int_s^T [D^{-1}b\,d\hat{X}(t) - \tfrac{1}{2}||b||^2_{D^{-1}}\,dt]\right\}. \tag{19}$$

With the aid of the drift decomposition (2) and formulas (12) and (13), the probability measure density (19) can be written in the form

$$\frac{d\tilde{\mu}}{d\hat{\mu}}(\hat{X}(\cdot)) = \exp\left\{(2\epsilon^2)^{-1}\left[S(\hat{X}_T) - S(x) - \int_s^T (V(\hat{X}(t))\,dt - A\circ d\hat{X}(t))\right]\right\}. \tag{20}$$

The probability $\mathbb{P}$ that the solution of Eq. (1), which we

denote as $\tilde{X}_{xs}(T)$, will be found in a Borel set $\mathscr{B}$ coincides with the transition probability $\tilde{P}$, viz.,[11]

$$\tilde{P}(\mathscr{B},T|x,s) = \mathbb{P}\{\tilde{X}_{xs}(T)\in\mathscr{B}\}. \tag{21}$$

$\tilde{P}$ is related to the transition probability $\hat{P}$ of the free diffusion process (18) by

$$\tilde{P}(\mathscr{B},T|x,s) = \int_{\mathscr{B}} \mathbb{E}\left\{\frac{d\tilde{\mu}}{d\hat{\mu}}(\hat{X}(\cdot))|\hat{X}_{xs}(T)=y\right\}\hat{P}(dy,T|x,s), \tag{22}$$

where $\hat{X}_{xs}(T)$ is the solution of Eq. (18) having the same initial conditions as $X_{xs}(T)$. If $\tilde{P}$ has a density $\tilde{p}$ and $\hat{P}$ has a density $\hat{p}$ then

$$\tilde{p}(y,T|x,s) = \exp\{(2\epsilon^2)^{-1}[S(y)-S(x) + \sigma_J(y,T;x,s)]\}, \tag{23}$$

where the joint entropy σ_j is defined as

$$\sigma_J(y,T;x,s) \equiv 2\epsilon^2 \ln\left[\mathbb{E}\left\{\exp\left[(2\epsilon^2)^{-1}\int_s^T (A\circ d\hat{X}(t) - V(\hat{X}(t))\,dt)\right]|\hat{X}_{xs}(T)=y\right\}\hat{p}(y,T|x,s)\right] \tag{24}$$

and $\hat{p}$ is the transition probability density of the Wiener process.

We have previously referred to (23) as the kinetic analog of Boltzmann's principle.[3] Whereas Boltzmann's principle (3) determines the probability of a state in terms of its entropy, its kinetic analog (23) relates the probability of a temporal succession of states to their entropy difference and joint entropy. The joint entropy is a quasithermodynamic potential inasmuch as it is a function of the endpoints of transition as well as the time of transition for time homogeneous diffusion processes. Given enough time, all predominantly dissipative systems "forget" and in the long time limit the states will become statistically independent. Then in order for (23) to reduce to (3) in the long time limit, the joint entropy must have the property that

$$\lim_{T-s\to\infty} \sigma_J(y,T;x,s) = S(x)+S(y). \tag{25}$$

To prove (25) it suffices to determine the stationary solutions of the pair of generalized Hamilton–Jacobi equations which the joint entropy satisfies.[3]

In dynamic programming, the optimal expected cost is considered as a function of the initial data and in this sense the backward generalized Hamilton–Jacobi equation

$$\partial_s\sigma_J + \tfrac{1}{2}||\nabla\sigma_J + A||_D^2 + \epsilon^2 D:\nabla(\nabla\sigma_J + A) = V(x) \tag{26}$$

has a privileged role in optimal stochastic control theory. We shall now derive Eq. (26) via dynamic programming and show that the joint entropy, when considered as a function of the initial data, coincides with the negative of the optimum expected total cost.

Let $\mathbb{D}\subset\mathbb{R}^n$ be an open set in which the diffusion process is controlled. Define the optimal expected total cost by

$$W^*(x,s) = \inf_u C^{*u}(x,s) \tag{27}$$

considered as a function of the initial data in the cylinder $[s,T]\times\mathbb{D}$ such that W^* is in $C^{1,2}(\mathbb{D})$ and continuous on the closure $\bar{\mathbb{D}} = \mathbb{D}\cup\partial\mathbb{D}$. Then $W^*(x,s)\leqslant C^{*u}(x,s)$ for any admissible control u and any initial data $(x,s)\in\mathbb{D}$. The optimal stochastic drift control u^0 is such that

$$G^{u^0}W^* + L^*(u^0,x) = \min_u\{G^uW^* + L^*(u,x)\} \tag{28}$$

for all $(x,s)\in\mathbb{D}$ and consequently $W^*(x,s) = C^{*u^0}(x,s)$ for all $(x,s)\in\mathbb{D}$.

By virtue of the definition of the expected total cost (9) and the mean forward stochastic derivative of the optimal expected total cost,

$$\begin{aligned}\mathscr{D}W^*(x,s) &= \lim_{\tau\to 0^+}\frac{1}{\tau}\mathbb{E}_{xs}\{W^*(X(\tau+s),\tau+s) - W^*(X(s),s)\}\\ &= (\partial_s W^* + G^uW^*)(x,s)\end{aligned} \tag{29}$$

taken along a sample path of the controlled diffusion process, we obtain

$$\mathscr{D}W^*(x,s) \geqslant -L^*(u,x) \tag{30}$$

or

$$\partial_s W^* + \min_u\{G^uW^* + L^*(u,x)\} = 0. \tag{31}$$

Equation (31) will be recognized as the dynamic programming equation of optimal stochastic control theory. And since the problem is of the Lagrange type [cf. (27) and (9)], the boundary condition is

$$W^*(y,T) = 0. \tag{32}$$

The minimum of (31) is achieved when the gradient in u is 0. The minimum occurs for $u = u^0$, with

$$u^0 = D(A - \nabla W^*) \tag{33}$$

which when introduced into the dynamic programming equation (31) leads to

$$-\partial_s W^* + \tfrac{1}{2}||\nabla W^* - A||_D^2 - \epsilon^2 D:\nabla(\nabla W^* - A) = V(x). \tag{34}$$

A comparison of the generalized Hamilton–Jacobi equations (26) and (34) leads to the conclusion that

$$W^*(x,s) = -\sigma_J(y,T;x,s) \tag{35}$$

when the joint entropy is considered as a function of the initial data. This establishes the role of the joint entropy in the realm of optimal stochastic control theory. Furthermore, by virtue of the asymptotic property of the joint entropy (25), we can show that the optimal expected total cost reduces to the expected entropy difference in the asymptotic time limit.[12]

For a smooth set of drift controls u, the generalized Hamilton–Jacobi equation (26) can be written as

$$\partial_s\sigma_J + G^u\sigma_J \leqslant L^*(u,x), \tag{36}$$

or equivalently as the dynamic programming equation

$$\partial_s\sigma_J + \max_u\{G^u\sigma_J - L^*(u,x)\} = 0. \tag{37}$$

Setting the gradient of (37) with respect to u equal to 0 we obtain the optimal drift control

$$u^0 = D(\nabla\sigma_J + A), \tag{38}$$

which when substituted back into the dynamic programming equation (37) yields the generalized Hamilton–Jacobi equation (26). The equivalence between the optimal expected total cost and the joint entropy has now been established.

Integrating both sides of (36) in $[s,T]$, using the optimal drift control (38), and taking the conditional expectation, we obtain

$$\mathbb{E}_{xs}\{\sigma_J(X(T),T;x,s)\} = \mathbb{E}_{xs}\left\{\int_s^T L^*(u^0,X(t))\,dt\right\} + c(x), \quad (39)$$

where the constant c can depend upon the initial state. In the limit as $T-s\to\infty$, we find

$$\overline{\lim_{T-s\to\infty}}\ \mathbb{E}_{xs}\left\{\int_s^T L^*(u^0,X(t))\,dt\right\} = \int_{\mathbb{D}} S(y)\,d\mu^0(y) - S(x) \geqslant 0, \quad (40)$$

where μ^0 is the invariant steady-state probability measure. Then in view of the asymptotic property of the joint entropy (25) we conclude that $c(x) = 2S(x)$. Introducing the conditional entropy as[3]

$$\sigma_C(y,T\,|x,s) = \sigma_J(y,T;x,s) - S(x), \quad (41)$$

Eq. (39) can now be written as

$$\mathbb{E}_{xs}\{\sigma_C(X(T),T\,|x,s)\} - S(x) = \mathbb{E}_{xs}\left\{\int_s^T L^*(u^0,X(t))\,dt\right\}. \quad (42)$$

Taking the asymptotic time limit of (42) and using (40) we find

$$\overline{\lim_{T-s\to\infty}}\ \mathbb{E}_{xs}\{\sigma_C(X(T),T\,|x,s)\} = \int_{\mathbb{D}} S(y)d\mu^0(y). \quad (43)$$

Given enough time so that the initial conditions have worn off, the expected value of the conditional entropy reduces to the expected value of the entropy with respect to the invariant probability measure. In the asymptotic time limit statistical independence is achieved and this can be interpreted in terms of the asymptotic optimal expected total cost: In the long time limit, the optimal expected total cost reduces to the expected difference in the entropy and its positive semidefiniteness follows from the second law. In other words, any additional costs arising from the statistical correlations between nonequilibrium states do not contribute to the asymptotic optimal expected cost since statistical independence is regained in the long time limit. It is precisely to this limit that Yasue[1] has addressed himself when he concluded that $u^0 = b$ is the optimal control.

IV. OPTIMAL CONTROL FOR SMALL NOISE INTENSITIES

In the last section we saw that optimal stochastic control coincides with deterministic control in the asymptotic time limit. This was attributed to the presence of nonequilibrium statistical correlations which prevent optimal deterministic control from being used. There is, however, another limit in which deterministic control can be achieved, namely in the thermodynamic limit as $\epsilon\to 0^+$ of vanishing noise intensity. In this limit, the variational problem becomes a control problem simply by taking $u = \dot{x}$ as the control.

In the limit as $\epsilon\to 0^+$, the OM function

$$C^u(x,s) = \int_s^T \frac{1}{2}\,||u-b||_D^2\,dt = \int_s^T L(u,x)\,dt \quad (44)$$

is a cost function for the control $u = \dot{x}$.[1] No expectation in (44) appears because the control problem is now deterministic. The loss function L has the following properties:

(a) $L(u,x)$ is strictly convex in the sense that $v^+\nabla_u^2 Lv > 0$ for any arbitrary vector $v\in\mathbb{R}^n$,

(b) $L(u^0,x) = 0$ for $u^0 = b$, the optimal or thermodynamic drift control, and

(c) $L(u,x) > 0$ for any admissible drift control $u\neq u^0$.

Property (c) can be easily verified by observing that $L = E$, the Weierstrass excess function (16) which is a necessary condition for optimality in the calculus of variations.

The function

$$H(u,x,p) = pu - L(u,x) \quad (45)$$

is known as the Pontryagin function in deterministic optimal control theory.[13] $p\in\mathbb{R}^n$ are usually referred to as the "momenta" in analogy with classical mechanics. Introducing (45) into (44), the extremum problem can be formulated as

$$\Delta C^u(x,s) = \delta\int_s^T (pu - H)\,dt + (pu - H)\Delta t\,|_s^T = 0, \quad (46)$$

where the Δ and δ variations are related by $\Delta x = \delta x + \dot{x}\Delta t$. Upon performing the indicated variations in (46) we get

$$\Delta C^u(x,s) = \int_s^T \{(u-\nabla_p H)\delta p - (\dot{p} + \nabla H)\delta x\}\,dt + p\Delta x|_s^T - H\Delta t\,|_s^T = 0. \quad (47)$$

From (47), we find the following extremum conditions for C^u (cf. Ref. 4):

(A) $\begin{cases}\dot{x} = \nabla_p H = u,\\ \dot{p} = -\nabla H = \nabla L,\end{cases}$

(B) $H = 0$ if $\Delta t\,|_s^T \neq 0$,

(C) $p = 0$ if $\Delta x|_s^T \neq 0$.

Let us first consider condition (A).

The optimal drift control u^* makes H an extremum since

$$\nabla_u H(u^*,x,p) = p - \nabla_u L(u^*,x) = p - D^{-1}(u^* - b) = 0 \quad (48)$$

which determines u^* as a single valued function of x and p. Introducing (48) into the second set of Hamiltonian equations (A) results in

$$\dot{x} = u^*, \quad d_t\nabla_u L(u^*,x) = \nabla L(u^*,x) \quad (49)$$

which are the Euler–Lagrange equations for the optimal control trajectory. They are reduced to a set of first-order differential equations by introducing the optimal control as a new set of functions. The Hamiltonian for the optimal control trajectory is

$$H(u^*,x,p) = \tfrac{1}{2}\,||p||_D^2 + bp \quad (50)$$

and consequently the Euler–Lagrange equations (49) for the optimal trajectory are

$$\dot{x} = u^*, \quad \dot{p} = -(p\cdot\nabla)b. \tag{51}$$

It will now be appreciated that

$$p = 0 \quad \text{and} \quad \hat{u}^* = D(\nabla S + A) \tag{52}$$

satisfy the extremum conditions for the relative cost (A)–(C); corresponding to a variational problem with a free terminal endpoint. If both terminal endpoints are fixed, (C) cannot hold and we find that

$$p = -2\nabla S \quad \text{and} \quad \tilde{u}^* = D(A - \nabla S) \tag{53}$$

satisfies conditions (A) and (B) with (C) replaced by $\Delta x|_s^T = 0$, provided the transversality condition

$$D{:}\nabla S A^{+} = 0 \tag{54}$$

holds. Several comments will help to clarify the meaning of the optimal drift controls (52) and (53).

Whereas the Euler–Lagrange equations are second order differential equations, the phenomenological equations of irreversible thermodynamics are of first order. This means that we cannot specify two initial conditions or equivalently two endpoint conditions, as is usually the case in the calculus of variations. Hence, the optimal drift control (53) must be interpreted in the following sense. If condition (C) is not satisfied then it will be possible to reach $\inf_u C^u$ only for $s \to -\infty$ when the final state of transition is specified at time T.[14] For then as $s \to -\infty$, the system will reach any neighborhood of the (stable) steady state. This means that an arbitrary nonequilibrium state, in the limit as $\epsilon \to 0^+$, cannot be realized in a finite time if the system is initially found in any neighborhood of the steady state where it spends an unlimited portion of its time. The variable time of transit implies that

$$H(u^*, x, p) = 0 \tag{55}$$

along both classes of optimal system trajectories which are solutions of Eqs. (52) and (53).

The optimal drift control (52) is seen to coincide with the thermodynamic drift control. We have previously shown that this applies to the asymptotic time limit where statistical independence is regained. Here we have shown that it also applies to the thermodynamic limit as $\epsilon \to 0^+$ and (52) is the optimal control for the decay of a nonequilibrium fluctuation. We have previously referred to the optimal path trajectory for the decay of a fluctuation as the "thermodynamic" path.[15]

Under time inversion we have $t \to -t$, $\dot{x} \to -\dot{x}$, and $A \to -A$ so that we can appreciate the optimal drift control (53) as the mirror image in time of the thermodynamic control (52). Since $\inf_u C^u$ can only be achieved by letting $s \to -\infty$, it is clear that (53) is the optimal drift control for the growth of a fluctuation. Its corresponding optimal trajectory has been referred to as the "antithermodynamic" path.[15] And in order that (53) be the optimal or antithermodynamic control for the growth of a fluctuation, the transversality condition (54) must be satisfied. If Boltzmann's principle (3) is to hold and in view of the drift field decomposition (2), the transversality condition (54) becomes a necessary condition for the existence of the invariant probability density in the limit as $\epsilon \to 0^+$ as can be seen from the time-independent continuity equation (5). The optimal drift control (53) is intimately connected with the problem of stochastic exit in the limit as $\epsilon \to 0^+$, as will now be shown.

V. OPTIMAL TRAJECTORIES FOR STOCHASTIC EXIT

Suppose that the steady state is found in a bounded domain $\mathbb{D} \subset \mathbb{R}^n$ with boundary $\partial\mathbb{D}$. In the limit as $\epsilon \to 0^+$ we have the following picture of the optimal trajectories of the system which is initially found in $\mathbb{D}$. The overwhelming tendency of the system is to approach any close neighborhood of the steady state by sliding down a solution of the optimal or thermodynamic control (52). Along the thermodynamic path, the optimum relative cost vanishes and the asymptotic optimal total cost is

$$C^{*\hat{u}^*}(x,s) = \int_s^\infty L^*(\hat{u}^*, x(t))\, dt = S^0 - S(x) \geqslant 0, \tag{56}$$

where S^0 is the steady-state value of the entropy. Hence, the optimal total cost reduces to the difference in the terminal costs, as measured in terms of the entropy.

The system will remain in a small neighborhood of the steady state for an unlimited amount of time. However, on account of random thermal fluctuations, the system is able to make excursions to those states y in $\mathbb{D}$ such that $S(y) > \max_{z\in\partial\mathbb{D}} S(z)$.[4,14] Sooner or later, the system will reach the boundary $\partial\mathbb{D}$ and there is maximum likelihood for exit to be made at that state on the boundary which possesses maximum entropy, provided that such a unique state exists. To ensure that the system was initially in a small neighborhood of the steady state, we must change our perspective and take as the initial time some distant time in the past (i.e., $s \to -\infty$). Then noting

$$S(y) - S(x) = \int_s^T u\cdot\nabla S\, dt \tag{57}$$

and

$$C^u(x,s) = \int_s^T \frac{1}{2}\,||u - \tilde{u}^*||^2_{D^{-1}}\, dt - 2\int_s^T u\cdot\nabla S\, dt \geqslant 2\{S(x) - S(y)\} \tag{58}$$

on account of the transversality condition (54), the optimum relative cost to transfer the system from any small neighborhood of the steady state to that state with maximum entropy on the boundary is

$$C^{\tilde{u}^*}(x, -\infty) = -2\int_{-\infty}^T \tilde{u}^*\cdot\nabla S\, dt = 2\left\{S(x) - \max_{z\in\partial\mathbb{D}} S(z)\right\} \geqslant 0. \tag{59}$$

Under the same conditions, the optimal total cost for the antithermodynamic drift control (53) is

$$C^{*\tilde{u}^*}(x, -\infty) = S(x) - \max_{z\in\partial\mathbb{D}} S(z) \tag{60}$$

which follows from

$$C^{*\tilde{u}^*}(x, -\infty) = C^{\tilde{u}^*}(x, -\infty) + \max_{z\in\partial\mathbb{D}} S(z) - S(x). \tag{61}$$

Expression (60) constitutes a *minimum relative entropy principle* for the optimal cost of transferring the system from any small neighborhood of the steady state to the most likely place of exit on the boundary in the thermodynamic limit as $\epsilon \to 0^+$.

VI. OPTIMAL STOCHASTIC VERSUS THERMODYNAMIC CONTROL

Suppose that the controller does not solve the optimal stochastic control problem but rather simply applies the deterministic control. How good is the optimal deterministic control in the stochastic control problem? It is rather intuitive that for small noise intensities, the deterministic control should be a rather good approximation to optimal stochastic control. We now make this statement more precise.

The minimum expected relative cost is written as

$$W^\epsilon(x,s) = \inf_u C^u(x,s) \tag{62}$$

in order to display the dependence of the minimum expected relative cost on the noise intensity. $W^\epsilon(x,s)$ satisfies the dynamic programming equation[16]

$$\partial_s W^\epsilon + \min_u \{ G^u W^\epsilon + \tfrac{1}{2}||u-b||^2_{D^{-1}} + \epsilon^2 \nabla\cdot b \} = 0 \tag{63}$$

which is to be solved subject to the boundary condition [cf. (32)]

$$W^\epsilon(y,T) = 0. \tag{64}$$

The minimum of (63) occurs for $u = u^\epsilon$, with

$$u^\epsilon = b - D\nabla W^\epsilon, \tag{65}$$

which when substituted back into the dynamic programming equation (63) gives

$$\partial_s W^\epsilon + b\cdot\nabla W^\epsilon - \tfrac{1}{2}||\nabla W^\epsilon||^2_D + \epsilon^2(D:\nabla\nabla W + \nabla\cdot b) = 0. \tag{66}$$

A solution to the generalized Hamilton–Jacobi equation (66) is sought in the form

$$W^\epsilon = W^0 + \epsilon^2 W' + O(\epsilon^2), \tag{67}$$

which will, in general, be valid for a finite number of terms.[17] Introducing the series expansion (67) into Eq. (66) and equating to 0 terms of the same order in ϵ, we obtain to lowest orders,

$$\partial_s W^0 + b\cdot\nabla W^0 + \tfrac{1}{2}||\nabla W^0||^2_D = 0 \tag{68}$$

and

$$\partial_s W' + b\cdot\nabla W' = -D:\nabla\nabla W^0 - \nabla\cdot b. \tag{69}$$

Equation (68) is the classical Hamilton–Jacobi equation and in the realm of geometrical optics, it provides an alternative description of the motion than that given by the Euler–Lagrange equations (49). In geometrical optics, the Euler–Lagrange equations give a ray description of the motion while the Hamilton–Jacobi equation describes the motion of the wave front.

Denoting

$$H(u^0,x,W^0) = \tfrac{1}{2}||\nabla W^0||^2_D - b\cdot W^0 \tag{70}$$

as the Hamiltonian for optimal control, Eq. (68) can be written as

$$-\partial_s W^0 + H(u^0,x,\nabla W^0) = 0. \tag{71}$$

On the strength of the definition of the canonical momenta as $p \equiv -\nabla W^0$, the Hamiltonian (70) is seen to coincide with (50) and along the optimal control trajectories, it vanishes [cf. (55)]. Then to lowest order, the minimum expected relative cost is not an explicit function of time along the optimal control trajectories. The trivial solution

$$\hat{W}^0 = 0 \tag{72}$$

of the time-independent Hamilton–Jacobi equation corresponds to the optimal or thermodynamic control $u^0 = b$ for the regression of a fluctuation from a given nonequilibrium state.

Equation (69) then becomes

$$d_s W' = -\nabla\cdot b, \tag{73}$$

where d_s denotes differentiation along the characteristic $\dot{x} = b$. Denote $y = y(x,s)$ as the characteristic with initial data (x,s) and its inverse solution by $x = x(y,T)$. Then the solution of Eq. (73) is formally expressed by

$$W'(x(y,T),s) = \left[\int_s^T \nabla\cdot b(y(x,t))\,dt\right]_{x=x(y,T)} = \ln\left[\text{Jacobian}\left(\frac{\partial x}{\partial y}\right)_{x=x(y,T)}\right], \tag{74}$$

where the integral is taken along the optimal trajectory with initial endpoint (x,s). Use has also been made of the boundary condition (64). Introducing (72) and (74) into (67) we get

$$W^\epsilon(x,s) = \epsilon^2 \ln\left[\text{Jacobian}\left(\frac{\partial x}{\partial y}\right)_{x=x(y,T)}\right] + O(\epsilon^2). \tag{75}$$

Formula (75) shows that the thermodynamic control gives *within order ϵ^2 of the optimum in the stochastic control problem*. The integrand in (74) is nonpositive; $W^\epsilon > 0$ and $W^\epsilon \to 0^+$ uniformly as $\epsilon \to 0^+$. Therefore, (72) is the lower bound of the optimal expected relative cost.

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The stochastic H-theorem

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(Received 31 July 1981; accepted for publication 11 June 1982)

The stochastic analogue of the generalized H-theorem is formulated for multidimensional, time homogeneous diffusion processes which asymptotically are characterized by an invariant probability distribution. It applies to both isolated and open thermodynamic systems, the latter being characterized by rotational probability currents. The physical mechanism for the monotonic behavior of the stochastic H-function in time is linked to the decay of statistical correlations between a given nonequilibrium state and those through which the system passes at successive instants in time.

PACS numbers: 05.40. + j, 05.70.Ln, 02.30.Hq

I. INTRODUCTION

There are two formulations of the second law of thermodynamics.[1] In the Boltzmann formulation, thermodynamic equilibrium refers to the state of maximum probability which corresponds to the state of maximum entropy. In the Gibbs formulation, the term equilibrium is used in connection with a distribution over all possible states. However, the averaging is performed with respect to a probability distribution for which the Gibbs entropy is maximum. Both Boltzmann and Gibbs attempted to prove that the entropy of an isolated system increases in some sense.

The Boltzmann definition of entropy does not, in general, show a monotonic tendency to increase in the course of time. The problem with the state definition of equilibrium is that if the initial conditions coincide with the state of maximum entropy then there will be a finite probability to find states of lower entropy as the system evolves in time.[2] In the Boltzmann formulation, we must take the magnitude of the equilibrium fluctuations as a measure of the uncertainty by which we can specify a macroscopic state.[3]

The Gibbs entropy for an isolated system does not depend on time. Therefore, in what sense should it show a tendency to increase in the course of time remains obscure. Ehrenfest[4] was the first to provide a meaning to the increase in entropy of an isolated system by introducing the notion of a "coarse-grained" density. The coarse-grained density is obtained by averaging the "fine-grained" density of the distribution over small, fixed cells in phase space. This method has been likened to the time averaging techniques of nonlinear mechanics.[5] Just as nonlinear, periodic systems tend to a limiting behavior, independent of the initial conditions, so too will isolated thermodynamic systems approach equilibrium irrespective of their initial conditions. However, the physical mechanisms are entirely different in the two cases: in nonlinear mechanics, limiting behavior is achieved by a periodic balance of negative, linear and positive, nonlinear dissipation while irreversible thermodynamic processes tend to forget their past. This continual loss of information is the motivation behind the coarse-graining of the probability density.

After a long lapse in time, we expect stationary diffusion processes, in the wide sense, to become subject to stationary probability laws (i.e., stationary in the strict sense). For time homogeneous diffusion processes, the transition probability is a function of the time interval only while the probability distribution is time-independent. If there exists an invariant probability distribution, then the transition probability will approach this function in the asymptotic time limit. Thus, for stationary diffusion processes in the wide sense, the coarse-grained density cannot be an explicit function of time and we know that it does *not* approach, in the strict sense, the invariant probability density.[6] This is certainly not implied by the monotonic behavior of the Gibbs entropy which is defined in terms of the coarse grained probability density. It is simply a consequence of the convexity of $x \ln x$. We emphasize that if the process was initially nonstationary then it will remain so for all times.

There have been more recent attempts at constructing an expression for a nonequilibrium H-function.[7-10] The common idea behind these attempts has been to show that different, normalized probability densities approach each other in the course of time. However, these analyses compromise the time homogeneity of the diffusion process that is a necessary condition in order to achieve a state characterized by an invariant probability distribution in the asymptotic time limit. Hence, these attempts suffer from the same dilemma as the generalized H-theorem.

It is therefore of interest to ask what function, in the stochastic theory of time homogeneous diffusion processes, would correspond to the coarse-grained density in the generalized H-theorem. In equilibrium statistical mechanics, the ensemble average of the H-function is identified as the negative of the Gibbs entropy, in units where Boltzmann's constant is equal to unity.[4] By replacing the coarse-grained probability density by the transition probability density, we are able to construct a stochastic H-function which provides a physical mechanism for the time evolution of time homogeneous diffusion processes to an asymptotic state of the motion, characterized by an invariant probability distribution. Such a physical mechanism is lacking in the generalized H-theorem.

 0022-2488/82/122452-09$02.50

II. DERIVATION OF THE TRANSITION PROBABILITY FOR MULTIDIMENSIONAL DIFFUSION PROCESSES

The derivation of a transformation formula, relating transition probabilities for diffusion processes with the same local variance matrices but with different drift parameters, is based upon the absolutely continuous substitution of probability measures.[11] The results of this section generalize our previous results[12] to multidimensional diffusion processes in which rotational probability flows can occur. The mathematical idea of this section is originally due to Ezawa, Klauder, and Shepp.[13]

Consider a probability space Ω with a given, increasing family of σ-algebras $\{\mathcal{F}_t\}$ which is generated by all finite-dimensional Borel cylinder subsets of Ω. However, different probability measures on $\mathcal{F}$ can arise through the application of nonequilibrium, external constraints which, apart from perhaps a stationary component, are suddenly released.

Let X_t be an n-dimensional, time homogeneous diffusion process which is $\mathcal{F}_t$-measurable and a solution of the stochastic differential equation

$$dX_t = \sigma\, dW_t; \quad X_0 = x_0, \tag{1}$$

where $W = (W_1,...,W_n)$ is a standard Brownian motion. To the stochastic process X_t, there corresponds the probability measure $\mathcal{P}$. The coefficient matrix σ, with σ_{ij} $(i,j = 1,...,n)$, is related to the symmetric local variance or diffusion matrix D by $D = \frac{1}{2}\sigma\sigma^\dagger$ which is assumed to be both state and time-independent. Henceforth, the dagger will denote the transpose.

As a result of the application of a nonequilibrium, external constraint which, apart from a stationary component, is suddenly removed, a finite drift is created which tends to restore the system to its stationary state. If the entire external constraint is released then the system will evolve toward the state of thermodynamic equilibrium. Since the external constraint will have no influence on the diffusion matrix, because it is a characteristic of the medium, the process X_t will be converted into the process $\tilde{X}_t$ which is a solution of the stochastic differential equation

$$d\tilde{X}_t = J(\tilde{X}_t)\, dt + \sigma\, dW_t; \quad \tilde{X}_0 = x_0, \tag{2}$$

where J is the thermodynamic flux which has been created by the nonequilibrium constraint.

The decomposition of the thermodynamic flux must be consistent with: (i) the time-independent Fokker–Planck equation for the invariant probability density, $\tilde{p}_\infty$, from which we define the current velocity as

$$J(x) - D\nabla \ln \tilde{p}_\infty(x) \equiv \tilde{v}_\infty(x), \tag{3}$$

and (ii) Boltzmann's principle

$$\ln \tilde{p}_\infty(x) = S(x) + \text{const} \tag{4}$$

which relates the probability of a state to its entropy S. For $n > 1$, the probability current, $\tilde{p}_\infty \tilde{v}_\infty$, does not have to vanish in R^n even if it satisfies zero boundary conditions since *rotational* probability flows can occur.[14] The presence of rotational probability flows can be used in the characterization of *open*, as opposed to *isolated*, thermodynamic processes since there must be some form of energy transfer in order to sustain such flows.

The introduction of Boltzmann's principle (4) into the definition of the current velocity, (3), results in

$$J(x) = D\nabla S + \tilde{v}_\infty = D\chi(x), \tag{5}$$

where χ is the thermodynamic force,

$$\chi \equiv \nabla S + A, \tag{6}$$

writing $A \equiv D^{-1}\tilde{v}_\infty$. The thermodynamic force $\chi = (\chi_1,...,\chi_n)$ is assumed to be a nonanticipating process that causes the thermodynamic flux J. If the nonequilibrium constraint were to be removed completely, the rotational probability current would vanish and χ would coincide with the entropy gradient, tending to restore the system to thermodynamic equilibrium. If, however, there is a finite stationary constraint which prevents the system from relaxing to full equilibrium, rotational probability fluxes can develop.

Expression (6) is not to be intended as a vectorial decomposition of the thermodynamic force. Although the most interesting case is that in which A is completely solenoidal, it need not, in general, be the only case of physical interest. In regard to the expression for the thermodynamic flux, (5), it permits us to cast the continuity equation for the invariant probability density in the form

$$\nabla\cdot\tilde{p}_\infty \tilde{v}_\infty = (\tilde{v}_\infty\cdot\nabla S + \nabla\cdot\tilde{v}_\infty)\tilde{p}_\infty = 0\,. \tag{7}$$

Sufficient, but not necessary, conditions for satisfying the continuity equation (7) require the vanishing of both terms separately. The vanishing of the first term is commonly referred to as the "transversality" condition which necessarily implies the incompressibility condition. If J can be decomposed into a field that is essentially a gradient of a potential and a field that is both orthogonal to the gradient field and is divergence free then it can be shown that Boltzmann's principle is verified on the basis of an asymptotic expansion in terms of Boltzmann's constant.[15] However, our results are independent of the size of Boltzmann's constant, which can be used as a measure of the strength of the thermal fluctuations, and consequently we require only that the continuity equation (7) be satisfied. Nevertheless, the metrical transitivity property of the (stochastic) entropy imposes the condition of transversality, *on the average*, in the asymptotic time limit. Furthermore, we shall see that, in the Gaussian limit, the transversality condition is satisfied on the average at every instant in time provided the fluctuation-dissipation relation holds which is a sufficient condition for the stability of the second order moments of the distribution.

Although the current velocity has the formal appearance of a classical mechanical velocity, i.e., $\tilde{v}_\infty \to -\tilde{v}_\infty$ under time inversion, we cannot conclude, in general, that (5) is a decomposition of the flux into components that are even and odd against time reversal.[9] For then, the current velocity would be a Hamiltonian flow (derivable from a Hamiltonian) and therefore satisfy the incompressibility condition everywhere. Rather, the current velocity is to be associated with rotational probability currents that occur in open thermodynamic systems; it behaves in much the same way as the magnetic induction in electrodynamics. In isolated systems, $\tilde{v}_\infty$ vanishes and (5) reduces to the well-known phenomenological relations of linear irreversible thermodynamics that satisfy the Onsager reciprocity relations.

We are, therefore, considering multidimensional diffusion processes which are stationary in the wide sense and become strictly stationary with the passage of time. If all the nonequilibrium constraints are not released we cannot exclude the possibility of rotational probability flows. However, we do not make the Gaussian assumption which is tantamount to expressing the thermodynamic force as a linear function of the generalized displacements. Nevertheless, it will frequently be instructive to take the Gaussian limit where explicit results can be obtained. For non-Gaussian processes we rely on the decisive property of diffusion processes: The transition probability is, under certain regularity conditions, uniquely determined by the drift field J and the diffusion matrix D.[16] This is far from being a triviality since J and D are determined from the first two moments of a conditional distribution and a distribution is not, in general, determined solely by any two of its moments.

The application of a nonequilibrium constraint, which is subsequently and partially removed, leads us to consider a new probability measure $\tilde{\mathscr{P}}$ for the nonequilibrium thermodynamic process $\tilde{X}_t$ on the σ-algebra of the subsets of Ω. In other words, the diffusion processes X_t and $\tilde{X}_t$ possess the same sample functions but are considered as distinct stochastic processes with respect to their probability measures $\mathscr{P}$ and $\tilde{\mathscr{P}}$. Given the transition probability for the process X_t, we are able to derive the transition probability for the process $\tilde{X}_t$ in terms of it.

Since the probability measures $\mathscr{P}$ and $\tilde{\mathscr{P}}$ correspond to diffusion processes which can be obtained from one another by means of an absolutely continuous substitution of the probability measures on the probability space Ω, there exists the probability density

$$\frac{d\tilde{\mathscr{P}}}{d\mathscr{P}}(X(\omega)) = \rho_\tau(\omega), \tag{8}$$

known as the Radon–Nikodym derivative.[17] Here, $X_\cdot(\omega)$ stands for a sample function of the process X_t on the closed interval $[0,\tau]$ and ω is the sample tag. For any Borel set $\mathscr{B}$ belonging to the σ-algebra $\mathscr{F}_s$ at time $s<\tau$, we have

$$\int_{\mathscr{B}} \rho_s \, d\mathscr{P} = \tilde{\mathscr{P}}(\mathscr{B}) = \int_{\mathscr{B}} \rho_\tau \, d\mathscr{P}, \tag{9}$$

which means that the probability measure density ρ is a *martingale*, i.e, $\rho_s = E\{\rho_\tau|\mathscr{F}_s\}, \tau > s$. $E\{\cdot|\mathscr{F}_s\}$ denotes the conditional expectation with respect to the σ-algebra $\mathscr{F}_s$. In addition we have the normalization condition

$$E\{\rho_\tau\} = \int_\Omega \rho_\tau d\mathscr{P} = 1, \tag{10}$$

where $E\{\cdot\}$ denotes the mathematical expectation with respect to the probability measure $\mathscr{P}$. An explicit formula for the conditional expectation of the probability measure density can now be derived on the basis of a nonequilibrium thermodynamic principle. This will provide a transformation formula which relates the transition probability densities of the two diffusion processes.

The relative probability of observing a sample path belonging to the diffusion process $\tilde{X}_\tau$ in the infinitesimal range dX_τ is given by the nonequilibrium thermodynamic principle[12]

$$\frac{d\rho_\tau}{\rho_\tau} = \tfrac{1}{2}\chi^\dagger(X_\tau) dX_\tau. \tag{11}$$

In essence, we are deriving the statistics of the process $\tilde{X}_t$ in terms of the known process X_t. Apart from a numerical factor of $\frac{1}{2}$, which arises from the compatibility with equilibrium statistical thermodynamics in the asymptotic time limit, the right side of (11) can be interpreted physically as the increment in the virtual work that is required to convert the "free" diffusion process X_t into the nonequilibrium thermodynamic process $\tilde{X}_t$. The work is *virtual* inasmuch as the line integral of (11) is not the difference of a function of state. Thermodynamically speaking, the existence of statistical correlations between nonequilibrium states that are not well-separated in time destroys the additivity of $\ln\rho_\tau$ so that we cannot simply replace $d\rho_\tau/\rho_\tau$ by $d\ln\rho_\tau$. Stochastically speaking, the statistical correlations are described in terms of Brownian motion sample functions which although are continuous are nevertheless locally erratic. The increment dX_τ is not of the order $d\tau$, as it would be for a smooth differentiable function, but rather it is of order $\sqrt{d\tau}$ while its variance is

$$E\{dX_\tau dX_\tau^\dagger\} = 2D\, d\tau. \tag{12}$$

Hence, the presence of statistical correlations between nonequilibrium states that are not well-separated in time requires the use of stochastic rather than ordinary calculus.

In order to evaluate $d\ln\rho_\tau$, we apply the Itô chain rule of stochastic calculus[18] to obtain

$$d\ln\rho_\tau = d\rho_\tau/\rho_\tau - \tfrac{1}{2}(d\rho_\tau/\rho_\tau)^2, \tag{13}$$

where the second term in (13) is a concrete manifestation of the Brownian motion phenomenon (12). Introducing the nonequilibrium thermodynamic principle (11) into expression (13) and taking into account (12) leads to

$$d\ln\rho_\tau = \tfrac{1}{2}(\chi^\dagger dX_\tau - \tfrac{1}{2}D{:}\chi\chi^\dagger d\tau). \tag{14}$$

Integrating (14) on the closed interval $[0,\tau]$ results in

$$\ln\rho_\tau = \tfrac{1}{2}\int_0^\tau (\chi^\dagger dX_t - \tfrac{1}{2}D{:}\chi\chi^\dagger dt). \tag{15}$$

Expression (15) for the probability measure density is somewhat inconvenient since the first integral is an Itô stochastic integral. Physically, it expresses the fact that the nonequilibrium states are correlated statistically. A physically more transparent form can be derived in the following way. According to the Itô formula, the total derivative of the stochastic entropy, considered as a function of the diffusion process X_t, is

$$dS(X_t) = \nabla S^\dagger dX_t + D{:}\nabla\nabla S\, dt. \tag{16}$$

Note that on account of the time homogeneity of the diffusion process and Boltzmann's principle (4), the stochastic entropy cannot be an explicit function of time. Although the vector field A is not derivable from a scalar potential, we can however use the symmetric multiplication[19]

$$A^\dagger \circ dX_t = A^\dagger dX_t + \tfrac{1}{2}dA^\dagger dX_t = A^\dagger dX_t + D{:}\nabla A\, dt, \tag{17}$$

to transform the vector, Itô stochastic integral in (15) into the Fisk–Stratonovich symmetric stochastic integral. Introduc-

ing expressions (6), (16), and (17) into (15) results in

$$\ln \rho_\tau = \tfrac{1}{2}\{S(X_\tau) - S(x_0) + \int_0^\tau A^\dagger \circ dX_t - \int_0^\tau D{:}(\tfrac{1}{2}\chi\chi^+ + \nabla\chi)dt\}. \quad (18)$$

For future reference we shall refer to

$$V(x) = D{:}(\tfrac{1}{2}\chi\chi^\dagger + \nabla\chi) = \tfrac{1}{2}D{:}(\nabla S\nabla S^\dagger + AA^\dagger) + D{:}\nabla\nabla S, \quad (19)$$

as the Onsager–Machlup (OM) potential.[20] The second equality in (19) has been obtained by employing the continuity equation (7). Finally we remark that in those cases in which the incompressibility condition is satisfied, the two definitions of the stochastic integral coincide, since the last term in (17) vanishes.

The transition probability for the diffusion process $\tilde{X}_t$ is defined by[21]

$$\tilde{P}(\mathscr{B},\tau|x_0) = \tilde{\mathscr{P}}(\tilde{X}_\tau \in \mathscr{B}), \quad (20)$$

for any Borel subset $\mathscr{B}$ and $\tilde{X}_\tau$ is a solution of the stochastic differential equation (2) with initial condition $\tilde{X}_0 = x_0$. It now follows from (9) that

$$\tilde{P}(\mathscr{B},\tau|x_0) = \int_{X_\tau \in \mathscr{B}} \rho_\tau(\omega) d\mathscr{P}(\omega) = \int_{\mathscr{B}} \Phi(x,\tau|x_0) p(x,\tau|x_0)\, dx, \quad (21)$$

where

$$\Phi(x,\tau|x_0) = E\{\rho_\tau(\omega)|\mathscr{F}_\tau\}. \quad (22)$$

In addition, we know that the transition probability of the free diffusion process,

$$P(\mathscr{B},\tau|x_0) = \mathscr{P}(X_\tau \in \mathscr{B}), \quad (23)$$

has a density

$$p(x,\tau|x_0) = \{4\pi|D|\tau\}^{-1/2} \times \exp\{-(x-x_0)^\dagger (4\tau D)^{-1}(x-x_0)\}, \quad (24)$$

where $|\cdot|$ denotes the determinant. Expression (21) clearly shows that there exists a transition probability density $\tilde{p}$ corresponding to the transition probability $\tilde{P}$, viz.,

$$\tilde{P}(\mathscr{B},\tau|x_0) = \int_{\mathscr{B}} \tilde{p}(x,\tau|x_0)\, dx, \quad (25)$$

where

$$\tilde{p}(x,\tau|x_0) = \Phi(x,\tau|x_0)\cdot p(x,\tau|x_0) = \exp\{\tfrac{1}{2}[S(x) - S(x_0)]\} \cdot E\{\exp\left[\tfrac{1}{2}\int_0^\tau (A^\dagger \circ dX_t - V dt)\right] | X_\tau = x\} \cdot p(x,\tau|x_0). \quad (26)$$

In the second line of (26), we have explicitly written the endpoint condition in lieu of the σ-algebra in order to emphasize that Φ is a conditional Wiener integral with respect to the fixed endpoints of transitions.

Parenthetically, we note that the stochastic derivation of the transition probability density offers a rigorous justification for Feynman's choice of representing the vector potential integral as a symmetric integral where the vector potential is evaluated at the midpoint of each interval.[22] Expression (26) bears a formal similarity to the Feynman kernel for a charged particle in an electromagnetic field.

In the following section, we study the asymptotic behavior of the transition probability density (26) and introduce *quasithermodynamic* potentials in order to describe the statistical correlations between nonequilibrium states that are contained in the conditional Wiener integral (26).

III. ASYMPTOTIC BEHAVIOR AND QUASI-THERMODYNAMIC POTENTIALS

Although their probability measures are absolutely continuous with respect to one another, the two diffusion processes show completely different asymptotic behavior. For the Brownian motion process (1), the transition probability tends to zero in the course of time while the nonequilibrium process (2) is characterized by strictly stationary probability laws in the asymptotic time limit, provided there exists a physically acceptable solution to the continuity equation (7).

The transition probability $\tilde{P}$ will then admit an invariant or stationary probability distribution $\tilde{P}_\infty$ such that

$$\tilde{P}_\infty(\mathscr{B}) = \int_{R^n} \tilde{P}(\mathscr{B},\tau|x_0)\tilde{P}_\infty(dx_0). \quad (27)$$

It follows that the transition probability of the process $\tilde{X}_t$ has the property that

$$\lim_{\tau\to\infty} \tilde{P}(\mathscr{B},\tau|x_0) = \tilde{P}_\infty(\mathscr{B}), \quad (28)$$

expressing the fact that a dissipative system tends to forget its past. Since the invariant distribution $\tilde{P}_\infty$ has a density $\tilde{p}_\infty$, it follows from (28) that

$$\lim_{\tau\to\infty} \tilde{p}(x,\tau|x_0) = \tilde{p}_\infty(x), \quad (29)$$

where the invariant probability density is defined in terms of the entropy in accordance with Boltzmann's principle (4). The asymptotic form of the transition probability density (29) and Boltzmann's principle (4) can now be shown to lead to the introduction of quasithermodynamic potentials when there is not a long time lapse between nonequilibrium states. We shall further show that the quasi-thermodynamic potentials reduce to thermodynamic state functions in the asymptotic time limit where the statistical correlations have had ample time to have worn off.

The diffusion operator

$$\mathscr{L} = J(x)\cdot\nabla + D{:}\nabla\nabla, \quad (30)$$

is assigned to the process $\tilde{X}_t$. The transition probability density $\tilde{p}$ satisfies both the backward

$$\partial_\tau \tilde{p} = \mathscr{L}_0 \tilde{p}, \quad (31)$$

and forward

$$\partial_\tau \tilde{p} = \mathscr{L}^\dagger \tilde{p}. \quad (32)$$

Kolmogorov equations with initial condition

$$\tilde{p}(x,\tau|x_0) = \delta(x - x_0) \quad \text{as } \tau\downarrow 0. \quad (33)$$

The subscript on the diffusion operator in (31) indicates differentiation with respect to the initial coordinates of the transition and $\mathscr{L}^\dagger$ is the adjoint, viz.,

$$\mathscr{L}^\dagger = -\nabla\cdot J(x) + D{:}\nabla\nabla. \quad (34)$$

In an analogous way that we have defined the current velocity from the time independent Fokker–Planck equation for the invariant probability density, we now define the transitional velocity[12]

$$\tilde{v}(x,\tau|x_0)\equiv J(x) - D\nabla \ln \tilde{p}(x,\tau|x_0), \tag{35}$$

from the Fokker–Planck equation (32). Observe that, unlike J, $\tilde{v}$ is a *nonlocal* function. Furthermore, $\tilde{v}$ transforms as $\tilde{v}\rightarrow -\tilde{v}$ under time reversal while the transitional velocity

$$\tilde{u}(x,\tau|x_0)\equiv D\nabla \ln \tilde{p}(x,\tau|x_0), \tag{36}$$

is invariant under time inversion. By virtue of the asymptotic condition (29),

$$\lim_{\tau\to\infty}\tilde{v}(x,\tau|x_0) = \tilde{v}_\infty(x); \quad \lim_{\tau\to\infty}\tilde{u}(x,\tau|x_0) = \tilde{u}_\infty(x), \tag{37}$$

$\tilde{u}_\infty$ is referred to as the "fluctuating" or "osmotic" velocity in the Einstein theory of equilibrium fluctuations.[23]

The pair of Kolmogorov equations, (31) and (32), can be transformed into a pair of self-adjoint equations that is closely allied with the Schrödinger equation. To this end, we write

$$\tilde{p}(x,\tau|x_0) = \exp\{\tfrac{1}{2}[S(x) - S(x_0)]\}\cdot K(x,\tau|x_0), \tag{38}$$

where the kernel, K, is defined as the conditional Wiener integral:

$$K(x,\tau|x_0) = E\left\{\exp\left[\tfrac{1}{2}\int_0^\tau (A^\dagger \circ dX_t - V\,dt)\right]|X_\tau = x\right\} \cdot p(x,\tau|x_0). \tag{39}$$

The kernel expression (39) can be considered as a generalization of the Feynman–Kac formula[24] insofar as it expresses the kernel as a conditional Wiener integral of a vector A as well as a scalar potential V. Since the transition probability satisifies the pair of Kolmogorov equations, (31) and (32), the kernel satisfies the pair of diffusion equations:

$$\partial_\tau K = (\nabla_0 + \tfrac{1}{2}A)^\dagger D(\nabla_0 + \tfrac{1}{2}A)K - \tfrac{1}{2}V(x_0)K, \tag{40}$$

$$\partial_\tau K = (\nabla - \tfrac{1}{2}A)^\dagger D(\nabla - \tfrac{1}{2}A)K - \tfrac{1}{2}V(x)K, \tag{41}$$

with the initial condition

$$K(x,\tau|x_0) = \delta(x - x_0) \text{ as } \tau\downarrow 0. \tag{42}$$

The derivation of the pair self-adjoint diffusion equations, (40) and (41), has made use of the continuity equation (7). They bear a formal similarity to the Schrödinger equation for a charged particle in an electromagnetic field A with scalar potential V.

The "gradient" transformation (38) has served to transform the original problem, (31) and (32), into a Sturm–Liouville problem, (40) and (41); with "natural" boundary conditions.[25] The asymptotic analysis can now be carried out in terms of a hierarchy of eigenvalues whose inverse represents the set of characteristic relaxation times of the nonequilibrium thermodynamic diffusion process. Provided that all eigenvalues are distinct and bounded from below by the zero eigenvalue, an invariant probability distribution exists which is approached asymptotically in time by the transition probability. In consideration of Boltzmann's principle, this means that

$$\lim_{\tau\to\infty} K(x,\tau|x_0) = \tfrac{1}{2}\{S(x) + S(x_0)\} + \text{const.} \tag{43}$$

The asymptotic form (43) implies that a long lapse in time leaves the nonequilibrium states statistically independent (i.e., asymptotic independence). It should therefore be expected that the probability of a given state, at different instants in time, be equal to the product of their probabilities an *any* instant in time (i.e., strong mixing). In conjunction with Boltzmann's principle (4), the strong mixing property implies that the entropy be metrically transitive or ergodic in the asymptotic time limit.

If, however, the time lapse is not long, the nonequilibrium states through which the processes passes at successive instants in time will be correlated statistically. It is apparent that these statistical correlations cannot be described by thermodynamic functions of state; that is, the kernel will enjoy the thermodynamic additive property (43) only in the asymptotic time limit. This consideration motivates the definition of a quasi-thermodynamic potential, viz.,[12]

$$\ln K(x,\tau|x_0)\equiv \tfrac{1}{2}\sigma_J(x,\tau;x_0) + \text{const.} \tag{44}$$

σ_J is known as the "joint" entropy; it is a quasithermodynamic potential inasmuch as it is a function of both endpoints of transition as well as the time interval of transition in the case of time homogeneous diffusion processes. The joint entropy accounts for the statistical correlations between nonequilibrium states that are not well-separated in time. Nevertheless, the asymptotic form of the kernel (43) and the definition of joint entropy (44) require

$$\lim_{\tau\to\infty}\sigma_J(x,\tau;x_0) = S(x) + S(x_0). \tag{45}$$

How this limit is approached is embodied in the stochastic H-theorem which is given in the next section.

To prove (45), we introduce the logarithmic transformation (44) into the pair of diffusion equations, (40) and (41). We then obtain the pair of generalized Hamilton–Jacobi equations

$$-\partial_\tau\sigma_J + \tfrac{1}{2}(\nabla_0\sigma_J + A)^\dagger D{:}(\nabla_0\sigma_J + A) + D{:}\nabla_0(\nabla_0\sigma_J + A) = V(x_0), \tag{46}$$

$$-\partial_\tau\sigma_J + \tfrac{1}{2}(\nabla\sigma_J - A)^\dagger D(\nabla\sigma_J - A) + D{:}\nabla(\nabla\sigma_J - A) = V(x), \tag{47}$$

where it will be appreciated that the joint entropy plays the role of a generalized classical action. We now solve Eqs. (46) and (47) and their common, particular, stationary solution ($\partial_\tau\sigma_J = 0$).

The stationary solution of Eq. (46) is imposed by the form of OM potential (19). Integrating, we obtain

$$\sigma_J(x,\tau = \infty;x_0) = S(x_0) + C(x). \tag{48}$$

The constant of integration, C, is to be determined by the stationary solution of (47). By virture of the continuity equation (7) for invariant probability density, we obtain $S(x)$ + const as the stationary solution Eq. (47) and on matching the constants of integration, we have

$$\sigma_J(x,\tau = \infty;x_0) = S(x) + S(x_0). \tag{49}$$

The only condition, used in the derivation of (49), is that the invariant probability density satisfy the continuity equation (7).

Introducing definition (44) into expression (38) and taking the logarithm of both sides give

$$\ln \tilde{p}(x,\tau|x_0) = \tfrac{1}{2}\{S(x) - S(x_0) + \sigma_J(x,\tau;x_0)\} + \text{const} \tag{50}$$

which we have shown to yield the correct asymptotic form, namely Boltzmann's principle (4). It is in this limit that we regain statistical independence. Over smaller time intervals, (50) provides information regarding the statistical correlations between nonequilibrium states. It is in this sense that we have referred to (50) as the *kinetic* analogue of Boltzmann's principle.[12] Here, we have generalized it to include rotational probability currents which can only occur in multidimensional diffusion processes occurring in open thermodynamic systems.

In the next section we show how asymptotic independence is approached in the asympotic time limit in terms of the quasi-thermodynamic potential

$$\sigma_C(x,\tau|x_0) \equiv \sigma_J(x,\tau;x_0) - S(x_0), \tag{51}$$

which is known as the "conditional" entropy.[12] On the strength of (45), we have

$$\lim_{\tau\to\infty} \sigma_C(x,\tau|x_0) = S(x) \tag{52}$$

affirming that a dissipative system forgets its past. The average behavior of the conditional entropy in respect to the entropy comprises the stochastic H-theorem. We preface our derivation by noting that results—which have a similar formal appearance to ours—have appeared in the literature.[7-10] This formal similarity stems from the fact that a time dependent probability density is used in place of the transition probability density. The stationarity property of the diffusion process has been artifically relinquished and this attests to the absence of a physical mechanism governing the proposed H-theorems. We shall remedy this situation by showing that the statistical correlations are, *on the average*, a decreasing function of the time interval of separation of the nonequilibrium states.

IV. STOCHASTIC EVOLUTION CRITERION

A stochastic evolutionary criterion is now derived which is valid for both isolated and open thermodynamic systems provided that the continuity equation (7) is satisfied. In spirit, it is closely allied to the Gibbs generalized H-theorem with the important difference that the transition probability density is used in place of the coarse-grained density. By virtue of the kinetic analogue of Boltzmann's principle (50), a physical mechanism can be invoked that is responsible for the evolution of the nonequilibrium thermodynamic process toward either thermodynamic equilibrium or a nonequilibrium stationary state, depending on the imposed constraints.

de Groot and Mazur[26] refer to the negative of the quantity

$$H_\tau = \int_{R^n} \tilde{p}(x,\tau|x_0)\cdot\ln\{\tilde{p}(x,\tau|x_0)/\tilde{p}_\infty(x)\}dx, \tag{53}$$

as the "Gibbs entropy postulate." They identify the left side of (53) with $-\Delta S^G$. We prefer to identify H_τ with

$$H_\tau = \tfrac{1}{2}\tilde{E}\{\sigma_C(\tilde{X}_\tau,\tau|x_0) - S(\tilde{X}_\tau)\} \tag{54}$$

on the strength of the kinetic analogue of Boltzmann's principle, (50). According to (52), this quantity is expected to asymptotically tend to zero. The manner in which H_τ tends to zero constitutes the stochastic evolutionary criterion.

In the first place, we establish

$$H_\tau \geqslant 0. \tag{55}$$

This is accomplished by adding $\tilde{p}(\tilde{p}_\infty/\tilde{p} - 1)$ to the integrand of (53) since the effect of these two terms cancel out on integration. Then, from the simple inequality

$$\ln(1/x) + x - 1 \geqslant 0, \tag{56}$$

it follows that the stochastic H-function is positive semidefinite. Physically this means that

$$\tilde{E}\{\sigma_J(\tilde{X}_\tau,\tau;x_0)\} \geqslant \tilde{E}\{S(\tilde{X}_\tau)\} + S(x_0), \tag{57}$$

stating that the statistical correlations between nonequilibrium states produce an entropy in addition to that of the nonequilibrium states.

In the second place, we establish that the stochastic H-function is a monotonically decreasing function of the time lapse between nonequilibrium states. Let $g(x,\tau)$ be a bounded measurable function and define the mean forward stochastic derivative of g as

$$\begin{aligned}\mathscr{D}g(\tilde{X}_\tau,\tau) &= \lim_{s\downarrow 0} s^{-1}\{\mathscr{T}_s g(x,\tau) - g(x,\tau)\} \\ &= (\partial_\tau + \mathscr{L})g(\tilde{X}_\tau,\tau),\end{aligned} \tag{58}$$

where $\mathscr{L}$ is the diffusion operator, defined by (30), and $\mathscr{T}$ is the shift operator

$$\begin{aligned}\mathscr{T}_s g(x,\tau) &= \tilde{E}\{g(\tilde{X}_{\tau+s},\tau+s)|\tilde{X}_\tau = x\} \\ &= \int_{R^n} g(y,\tau+s)\tilde{P}(dy,\tau+s|x,\tau).\end{aligned} \tag{59}$$

The random variable $\mathscr{D}g(\tilde{X}_\tau,\tau)$ is automatically $\tilde{\mathscr{P}}$-measurable. It will now be appreciated that the total time derivative of H_τ coincides with the conditional expectation of the mean forward derivative of the quantity, $\frac{1}{2}(\sigma_C - S)$, viz.,

$$d_\tau H_\tau = \tfrac{1}{2}\tilde{E}\{\mathscr{D}[\sigma_C(\tilde{X}_\tau,\tau|x_0) - S(\tilde{X}_\tau)]\}, \tag{60}$$

which is equivalent to

$$d_\tau H_\tau = \int_{R^n} \partial_\tau \tilde{p}(x,\tau|x_0)\cdot\ln\{\tilde{p}(x,\tau|x_0)/\tilde{p}_\infty(x)\}dx. \tag{61}$$

Introducing the Fokker–Planck equation and integrating by parts, we obtain the fundamental inequality

$$d_\tau H_\tau = -\int_{R^n} (\nabla \ln \tilde{p}/\tilde{p}_\infty)^\dagger D(\nabla \ln \tilde{p}/\tilde{p}_\infty)\tilde{p}(x,\tau|x_0)dx \leqslant 0, \tag{62}$$

on account of the natural boundary conditions. In the derivation of (62) we have written the transitional velocity $\tilde{v}$ in the form

$$\tilde{v}(x,\tau|x_0) = \tilde{v}_\infty(x) + D\nabla \ln(\tilde{p}_\infty/\tilde{p}) \tag{63}$$

and made use of the continuity equation (7). In the next section we shall see that thanks to the continuity equation (7), all terms in which the rotational probability current appears explicitly cancel out. The quadratic form (62) attests to the fact that H_τ changes *essentially* by dissipation. The wearing off of the statistical correlations between nonequilibrium states means that a predominantly dissipative system tends

to forget its past and this is what is responsible for the transformation of the transition probability into the invariant probability distribution in the asymptotic time limit.

The same cannot be said of the Gibbs entropy, defined in terms of the coarse-grained probability density, or of a nonequilibrium H-function which uses a time dependent probability density in its definition.[7-10] *A nonstationary diffusion process, in the wide sense, does not become stationary, in the strict sense simply with the passage of time.* Furthermore, the stochastic H-theorem tells us how the approach to the invariant probability distribution is achieved: The additional entropy due to the statistical correlations between nonequilibrium states is, *on the average*, a decreasing function of the time interval of separation. This appears as a universal characteristic of all predominantly dissipative systems.

V. COMPARISON WITH THE SECOND LAW

The question now arises as to the connection between the stochastic H-function and the second law of thermodynamics. To this end, we write the stochastic H-function in the form

$$H_\tau = \tilde{E}\{\ln \tilde{p}(\tilde{X}_\tau,\tau|x_0) - \ln \tilde{p}_\infty(\tilde{X}_\tau)\} \tag{64}$$

and analyze the time derivative of each term separately. The mean forward derivative of $\ln \tilde{p}$ is

$$\begin{aligned}\mathscr{D}\ln\tilde{p} = & -\tilde{p}^{-1}\nabla\cdot\tilde{p}\tilde{v} + \tilde{p}^{-1}D:\nabla\nabla\tilde{p} \\ & + J\cdot\nabla\ln\tilde{p} - D:(\nabla\ln\tilde{p})(\nabla\ln\tilde{p})^\dagger,\end{aligned} \tag{65}$$

where we have used the Fokker–Planck equation (32) and the Itô chain rule of stochastic calculus

$$d\ln\tilde{p} = d\tilde{p}/\tilde{p} - \tfrac{1}{2}(d\tilde{p}/\tilde{p})^2. \tag{66}$$

The conditional expectation of (65) is

$$\begin{aligned}\tilde{E}\{\mathscr{D}\ln\tilde{p}\} = \int_{R^n}\{&\tilde{v}_\infty\cdot\nabla\ln\tilde{p} \\ & + D:\nabla\ln\tilde{p}(\nabla\ln\tilde{p}_\infty/\tilde{p})^\dagger\}\tilde{p}\,dx.\end{aligned} \tag{67}$$

Integrating the first time by parts and on account of the natural boundary conditions, we obtain

$$d_\tau\tilde{E}\{\ln\tilde{p}\} = -\tilde{E}\{\nabla\cdot\tilde{v}_\infty + D:\nabla\ln\tilde{p}(\nabla\ln\tilde{p}/\tilde{p}_\infty)^\dagger\}. \tag{68}$$

The total time derivative of the second time term in (64),

$$d_\tau\tilde{E}\{\ln\tilde{p}_\infty\} - \tilde{E}\{\tilde{\nabla}_\infty\cdot\nabla\ln\tilde{p}_\infty + D:\nabla\ln\tilde{p}_\infty(\nabla\ln\tilde{p}_\infty/\tilde{p})^\dagger\},$$

is precisely what is needed in order to complete the square in (68) and to eliminate the first term by virtue of the continuity equation (7). The difference between (68) and (69) is the negative semidefinite quadratic form (62).

According to Boltzmann's principle (4), expression (69) is the time derivative of the conditional expectation of the stochastic entropy. In the asymptotic time limit we have

$$\begin{aligned}&\lim_{\tau\to\infty} d_\tau\tilde{E}\{S(\tilde{X}_\tau)\} \\ &\quad = \lim_{\tau\to\infty}\tilde{E}\{\mathscr{D}S(\tilde{X}_\tau)\} = \tilde{E}\{v_\infty\cdot\nabla S\} = -\tilde{E}\{\nabla\cdot\tilde{v}_\infty\}.\end{aligned} \tag{70}$$

The invariant probability distribution has the property that

$$\tilde{P}^\tau_\infty(\mathscr{B}) = \tilde{\mathscr{P}}(\tilde{X}_\tau\in\mathscr{B}) = \tilde{P}^0_\infty(\mathscr{B}) \tag{71}$$

in the asymptotic time limit. In this limit, the process becomes strictly stationary so that the limiting distribution is left invariant under arbitrary shift transformations. In terms of Boltzmann's principle, this means that the stochastic entropy will become metrically transitive or ergodic in the asymptotic time limit. The condition which guarantees the metrical transitive property of the stochastic entropy is given by (70): The transversality condition is satisfied, *on the average*,

$$\tilde{E}\{\tilde{v}_\infty\cdot\nabla S\} = 0, \tag{72}$$

where $\tilde{E}$ is the mathematical expectation with respect to the invariant probability density.

It is clear from (69) that the conditional expectation of the stochastic entropy will not, in general, display a monotonic tendency to increase in time. Specializing to Gaussian fluctuations, we show this hinges on an appropriate choice of the initial conditions. The reason is that the entropy has been defined in terms of a single state in contrast to the Gibbs definition as a distribution over states. In other words, if the initial state could be made to coincide with the most probable state, compatible with the external constraints, then there would be a finite probability to observe states with lower entropy in the course of time.

Gaussian diffusion processes have a drift field given by

$$J(x) = Gx, \tag{73}$$

and an entropy difference

$$S(x) - S_0 = -\tfrac{1}{2}Q_\infty^{-1}:xx^\dagger, \tag{74}$$

where G is a state and time independent transport matrix, with no particular symmetry properties, and Q_∞ is the asymptotic form of the matrix of the second order moments. The existence of Q_∞ depends on whether there is a stationary, unique and bounded solution to the matrix equation

$$d_\tau Q_\tau = GQ_\tau + Q_\tau G^\dagger + 2D; \quad Q_{t=0} = Q_0 > 0, \tag{75}$$

where Q_τ is the matrix of the second order moments that are defined as the conditional expectation

$$Q_\tau \equiv \tilde{E}_{x_0}\{\tilde{X}_\tau\tilde{X}_\tau^\dagger\}. \tag{76}$$

The condition of stationarity is

$$GQ_\infty + Q_\infty G^\dagger = -2D, \tag{77}$$

which is known as the fluctuation-dissipation relation.[27] Provided G is a stability matrix, i.e., all of its characteristic roots have negative real parts, there will exist the unique and bounded solution

$$Q_\infty = 2\int_0^\infty \Lambda_t D\Lambda_t^\dagger dt, \tag{78}$$

to the fluctuation-dissipation relation (77) where Λ_t is the fundamental matrix associated with G, viz., $\Lambda_t = \exp(Gt)$:

For Gaussian diffusion processes, (78) provides the link between kinetics and thermodynamics. For a given diffusion matrix D, the equilibrium second order moments are uniquely defined in terms of the phenomenological transport matrix, G. Moreover, (78) relates the asymptotic properties of Gaussian diffusion processes to their asymptotic stability properties. This can be substantiated further by considering the stochastic H-function.

The mean and covariance functions of the nonequilibrium thermodynamic process X_t are

$$E_{x_0}\{\tilde{X}_t\} = \Lambda_t x_0; \quad \tilde{E}_{x_0}\{(\tilde{X} - \Lambda_t x_0)(\tilde{X} - \Lambda_t x_0)^\dagger\} = C_t,$$

where $C_t = Q_\infty - \Lambda_t Q_\infty \Lambda_t^\dagger$. The two moments determine the transition probability density, viz.,

$$\tilde{p}(x,\tau|x_0) = \{(2\pi)^n |C_\tau|\}^{-1/2} \cdot \exp\{-\tfrac{1}{2} C_\tau^{-1} : (x - \Lambda_\tau x_0)(x - \Lambda_\tau x_0)^\dagger\}, \quad (79)$$

while Boltzmann's principle determines the invariant probability density,

$$\tilde{p}_\infty(x) = \{(2\pi)^n |Q_\infty|\}^{-1/2} \cdot \exp(-\tfrac{1}{2} Q_\infty^{-1} : xx^\dagger). \quad (80)$$

Equipped with expressions (79) and (80), we can now construct the stochastic H-function.

The stochastic H-function reads

$$H_\tau = -\tfrac{1}{2}\ln(|Q_\infty^{-1}||C_\tau|) + \tfrac{1}{2} Q_\infty^{-1} : \Lambda_\tau (Q_0 - Q_\infty)\Lambda_\tau^\dagger. \quad (81)$$

In order to show that (81) is positive semidefinite—independent of the choice of the initial conditions—we write it in the form

$$H_\tau = -\tfrac{1}{2}\ln(|I - A|) - \tfrac{1}{2}\mathrm{tr}(A - A_0), \quad (82)$$

where I is the identity matrix, $A \equiv Q_\infty^{-1}\Lambda_\tau Q_\infty \Lambda_\tau^\dagger$, and $A_0 \equiv Q_\infty^{-1}\Lambda_\tau Q_0 \Lambda_\tau^\dagger$. Setting $Y = I - A$ and using the determinant inequality, $|Y| \leqslant \Pi_{i=1}^n y_{ii}$, we conclude that (81) is positive semidefinite for arbitrary initial conditions because

$$\sum_i^n (y_{ii} - \ln y_{ii}) - n \geqslant 0.$$

In comparison to (81), the condition expectation of the stochastic entropy is

$$\Delta S^B \equiv \tilde{E}_{x_0}\{S(\tilde{X}_\tau) - S_0\} = \tfrac{1}{2}\mathrm{tr}(A - A_0). \quad (83)$$

de Groot and Mazur[28] argue that $\Delta S^G \to \Delta S^B$, where the former is the Gibbs entropy difference which they have set equal to the negative of expression (81), for "macroscopic" initial conditions and for finite time intervals. They contend that whereas $\mathrm{tr}A_0$ is of the order of the number of particles in the system, $\mathrm{tr}A$ is of the order of the number of independent, fluctuating thermodynamic variables that are required to characterize the system thermodynamically. Since the former is overwhelmingly greater than the latter and for finite time intervals where the logarithmic term in (81) becomes negligible, the Boltzmann and Gibbs definitions of the entropy coincide.

On the one hand, the time derivative of the stochastic H-function, (81), is

$$d_\tau H_\tau = \tfrac{1}{2}\mathrm{tr}\{(I - A)^{-1} A\, d_\tau A + d_\tau A_0\} \leqslant 0, \quad (84)$$

provided G is a stability matrix since then both $d_\tau A_0 = Q_\infty^{-1}\Lambda_\tau (GQ_0 + Q_0 G^\dagger)\Lambda_\tau^\dagger \leqslant 0$ and $d_\tau A = -2Q_\infty^{-1}\Lambda_\tau D \Lambda_\tau^\dagger \leqslant 0$ on the strength of the fluctuation-dissipation relation (77). On the other hand, the time derivative of the Boltzmann entropy is

$$d_\tau \Delta S^B = \tfrac{1}{2}\mathrm{tr}(d_\tau A - d_\tau A_0),$$

which cannot be shown to possess a definite sign unless recourse is made to arguments involving "macroscopic" initial conditions.[28] Indeed, if there existed an unlimited precision by which the initial state could be made to coincide with the most probable state (i.e., $Q_0 = 0$), then the stochastic H-function would *still* show a monotonic tendency to decrease in the course of time while ΔS^B, according to (85), would show the same tendency. If the identification $H_\tau \leftrightarrow -\Delta S^G$ were now made, we would obtain the paradoxical result that the Gibbs entropy would continue to increase in time even though the system was initially found in the most probable state! Therefore, for certain initial conditions, the Boltzmann and Gibbs entropies show opposing tendencies. It is only for nearly deterministic systems (i.e., "macroscopic" initial conditions), where the effects of fluctuations have a secondary role, that the Boltzmann and Gibbs definitions of the entropy can be shown to be compatible. Thus, in order to account for nonequilibrium fluctuations, the stochastic H-function must be interpreted in accordance with the kinetic analogue of Boltzmann's principle (50).

de Groot and Mazur have further argued that over finite time intervals, the logarithmic term in the stochastic H-function expression (81) is of negligible importance. On the strength of the kinetic analogue of Boltzmann's principle, we can appreciate that the time rate of change of this term is a measure of the rate of decay of the statistical correlations. For the Gaussian diffusion process under consideration, we have

$$\tilde{E}\{\mathscr{D}\sigma_C\} = -\tilde{E}\{\mathscr{D}S\} + (I - A)^{-1} : d_\tau A. \quad (86)$$

Recalling the physical significance of the conditional entropy, we can appreciate that the second term in (86) is the rate at which the statistical correlations decay. It therefore becomes clear that de Groot and Mazur have addressed themselves to the case in which the deterministic factors predominate on account of the large initial displacement from thermodynamic equilibrium and sufficiently large time intervals are considered so that the statistical correlations between nonequilibrium states have had ample time to have worn off. In this case, (86) shows that the average rates of change of the conditional and stochastic entropies are approximately equal in magnitude and opposite in sign. The rate of change of the stochastic H-function therefore becomes approximately equal to the negative of the time rate of change of conditional expectation of the stochastic entropy.

In conclusion, we note that the transversality condition will be satisfied, *on the average at every instant in time*, by the Gaussian process under consideration. That is,

$$\begin{aligned}&\tilde{E}_{x_0}\{\tilde{v}_\infty \cdot \nabla S(\tilde{X}_\tau)\} \\ &= \tilde{E}_{x_0}\{(Q_\infty^{-1}\tilde{X}_\tau)^\dagger G \tilde{X}_\tau\} - \tilde{E}_{x_0}\{(Q_\infty^{-1}\tilde{X}_\tau)^\dagger D (Q_\infty^{-1}\tilde{X}_\tau)\} \\ &= Q_\tau : \{Q^{-1}G + Q_\infty^{-1} D Q_\infty^{-1}\} = 0, \end{aligned} \quad (87)$$

where the matrix of the second order moments has been defined according to (76). Since Q_τ is a positive definite symmetric matrix, it follows that the symmetric part of the second factor must vanish. This is precisely the fluctuation-dissipation relation (77). Recalling that a unique and bounded solution to the fluctuation-dissipation relation exists only in the case that G is a stability matrix [cf. Eq. (78)], we conclude that (87) is a *sufficient* condition for the asymptotic stability of the Gaussian process.[29]

ACKNOWLEDGMENT

We would like to thank an unknown referee for having pointed out that the stochastic H-theorem is more general than we had previously imagined.

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Mean field approximations for U(*N*) and SU(*N*) lattice gauge theories

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(Received 28 January 1982; accepted for publication 13 May 1982)

A particular parametrization of the groups U(N) and SU(N) is constructed by observing that the sphere S^{2N-1} is homeomorphic to the factor spaces U(N)/U($N-1$) or SU(N)/SU($N-1$) and continuing the corresponding fibration. The spheres are naturally embedded into Euclidean spaces and thus allow an extension of the mean field approximation by a saddle-point method to U(N) and SU(N) lattice gauge theories. It differs from the standard variational approach, the result of which can also be obtained by embedding the group into the Euclidean space of matrices. For both approaches the phase transition points are calculated and compared with the results of Monte-Carlo simulations. The best agreement is obtained for the standard variational approach with axial gauge fixing.

PACS numbers: 05.50. + q

I. INTRODUCTION

The functional approach to the mean field theory[1] of chiral or gauge models on lattices makes use of an embedding of the group manifold into a real linear space. This linear space is needed for a Fourier transformation with a subsequent deformation of the integration contours. The most elementary cases are the group U(1) whose manifold S^1, the unit circle, is trivially embedded into C^1 or R^2, and the group SU(2) whose manifold is considered as the unit sphere S^3 in R^4. For groups U(N), $N>1$, and SU(N), $N>2$, it is no longer obvious how to perform the embedding.

We emphasize that the construction of the real linear space is by no means unique if no further constraint is imposed. For example, we can always use an $N\times N$ complex matrix realization of the groups U(N) or SU(N), which suggests the trivial embedding of these groups into the $2N^2$ dimensional real vector space of complex $N\times N$ matrices. The standard variational approach[2] can be viewed as such an embedding with the translation invariant mean field proportional to the unit matrix. We show in this article that U(N) [SU(N)] can locally be embedded into an $N^2+N(N^2+N-2)$ dimensional linear space. This embedding is local in the sense of nontrivial fiber bundles, and entails that the mean field itself is expressed in terms of a local coordinate system.

Our construction[3] is based on the fact that the group manifold U(N) [SU(N)] can be represented as a fiber bundle with the factor space U(N)/U($N-1$) [SU(N)/SU($N-1$)] as base space and U($N-1$) [SU($N-1$)] as fibers, and that this fibration can be continued with U($N-1$) [SU($N-1$)]. It ends with U(1), respectively, SU(2). The base space U(N)/U($N-1$) [SU(N)/SU($N-1$)] is homeomorphic to the sphere S^{2N-1}, which can trivially be embedded into R^{2N} or C^N.

The functional approach uses a reparametrization of the Gibbs measure to obtain an extremal field configuration, which is called "mean field" in this context. A systematic asymptotic expansion can be derived if fluctuations of increasing order are taken into account. For a given system of parameters, on the other hand, an upper bound for the free energy density (lower bound for ln Z) can be derived by a variational principle.[2] Again we call the extremal configuration "mean field." Of course, the mean fields resulting from the functional and the variational approach need not be identical. They are identical in the case of the embedding of the group into $2N^2$ dimensional matrix space, but they turn out to be different for the case of local spherical coordinates, which we study in this article.

In view of Elitzur's theorem[4] the question whether the mean field methods are compatible with gauge invariance have provoked some confusion. In a gauge invariant formulation a mean field configuration is in general a representative of an orbit generated by the local gauge group or even a larger gauge invariant manifold, and expectations ought to be identified in the mean field approximation with averages over this manifold. After a complete gauge fixing the mean field may become unique with respect to the method adopted. In general a systematic saddle-point expansion involves similar problems with gauge fixing as standard perturbation theory. Another question is whether gauge fixing improves the mean field approximation.

Mean field approximations for U(N) and SU(N) lattice gauge theories yield first order phase transitions at some points $\beta_c(d,N)$ for all dimensions $d>2$ and all N. Monte-Carlo simulations reveal for $d=4$ a second order phase transition in the case of U(1)[5] and first order phase transitions for U(N), $N\geqslant 2$[6] and SU(N), $N\geqslant 4$.[7] Numerical values of the standard variational approach without gauge fixing have been published in a series of articles.[8] These authors calculate a point which has no thermodynamical meaning in the mean field approximation, denote it β_c, and call it "phase transition point" (in the earliest article) or "critical point" and "transition point" (in the later articles) though it has no relation to the phase transition point. They compare it with the "crossover point" or the phase transition points known from the Monte-Carlo results and claim an excellent agreement.

In this paper we develop the spherical embedding method and compare its phase transition points with those obtained from the standard matrix embedding approach. Confronting these numerically calculated phase transition points with published Monte-Carlo simulations it turns out that the Monte-Carlo phase transitions are best—and in fact remarkably closely—reproduced by the standard matrix

 0022-2488/82/122461-06$02.50

embedding method with axial gauge fixing imposed. In Sec. II the spherical embedding of the groups U(N) and SU(N) is constructed. Based on this embedding mean field approximations for gauge models within a functional approach are worked out and analyzed in Sec. III. An independent link variational mean field derived from the same parametrization is shown to be different in Sec. IV. Finally, in Sec. V the critical values of the standard matrix embedding mean field for U(N) are calculated. The numerical results following from both embedding procedures are compared with Monte-Carlo simulations.

II. GROUP FIBERING AND EMBEDDING

Consider the group U(N) [SU(N)] as acting on the complex vector space C^N. This space decomposes into orbits which are spheres of radius

$$|z| = \left(\sum_{i=1}^{N} |z_i|^2 \right)^{1/2} \tag{1}$$

or the null orbit $\{z = 0\}$. Each sphere is homeomorphic to the factor space U(N)/U($N-1$)[SU(N)/SU($N-1$)]. Indeed, let ζ, $z \in C^N$

$$\zeta = (1,0,0,\ldots,0), \tag{2}$$

$$z = (z_1,z_2,z_3,\ldots,z_N); \quad |z| = 1. \tag{3}$$

Then any $u \in$ U(N) [SU(N)] satisfying

$$z = u\zeta \tag{4}$$

implies

$$\begin{aligned} &u = u_z v, \\ &u_z, v \in \mathrm{U}(N)\ [\mathrm{SU}(N)], \end{aligned} \tag{5}$$

with

$$u_z = \begin{pmatrix} z_1 & \cdots & \cdot \\ z_2 & \cdots & \cdot \\ \vdots & & \\ z_N & \cdots & \cdot \end{pmatrix}, \tag{6}$$

$$v = \begin{pmatrix} 1 & 0 \\ 0 & \tilde{v} \end{pmatrix}, \tag{7}$$

$\tilde{v} \in$ U($N-1$) [SU($N-1$)].

The factor v depends of course on how the remaining columns of u_z are defined as functions of z. Each definition represents a local coordinate system (chart) on U(N)/U($N-1$) [SU(N)/SU($N-1$)].

For definiteness we construct a covering set of charts (an atlas). Denote

$$\gamma_n = \left(\sum_{i=1}^{n} |z_i|^2 \right)^{1/2} \tag{8}$$

and set

$$u_z = \begin{bmatrix} z_1 & -\bar{z}_2/\gamma_2 & -z_1\bar{z}_3/\gamma_2\gamma_3 & \cdots & -z_1\bar{z}_N/\gamma_{N-1} \\ z_2 & \bar{z}_1/\gamma_2 & -z_2\bar{z}_3/\gamma_2\gamma_3 & \cdots & -z_2\bar{z}_N/\gamma_{N-1} \\ z_3 & 0 & \gamma_2/\gamma_3 & \cdots & -z_3\bar{z}_N/\gamma_{N-1} \\ \cdot & \cdot & & & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ z_N & 0 & 0 & \cdots & \gamma_{N-1} \end{bmatrix}. \tag{9}$$

Note that u_z is null below the diagonal and to the right of the first column. It is easy to prove that $u_z \in$ SU(N). Obviously this chart extends to all points on the sphere with $\gamma_2 \neq 0$. If we permute the last $N-1$ components of z and construct u_z for this permuted vector, we obtain another chart. $N-1$ of these charts suffice to cover the whole sphere.

It is important to note that the Haar measure on U(N) [SU(N)] can be decomposed similarly [see (5)]:

$$du = d^{2N-1}\omega(z) d\tilde{v}, \tag{10}$$

where $d^{2N-1}\omega(z)$ is the uniform normalized measure on the sphere $|z| = 1$ in C^N,

$$d^{2N-1}\omega(z) = \frac{1}{\Omega_{2N-1}} \left(\prod_{i=1}^{N} d\,\mathrm{Re}\, z_i\, d\,\mathrm{Im}\, z_i \right) \delta(|z| - 1), \tag{11}$$

$$\Omega_{2N-1} = 2\frac{\pi^N}{(N-1)!}. \tag{12}$$

The proof of (10) follows from left-invariance of the rhs of (10) under translation on the group.

For a given $u \in$ U(N) [SU(N)] we have thus obtained a factorization

$$\begin{aligned} u = {} & u_{z^{(N)}} u_{z^{(N-1)}} \cdots u_{z^{(2)}} u_{z^{(1)}} \\ & (\cdots u_{z^{(3)}} u_{z^{(2)}}), \end{aligned} \tag{13}$$

where $z^{(k)} \in C^k$, $|z^{(k)}| = 1$, and

$$u_{z^{(k)}} = \begin{pmatrix} \mathbb{1}_{N-k} & & 0 \\ & z_1^{(k)} & \cdots & \cdot \\ 0 & z_2^{(k)} & \cdots & \cdot \\ & z_k^{(k)} & \cdots & \cdot \end{pmatrix}. \tag{14}$$

In (13) the vectors $z^{(k)}$, $k < N$, depend on the chart used.

The embedding of the spheres S^{2N-1} into the space C^N of complex vectors p is established by

$$z_i = \frac{1}{|p|} p_i, \quad |p| = \left(\sum_{i=1}^{N} |p_i|^2 \right)^{1/2}. \tag{15}$$

For any vector $p^{(k)} \in C^k$ introduce the matrix $w_{p^{(k)}}$ by

$$\begin{aligned} &w_{p^{(k)}} = |p^{(k)}| u_z, \\ &z = p^{(k)}/|p^{(k)}|. \end{aligned} \tag{16}$$

Then the matrix function u(13) with support on

$$S^{2N-1} \times S^{2N-3} \times S^{2N-5} \ldots \times S^{1(3)}$$

can be extended to the matrix function

$$w = w_{p^{(N)}} w_{p(N-1)} \cdots w_{p^{(1)}((2))} \tag{17}$$

with support on

$$R^{2N} \times R^{2N-2} \times R^{2N-4} \ldots \times R^{2(4)}$$

by means of (16).

Consider now an action function $S(u)$ depending on field variables $u \in$ U(N) [SU(N)] which are carried by a set of simplices σ on the lattice. The partition function of the model is

$$Z = \int \prod_{\sigma} du_\sigma e^{S(u)}. \tag{18}$$

The action depends polynomially on all matrix elements of the u_σ and can correspondingly be extended to a function of w_σ using (13) and (17).

For test functions on the group manifold with support covered by one chart we can use the delta function representation

$$\delta(u-w)=\int\prod_{k=1(2)}^{N}\left(\prod_{i=1}^{k}\frac{d\,\mathrm{Re}\,q_i^{(k)}}{2\pi}\frac{d\,\mathrm{Im}\,q_i^{(k)}}{2\pi}\right)\times\exp\left[i\,\mathrm{Re}\,(z^{(k)}-p^{(k)})\cdot\overline{q^{(k)}}\right],\tag{19}$$

where w is the matrix function (17) and

$$z^{(k)}\cdot\overline{q^{(k)}}=\sum_{i=1}^{k}z_i^{(k)}\,\overline{q_i^{(k)}}.\tag{20}$$

In (18) the integration $\int du_\sigma$ extends over several charts. However, since one chart covers the whole group U(N) [SU(N)] up to a set of Haar measure zero whose dimension is that of the group less four, and the resulting mean field is a particular fixed configuration which can be chosen in the interior of the domain of a chart, we will neglect this peculiarity. According to the functional approach[1] we insert the delta function (19) into (18), introduce additional integrations over the variables w, replace $S(u)$ by $S(w)$, and change the order of integration. Since

$$du_\sigma=\prod_{k=1(2)}^{N}d^{2k-1}\omega(z_\sigma^{(k)}),\tag{21}$$

we can perform these integrations and obtain

$$\int\prod_{k=1(2)}^{N}\{d^{2k-1}\omega(z_\sigma^{(k)})\exp i\,\mathrm{Re}\,z_\sigma^{(k)}\cdot\bar{q}_\sigma^{(k)}\}=\prod_{k=1(2)}^{N}\left\{(k-1)!\left(\frac{2}{|q_\sigma^{(k)}|}\right)^{k-1}J_{k-1}(|q_\sigma^{(k)}|)\right\},\tag{22}$$

where J_n is the Bessel function of order n. Then we have

$$Z=\int\left\{\prod_\sigma\prod_{k=1(2)}^{N}\left(\prod_{i=1}^{k}\frac{d\,\mathrm{Re}\,q_{i,\sigma}^{(k)}d\,\mathrm{Im}\,q_{i,\sigma}^{(k)}}{(2\pi)^2}d\,\mathrm{Re}\,p_{i,\sigma}^{(k)}d\,\mathrm{Im}\,p_{i,\sigma}^{(k)}\right)(k-1)!\left(\frac{2}{|q_\sigma^{(k)}|}\right)^{k-1}J_{k-1}(|q_\sigma^{(k)}|)\exp(-i\,\mathrm{Re}\,p_\sigma^{(k)}\overline{q}_\sigma^{(k)})\right\}e^{S(w)}.\tag{23}$$

Denote

$$\eta_{i,\sigma}^{(k)}=\mathrm{Re}\,q_{i,\sigma}^{(k)},\qquad\xi_{i,\sigma}^{(k)}=\mathrm{Im}\,q_{i,\sigma}^{(k)}.\tag{24}$$

The integration contours in $\eta_{i,\sigma}^{(k)}$, $\xi_{i,\sigma}^{(k)}$ can be deformed arbitrarily in compact domains. We let them pass through the stationary points, which obviously lie on the imaginary axis. Thus we put at these points

$$\eta_{i,\sigma}^{(k)}=i\,\mathrm{Re}\,m_{i,\sigma}^{(k)},\qquad\xi_{i,\sigma}^{(k)}=i\,\mathrm{Im}\,m_{i,\sigma}^{(k)}\tag{25}$$

and get as conditions for the extremal points

$$p_{i,\sigma}^{(k)}=-m_{i,\sigma}^{(k)}\frac{1}{\mu_\sigma^{(k)}}\Psi_k'(\mu_\sigma^{(k)}),\tag{26}$$

where

$$\mu_\sigma^{(k)}=\left(\sum_{i=1}^{k}|m_{i,\sigma}^{(k)}|^2\right)^{1/2},\tag{27}$$

$$\Psi_k(\xi)=\ln\{(k-1)!(2/\xi)^{k-1}I_{k-1}(\xi)\},\tag{28}$$

I_n is the modified Bessel function of order n.

Instead of solving (26) for the $m_{i,\sigma}^{(k)}$ we define an effective action by inserting $p_{i,\sigma}^{(k)}$ into the exponent of (23),

$$S_{\mathrm{eff}}(m)=S(\tilde{w})+\sum_\sigma\sum_{k=1(2)}^{N}[\Psi_k(\mu_\sigma^{(k)})-\mu_\sigma^{(k)}\Psi_k'(\mu_\sigma^{(k)})].\tag{29}$$

Here

$$\tilde{w}_\sigma=\left(\prod_{k=1(2)}^{N}\Psi_k'(\mu_\sigma^{(k)})\right)R_\sigma,\tag{30}$$

where R_σ is the function u(13) with arguments

$$z^{(k)}=-m_\sigma^{(k)}/\mu_\sigma^{(k)}.\tag{31}$$

III. GAUGE MODELS

In the case of gauge models on a cubic lattice in d dimensions the field variables are carried by the links and without gauge fixing,

$$S(u)=\beta\sum_P\frac{1}{N}\,\mathrm{Re}\,\mathrm{Tr}\,u_P,\tag{32}$$

where u_P is the ordered product of the u_σ along the border of the plaquette P. Let V denote the number of sites and

$$\beta^*=\tfrac{1}{2}(d-1)\beta.\tag{33}$$

S_{eff} assumes a maximal value if the products of the R_σ forming the plaquette variables R_P equal 1. Moreover, we assume $\mu_\sigma^{(k)}$ not to depend on the link σ. Then

$$\frac{1}{Vd}S_{\mathrm{eff}}=\beta^*\left[\prod_{k=1(2)}^{N}\Psi_k'(\mu^{(k)})\right]^4+\sum_{k=1(2)}^{N}[\Psi_k(\mu^{(k)})-\mu^{(k)}\Psi_k'(\mu^{(k)})].\tag{34}$$

We can further maximize S_{eff} in the remaining parameters $\mu^{(k)}$.

From (28) we find

$$\Psi_k'(\xi)=I_k(\xi)/I_{k-1}(\xi)\tag{35}$$

and

$$\Psi_k''(\xi)>0,\quad 0\leqslant\xi<\infty.\tag{36}$$

The stationarity condition for S_{eff} then reads

$$4\beta^*\left[\prod_{n=1(2)}^{N}\Psi_n'(\mu^{(n)})\right]^4=\mu^{(k)}\Psi_k'(\mu^{(k)}),$$
$$1(2)\leqslant k\leqslant N. \tag{37}$$

This set of equations has two solutions:

(1) all $\mu^{(k)}=0$;

(2) all $\mu^{(k)}\neq 0$.

The absolute maximum of S_{eff} (34) with respect to the parameters $\mu^{(1)2},\ldots,\mu^{(N)}$ gives the logarithm of the partition function Z. The first solution yields the absolute maximum for sufficiently small β, the second for sufficiently large β. There is a first order phase transition at $\beta_c(N)$ in between. For $0\leqslant\beta\leqslant\beta_c$ $\ln Z$ is zero and increases for $\beta>\beta_c$. The second solution can be found numerically and in addition asymptotically for $\beta\to\infty$.

We first consider the asymptotic expansion. Set

$$\alpha=\mu^{(k)}\Psi_k'(\mu^{(k)}) \tag{38}$$

and solve for $\mu^{(k)}$,

$$\mu^{(k)}=\mu^{(k)}(\alpha). \tag{39}$$

For $\alpha\to\infty$ we find

$$\mu^{(k)}(\alpha)=\alpha+k-\tfrac{1}{2}-\frac{1}{2\alpha}(k-\tfrac{1}{2})(k-\tfrac{3}{2})+O\left(\frac{1}{\alpha^2}\right). \tag{40}$$

On the other hand, we get from (37)

$$4\beta^*=\alpha\left[\prod_{k=1(2)}^{N}\frac{\mu^{(k)}(\alpha)}{\alpha}\right]^4, \tag{41}$$

which for $\alpha\to\infty$ yields

$$4\beta^*=\alpha+a_0+\frac{a_1}{\alpha}+O\left(\frac{1}{\alpha^2}\right), \tag{42}$$

with

$$a_0=2\Delta, \tag{43}$$

$$a_1=2\Delta^2-\tfrac{1}{3}N(N-1)(4N+1). \tag{44}$$

Here we introduced the dimension Δ of the group manifold,

$$\Delta=\begin{cases}N^2, & \text{for U}(N),\\ N^2-1, & \text{for SU}(N).\end{cases} \tag{45}$$

We recognize that $\alpha\to\infty$ implies $\beta^*\to\infty$ and vice versa.

Inversion of (41), (42) gives

$$\alpha=4\beta^*-a_0-\frac{a_1}{4\beta^*}+O((\beta^*)^{-2}) \tag{46}$$

and furthermore, by (40)

$$\mu^{(k)}=4\beta^*-a_0+k-\tfrac{1}{2}-(1/4\beta^*)\left[a_1+\tfrac{1}{2}(k-\tfrac{1}{2})(k-\tfrac{3}{2})\right]+O((\beta^*)^{-2}). \tag{47}$$

This expression can be inserted into S_{eff} (34) and gives its extremal value

$$S_{\text{eff,extr}}=Vd\left\{\beta^*-\frac{\Delta}{2}\ln 2\beta^*+\sum_{k=1(2)}^{N}\ln\frac{(k-1)!}{(4\pi)^{1/2}}+\frac{1}{16\beta^*}a_1+O((\beta^*)^{-2})\right\}. \tag{48}$$

As a typical shortcoming of mean field approximations without gauge fixing we observe that the coefficient of $\ln\beta^*$ in $S_{\text{eff,extr}}$ is proportional to d whereas a similar treatment with gauge fixing would make it proportional to $d-1$.

In order to calculate β_c numerically we remember that β_c is the largest value of β for which

$$S_{\text{eff,extr}}=0. \tag{49}$$

The stationarity conditions (37) and this equation determine the critical parameters $\beta_c(d,N)$ and $\mu_c^{(1)2}(d,N)\cdots\mu_c^{(N)}(d,N)$. It is moreover convenient to scale β_c by Δ (45) and define

$$\eta_c=\beta_c^*/\Delta. \tag{50}$$

Numerical values of η_c are given in Table I.

For sufficiently large N the expansion (48) remains even valid for $\beta^*=\beta_c^*$ and can then be solved to give

$$\eta_c=\tfrac{1}{2}\ln 2N+\tfrac{1}{2}\ln(\tfrac{1}{2}\ln 2N)+\tfrac{3}{4}+O\left(\frac{\ln(\ln N)}{\ln N}\right). \tag{51}$$

η_c increases with N and assumes no limit at $N=\infty$.

IV. THE VARIATIONAL APPROACH

By means of Jensen's inequality

$$\int dm\, e^f\geqslant e^{\int dm f}, \tag{52}$$

valid for any probability measure m and real-valued function

TABLE I. $\eta_c=((d-1)/2\Delta)\beta_c$, $\Delta=N^2$ for U(N) and N^2-1 for SU(N) calculated without gauge fixing. The Monte-Carlo results are valid only for $d=4$.

N	U(N) matrices	U(N) spheres	SU(N) spheres	U(N) Monte Carlo
1	1.823353	1.823353	...	1.507[5]
2	1.681680	1.939844	1.413114	1.24 ± 0.02[6]
3	1.645080	2.101356	1.860603	1.15 ± 0.08[6]
4	1.629917	2.239659	2.097655	1.14 ± 0.07[6]
5	1.6222	2.355515	2.260836	1.13 ± 0.07[6]
6	1.6177	2.454012	2.385978	1.13 ± 0.11[6]
7	1.6147		2.487805	
8	1.61275			
9	1.61133			
10	1.61028			
∞	1.60506959			

f, we can derive a lower bound for the partition function. With a local chart (13) and the Haar measure represented in the form (21) we define the probability measure

$$dm = \prod_{\sigma} \left\{ \prod_{k=1(2)}^{N} [d^{2k-1}\omega(z_\sigma^{(k)}) \times \exp(\mathrm{Re}\, z_\sigma^{(k)} \bar{m}^{(k)} - \Psi_k(\mu^{(k)}))] \right\}, \tag{53}$$

with Ψ_k from (28), σ labelling the links, and arbitrary vectors $m^{(k)} \in C^k$ and $\mu^{(k)} = |m^{(k)}|$. In addition we set

$$f = \beta \sum_P \frac{1}{N} \mathrm{Re}\, \mathrm{Tr}\, u_P + \sum_{k,\sigma} \{\Psi_k(\mu^{(k)}) - \mathrm{Re}\, z_\sigma^{(k)} \bar{m}^{(k)}\}. \tag{54}$$

Inserting (53) and (54) into (52) yields

$$\frac{1}{Vd} \ln Z \geqslant \beta^* \frac{1}{N} \mathrm{Tr}\,(M^2 M^{+2}) + \sum_{k=1(2)}^{N} \{\Psi_k(\mu^{(k)}) - \mu^{(k)} \Psi_k'(\mu^{(k)})\}. \tag{55}$$

The matrix M factorizes,

$$M = \prod_{\substack{k=1(2) \\ \text{ordered}}}^{N} M_k(m^{(k)}), \tag{56}$$

where the order of the factors is the same as in (13). Each factor is defined by the integral

$$M_k(m^{(k)}) = \int d^{2k-1}\omega(z^{(k)}) u_{z^{(k)}} \times \exp\{\mathrm{Re}\, z^{(k)} \bar{m}^{(k)} - \Psi_k(\mu^{(k)})\}, \tag{57}$$

with $u_{z^{(k)}}$ as in (9) and (14).

Again we can maximize the rhs of (55) with respect to all the vectors $m^{(k)} \in C^k$. Except for the smallest N this seems quite a hard task. A weaker bound can be obtained if we assume

$$m^{(k)} = \begin{pmatrix} \mu^{(k)} \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{58}$$

Then $M_k(m^{(k)})$ is diagonal,

$$M_k(m^{(k)}) = \begin{pmatrix} \sigma_1^{(k)} & & 0 \\ & \ddots & \\ 0 & & \sigma_N^{(k)} \end{pmatrix} \tag{59}$$

and we obtain

$$\sigma_n^{(k)} = 1 \quad \text{for } n \leqslant N-k,$$
$$\sigma_{N-k+1}^{(k)} = \Psi_k'(\mu^{(k)}),$$
$$\sigma_{N-k+2}^{(k)} = \tfrac{1}{2}\mu^{(k)} \exp\{-\Psi_k(\mu^{(k)})\} \Gamma(k) \times \sum_{m=0}^{\infty} \frac{\Gamma(m+\frac{5}{2})(\mu^{(k)}/2)2m}{m!(m+2)!\Gamma(k+m+\frac{1}{2})},$$
$$\sigma_{N-k+n}^{(k)} = 1 - \frac{\int_0^{\mu^{(k)}} dt\, t^{2n-2} \exp\{\Psi_k(t) - \Psi_k(\mu^{(k)})\}}{(\mu^{(k)})^{2n-1}}, \quad n \geqslant 3. \tag{60}$$

This result obviously differs from (34) obtained by the functional approach.

V. NUMERICAL RESULTS FOR PHASE TRANSITION POINTS

In this section we compare numerical values of the phase transition points β_c obtained by different mean field approaches with the results of Monte-Carlo simulations for U(N) groups.[5,6] First we do not impose gauge fixing. The functional approach based on embedding of spheres has already been discussed in Sec. III. The standard variational method (which can be viewed as a functional approach by $N \times N$ matrix embedding) leads to

$$\frac{\ln Z}{Vd} \geqslant \max_{x \in R_+} \left\{ \beta^* \left(\frac{w'(x)}{N} \right)^4 + w(x) - x w'(x) \right\} \tag{61}$$

with

$$w(x) = \ln \int du\, e^{x\, \mathrm{Re}\, \mathrm{Tr}\, u}. \tag{62}$$

We restrict the discussion to the case of U(N) groups, where

$$w(x) = \ln \det M\ , \qquad M_{kl} = I_{k-l}(x), \quad k,l = 1,\ldots,N. \tag{63}$$

For large N an asymptotic expansion of (61) can be performed using, for $x = N\xi$, $\xi > 1$ fixed,[9,10]

$$\frac{1}{N^2} w(x) = \xi - \tfrac{1}{2} \ln \xi - \tfrac{3}{4} + \frac{1}{N^2} \left(\tfrac{1}{12} - A - \tfrac{1}{12} \ln N + \tfrac{1}{8} \ln \frac{\xi}{\xi - 1} \right) + \frac{1}{N^4} \left(\tfrac{3}{128} \cdot \frac{1}{(\xi-1)^3} - \tfrac{1}{240} \right) + O(N^{-6}), \tag{64}$$

with $A = 0.248\,754\,477\,0$. For large N we can even obtain the critical parameters x_c, β_c^* in the form of asymptotic expansions. Defining

$$x_c = N\xi_c, \tag{65}$$
$$\beta_c^* = \Delta \eta_c, \tag{66}$$

we first determine from (61) the expansion

$$\xi_c = \xi_0 + \frac{1}{N^2}(a_1 \ln N + b_1) + \frac{1}{N^4}(a_2 \ln^2 N + b_2 \ln N + c_2) + O(N^{-6}) \tag{67}$$

and therefore obtain

$$\eta_c = \tfrac{1}{4} \xi_c \left(1 - \frac{1}{2\xi_c}\right)^{-3} \times \left\{ 1 + \frac{1}{N^2} \frac{3}{4(\xi_c - 1)(2\xi_c - 1)} + \frac{1}{N^4} \left[\frac{3}{8(\xi_c-1)^2(2\xi_c-1)^2} + \frac{27\xi_c}{64(\xi_c-1)^4(2\xi_c-1)} \right] + \cdots \right\}. \tag{68}$$

It is crucial that $\xi_0 > 1$ in order that the expansion (64) is applicable; we find $\xi_0 = 4.514\,659\,57$.

In Table I we list the values for η_c. For U(N) and the matrix embedding method (standard variation method) the η_c are calculated numerically for $1 \leqslant N \leqslant 4$ and are obtained from (68) for $N \geqslant 5$. In the case of the sphere embedding method all numbers for U(N) and SU(N) are obtained by numerical computations. For extremely large N we could also use the expansion (51). In the same table we list the results of Lautrup and Nauenberg[5] and Creutz and Moriarty[6] obtained by Monte-Carlo simulations for $d = 4$ dimensions but re-expressed in terms of the parameter η_c together with the errors quoted by these authors. Obviously both the matrix and the spherical embedding approach provide too large numbers. The latter one is even worse since it yields values of η_c increasing with N whereas the Monte-Carlo results seem to tend to a constant limit.

We next impose axial gauge fixing. We study only the standard variational approach (matrix embedding) since we expect that the qualitative behavior for $N \to \infty$ is conserved under gauge fixing. Then instead of Eq. (6) we have

$$\frac{1}{V} \ln Z \geqslant \max_x \left\{ \binom{d-1}{2} \beta \left(\frac{w'(x)}{N} \right)^4 + (d-1)\beta \left(\frac{w'(x)}{N} \right)^2 + (d-1)[w(x) - xw'(x)] \right\}. \tag{69}$$

The critical point β_c is again obtained from condition (49). We consider only $d = 4$ and list the results for $(1/N^2)\beta_c$ in Table II. For $N \geqslant 5$ we again employ the asymptotic expansions (67), (68). In this case $\xi_0 = 2.415\,278\,13$. Comparison of Tables I and II shows that gauge fixing reduces β_c considerably. Moreover, the results for β_c of Table II are in surprisingly good agreement with the Monte-Carlo simulations. For SU(2) we obtain $\frac{1}{3}\beta_c = 0.560\,575\,53$. We expect $(1/\Delta)\beta_c$ for SU(N) to converge with N from below to the same limit as for U(N).

The latent heat per plaquette,

$$q = \frac{1}{\binom{d}{2} V} \frac{\partial}{\partial \beta} \ln Z \,|_{\beta = \beta_c + 0}, \tag{70}$$

is more sensitive than β_c. For $N = \infty$ we obtain for the latent heat per plaquette

$$q|_{N=\infty} = \tfrac{1}{2}\left[\left(1 - \frac{1}{2\xi_0} \right)^4 + \left(1 - \frac{1}{2\xi_0} \right)^2 \right], \tag{71}$$

which for $d = 4$ gives

TABLE II. $(1/\Delta)\beta_c$, $\Delta = N^2$ for U(N) calculated with axial gauge fixing. All numbers are for $d = 4$.

N	U(N) matrices	U(N) Monte Carlo
1	0.776662	1.005[5]
2	0.712823	0.825 ± 0.013[6]
3	0.695149	0.76 ± 0.06[6]
4	0.687593	0.76 ± 0.04[6]
5	0.6837	0.75 ± 0.04[6]
6	0.6813	0.75 ± 0.07[6]
7	0.6798	
8	0.67871	
9	0.67795	
10	0.67739	
∞	0.67455297	

$$q|_{N=\infty} = 0.512\,122.$$

This is more than twice the value which can be read off the data of Ref. 6 for U(6). Since $\ln Z = 0$ for $\beta \leqslant \beta_c$ in the mean field approximation it is not surprising that q is too large.

ACKNOWLEDGMENT

The authors thank T. Raddatz for performing most of the numerical computations.

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Real solutions of the Yang–Mills field equations in Minkowski space

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(Received 15 April 1981; accepted for pubication 10 August 1981)

A system of nonlinear partial differential equations is obtained by considering complex self-dual Yang–Mills fields in Minkowski space and then selecting those fields whose real part is again a solution of the Yang–Mills field equations. From solutions of this system families of real solutions of the Yang–Mills field equations in Minkowski space are obtained, which depend on one or more arbitrary solutions of the two-dimensional Laplace equation and one or more arbitrary functions.

PACS numbers: 11.10.Np

I. INTRODUCTION

The important role of Yang–Mills theory in particle physics led people to a detailed investigation of this theory. Several attempts were made to find real classical solutions of a pure Yang–Mills theory in Minkowski space, but the number of solutions, which have been found explicitly, is limited.[1–8] On the other hand, the number of the corresponding solutions in Euclidean space is quite large.[8] This is mainly due to the fact that a self-dual field can be real in Euclidean space, while it is necessarily complex in Minkowski space. It is obvious that it is much easier to solve the equations coming from the self-duality condition, than those coming from the Yang–Mills field equations, since the order of the former is lower than the order of the latter.

The standard way of getting real solutions in Minkowski space is by using directly the equations of motion. We shall not apply this method. Instead we shall try to find complex self-dual solutions, whose real parts are again solutions of the Yang–Mills field equations. One solution with this property has been found before.[5] In Sec. II we express complex self-dual solutions by a real function φ and a complex function ρ. These functions must satisfy a system of nonlinear partial differential equations. In Sec. III we select those self-dual fields, whose real part is again a solution. Then we are led to an additional set of differential equations for the functions φ and ρ. In Sec. IV by solving the system of differential equations found in Secs. II and III, a number of real Minkowski space solutions is obtained, which depend on one or more arbitrary solutions of the two-dimensional Laplace equation and one or more arbitrary functions.

II. SELF-DUAL SU(2) GAUGE FIELDS IN MINKOWSKI SPACE

To proceed in the description of self-dual SU(2) gauge field in Minkowski space we introduce the variables $y, \bar{y}, z, \bar{z}$ by the relations

$$y = (1/\sqrt{2})(x_1 + ix_2), \quad \bar{y} = (1/\sqrt{2})(x_1 - ix_2),$$
$$z = (1/\sqrt{2})(x_3 + x_0), \quad \bar{z} = (1/\sqrt{2})(x_3 - x_0). \tag{2.1}$$

Also, if b^i_μ, $i = 1,2,3, \mu = 0,1,\ldots,3$ are the gauge field and $f^i_{\mu\nu}$ the field strengths

$$f^i_{\mu\nu} = \partial_\nu b^i_\mu - \partial_\mu b^i_\nu - e\epsilon^{ijk} b^j_\mu b^k_\nu, \tag{2.2}$$

we introduce the matrices $B_\mu = (e/2i)\sigma^j b^j_\mu$ and $F_{\mu\nu} = (e/2i)\sigma^j f^j_{\mu\nu}$, where σ^j are the Pauli matrices. Then we get

$$F_{\mu\nu} = \partial_\nu B_\mu - \partial_\mu B_\nu - [B_\mu, B_\nu]. \tag{2.3}$$

Finally we define the variables $B_y, B_{\bar{y}}, B_z, B_{\bar{z}}$ by the relations

$$B_y = (1/\sqrt{2})(B_1 - iB_2), \quad B_{\bar{y}} = (1/\sqrt{2})(B_1 + iB_2),$$
$$B_z = (1/\sqrt{2})(B_3 + B_0), \quad B_{\bar{z}} = (1/\sqrt{2})(B_3 - B_0). \tag{2.4}$$

A Yang–Mills field in Minkowski space is called self-dual if it satisfies the relations

$$F_{\mu\nu} = (i/2)\epsilon_{\mu\nu\rho\sigma} F^{\rho\sigma}, \tag{2.5}$$

where $\epsilon_{\mu\nu\rho\sigma}$ is totally antisymmetric and $\epsilon_{1230} = 1$. It is obvious from Eq. (2.5) that every self-dual Yang–Mills field in Minkowski space is necessarily complex. Equation (2.5) implies the relations $F_{12} = -iF_{30}$, $F_{13} = iF_{20}$, and $F_{23} = -iF_{10}$. From these expressions and Eqs. (2.4) and (2.5) we get

$$F_{yz} = F_{\bar{y}\bar{z}} = 0, \tag{2.6}$$

$$F_{y\bar{y}} + F_{\bar{z}\bar{z}} = 0. \tag{2.7}$$

Equations (2.6) and (2.7) are equivalent to Eq. (2.5).

Equation (2.6) is solved by the expressions

$$B_y = D^{-1}\partial_y D, \quad B_{\bar{y}} = \bar{D}^{-1}\partial_{\bar{y}}\bar{D}, \tag{2.8}$$

$$B_z = D^{-1}\partial_z D, \quad B_{\bar{z}} = \bar{D}^{-1}\partial_{\bar{z}}\bar{D}, \tag{2.9}$$

where D and $\bar{D}$ are 2×2 matrices. We are interested in finding solutions for which b^j_α, $\alpha = 1$ and 2, are real. For such solutions the matrices BV_β are anti-Hermitian. Then from Eqs. (2.8) we get

$$\bar{D} = (D^+)^{-1}. \tag{2.10}$$

As in the Euclidean space case[9] we can go in the R gauge, defined by the relation

$$D = R = \frac{1}{\sqrt{\varphi}}\begin{pmatrix} 1, & 0 \\ \rho, & \varphi \end{pmatrix}, \tag{2.11}$$

where φ is real and ρ is complex in general. Then from Eqs. (2.8) and (2.9) we find the following expressions for the fields:

$$e\mathbf{b}_1 = (1/2\varphi)[\rho_2 + \bar{\rho}_2 + i(\rho_1 - \bar{\rho}_1), \rho_1 + \bar{\rho}_1 - i(\rho_2 - \bar{\rho}_2), -2\varphi_2], \tag{2.12}$$

$$e\mathbf{b}_2 = (i/2\varphi)[\rho_2 - \bar{\rho}_2 + i(\rho_1 + \bar{\rho}_1), \rho_1 - \bar{\rho}_1 - i(\rho_2 + \bar{\rho}_2), -2i\varphi_1], \tag{2.13}$$

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$$e\mathbf{b}_3 = (1/2\varphi)[i(\rho_3 - \bar{\rho}_3 + \rho_0 + \bar{\rho}_0),$$
$$\rho_3 + \bar{\rho}_3 + \rho_0 - \bar{\rho}_0, -2i\varphi], \tag{2.14}$$
$$e\mathbf{b}_0 = (1/2\varphi)[i(\rho_3 + \bar{\rho}_3 + \rho_0 - \bar{\rho}_0),$$
$$\rho_3 - \bar{\rho}_3 + \rho_0 + \bar{\rho}_0, -2i\varphi_3], \tag{2.15}$$

where the index in the functions ρ and φ means differentiation with respect to the corresponding variable x_μ. We see immediately from Eqs. (2.12)–(2.15) that the fields $\mathbf{b}_1$ and $\mathbf{b}_2$ are real while the field $\mathbf{b}_3$ and $\mathbf{b}_0$ are complex. Therefore let us write

$$\mathbf{b}_\mu = \mathbf{b}_\mu^R + i\mathbf{b}_\mu^I, \tag{2.16}$$

where $\mathbf{b}_\mu^R$ is the real part of the field and $i\mathbf{b}_\mu^I$ the imaginary part. To simplify the notation let us introduce the Hermitian matrices H and K by the relations

$$H = \begin{pmatrix} -\varphi & \bar{\rho} \\ \rho, & \varphi \end{pmatrix}, \tag{2.17}$$

$$G = \begin{pmatrix} 0, & -i\bar{\rho} \\ i\rho, & 0 \end{pmatrix}, \tag{2.18}$$

and let us write

$$B_\mu^R = (e/2i)\boldsymbol{\sigma}\cdot\mathbf{b}_\mu^R, \tag{2.19}$$

$$B_\mu^I = (e/2i)\boldsymbol{\sigma}\cdot\mathbf{b}_\mu^I, \tag{2.20}$$

in which case we have

$$B_\mu = B_\mu^R + iB_\mu^I. \tag{2.21}$$

From Eqs. (2.12)–(2.20) we get

$$B_\alpha = B_\alpha^R = (1/2i\varphi)\epsilon_{\alpha\beta}H_\beta + (1/2i\varphi)G_\alpha, \quad \alpha,\beta = 1,2, \tag{2.22}$$

$$B_3^R = (1/2i\varphi)G_3, \quad B_3^I = (1/2\varphi)H_0, \tag{2.23}$$

$$B_0^R = (1/2i\varphi)G_0, \quad B_0^I = (1/2\varphi)H_3, \tag{2.24}$$

where the index in a matrix means differentiation of all the matrix elements of that matrix with respect to the corresponding variable x_μ.

From Eqs. (2.8), (2.9), and (2.11) we get

$$F_{a\bar{b}} = \frac{1}{\varphi^2}\begin{pmatrix} -\varphi\varphi_{a\bar{b}} + \varphi_a\varphi_{\bar{b}} - \rho_a\bar{\rho}_{\bar{b}}, & \varphi\bar{\rho}_{a\bar{b}} - 2\varphi_a\bar{\rho}_{\bar{b}} \\ \varphi\rho_{a\bar{b}} - 2\varphi_{\bar{b}}\rho_a, & \varphi\varphi_{a\bar{b}} - \varphi_a\varphi_{\bar{b}} + \rho_a\bar{\rho}_{\bar{b}} \end{pmatrix}, \quad a,b = y,z. \tag{2.25}$$

Combining Eqs. (2.7) and (2.25) we find that the functions φ and ρ must satisfy the system

$$\varphi(\varphi_{y\bar{y}} + \varphi_{z\bar{z}}) - \varphi_y\varphi_{\bar{y}} - \varphi_z\varphi_{\bar{z}} + \rho_y\bar{\rho}_{\bar{y}} + \rho_z\bar{\rho}_{\bar{z}} = 0, \tag{2.26}$$

$$\varphi(\rho_{y\bar{y}} + \rho_{z\bar{z}}) - 2\rho_y\varphi_{\bar{y}} - 2\rho_z\varphi_{\bar{z}} = 0, \tag{2.27}$$

$$\varphi(\bar{\rho}_{y\bar{y}} + \bar{\rho}_{z\bar{z}}) - 2\bar{\rho}_{\bar{y}}\varphi_y - 2\bar{\rho}_{\bar{z}}\varphi_z = 0. \tag{2.28}$$

If we express Eqs. (2.26)–(2.28) in the variables x_μ we get respectively

$$\varphi\partial^\mu\partial_\mu\varphi - \partial^\mu\varphi\partial_\mu\varphi + \partial^\mu\rho\partial_\mu\bar{\rho} + i(\rho_1\bar{\rho}_2 - \rho_2\bar{\rho}_1) - (\rho_3\bar{\rho}_0 - \rho_0\bar{\rho}_3) = 0, \tag{2.29}$$

$$\varphi\partial^\mu\partial_\mu\rho - 2\partial^\mu\varphi\partial_\mu\rho + 2i(\varphi_1\rho_2 - \varphi_2\rho_1) - 2(\varphi_3\rho_0 - \varphi_0\rho_3) = 0, \tag{2.30}$$

$$\varphi\partial^\mu\partial_\mu\bar{\rho} - 2\partial^\mu\varphi\partial_\mu\bar{\rho} - 2i(\varphi_1\bar{\rho}_2 - \varphi_2\bar{\rho}_1) + 2(\varphi_3\bar{\rho}_0 - \varphi_0\bar{\rho}_3) = 0. \tag{2.31}$$

The imaginary part of Eq. (2.29) which is $\bar{\rho}_3\rho_0 - \bar{\rho}_0\rho_3$ must be zero. Also taking the complex conjugate of Eq. (2.31) and subtracting it from Eq. (2.30) we find that the expression $\varphi_3\rho_0 - \varphi_0\rho_3$ must be zero. Therefore the system of Eqs. (2.29)–(2.31) is equivalent to the system

$$\varphi\partial^\mu\partial_\mu\varphi - \partial^\mu\varphi\partial_\mu\varphi + \partial^\mu\rho\partial_\mu\bar{\rho} + i(\rho_1\bar{\rho}_2 - \rho_2\bar{\rho}_1) = 0, \tag{2.32}$$

$$\varphi\partial^\mu\partial_\mu\rho - 2\partial^\mu\varphi\partial_\mu\rho + 2i(\varphi_1\rho_2 - \varphi_2\rho_1) = 0, \tag{2.33}$$

$$\varphi_3\rho_0 - \varphi_0\rho_3 = 0, \tag{2.34}$$

$$\rho_3\bar{\rho}_0 - \rho_0\bar{\rho}_3 = 0. \tag{2.35}$$

III. CONDITIONS UNDER WHICH THE REAL PART OF THE COMPLEX SELF-DUAL SOLUTION IS AGAIN A SOLUTION

We shall determine in this section the conditions under which the real part of the complex self-dual solution (2.22)–(2.24) is again a solution of the Yang–Mills field equations in Minkowski space

$$\partial^\mu F_{\mu\nu} + [B^\mu, F_{\mu\nu}] = 0. \tag{3.1}$$

To do that we introduce the expression (2.21) into Eq. (2.3), in which case we get

$$F_{\mu\nu} = F_{\mu\nu}^R + iF_{\mu\nu}^I, \tag{3.2}$$

where $F_{\mu\nu}^R$ is the anti-Hermitian part of the matrix $F_{\mu\nu}$ and $iF_{\mu\nu}^I$ is its Hermitian part. Explicitly we get

$$F_{\mu\nu}^R = M_{\mu\nu} + [B_\mu^I, B_\nu^I], \tag{3.3}$$

$$F_{\mu\nu}^I = \partial_\nu B_\mu^I - \partial_\mu B_\nu^I - [B_\mu^R, B_\nu^I] - [B_\mu^I, B_\nu^R], \tag{3.4}$$

where $M_{\mu\nu}$ are the field strengths coming from the real part of the complex field namely

$$M_{\mu\nu} = \partial_\nu B_\mu^R - \partial_\mu B_\nu^R - [B_\mu^R, B_\nu^R]. \tag{3.5}$$

From Eqs. (2.21), (3.1), and (3.2) we get

$$\partial^\mu F_{\mu\nu}^R + i\partial^\mu F_{\mu\nu}^I + [(B^R)^\mu, F_{\mu\nu}^R] - [(B^I)^\mu, F_{\mu\nu}^I] + i[(B^R)^\mu, F_{\mu\nu}^I] + i[(B^I)^\mu, F_{\mu\nu}^R] = 0, \tag{3.6}$$

from which we find that we must have

$$\partial^\mu F_{\mu\nu}^R + [(B^R)^\mu, F_{\mu\nu}^R] - [(B^I)^\mu, (F^I)_{\mu\nu}] = 0. \tag{3.7}$$

Using Eqs. (3.3) and (3.4) to eliminate $F_{\mu\nu}^R$ and $F_{\mu\nu}^I$ from Eq.

(3.7) we get

$$\partial^\mu M_{\mu\nu} + \partial^\mu [B^I_\mu, B^I_\nu] + [(B^R)^\mu, M_{\mu\nu} + [B^I_\mu, B^I_\nu]] - [(B^I)^\mu, \partial_\nu B^I_\mu - \partial_\mu B^I_\nu - [B^R_\mu, B^I_\nu] - [B^I_\mu, B^R_\nu]] = 0. \tag{3.8}$$

We want the real part of the complex self-dual solution to be again a solution, namely, we want to have

$$\partial^\mu M_{\mu\nu} + [(B^R)^\mu, M_{\mu\nu}] = 0. \tag{3.9}$$

Since Eq. (3.8) is satisfied we get if we subtract Eq. (3.9) from Eq. (3.8)

$$\partial^\mu [B^I_\mu, B^I_\nu] + [(B^R)^\mu, [B^I_\mu, B^I_\nu]] - [(B^I)^\mu, \partial_\nu B^I_\mu - \partial_\mu B^I_\nu - [B^R_\mu, B^I_\nu] - [B^I_\mu, B^R_\nu]] = 0. \tag{3.10}$$

Therefore, we find that if a self-dual Yang–Mills field satisfies Eq. (3.10) its real part is again a solution of the Yang–Mills field equations. We shall take this as the basic equation which the field has to satisfy. Of course we could directly require the field to satisfy Eq. (3.9). This however, leads to a higher-order system of nonlinear partial differential equations.

Let us assume that the field is of the form of Eqs. (2.22)–(2.24). Then for $\nu = \alpha = 1$ or 2 since $B^I_\alpha = 0$ we get from Eq. (3.10)

$$[B^I_3, \partial_\alpha B^I_3] - [B^I_0, \partial_\alpha B^I_0] - [B^I_3, [B^I_3, B^R_\alpha]] + [B^I_0, [B^I_0, B^R_\alpha]] = 0, \tag{3.11}$$

which becomes if we use the explicit expressions for the fields B^I_3, B^I_0, and B^R_α given by Eqs. (2.22)–(2.24)

$$[H_0, H_{0\alpha}] - [H_3, H_{3\alpha}] - (1/2i\varphi)\epsilon_{\alpha\beta}[H_0, [H_0, H_\beta]] - (1/2i\varphi)[H_0, [H_0, G_\alpha]] + (1/2i\varphi)\epsilon_{\alpha\beta}[H_3, [H_3, H_\beta]] + (1/2i\varphi)[H_3, [H_3, G_\alpha]] = 0. \tag{3.12}$$

Equation (3.12) is satisfied if the functions φ and ρ satisfy the following relations:

$$\bar\rho_0(\varphi\rho_{0\alpha} - \varphi_0\rho_\alpha) - \rho_0(\varphi\bar\rho_{0\alpha} - \varphi_0\bar\rho_\alpha) - \bar\rho_3(\varphi\rho_{3\alpha} - \varphi_3\rho_\alpha) + \rho_3(\varphi\bar\rho_{3\alpha} - \varphi_3\bar\rho_\alpha) + i\epsilon_{\alpha\beta}\{\varphi_0(\bar\rho_0\rho_\beta + \bar\rho_\beta\rho_0) - \varphi_3(\bar\rho_3\rho_\beta + \bar\rho_\beta\rho_3) - 2\varphi_\beta(\rho_0\bar\rho_0 - \rho_3\bar\rho_3)\} = 0, \tag{3.13}$$

$$2\varphi_0(\varphi\rho_{0\alpha} - \varphi_0\rho_\alpha) - 2\varphi_3(\varphi\rho_{3\alpha} - \varphi_3\rho_\alpha) - \rho_0(2\varphi\varphi_{0\alpha} + \rho_0\bar\rho_\alpha + \rho_\alpha\bar\rho_0) + \rho_3(2\varphi\varphi_{3\alpha} + \rho_3\bar\rho_\alpha + \rho_\alpha\bar\rho_3) + i\epsilon_{\alpha\beta}\{2\rho_\beta(\varphi_0^2 - \varphi_3^2) - 2\varphi_\beta(\varphi_0\rho_0 - \varphi_3\rho_3) + \rho_\beta(\rho_0\bar\rho_0 - \rho_3\bar\rho_3) - \bar\rho_\beta(\rho_0^2 - \rho_3^2)\} = 0. \tag{3.14}$$

For $\nu = 3$ Eq. (3.10) gives

$$\partial^0 [B^I_0, B^I_3] + [(B^R)^0, [B^I_0, B^I_3]] - [(B^I)^0, \partial_3 B^I_0 - \partial_0 B^I_3] + [(B^I)^0, [B^R_0, B^I_3] + [B^I_0, B^R_3]] = 0. \tag{3.15}$$

From this equation we get

$$\partial_0[H_3, H_0] - (3\varphi_0/\varphi)[H_3, H_0] - [H_3, H_{33} - H_{00}] + (1/2i\varphi)\{[G_0, [H_3, H_0]] + [H_3, [G_0, H_0]] + [H_3, [H_3, G_3]]\} = 0, \tag{3.16}$$

which is satisfied if the following relations hold

$$\varphi[2(\bar\rho_3\rho_{00} - \rho_3\bar\rho_{00}) + \rho_0\bar\rho_{30} - \bar\rho_0\rho_{30} + \rho_3\bar\rho_{33} - \bar\rho_3\rho_{33}] + 5\varphi_0(\rho_3\bar\rho_0 - \rho_0\bar\rho_3) = 0, \tag{3.17}$$

$$2\varphi[\partial_0(\varphi_3\bar\rho_0 - \varphi_0\bar\rho_3) + \varphi_3(\bar\rho_{00} - \bar\rho_{33}) - \bar\rho_3(\varphi_{00} - \varphi_{33})] - 6\varphi_0(\varphi_3\bar\rho_0 - \varphi_0\bar\rho_3) - 2\varphi_3(\varphi_0\bar\rho_0 - \varphi_3\bar\rho_3) - 2\bar\rho_3(\rho_0\bar\rho_0 - \rho_3\bar\rho_3) + \bar\rho_0(\rho_3\bar\rho_0 - \rho_0\bar\rho_3) = 0. \tag{3.18}$$

If we take into account Eqs. (2.34) and (2.35), Eqs. (3.17) and (3.18) becomes, respectively,

$$2(\bar\rho_3\rho_{00} - \rho_3\bar\rho_{00}) + \rho_0\bar\rho_{30} - \bar\rho_0\rho_{30} + \rho_3\bar\rho_{33} - \bar\rho_3\rho_{33} = 0, \tag{3.19}$$

$$\varphi[\varphi_3(\bar\rho_{00} - \bar\rho_{33}) - \bar\rho_3(\varphi_{00} - \varphi_{33})] - \varphi_3(\varphi_0\bar\rho_0 - \varphi_3\bar\rho_3) - \bar\rho_3(\rho_0\bar\rho_0 - \rho_3\bar\rho_3) = 0. \tag{3.20}$$

For $\nu = 0$ Eq. (3.10) gives

$$\partial_3[B^I_3, B^I_0] + [B^I_3, [B^R_3, B^I_0]] - [B^I_3, \partial_0 B^I_3 - \partial_3 B^I_0] + [B^I_3, [B^R_3, B^I_0] + [B^I_3, B^R_0]] = 0, \tag{3.21}$$

or

$$\partial_3[H_0, H_3] - (3\varphi_3/\varphi)[H_0, H_3] - [H_0, H_{00} - H_{33}] + (1/2i\varphi)\{[G_3, [H_0, H_3]] + [H_0, [G_3, H_3]] + [H_0, [H_0, G_0]]\} = 0. \tag{3.22}$$

The above equation is satisfied if the following relations hold:

$$\varphi[2(\bar\rho_0\rho_{33} - \rho_0\bar\rho_{33}) + \rho_3\bar\rho_{03} - \bar\rho_3\rho_{03} + \rho_0\bar\rho_{00} - \bar\rho_0\rho_{00}] + 5\varphi_3(\rho_0\bar\rho_3 - \rho_3\bar\rho_0) = 0, \tag{3.23}$$

$$2\varphi[\partial_3(\varphi_0\bar\rho_3 - \varphi_3\bar\rho_0) + \varphi_0(\bar\rho_{33} - \bar\rho_{00}) - \bar\rho_0(\varphi_{33} - \varphi_{00})] - 6\varphi_3(\varphi_0\bar\rho_3 - \varphi_3\bar\rho_0) - 2\varphi_0(\varphi_3\bar\rho_3 - \varphi_0\bar\rho_0) - 2\bar\rho_0(\rho_3\bar\rho_3 - \rho_0\bar\rho_0) + \bar\rho_3(\rho_0\bar\rho_3 - \rho_3\bar\rho_0) = 0. \tag{3.24}$$

Since the functions φ and ρ must satisfy Eqs. (2.34) and (2.35) Eqs. (3.23) and (3.24) become, respectively,

$$2(\bar\rho_0\rho_{33} - \rho_0\bar\rho_{33}) + \rho_3\bar\rho_{03} - \bar\rho_3\rho_{03} + \rho_0\bar\rho_{00} - \bar\rho_0\rho_{00} = 0, \tag{3.25}$$

$$\varphi[\varphi_0(\bar\rho_{33} - \bar\rho_{00}) - \bar\rho_0(\varphi_{33} - \varphi_{00})] - \varphi_0(\varphi_3\bar\rho_3 - \varphi_0\bar\rho_0) - \bar\rho_0(\rho_3\bar\rho_3 - \rho_0\bar\rho_0) = 0. \tag{3.26}$$

Therefore we find that the functions φ and ρ must satisfy Eqs. (2.32)–(2.35), (3.13), (3.14), (3.19), (3.20), (3.25), and (3.26).

The system of equations which the function φ and ρ must satisfy is considerably simplified if ρ is real. In this case the system (2.32)–(2.35) is replaced by the system

$$\varphi\partial^\mu\partial_\mu\varphi - \partial^\mu\varphi\partial_\mu\varphi + \partial^\mu\rho\partial_\mu\rho = 0, \tag{3.27}$$

$$\varphi\partial^\mu\partial_\mu\rho - 2\partial^\mu\varphi\partial_\mu\rho = 0, \tag{3.28}$$

$$\varphi_1\rho_2 - \varphi_2\rho_1 = 0, \tag{3.29}$$

$$\varphi_3\rho_0 - \varphi_0\rho_3 = 0. \tag{3.30}$$

Also, in this case we get from Eq. (3.14)

$$\varphi_0(\varphi\rho_{0\alpha} - \varphi_0\rho_\alpha) - \varphi_3(\varphi\rho_{3\alpha} - \varphi_3\rho_\alpha) - \rho_0(\varphi\varphi_{0\alpha} + \rho_0\rho_\alpha) + \rho_3(\varphi\varphi_{3\alpha} + \rho_3\rho_\alpha) = 0, \tag{3.31}$$

$$(\varphi_3\rho_3 - \varphi_0\rho_0)\varphi_\alpha - (\varphi_3^2 - \varphi_0^2)\rho_\alpha = 0, \quad \alpha = 1,2 \tag{3.32}$$

From Eqs. (3.20) and (3.13)

$$\varphi_3[\varphi(\rho_{00}-\rho_{33})+\varphi_3\rho_3-\varphi_0\rho_0]$$
$$-\rho_3[\varphi(\varphi_{00}-\varphi_{33})+\rho_0\rho_0-\rho_3\rho_3]=0, \quad (3.33)$$
$$(\rho_3\rho_3-\rho_0\rho_0)\varphi_\alpha-(\varphi_3\rho_3-\varphi_0\rho_0)\rho_\alpha=0, \quad (3.34)$$

while Eqs. (3.19) and (3.25) are satisfied. We find that Eq. (3.34) holds if Eqs. (3.30) and (3.32) are satisfied, except if $\varphi_0=\varphi_3=0$. Finally the relation we get from Eq. (3.26) follows from Eqs. (3.30) and (3.33) except if $\varphi_3=\rho_3=0$, which is a noninteresting case. Therefore, if ρ is real the real part of the complex expressions (2.22)–(2.24) is a solution of the Yang–Mills field equations in Minkowski space if Eqs. (3.27)–(3.34) are satisfied and we do not have $\varphi_3=\rho_3=0$.

IV. REAL MINKOWSKI SPACE SOLUTIONS

In this section we shall present a number of Minkowski space Yang–Mills fields, which are obtained by solving the system of nonlinear partial differential equations, found in Secs. II and III. We shall consider solutions of the following two types.

A. Solutions of the first type

We shall call solutions of the first type the solutions of the form

$$\varphi=\varphi(x_1,x_2), \quad \rho=\bar\rho=\rho(x_3,x_0). \quad (4.1)$$

In this case Eqs. (3.29)–(3.32) are satisfied and (3.27), (3.28), and (3.33) become, respectively,

$$\varphi(\varphi_{11}+\varphi_{22})-\varphi_1\varphi_1-\varphi_2\varphi_2+\rho_3\rho_3-\rho_0\rho_0=0, \quad (4.2)$$
$$\varphi(\rho_{33}-\rho_{00})=0, \quad (4.3)$$
$$\rho_3(\rho_3\rho_3-\rho_0\rho_0)=0, \quad (4.4)$$

while Eq. (3.34) gives $(\rho_3\rho_3-\rho_0\rho_0)\varphi_\alpha=0$. The general solution of this system is

$$\varphi=e^{v}, \quad \rho=h(z) \quad \text{or} \quad \tau(\bar z), \quad (4.5)$$

where v is an arbitrary solution of the two-dimensional Laplace equation

$$v_{11}+v_{22}=0, \quad (4.6)$$

and h and τ are arbitrary real functions of their arguments. For $\rho=h(z)$ if we write $q=(1/\sqrt{2})h_z$ we get from Eqs. (2.12)–(2.16)

$$e\mathbf{b}^R_\alpha=(0,0,-\epsilon_{\alpha\beta}v_\beta), \quad e\mathbf{b}^R_\xi=(0,qe^{-v},0). \quad (4.7)$$

These potentials give the field strengths

$$e\mathbf{f}^R_{12}=e\mathbf{f}^R_{30}=0, \quad e\mathbf{f}^R_{\alpha\xi}=qe^{-v}(-\epsilon_{\alpha\beta}v_\beta,v_\alpha,0). \quad (4.8)$$

Similar expressions are obtained if we take $\rho=\tau(\bar z)$. The expressions (4.7) and (4.8) give a class of real solutions of the Yang–Mills field equations in Minkowski space, which depends on an arbitrary solution v of Eq. (4.6) and an arbitrary function $q=q(z)$.

The action density S is given by the expression

$$S=-\tfrac{1}{4}(\mathbf{f}^R)^{\mu\nu}(\mathbf{f}^R)_{\mu\nu}=(1/2e^2)\,\mathrm{Tr}[(F^R)^{\mu\nu}(F^R)_{\mu\nu}]. \quad (4.9)$$

Also the energy-momentum tensor $\theta_{\mu\nu}$ is

$$\theta_{\mu\nu}=-(\mathbf{f}^R)_{\mu\lambda}(\mathbf{f}^R)_\nu{}^\lambda+\tfrac{1}{2}g_{\mu\nu}(\mathbf{f}^R)^{\rho\sigma}(\mathbf{f}^R)_{\rho\sigma}, \quad (4.10)$$

from which we find the energy density $\mathscr{E}$.

$$\mathscr{E}=\theta_{00}=\tfrac{1}{2}(\mathbf{f}^R)_{0j}(\mathbf{f}^R)_{0j}+\tfrac{1}{4}(\mathbf{f}^R)_{jk}(\mathbf{f}^R)_{jk}. \quad (4.11)$$

The total energy E is the space integral of the above expression.

The action density which is obtained from the expressions (4.8) is zero and the energy density is

$$\mathscr{E}=(2/e^2)q^2e^{-2v}v_\alpha v_\alpha. \quad (4.12)$$

B. Solutions of the second type

We shall call solutions of the second type the solutions of the form

$$\varphi=\varphi(x_1,x_2,x_3+x_0), \quad \rho=\rho(x_1,x_2,x_3+x_0). \quad (4.13)$$

For such solutions we have $\varphi_{\bar z}=\rho_{\bar z}=\bar\rho_{\bar z}=0$, $\varphi_3=\varphi_0$, $\rho_3=\rho_0$, $\bar\rho_3=\bar\rho_0$. Then Eqs. (3.13), (3.14), (3.19), (3.20), (3.25), and (3.26) are satisfied, while Eqs. (2.26) and (2.27) give, respectively,

$$\varphi\varphi_{y\bar y}-\varphi_y\varphi_{\bar y}+\rho_y\bar\rho_{\bar y}=0, \quad (4.14)$$
$$\varphi\rho_{y\bar y}-2\rho_y\varphi_{\bar y}=0. \quad (4.15)$$

Also, Eq. (2.28) gives the complex conjugate of Eq. (4.15). Therefore, the only equations the function φ and ρ must satisfy are (4.14) and (4.15). We shall consider the following families of solutions.

1. First family of solutions

This is the family in which

$$\varphi=\tilde\varphi(g)h(z), \quad \rho=\bar\rho=\tilde\rho(g)h(z), \quad g=g(x_1,x_2). \quad (4.16)$$

Then, Eqs. (4.14) and (4.15) become, respectively,

$$g_{y\bar y}\tilde\varphi\tilde\varphi'+g_y\,g_{\bar y}[\tilde\varphi\tilde\varphi''-(\tilde\varphi')^2+(\tilde\rho')^2]=0, \quad (4.17)$$
$$\tilde g_{y\bar y}\tilde\varphi\tilde\rho'+g_y\,g_{\bar y}(\tilde\varphi\tilde\rho''-2\tilde\varphi'\tilde\rho')=0, \quad (4.18)$$

where the prime denotes differentiation with respect to g. Proceeding as in Ref. 10 we find that the general solution of the above system is

$$\tilde\varphi=\pm b/\cosh v, \quad \tilde\rho=b\tanh v+c, \quad (4.19)$$

where v is an arbitrary solution of the two-dimensional Laplace equation (4.6) and b and c are arbitrary real constants. From Eqs. (2.12)–(2.16), (4.16) and (4.19) we get

$$e\mathbf{b}^R_\alpha=\left(\pm\epsilon_{\alpha\beta}\frac{v_\beta}{\cosh v},\ \pm\frac{v_\alpha}{\cosh v},\ \epsilon_{\alpha\beta}v_\beta\tanh v\right), \quad \alpha=1,2, \quad (4.20)$$

$$e\mathbf{b}^R_\xi=[0,\pm(h_z/2^{1/2}h)(\sinh v+l\cosh v),0], \quad \xi=3,0, \quad (4.21)$$

where $l=c/b$ and h is an arbitrary function of z. The field strengths which are obtained from the expressions (4.20) and (4.21) are

$$e\mathbf{f}^R_{12}=e\mathbf{f}^R_{30}=0, \quad (4.22)$$
$$e\mathbf{f}^R_{\alpha\xi}=(h_z/2^{1/2}h)\{\pm\epsilon_{\alpha\beta}v_\beta(\sinh v+l\cosh v)\tanh v, \mp v_\alpha(\cosh v+l\sinh v),-\epsilon_{\alpha\beta}v_\beta(\tanh v+l)\}. \quad (4.23)$$

Equations (4.20)–(4.23), where v is an arbitrary solution of the two-dimensional Laplace equation, h is an arbitrary function of z and l an arbitrary constant, give a real solution of the Yang–Mills field equations in Minkowski space.

For the solution (4.20)–(4.23) we get from Eqs. (4.9) and (4.11)

$$S = 0,$$
$$\mathscr{E} = \tfrac{1}{2}(h_z/h)^2 v_\alpha v_\alpha [(1 + l^2)\cosh 2v + 2l \sinh 2v]. \tag{4.24}$$

2. Second family of solutions

This is the family in which

$$\varphi = \varphi(x_1, x_2, z), \tag{4.25a}$$
$$\rho = \rho(\bar{y}, z). \tag{4.25b}$$

Then, Eq. (4.15) is satisfied and Eq. (4.14) becomes $\varphi\varphi_{y\bar{y}} - \varphi_y\varphi_{\bar{y}} = 0$. The general solution of this equation is

$$\varphi = e^v, \quad v = \sum_k v^{(k)}(x_1, x_2) h^{(k)}(z), \quad k = 1,2,3..., \tag{4.26}$$

where the functions $v^{(k)}$ are arbitrary solutions of the two-dimensional Laplace equation, and the $h^{(k)}$ are arbitrary functions of z. From Eqs. (2.12)–(2.16), (4.25b), and (4.26) we get the following expressions for the potentials:

$$e\mathbf{b}^R_\alpha = (0,0, -\epsilon_{\alpha\beta} v_\beta), \tag{4.27}$$
$$e\mathbf{b}^R_\xi = \frac{1}{2\sqrt{2}} e^{-v}[i(\rho_z - \bar{\rho}_z), \rho_z + \bar{\rho}_z, 0]. \tag{4.28}$$

From these potentials we get

$$e\mathbf{f}^R_{12} = e\mathbf{f}^R_{30} = 0, \tag{4.29}$$
$$\begin{aligned} e\mathbf{f}^R_{\alpha\xi} = \{&(1/2\sqrt{2}) e^{-v} \\ &\times [iv_\alpha(\rho_z - \bar{\rho}_z) - i(\rho_{z\alpha} - \bar{\rho}_{z\alpha}) - \epsilon_{\alpha\beta} v_\beta(\rho_z + \bar{\rho}_z)], \\ &(1/2\sqrt{2}) e^{-v}[v_\alpha(\rho_z + \bar{\rho}_z) \\ &- (\rho_{z\alpha} + \bar{\rho}_{z\alpha}) + i\epsilon_{\alpha\beta} v_\beta(\rho_z - \bar{\rho}_z)], -(1/\sqrt{2})\epsilon_{\alpha\beta} v_{\beta z}\}. \end{aligned} \tag{4.30}$$

The action density S obtained from this solution is zero, and the energy density $\mathscr{E}$ is given by the expression

$$\begin{aligned} \mathscr{E} = &(1/2e^2) \\ &\times \{v_{\alpha z} v_{\alpha z} + e^{-2v}[2v_\alpha v_\alpha \rho_z \bar{\rho}_z - v_\alpha(\rho_z \bar{\rho}_{z\alpha} + \bar{\rho}_z \rho_{z\alpha}) \\ &+ i\epsilon_{\alpha\beta} v_\beta(\rho_{z\alpha}\bar{\rho}_z - \bar{\rho}_{z\alpha}\rho_z) + \rho_{z\alpha}\bar{\rho}_{z\alpha}]\}. \end{aligned} \tag{4.31}$$

3. Third family of solutions

This contains the solutions of the system (4.14)–(4.15), whose ρ is complex in general, and satisfies the relation $\rho_y \neq 0$. In this case Eq. (4.15) gives $(\ln \rho_y)_{\bar{y}} = (\ln \varphi^2)_{\bar{y}}$. Therefore,

$$\rho_y = \varphi^2 u(y, x_3 + x_0), \tag{4.32}$$

where u is an arbitrary function of its arguments. Substituting in Eq. (4.14) we get

$$(\ln \varphi)_{y\bar{y}} + u\bar{u}\varphi^2 = 0, \tag{4.33}$$

or if we write $w = \ln \varphi + \frac{1}{2}\ln u\bar{u}$ the above equation becomes

$$(\partial_1\partial_1 + \partial_2\partial_2)w + 2e^{2w} = 0. \tag{4.34}$$

This is the two-dimensional Liouville's equation. Its solution is

$$e^{2w} = g_y \bar{g}_{\bar{y}}/(g\bar{g} + 1)^2, \tag{4.35}$$

where $g = g(y)$ is an arbitrary function of y. Therefore we get

$$\varphi = \left(\frac{g_y \bar{g}_{\bar{y}}}{u\bar{u}}\right)^{1/2} \frac{1}{g\bar{g} + 1}. \tag{4.36}$$

From Eqs. (4.32) and (4.36) we get

$$\rho = -\frac{\bar{g}_{\bar{y}}}{\bar{u}\bar{g}} \frac{1}{g\bar{g} + 1}. \tag{4.37}$$

An arbitrary function of $\bar{y}$ can be added on the right-hand side of the above expression, which however is unimportant and will be omitted.

To calculate the potentials we shall use Eqs. (2.12)–(2.16), (4.36), and (4.37). Then we find

$$e\mathbf{b}^R_1 = \left[\frac{i}{\sqrt{2}}\varphi(u - \bar{u}), \frac{1}{\sqrt{2}}\varphi(u + \bar{u}), -(\ln \varphi)_2\right], \tag{4.38}$$
$$e\mathbf{b}^R_2 = \left[-\frac{1}{\sqrt{2}}\varphi(u + \bar{u}), \frac{i}{\sqrt{2}}\varphi(u - \bar{u}), (\ln \varphi)_1\right], \tag{4.39}$$
$$\begin{aligned} e\mathbf{b}^R_3 &= e\mathbf{b}^R_0 \\ &= \frac{1}{2g\bar{g}(2g_y \bar{g}_{\bar{y}} u\bar{u})^{1/2}} \{i[g\bar{g}_{\bar{y}} u(\ln \bar{u})_z - \bar{g}g_y \bar{u}(\ln u)_z], \\ &\quad g\bar{g}_{\bar{y}} u(\ln \bar{u})_z + \bar{g}g_y \bar{u}(\ln u)_z, 0\}. \end{aligned} \tag{4.40}$$

The field strengths $e\mathbf{f}^R_{12}$ and $e\mathbf{f}^R_{30}$ we get from Eqs. (4.38)–(4.40) are

$$e\mathbf{f}^R_{12} = e\mathbf{f}^R_{30} = 0. \tag{4.41}$$

Also, since $\mathbf{f}^R_{13} + i\mathbf{f}^R_{23} = \mathbf{f}^R_{\bar{y}z}$ the field strengths $\mathbf{f}^R_{13}$ and $\mathbf{f}^R_{23}$ are the real and imaginary parts respectively of $\mathbf{f}^R_{\bar{y}z}$. The explicit expression of $\mathbf{f}^R_{\bar{y}z}$ can be calculated from (2.12)–(2.16). We get

$$\begin{aligned} e\mathbf{f}^R_{\bar{y}z} &= \left\{-i\frac{\varphi}{2}\left[\bar{u}_z + \left(\frac{\rho_z}{\varphi^2}\right)_{\bar{y}}\right], \frac{\varphi}{2}\left[\bar{u}_z - \left(\frac{\rho_z}{\varphi^2}\right)_{\bar{y}}\right], \right. \\ &\quad \left. i\left[-\frac{1}{2}\left(\frac{\bar{u}_z}{\bar{u}}\right)_{\bar{y}} + \bar{u}\rho_z\right]\right\} \\ &= \left\{-\frac{i}{2}\left(\frac{g_y \bar{g}_{\bar{y}}}{u\bar{u}}\right)^{1/2}\left[\frac{\bar{u}_z}{g\bar{g} + 1} + \frac{u}{g_y \bar{g}}\left(\frac{\bar{u}_z}{\bar{u}}\right)_{\bar{y}}\right.\right. \\ &\quad \left. - \frac{\bar{u}_z \bar{g}_{\bar{y}} u}{g_y \bar{u}\bar{g}^2(g\bar{g} + 1)}\right], \frac{1}{2}\left(\frac{g_y \bar{g}_{\bar{y}}}{u\bar{u}}\right)^{1/2} \\ &\quad \times \left[\frac{\bar{u}_z}{g\bar{g} + 1} - \frac{u}{g_y \bar{g}}\left(\frac{\bar{u}_z}{\bar{u}}\right)_{\bar{y}} + \frac{\bar{u}_z \bar{g}_{\bar{y}} u}{g_y \bar{u}\bar{g}(g\bar{g} + 1)}\right], \\ &\quad \left. i\left[-\frac{1}{2}\left(\frac{\bar{u}_z}{\bar{u}}\right)_{\bar{y}} + \frac{\bar{u}_z \bar{g}_{\bar{y}}}{\bar{u}\bar{g}(g\bar{g} + 1)}\right]\right\}. \end{aligned} \tag{4.42}$$

Also, we have $e\mathbf{f}^R_{\alpha 3} = e\mathbf{f}^R_{\alpha 0}$. Finally from Eqs. (4.9) and (4.11) we obtain $S = 0$ and

$$\mathscr{E} = \frac{1}{e^2}\mathbf{f}^R_{\bar{y}z} \cdot \mathbf{f}^R_{yz}. \tag{4.43}$$

If we use the expression (4.42) we get from Eq. (4.43)

$$\mathscr{E} = \frac{1}{e^2}\left[\frac{1}{2}\left(\frac{u_z}{ug}\right)_y \left(\frac{\bar{u}_z}{u\bar{g}}\right)_{\bar{y}} + \frac{1}{4}\left(\frac{u_z}{u}\right)_y \left(\frac{\bar{u}_z}{\bar{u}}\right)_{\bar{y}}\right]. \tag{4.44}$$

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An embedding of some Stiefel bundles

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(Received 21 May 1981; accepted for publication 1 August 1981)

We present an embedding of Stiefel manifolds $f_n: V_{2,1}(F)\to V_{n+1,n}(F)$, $(n\geqslant 2)$ with $F=\mathbb{C}$ or $\mathbb{R}$ having the property that the pullback via f_n of the curvature 2-form on $V_{n+1,n}(F)$ to $V_{2,1}(F)$ is an integer multiple n times the curvature 2-form on $V_{2,1}(F)$. We thus obtain the field of a magnetic pole of strength $g=n/2$.

PACS numbers: 11.10.Np, 02.40.Sf

1. INTRODUCTION

The unit sphere S_{2n+1}, $n=1, 2, 3, \cdots$ in $(2n+2)$-dimensional Euclidean space is given by the equation

$$\sum_{h=0}^{n}\bar{z}_h z_h = 1, \quad z_h\in\mathbb{C}\ (h=0, 1, 2, ..., n), \tag{1.1}$$

where the bar denotes complex conjugation. This is invariant under the right action of U(1) given by

$$z_h\to z_h e^{iX}, \quad X\in\mathbb{R}\ (h=0, 1, 2, ..., n). \tag{1.2}$$

These transformations are generated by the unit tangent vector field on S_{2n+1}:

$$\xi=\sum_{h=0}^{n}\left(x_h\frac{\partial}{\partial y_h}-y_h\frac{\partial}{\partial x_h}\right), \quad z_h=x_h+iy_h. \tag{1.3}$$

The 1-form dual to this is

$$\omega=\sum_{h=0}^{n}(x_h dy_h-y_h dx_h)=i\sum_{h=0}^{n}z_h d\bar{z}_h. \tag{1.4}$$

This is the connection 1-form on the Hopf bundle $S_{2n+1}\to\mathbb{C}P_n$ (see Trautman[1] for an alternative derivation). The corresponding curvature 2-form

$$\Omega=d\omega \tag{1.5}$$

satisfies, as well as the Bianchi identities

$$d\Omega=0 \tag{1.6}$$

the sourceless gauge equations (proved in Ref. 1),

$$d{}^*\Omega=0. \tag{1.7}$$

For the case $n=1$, the bundle space becomes the 3-sphere

$$S_3: \bar{z}_0 z_0+\bar{z}_1 z_1=1; \tag{1.8}$$

the connection 1-form is now

$$\omega_0=i(z_0 d\bar{z}_0+z_1 d\bar{z}_1) \tag{1.9}$$

and the pullback of ω_0 to the base space $\mathbb{C}P_1=S_2$, via a cross section of the bundle $S_3\to\mathbb{C}P_1$, is the potential of a magnetic pole (modulo a gauge transformation) of strength $g=\frac{1}{2}$.[1]

Writing (1.8) in the form

$$(\bar{z}_0 z_0+\bar{z}_1 z_1)^n=1, \quad n\geqslant 2 \tag{1.10}$$

and using the binomial expansion we obtain Trautman's[1] embedding

$$k_n: S_3\to S_{2n+1},$$

$$k_n(z_0, z_1)=(z_0^n, \tbinom{n}{1}^{1/2}z_0^{n-1}z_1, ..., \tbinom{n}{h}^{1/2}z_0^{n-h}z_1^h, ..., z_1^n), \tag{1.11}$$

which he expressed as an embedding of the base manifolds $\mathbb{C}P_1\to\mathbb{C}P_n$. The pullback of (1.4) by k_n is

$$k_n^*\omega=i\sum_{h=0}^{n}\tbinom{n}{h}z_0^{n-h}z_1^h d(\bar{z}_0^{n-h}\bar{z}_1^h)=n\omega_0, \tag{1.12}$$

which when pulled back to $\mathbb{C}P_1$, via a cross section of the bundle $S_3\to\mathbb{C}P_1$, corresponds to the potential of a magnetic pole of strength $g=n/2$. If $\Omega_0=d\omega_0$ then clearly

$$k_n^*\Omega=n\Omega_0. \tag{1.13}$$

In this paper we present an analog of (1.11) for embedding the bundle spaces $V_{2,1}(F)$, $F=\mathbb{R}$ or $\mathbb{C}$, in $V_{n+1,n}(F)$, $n\geqslant 2$, of Stiefel bundles over the Grassmannians $G_{2,1}(F)$ and $G_{n+1,n}(F)$, respectively (see Trautman and Nowakowski[2] who have shown that for the natural connections on Stiefel bundles[3,4] the curvature 2-forms satisfy the sourceless gauge equations). Here $G_{n+1,n}(\mathbb{R})=S_n$, $G_{n+1,n}(\mathbb{C})=\mathbb{C}P_n$, $V_{n+1,n}(\mathbb{R})=\mathrm{SO}(n+1)$ and $V_{n+1,n}(\mathbb{C})=\mathrm{SU}(n+1)$. Thus a representation of SO(2) or SU(2) by $(n+1)\times(n+1)$ matrices would constitute an embedding of the bundle spaces and this is in fact what we describe in the sequel. When the curvature 2-form on $V_{n+1,n}(F)$ is pulled back to $V_{2,1}(F)$, using our embedding we obtain a similar result to (1.13). The bundle $V_{2,1}(\mathbb{R})\to G_{2,1}(\mathbb{R})$ is trivial but we include it since our argument applies equally well to the case $F=\mathbb{R}$ as to the case $F=\mathbb{C}$.

2. EMBEDDING $V_{2,1}(F)$ IN $V_{n+1,n}(F)$

Let $a=(a_{\alpha\beta})$, $\alpha,\beta=1, 2$ be a 2×2 matrix with real or complex entries. Let $f_n(a)=A$ be an $(n+1)\times(n+1)$ matrix given by

$$\tbinom{n}{m}^{1/2}(a_{11}+a_{12}t)^{n-m}(a_{21}+a_{22}t)^m=\sum_{h=0}^{n}A_{mh}\tbinom{n}{h}^{1/2}t^h \tag{2.1}$$

for $m=0, 1, 2, ..., n$. Here t is arbitrary and may be real or complex while $\binom{n}{m}$ is the binomial coefficient. We first prove that f_n is a homomorphism which preserves the Hermitian conjugate operation, indicated by a dagger; thus we have

Lemma 1:

(i) $f_n(ba)=f_n(b)f_n(a)$,

(ii) $f_n(a^\dagger)=(f_n(a))^\dagger$.

Proof: (i) Let $f_n(a)=A$ given by (2.1) and $f_n(b)=B$ so that

$$\tbinom{n}{m}^{1/2}(b_{11}+b_{12}t)^{n-m}(b_{21}+b_{22}t)^m=\sum_{h=0}^{n}B_{mh}\tbinom{n}{h}^{1/2}t^h \tag{2.2}$$

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for $m = 0, 1, 2, \ldots, n$. Multiply this equation by

$$\binom{n}{m}^{1/2} s^m = \sum_{q=0}^{n} \delta_{mq} \binom{n}{q}^{1/2} s^q, \tag{2.3}$$

where s is an arbitrary real or complex variable and δ_{mq} is the Kronecker delta. Then sum the resulting equation with respect to m from 0 to n to obtain

$$\{b_{11} + b_{12}t + (b_{21} + b_{22}t)s\}^n = \sum_{h=0}^{n} \sum_{q=0}^{n} B_{qh} \binom{n}{q}^{1/2} \binom{n}{h}^{1/2} s^q t^h. \tag{2.4}$$

Differentiating m times with respect to t and putting $t = 0$ we have

$$\binom{n}{m}^{1/2} (b_{11} + b_{21}s)^{n-m} (b_{12} + b_{22}s)^m = \sum_{q=0}^{n} B_{qm} \binom{n}{q}^{1/2} s^q. \tag{2.5}$$

Multiply this equation by (2.1) and sum over m from 0 to n:

$$\{(b_{11} + b_{21}s)(a_{11} + a_{12}t) + (b_{12} + b_{22}s)(a_{21} + a_{22}t)\}^n = \sum_{h=0}^{n} \sum_{q=0}^{n} C_{qh} \binom{n}{q}^{1/2} \binom{n}{h}^{1/2} t^h s^q, \tag{2.6}$$

where

$$C_{qh} = \sum_{m=0}^{n} B_{qm} A_{mh} \tag{2.7}$$

or, in matrix notation, $C = BA$. Differentiating (2.6) r times with respect to s and putting $s = 0$ the resulting expression may be written

$$\binom{n}{r}^{1/2} (c_{11} + c_{12}t)^{n-r} (c_{21} + c_{22}t)^r = \sum_{h=0}^{n} C_{rh} \binom{n}{h}^{1/2} t^h, \tag{2.8}$$

where, in matrix notation, $c = ba$. Comparing this with the definition of f_n we have

$$f_n(ba) = C = BA = f_n(b) f_n(a). \tag{2.9}$$

(ii) Let $f_n(a^\dagger) = D$. Then by the definition (2.1) of f_n we have

$$\binom{n}{m}^{1/2} (\bar{a}_{11} + \bar{a}_{21}t)^{n-m} (\bar{a}_{12} + \bar{a}_{22}t)^m = \sum_{h=0}^{n} D_{mh} \binom{n}{h}^{1/2} t^h. \tag{2.10}$$

Repeating the argument which led from (2.2) to (2.5) we may obtain from (2.10) the equation

$$\binom{n}{m}^{1/2} (\bar{a}_{11} + \bar{a}_{12}s)^{n-m} (\bar{a}_{21} + \bar{a}_{22}s)^m = \sum_{h=0}^{n} D_{hm} \binom{n}{h}^{1/2} s^h \tag{2.11}$$

for $m = 0, 1, 2, \ldots, n$. Comparing this with the complex conjugate of (2.1) (with $\bar{t} = s$) we find that

$$D_{hm} = \bar{A}_{mh} = A^\dagger{}_{hm}. \tag{2.12}$$

Thus

$$f_n(a^\dagger) = A^\dagger = (f_n(a))^\dagger. \tag{2.13}$$

It clearly follows from the definition of f_n that $f_n(1) = 1$ and thus we have the

Corollary 1: If $a^\dagger a = 1$ then $(f_n(a))^\dagger f_n(a) = 1$ and so

$f_n: \mathrm{U}(2) \to \mathrm{U}(n+1)$ if $a_{\alpha\beta} \in \mathbb{C}$ $(\alpha, \beta = 1, 2)$,

$f_n: \mathrm{O}(2) \to \mathrm{O}(n+1)$ if $a_{\alpha\beta} \in \mathbb{R}$ $(\alpha, \beta = 1, 2)$.

The embedding f_n requires one further property before it can be applied to the Stiefel manifolds and this is obtained from the following

Lemma 2: If $a^\dagger a = 1$ and $A = f_n(a)$, then

$\det A = (\det a)^{n(n+1)/2}$.

Proof: Let b be a unitary 2×2 matrix with $f_n(b) = B$. By Lemma 1

$$f_n(b^\dagger a b) = B^\dagger A B \tag{2.14}$$

and by Corollary 1 A and B are unitary. Let

$$b^\dagger a b = c, \quad B^\dagger A B = C, \tag{2.15}$$

and by (2.14) we have

$$\binom{n}{m}^{1/2} (c_{11} + c_{12}t)^{n-m} (c_{21} + c_{22}t)^m = \sum_{h=0}^{n} C_{mh} \binom{n}{h}^{1/2} t^h \tag{2.16}$$

for $m = 0, 1, 2, \ldots, n$. Since a and b are unitary we may choose b so that c is diagonal. Thus,

$$\binom{n}{m}^{1/2} c_{11}^{n-m} c_{22}^m t^m = \sum_{h=0}^{n} C_{mh} \binom{n}{h}^{1/2} t^h \tag{2.17}$$

from which we conclude that C is diagonal with diagonal entries

$$C_{mm} = c_{11}^{n-m} c_{22}^m, \quad m = 0, 1, 2, \ldots, n. \tag{2.18}$$

Hence we have

$$\det C = (c_{11} c_{22})^{n(n+1)/2} = (\det c)^{n(n+1)/2}, \tag{2.19}$$

and since $\det C = \det A$ and $\det c = \det a$ we have established the result of the lemma.

It is interesting to note that the result of this lemma is also true if $a^\dagger a \neq 1$, but $a_{\alpha\beta} \in \mathbb{C}$, $\alpha, \beta = 1, 2$ for then the unitary matrix b can triangularize a and one can show then that $f_n(b) = B$ can triangularize A, i.e., C is triangular with diagonal elements given again by (2.18). Thus (2.19) holds once more and the result of the lemma is again established.

Corollary 2: If $a^\dagger a = 1$ and $\det a = 1$ then $A^\dagger A = 1$ and $\det A = 1$ where $A = f_n(a)$ and so

$f_n: \mathrm{SU}(2) \to \mathrm{SU}(n+1)$ if $a_{\alpha\beta} \in \mathbb{C}$ $(\alpha, \beta = 1, 2)$,

$f_n: \mathrm{SO}(2) \to \mathrm{SO}(n+1)$ if $a_{\alpha\beta} \in \mathbb{R}$ $(\alpha, \beta = 1, 2)$.

We may therefore write

$$f_n: V_{2,1}(F) \to V_{n+1,n}(F), \quad F = \mathbb{R} \text{ or } \mathbb{C}. \tag{2.20}$$

The homomorphism f_n provides an $(n+1)$-dimensional representation of the groups SU(2) and SO(2). In the complex case, putting $c_{11} = \sigma$, $c_{22} = \sigma^{-1}$, where $\sigma = e^{i\rho}$, $\rho \in \mathbb{R}$, in (2.18) we find

$$\mathrm{tr}\, C = \mathrm{tr}\, A = \sigma^n + \sigma^{n-2} + \cdots + \sigma^{-n+2} + \sigma^{-n}. \tag{2.21}$$

But this is $X^j(\rho)$, the character of the irreducible representation with index $j = n/2$. Thus f_n is an *irreducible* representation of SU(2) of dimension $2j + 1 = n + 1$ (cf. Talman, Ref. 5, p. 115).

3. THE CURVATURE 2-FORM

Following Trautman and Nowakowski[2] we begin with the Maurer–Cartan form on $V_{n+1,n}(F)$ given by

$$\omega = A^\dagger dA, \quad A \in V_{n+1,n}(F), \tag{3.1}$$

which has values in the Lie algebra $so(n+1)$ or $su(n+1)$. Its components ω_{mh} thus satisfy $\bar{\omega}_{hm} + \omega_{mh} = 0$, $m, h = 0, 1, 2, \ldots, n$. The components ω_{ab}, $a, b = 0, 1, 2, \ldots, (n-1)$ constitute the natural connection 1-form on $V_{n+1,n}(F)$. The corresponding curvature 2-form has components

$$\Omega_{ab} = d\omega_{ab} + \sum_{c=0}^{n-1} \omega_{ac} \wedge \omega_{cb} = \bar{\omega}_{na} \wedge \omega_{nb}. \tag{3.2}$$

We now establish the following

Lemma 3:

$$f_n^* \Omega_{ab} = n\Omega_0 \delta_{a,n-1} \delta_{b,n-1} \quad (n \geqslant 2),$$

where f_n^* denotes the pullback of forms via f_n from $V_{n+1,n}(F)$ to $V_{2,1}(F)$ while Ω_0 is the curvature 2-form on $V_{2,1}(F)$.

Proof: We begin by calculating

$$f_n^* \omega_{nb} = \sum_{h=0}^{n} A^{\dagger}_{nh}\, dA_{hb}, \quad b = 0, 1, 2, \ldots, (n-1), \tag{3.3}$$

where A_{hq} is given by (2.1). Beginning with

$$\binom{n}{m}^{1/2} (\bar{a}_{11} + \bar{a}_{21} t)^{n-m} (\bar{a}_{12} + \bar{a}_{22} t)^m = \sum_{h=0}^{n} A^{\dagger}_{mh} \binom{n}{h}^{1/2} t^h \tag{3.4}$$

and repeating the sequence of operations which led from (2.2) to (2.5) we obtain

$$\binom{n}{m}^{1/2} (\bar{a}_{11} + \bar{a}_{12} s)^{n-m} (\bar{a}_{21} + \bar{a}_{22} s)^m = \sum_{q=0}^{n} A^{\dagger}_{qm} \binom{n}{q}^{1/2} s^q. \tag{3.5}$$

From (2.1) we have

$$\begin{aligned} &\binom{n}{m}^{1/2} \{(n-m)(a_{11} + a_{12} t)^{n-m-1} (da_{11} + da_{12} t)(a_{21} + a_{22} t)^m \\ &\quad + m(a_{11} + a_{12} t)^{n-m} (a_{21} + a_{22} t)^{m-1} (da_{21} + da_{22} t)\} \\ &\quad = \sum_{h=0}^{n} dA_{mh} \binom{n}{h}^{1/2} t^h. \end{aligned} \tag{3.6}$$

Multiply (3.6) by (3.5) and sum over m from 0 to n. Then, using the property $a^{\dagger}a = 1$, we find

$$\begin{aligned} &n(1 + st)^{n-1} \{(a^{\dagger}da)_{11} + (a^{\dagger}da)_{21} s \\ &\quad + (a^{\dagger}da)_{12} t + (a^{\dagger}da)_{22} st\} \\ &\quad = \sum_{h=0}^{n} \sum_{q=0}^{n} (A^{\dagger} dA)_{qh} \binom{n}{h}^{1/2} \binom{n}{q}^{1/2} t^h s^q. \end{aligned} \tag{3.7}$$

Differentiating m times with respect to t and putting $t = 0$ gives

$$\begin{aligned} &\binom{n}{m}^{1/2} \{(n-m) s^m ((a^{\dagger}da)_{11} + (a^{\dagger}da)_{21} s) + m s^{m-1} ((a^{\dagger}da)_{12} \\ &\quad + (a^{\dagger}da)_{22} s)\} = \sum_{q=0}^{n} (A^{\dagger} dA)_{qm} \binom{n}{q}^{1/2} s^q \end{aligned} \tag{3.8}$$

for $m = 1, 2, 3, \ldots, n$. From this we see that

$$(A^{\dagger} dA)_{nm} = 0, \quad m = 1, 2, 3, \ldots, (n-2) \tag{3.9}$$

and

$$(A^{\dagger} dA)_{n,n-1} = n^{1/2} (a^{\dagger}da)_{21}. \tag{3.10}$$

We calculate directly from (3.5) that

$$A^{\dagger}_{nm} = \binom{n}{m}^{1/2} \bar{a}_{12}^{n-m} \bar{a}_{22}^m, \quad m = 0, 1, 2, \ldots, n \tag{3.11}$$

while (2.1) yields

$$A_{m0} = \binom{n}{m}^{1/2} a_{11}^{n-m} a_{21}^m, \quad m = 0, 1, 2, \ldots, n, \tag{3.12}$$

and so

$$\begin{aligned} (A^{\dagger} dA)_{n0} &= \sum_{m=0}^{n} \binom{n}{m} \bar{a}_{12}^{n-m} \bar{a}_{22}^m d(a_{11}^{n-m} a_{21}^m) \\ &= n(a^{\dagger}a)_{21}^{n-1} (a^{\dagger}da)_{21} = 0, \quad n \geqslant 2. \end{aligned} \tag{3.13}$$

Hence (3.3) becomes, using (3.9), (3.10), and (3.13),

$$f_n^* \omega_{nb} = n^{1/2} (a^{\dagger}da)_{21} \delta_{b,n-1} \tag{3.14}$$

for $b = 0, 1, 2, \ldots, (n-1)$. Thus we have

$$f_n^* \Omega_{ab} = n\Omega_0 \delta_{a,n-1} \delta_{b,n-1}, \tag{3.15}$$

with

$$\Omega_0 = \overline{(a^{\dagger}da)_{21}} \wedge (a^{\dagger}da)_{21}. \tag{3.16}$$

The connection 1-form ω_0 on $V_{2,1}(F)$ is

$$\omega_0 = (a^{\dagger}da)_{11} = \omega_{00} \tag{3.17}$$

and the curvature 2-form is [from (3.2) with $n = 1$]

$$\Omega_0 = \Omega_{00} = d\omega_0 = \bar{\omega}_{10} \wedge \omega_{10} \tag{3.18}$$

with $\omega_{10} = (a^{\dagger}da)_{21}$. We obtain agreement with (1.9) by choosing $\bar{a}_{11} = a_{22} = z_0$, $a_{12} = -\bar{a}_{21} = iz_1$ and making the replacement $\omega_0 \to i\omega_0$ in (3.17) and (3.18). Then (1.8) corresponds to $a^{\dagger}a = 1$.

We finally note that to obtain a result similar to (1.12) we should consider f_n as embedding $V_{2,1}(F)$ in $V_{n+1,1}(F)$. The connection 1-form on $V_{n+1,1}(F)$ is $(A^{\dagger} dA)_{00}$, and using

$$A^{\dagger}_{0m} = \binom{n}{m}^{1/2} \bar{a}_{11}^{n-m} \bar{a}_{21}^m, \quad m = 0, 1, 2, \ldots, n \tag{3.19}$$

together with A_{m0} given by (3.12), we see that

$$\begin{aligned} f_n^* (A^{\dagger} dA)_{00} &= \sum_{m=0}^{n} \binom{n}{m} \bar{a}_{11}^{n-m} \bar{a}_{21}^m d(a_{11}^{n-m} a_{21}^m) \\ &= n(a^{\dagger}a)_{11}^{n-1} (a^{\dagger}da)_{11} \\ &= n\omega_0. \end{aligned} \tag{3.20}$$

4. CONCLUSION

Trautman and Nowakowski[2] have suggested the interesting problem of taking a principal bundle with a connection and with structure group the orthogonal, unitary, or simplectic groups, embedding its base manifold in a Grassmannian (on account of the universality of these manifolds); calculating the connection on the original bundle induced by the embedding; and checking if it corresponds to a sourceless gauge field. We have described in this paper a simple example of this program. The curvature 2-form $f_n^* \Omega_{ab}$ clearly satisfies the sourceless gauge equations (1.7).

ACKNOWLEDGMENTS

I wish to thank Dr. M. Clancy, Dr. F. Gaines, Dr. J. McCrea, Dr. J. Pulè, and Professor J. T. Lewis for helpful and stimulating discussions.

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Spacetime metric and Yang–Mills fields unified in a Galilean subspace structure

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(Received 15 September 1981; accepted for publication 11 June 1982)

A novel approach to the unification of spacetime metric and Yang–Mills fields is presented. The spacetime metric field appears naturally as part of a first order G-structure, a Galilean subspace structure on a world manifold of higher dimension. There is an *a priori* distinction between internal space dimensions and spacetime dimensions. The prolongation of the first order Galilean subspace structure to second order is a principal bundle of second order coframes which has additional degrees of freedom in the second order part of its gauge group. The Yang–Mills fields are defined in a natural way as second order gauge fields by a reduction of the second order Galilean subspace structure. The Yang–Mills fields appear as part of a connection on the world manifold rather than on the spacetime manifold. The *kinematic* foundations of the new model are analyzed using the theory of G-structures and their prolongations. Kaluza–Klein models are also discussed from the G-structure viewpoint and compared with the Galilean subspace model.

PACS numbers: 11.10.Np, 11.30.Ly

1. INTRODUCTION

The hypothesis that there exist world dimensions in addition to the four dimensions of spacetime has been an important theme in the search for a unified field theory since the early work of Kaluza and Klein.[1,2] The idea that such additional world dimensions should exist became more plausible with the discovery of new internal degrees of freedom and the subsequent increasing importance of internal symmetry groups, particularly in connection with Yang–Mills gauge fields.[3] It is customary to interpret a Yang–Mills gauge field as a connection on a principal fiber bundle over spacetime with an internal symmetry group as typical fiber. The shift to a model of the Kaluza–Klein type consists in regarding the total space rather than the base space of the bundle as the real world manifold; consequently, in such a model, the group dimensions are assumed to be just as real as the spacetime dimensions. Moreover, the geometric structure of such models is that of a first order flat and involutive subspace structure[4–6] defined on a world manifold of higher dimension equipped with a pseudo-Riemannian metric of the Lorentz type. Although the subspace structure is introduced *a priori* in some presentations[7] and by means of a spontaneous symmetry breaking[8] mechanism in others,[9] the geometric structure ultimately obtained is the same. The essential point is that these models are based on a *first order* G-structure on the world manifold. In Sec. 7, the various approaches to the Kaluza–Klein models will be discussed, and models of this type will be contrasted with the type of model introduced in this paper.

The purpose of this paper is to describe a new model in which spacetime metric and Yang–Mills fields are unified. In this model an *a priori* distinction between spacetime dimensions and internal dimensions is made. This distinction is achieved by postulating a Galilean subspace structure on a world manifold of higher dimensions. The subspace dimensions are the internal dimensions and the other dimensions are the spacetime dimensions. In the case of the familiar Galilean spacetime structure, the subspace dimensions are space dimensions while the other dimension is the time dimension. It is natural to demand that the subspace structure (distribution) is involutive in order that the world manifold be foliated with exactly one leaf (maximal connected submanifold) of the foliation through each world point p such that the tangent space to the leaf at p is the subspace of the world tangent space at p picked out by the subspace structure. It is then possible to require that these internal submanifolds are compact by requiring that they be manifolds of constant positive curvature, a condition which may be expressed as a system of second order partial differential equations for the subspace metric g_S. The constant curvature may vary with the submanifold (depend on the spacetime variables). If the subspace structure is required to be first order flat (hence also involutive), then there exist locally (not just at a point) adapted coordinate systems with respect to which the spacetime metric g assumes a particularly simple form and depends only on the spacetime variables.

It is well known that a first order (pseudo) Riemannian structure completely determines the prolonged structure in second (and higher) order; that is, the connection (up to a torsion) is uniquely determined by the metric. However, a first order Galilean subspace structure does not completely determine a connection (even up to a torsion), a result that is widely known in the special case of Galilean spacetime structures analyzed in conjunction with Galilean general relativity theory.[10] For the particular assignment of internal and spacetime dimensions stated above, part of the Galilean subspace structure connection that is left undetermined may be assigned the role of a Yang–Mills gauge field; consequently, the Yang Mills gauge fields may be introduced by a reduc-

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 0022-2488/82/122475-13$02.50

tion of the second order Galilean subspace structure. In this model, the spacetime metric appears naturally as part of a first order G-structure, and the Yang–Mills fields appear equally naturally as part of a second order G-structure, as part of a connection. Note that here the Yang–Mills gauge fields are part of a *second order* G-structure on the world manifold while in models of the Kaluza–Klein type they are part of a *first order* G-structure on the world manifold.

The language for jets and G-structures and the particular approach to the prolongation of G-structures used in this paper has been explicated in detail in a previous paper by Coleman and Korte.[11] Simple first order subspace structures (without metrics) are described in Sec. 2 and the prolongation of such structures to second order is carried out in Sec. 3. The results of these two sections are generalized to the case of Galilean subspace structures in Sec. 4 with the details of the solution of the prolongation equations presented in Appendix A. Then the metric forms canonically associated with the first order Galilean subspace structure are discussed in Sec. 5. Finally, in Sec. 6, the preceding results as well as the discussion of first order integrability conditions presented in Appendix B are used to describe the new model in which spacetime metric and Yang–Mills fields are unified, and in Sec. 7, this model is compared and contrasted with the models of the Kaluza–Klein type.

In Appendix C, it is shown that under a transformation from one adapted coordinate system to another, the Yang–Mills fields do in fact transform according to the standard Yang–Mills gauge transformation.

Although Galilean subspace structures are also of interest in connection with the analysis of Galilean general relativity theory, the task of specializing our results to this particular case and of relating the resulting description to that of Künzle[10] is left for lack of space to the interested reader.

2. FIRST ORDER SUBSPACE STRUCTURES

Subspace structures appear as an integral part of a variety of geometric structures of interest to theoretical physicists. An absolute time or an absolute space structure is a subspace structure in a pure form. A connection on a principal or associated fiber bundle is a type of subspace structure. The essence of a model of the Kaluza–Klein type is a subspace structure on a pseudo-Riemannian manifold. A special type of subspace structure, the Galilean subspace structure, plays a key role in the model presented in this paper. In this section, subspace structures are presented from the G-structure viewpoint, which is then related to the more customary treatment.

Let M be a C^∞ manifold of dimension $N = n + m$. The conventions adopted for index ranges are as follows:

$$\begin{aligned} &I,J,K,L,\cdots \quad 1,2,\ldots,N, \\ &\kappa,\lambda,\mu,\nu,\cdots \quad 1,2,\ldots,n, \\ &a,b,c,e,f,\cdots \quad n+1,n+2,\ldots,N=n+m. \end{aligned} \tag{2.1}$$

Denote by $S^1_{n,m}$ the subgroup of G^1_N consisting of those elements

$$\partial^1_0\, I_N(a^I_J d^{\,1}_0\, I^J_N) \tag{2.2}$$

for which (a^I_J) has the block form

$$(s^I_J) = \begin{bmatrix} s^\mu_\nu & 0 \\ s^a_\nu & s^a_b \end{bmatrix}. \tag{2.3}$$

The kth order prolongation of $S^1_{n,m}$ will be denoted by $S^k_{n,m}$. If (s^I_J) and (t^I_J) are matrices of the form (2.3), then the product (r^I_J) where $r = st$ is explicitly given by

$$\begin{aligned} r^\mu_\nu &= s^\mu_\lambda t^\lambda_\nu, \\ r^a_\nu &= s^a_\lambda t^\lambda_\nu + s^a_c t^c_\nu, \\ r^a_b &= s^a_c t^c_b. \end{aligned} \tag{2.4}$$

The element inverse to (2.3) is

$$(s^{-1I}_J) = \begin{bmatrix} (s^\mu_\nu)^{-1} & 0 \\ -(s^a_c)^{-1} s^c_\lambda (s^\lambda_\nu)^{-1} & (s^a_b)^{-1} \end{bmatrix}, \tag{2.5}$$

where $(s^\mu_\nu)^{-1}$ and $(s^a_b)^{-1}$ denote the inverses of the submatrices (s^μ_ν) and (s^a_b), respectively. Note that $s^{-1\mu}_\nu$ denotes the n-dimensional part of the inverse of s^I_J. Also, since $s^\mu_b = 0$, $(s^{-1\mu}_\nu) = (s^\mu_\nu)^{-1}$.

Let $p \in U \subset M$ and let $h: U \to V \subset \mathbb{R}^N$ be a local diffeomorphism such that $h(p) = \mathbf{0}$. The 1-jet $j^1_p h$ is an N^1-coframe for M at p. Relative to any given chart (U,x), $j^1_p h$ may be represented in the form

$$j^1_p h = \partial^1_0 I_N(h^I_J d^{\,1}_p x^J), \tag{2.6}$$

where h^I_J is the partial derivative of $h^I \circ x_p^{-1}$ with respect to the Jth argument at $\mathbf{0} \in \mathbb{R}^n$ and $x_p = x - x(p)$. The bundle of N^1-coframes on M is denoted by

$$\mathscr{H}^1{}^*(M) = \langle H^1{}^*(M), \pi_{H^1*}, M, G^1_N \rangle. \tag{2.7}$$

The structure group G^1_N acts freely on the left of $\mathscr{H}^1{}^*(M)$. By restricting this action to the group $S^1_{n,m} \subset G^1_N$, one may construct the associated bundle of $S^1_{n,m}$ related N^1-coframes,

$$\begin{aligned} &S^1_{n,m} \backslash \mathscr{H}^1{}^*(M) \\ &= \langle S^1_{n,m} \backslash H^1{}^*(M), \pi_{S^1_{n,m} \backslash H^1*}, M, S^1_{n,m} \backslash G^1_N, \mathscr{H}^1{}^*(M) \rangle. \end{aligned} \tag{2.8}$$

An $S^1_{n,m}$-structure on M (a subspace structure) is defined by a cross section of $S^1_{n,m} \backslash \mathscr{H}^1{}^*(M)$, $\Sigma: M \to S^1_{n,m} \backslash \mathscr{H}^1{}^*(M)$, which determines at each $p \in M$ an equivalence class, $\Sigma(p)$, of $S^1_{n,m}$ related N^1-coframes.

It is more convenient, from a computational viewpoint, to work with a family of local cross sections of $\mathscr{H}^1{}^*(M)$, where for each such local cross section $h: U \to H^1{}^*(U)$, the N^1-coframe $h(p)$ for any $p \in U$ belongs to the equivalence class of N^1-coframes $\Sigma(p)$ determined by the $S^1_{n,m}$-structure. If $\tilde{h}: \tilde{U} \to H^1{}^*(\tilde{U})$ is any other such local cross section and $U \cap \tilde{U} \neq \emptyset$, then h and $\tilde{h}$ are related by a local $S^1_{n,m}$ gauge transformation, $s: U \cap \tilde{U} \to U \cap \tilde{U} \times S^1_{n,m}$ given by

$$s(p) = \partial^1_0\, I_N(s^I_J d^{\,1}_0\, I^J_N). \tag{2.9}$$

Thus, for $p \in U \cap \tilde{U}$,

$$\begin{aligned} \tilde{h}(p) &= s(p) \circ h(p) \\ &= \partial^1_0\, I_N(s^I_L h^L_J d^{\,1}_p x^J). \end{aligned} \tag{2.10}$$

From the expression

$$(\tilde{h}^I_J) = \begin{bmatrix} s^\mu_\lambda h^\lambda_\nu & s^\mu_\lambda h^\lambda_b \\ s^a_\lambda h^\lambda_\nu + s^a_c h^c_\nu & s^a_\lambda h^\lambda_b + s^a_c h^c_b \end{bmatrix}, \tag{2.11}$$

it is easy to see that a suitable standard representative for the equivalence classes may be selected by means of the coordinate dependent, gauge fixing conditions

$$h^{\mu}_{\nu} = \delta^{\mu}_{\nu}, \quad h^{a}_{\nu} = 0, \quad h^{a}_{b} = \delta^{a}_{b}. \tag{2.12}$$

The standard form of (h^{I}_{J}) will be denoted by (Σ^{I}_{J}).

To derive the coordinate transformation law for the standard representative Σ^{I}_{J}, consider a coordinate transformation from (U,x) to $(\bar{U},\bar{x})$. Then

$$\partial^{1}_{0} I_{N}(\Sigma^{I}_{J} d^{1}_{p} x^{J}) = \partial^{1}_{0} I_{N}(\Sigma^{I}_{J} X^{J}_{K} d^{1}_{p} \bar{x}^{K}) \tag{2.13}$$

and

$$(\Sigma^{I}_{J} X^{J}_{K}) = \begin{bmatrix} \delta^{\mu}_{\nu} & \Sigma^{\mu}_{b} \\ 0 & \delta^{a}_{b} \end{bmatrix} \begin{bmatrix} X^{\mu}_{\nu} & X^{\mu}_{b} \\ X^{a}_{\nu} & X^{a}_{b} \end{bmatrix}$$

$$= \begin{bmatrix} X^{\mu}_{\nu} + \Sigma^{\mu}_{c} X^{c}_{\nu} & X^{\mu}_{b} + \Sigma^{\mu}_{c} X^{c}_{b} \\ X^{a}_{\nu} & X^{a}_{b} \end{bmatrix}. \tag{2.14}$$

From (2.11) and (2.12), it is apparent that the standard representative $(\bar{\Sigma}^{I}_{J})$ is determined by

$$\bar{\Sigma}^{\mu}_{b} = (X^{\mu}_{\lambda} + \Sigma^{\mu}_{c} X^{c}_{\lambda})^{-1}(X^{\lambda}_{b} + \Sigma^{\lambda}_{e} X^{e}_{b}). \tag{2.15}$$

Clearly, by choosing $X^{a}_{b} = \delta^{a}_{b}$ and $X^{\mu}_{b} = -\Sigma^{\mu}_{b}$, one obtains $\bar{\Sigma}^{\mu}_{b} = 0$; consequently, for any $p \in M$, there exists a preferred coordinate system in which $(\Sigma^{I}_{J}) = (\delta^{I}_{J})$. Such a coordinate system is said to be adapted at $p \in M$. Moreover, if $\Sigma^{\mu}_{b} = 0$, then $\bar{\Sigma}^{\mu}_{b} = 0$ iff $X^{\mu}_{b} = 0$; consequently, the preferred coordinate system is determined only up to an $S^{1}_{n,m}$ transformation.

For every $p \in M$, the active microsymmetry group for an $S^{1}_{n,m}$-structure is isomorphic to $S^{1}_{n,m}$. Let $f: M \to M$ be a diffeomorphism such that $f(p) = p$. Then the microtransformation at p is

$$j^{1}_{p} f = \partial^{1}_{p} x(F^{I}_{J} d^{1}_{p} x^{J}), \tag{2.16}$$

where F^{I}_{J} is the partial derivative of $F^{I} = x^{I}_{p} \circ f \circ x^{-1}_{p}$ with respect to the Jth argument at $0 \in \mathbb{R}$. Under such a transformation, the standard representative transforms according to

$$\tilde{\Sigma}^{\mu}_{b} = (F^{\mu}_{\lambda} + \Sigma^{\mu}_{c} F^{c}_{\lambda})^{-1}(F^{\lambda}_{b} + \Sigma^{\lambda}_{e} F^{e}_{b}). \tag{2.17}$$

The invariance condition is just $\tilde{\Sigma}^{\mu}_{b} = \Sigma^{\mu}_{b}$, from which it readily follows that

$$F^{\mu}_{b} = F^{\mu}_{\lambda} \Sigma^{\lambda}_{b} + \Sigma^{\mu}_{c} F^{c}_{\lambda} \Sigma^{\lambda}_{b} - \Sigma^{\mu}_{c} F^{c}_{b}. \tag{2.18}$$

It is a routine matter to show that the transformations (2.16) with F_{b} given by (2.18) form a group isomorphic to $S^{1}_{n,m}$. Indeed, since the coordinate system may be freely chosen, one of the preferred systems in which $\Sigma^{\mu}_{b} = 0$ may be used. In such a system, F^{μ}_{ν}, F^{a}_{ν}, and F^{a}_{b} may be chosen freely while $F^{\mu}_{b} = 0$.

To recover the customary description of a subspace structure from the above G-structure treatment, note that the first n arguments of the standard N^{1}-coframe

$$\partial^{1}_{0} I_{N}(\Sigma^{I}_{J} d^{1}_{p} x^{J}) \tag{2.19}$$

determined by the $S^{1}_{n,m}$-structure determine n linearly independent 1^{1}-cospeeds (1-forms); namely,

$$\omega^{\mu} = \partial^{1}_{0} I(d^{1}_{p} x^{\mu} + \Sigma^{\mu}_{a} d^{1}_{p} x^{a}) \tag{2.20}$$

for each $\mu \in \{1,2,\ldots,n\}$. A 1^{1}-speed (vector) at $p \in M$ is a 1:jet $j^{1}_{0}\gamma$ of a map $\gamma: \mathbb{R} \to M$ for which $\gamma(0) = p$.

$$j^{1}_{0}\gamma = \partial^{1}_{p} x(\gamma^{I}_{1} d^{1}_{0} I). \tag{2.21}$$

The set of such 1^{1}-speeds at p forms a linear vector space $L^{1}_{1}(M_{p})$ [isomorphic to $T(M_{p})$]. The 1^{1}-cospeeds (2.20) define a linear subspace of $L^{1}_{1}(M_{p})$ consisting of those 1^{1}-speeds (2.21) which satisfy

$$\omega^{\mu} \cdot j^{1}_{0}\gamma = 0, \quad \mu = 1,2,\ldots,n. \tag{2.22}$$

It is easy to show that the subspace so defined is invariant under both coordinate and active microsymmetry transformations. In an adapted coordinate system, the $\gamma^{\mu}_{1} = 0$ while the γ^{a}_{1} are arbitrary.

3. SECOND ORDER SUBSPACE STRUCTURES

An $S^{1}_{n,m}$-structure determines at each $p \in M$ an equivalence class of N^{1}-coframes; namely, the N^{1}-coframes

$$\partial^{1}_{0} I_{N}(s^{J}_{J} \Sigma^{J}_{K} d^{1}_{p} x^{K}), \tag{3.1}$$

where (Σ^{I}_{J}) determines the standard representative and $(s^{I}_{J}) \in S^{1}_{n,m}$. Any N^{2}-coframe which projects onto the N^{1}-coframe (3.1) may be expressed in the form

$$\partial^{2}_{0} I_{N}\left(s^{I}_{R} \Sigma^{R}_{J} d^{2}_{p} x^{J} + \frac{1}{2!} s^{I}_{R} \Gamma^{R}_{JK} d^{2}_{p} x^{J} d^{2}_{p} x^{K}\right). \tag{3.2}$$

If $q \in M$ is a point infinitesimally near $p \in M$ and $w^{I} = x^{I}(q) - x^{I}(p)$, then the N^{2}-coframe (3.2) at p determines an N^{1}-coframe at q; namely,

$$\partial^{1}_{0} I_{N}\left[s^{I}_{R}(\Sigma^{R}_{J} + \Gamma^{R}_{JS} w^{S}) d^{1}_{q} x^{J}\right]. \tag{3.3}$$

The standard representative corresponding to the N^{1}-coframe (3.3) may be determined from

$$(\Sigma^{I}_{J} + \Gamma^{I}_{JS} w^{S})$$

$$= \begin{bmatrix} \delta^{\mu}_{\nu} + \Gamma^{\mu}_{\nu S} w^{S} & \Sigma^{\mu}_{b} + \Gamma^{\mu}_{bS} w^{S} \\ \Gamma^{a}_{\nu S} w^{S} & \delta^{a}_{b} + \Gamma^{a}_{bS} w^{S} \end{bmatrix}$$

$$= \begin{bmatrix} \delta^{\mu}_{\nu} + \Gamma^{\mu}_{\nu S} w^{S} & 0 \\ \Gamma^{a}_{\nu S} w^{S} & \delta^{a}_{b} + \Gamma^{a}_{bS} w^{S} - \Gamma^{a}_{\lambda S} \Sigma^{\lambda}_{b} w^{S} \end{bmatrix}$$

$$\times \begin{bmatrix} \delta^{\mu}_{\nu} & \Sigma^{\mu}_{b} + \Gamma^{\mu}_{bS} w^{S} - \Gamma^{\mu}_{\lambda S} \Sigma^{\lambda}_{b} w^{S} \\ 0 & \delta^{a}_{b} \end{bmatrix}. \tag{3.4}$$

Thus, the standard matrix for (3.3) is

$$\begin{bmatrix} \delta^{\mu}_{\nu} & \Sigma^{\mu}_{b} + \Gamma^{\mu}_{bS} w^{S} - \Gamma^{\mu}_{\lambda S} \Sigma^{\lambda}_{b} w^{S} \\ 0 & \delta^{a}_{b} \end{bmatrix}. \tag{3.5}$$

On the other hand, the $S^{1}_{n,m}$-structure determines at $q \in M$ an equivalence class of N^{1}-coframes, the standard representative of which is

$$\partial^{1}_{0} I_{N}(\Sigma^{I}_{J}(q) d^{1}_{q} x^{J}). \tag{3.6}$$

However, expanding $\Sigma^{I}_{J}(q)$ about p gives

$$\Sigma^{I}_{J}(q) = \Sigma^{I}_{J}(p) + \Sigma^{I}_{J,S}(p) w^{S}$$

$$= \begin{bmatrix} \delta^{\mu}_{\nu} & \Sigma^{\mu}_{b} + \Sigma^{\mu}_{b,S} w^{S} \\ 0 & \delta^{a}_{b} \end{bmatrix}, \tag{3.7}$$

which is already in standard form. The prolongation (3.2) is self-consistent iff (3.7) and (3.5) differ at most by a term of the form $(B^{I}_{JS} w^{S})$, where $B^{I}_{JK} = -B^{I}_{KJ}$. In block matrix form,

this term is

$$(B^I_{JS}w^S)=\begin{bmatrix} B^\mu_{\nu\lambda}w^\lambda + B^\mu_{\nu c}w^c & B^\mu_{b\lambda}w^\lambda + B^\mu_{bc}w^c \\ B^a_{\nu\lambda}w^\lambda + B^a_{\nu c}w^c & B^a_{b\lambda}w^\lambda + B^a_{bc}w^c \end{bmatrix}. \tag{3.8}$$

Both (3.5) and (3.7) have a zero matrix in the lower left block; consequently,

$$B^a_{\nu\lambda}=0, \quad B^a_{\nu c}=0. \tag{3.9}$$

Since the diagonal blocks of both (3.5) and (3.7) are δ^μ_ν and δ^a_b,

$$\begin{aligned} &B^\mu_{\nu\lambda}=0, \quad B^\mu_{\nu c}=0, \\ &B^a_{bc}=0, \quad B^a_{b\lambda}=0. \end{aligned} \tag{3.10}$$

By skew symmetry,

$$B^\mu_{b\lambda} = -B^\mu_{\lambda b}=0. \tag{3.11}$$

Thus, only B^μ_{bc} may differ from zero. Thus, the condition for self-consistency of the prolonged structure is

$$\Sigma^\mu_b + \Sigma^\mu_{b,S}w^S + B^\mu_{bc}w^c = \Sigma^\mu_b + \Gamma^\mu_{bS}w^S - \Gamma^\mu_{\lambda S}\Sigma^\lambda_b w^S. \tag{3.12}$$

Hence,

$$\begin{aligned} &\Sigma^\mu_{b,\nu}=\Gamma^\mu_{b\nu}-\Gamma^\mu_{\lambda\nu}\Sigma^\lambda_b, \\ &\Sigma^\mu_{b,c}+B^\mu_{bc}=\Gamma^\mu_{bc}-\Gamma^\mu_{\lambda c}\Sigma^\lambda_b. \end{aligned} \tag{3.13}$$

The first of these equations gives

$$\Gamma^\mu_{\nu b}=\Gamma^\mu_{b\nu}=\Sigma^\mu_{b,\nu}+\Gamma^\mu_{\lambda\nu}\Sigma^\lambda_b. \tag{3.14}$$

The symmetric part of the second equation of (3.13) and (3.14) together give

$$\begin{aligned} \Gamma^\mu_{bc} =& \tfrac{1}{2}(\Sigma^\mu_{b,c}+\Sigma^\mu_{c,b})+\tfrac{1}{2}(\Sigma^\mu_{b,\nu}\Sigma^\nu_c+\Sigma^\mu_{c,\nu}\Sigma^\nu_b) \\ &+\Gamma^\mu_{\nu\lambda}\Sigma^\nu_b\Sigma^\lambda_c. \end{aligned} \tag{3.15}$$

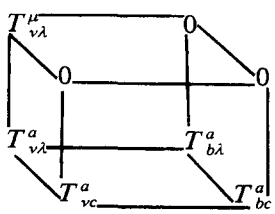
From the skew symmetric part of the second equation of (3.13) and from (3.14), it follows that

$$B^\mu_{bc} = -\tfrac{1}{2}(\Sigma^\mu_{b,c}-\Sigma^\mu_{c,b})+\tfrac{1}{2}(\Sigma^\mu_{b,\nu}\Sigma^\nu_c-\Sigma^\mu_{c,\nu}\Sigma^\nu_b). \tag{3.16}$$

Thus, the components $\Gamma^\mu_{\nu\lambda}$, $\Gamma^a_{\nu\lambda}$, $\Gamma^a_{\nu c}(=\Gamma^a_{c\nu})$, and Γ^a_{bc} are completely undetermined while the components $\Gamma^\mu_{\nu b}(=\Gamma^\mu_{b\nu})$ and Γ^μ_{bc} are determined by the first order structure, and $\Gamma^\mu_{\nu\lambda}$ and B^μ_{bc} depend only on the first order structure. The undetermined coefficients indicate that the prolonged group $S^2_{n,m}$ has more parameters than $S^1_{n,m}$.

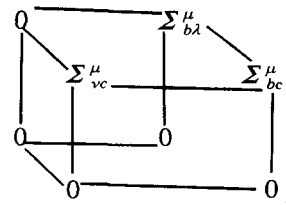
It will now be shown that the general N^2-coframe (3.2) which belongs to the $S^2_{n,m}$-structure factors into the product of an $S^2_{n,m}$ group element and a standard representative N^2-coframe.

Let T^I_{JK} have the block form



(3.17)

and define Σ^I_{JK} by



(3.18)

where

$$\begin{aligned} &\Sigma^\mu_{\nu c}=\Sigma^\mu_{c,\nu}, \quad \Sigma^\mu_{b\lambda}=\Sigma^\mu_{b,\lambda}, \\ &\Sigma^\mu_{bc}=\tfrac{1}{2}(\Sigma^\mu_{b,c}+\Sigma^\mu_{c,b})+\tfrac{1}{2}(\Sigma^\mu_{b,\alpha}\Sigma^\alpha_c+\Sigma^\mu_{c,\alpha}\Sigma^\alpha_b). \end{aligned} \tag{3.19}$$

Now consider the product of

$$\partial^2_0 I_N\left(d^2_0 I^I_N+\frac{1}{2!}T^I_{JK}d^2_0 I^J_N d^2_0 I^K_N\right) \tag{3.20}$$

and

$$\partial^2_0 I_N\left(\Sigma^I_J d^2_p x^J+\frac{1}{2!}\Sigma^I_{JK}d^2_p x^J d^2_p x^K\right). \tag{3.21}$$

One obtains

$$\partial^2_0 I_N\left(\Sigma^I_J d^2_p x^J+\frac{1}{2!}\Gamma^I_{JK}d^2_p x^J d^2_p x^K\right), \tag{3.22}$$

where

$$\Gamma^I_{JK}=\Sigma^I_{JK}+T^I_{LM}\Sigma^L_J\Sigma^M_K. \tag{3.23}$$

In block form, Eq. (3.23) becomes

$$\begin{aligned} &\Gamma^\mu_{b\lambda}=\Sigma^\mu_{b\lambda}+2T^\mu_{\alpha\lambda}\Sigma^\alpha_b, \\ &\Gamma^\mu_{\nu c}=\Sigma^\mu_{\nu c}+2T^\mu_{\alpha\nu}\Sigma^\alpha_c, \\ &\Gamma^\mu_{bc}=\Sigma^\mu_{bc}+T^\mu_{\alpha\beta}\Sigma^\alpha_b\Sigma^\beta_c, \\ &\Gamma^\mu_{\nu\lambda}=T^\mu_{\nu\lambda}, \\ &\Gamma^a_{\nu\lambda}=T^a_{\nu\lambda}, \\ &\Gamma^a_{\nu c}=2T^a_{\nu\alpha}\Sigma^\alpha_c+2T^a_{\nu c}, \\ &\Gamma^a_{b\lambda}=2T^a_{\alpha\lambda}\Sigma^\alpha_b+2T^a_{b\lambda}, \\ &\Gamma^a_{bc}=T^a_{\alpha\beta}\Sigma^\alpha_b\Sigma^\beta_c+T^a_{\alpha c}\Sigma^\alpha_b+T^a_{b\alpha}\Sigma^\alpha_c+T^a_{bc}. \end{aligned} \tag{3.24}$$

The first three of these equations coincide with (3.14) and (3.15). From the remaining equations, it is clear that the quantities $\Gamma^\mu_{\nu\lambda}$, $\Gamma^a_{\nu\lambda}$, $\Gamma^a_{\nu c}=\Gamma^a_{c\nu}$, and Γ^a_{bc} may be expressed in terms of the quantities $T^\mu_{\nu\lambda}$, $T^a_{\nu\lambda}$, $T^a_{\nu c}=T^a_{c\nu}$, and T^a_{bc} and conversely; consequently, if one set is arbitrary so is the other.

The product of

$$\partial^2_0 I_N(s^I_J d^2_0 I^J_N) \tag{3.25}$$

and (3.20) yields

$$\partial^2_0 I_N\left(s^I_J d^2_0 I^J_N+\frac{1}{2!}s^I_{JK}d^2_0 I^J_N d^2_0 I^K_N\right), \tag{3.26}$$

where s^a_{JK} and $s^\mu_{\nu\lambda}$ may be freely chosen and

$$\begin{aligned} &s^a_{\nu c}=s^a_e T^e_{\nu c}=s^a_{c\nu}, \\ &s^a_{bc}=s^a_e T^e_{bc}. \end{aligned} \tag{3.27}$$

The 2-jet (3.26) is the general element of the prolonged group $S^2_{n,m}$. The N^2-coframe (3.21) is the standard representative of

the equivalence class of N^2-coframes at $p \in M$ determined by the $S^2_{n,m}$-structure. The general N^2-coframe belonging to this equivalence class is given by (3.2), which is the composition of (3.26) and (3.21).

4. GALILEAN SUBSPACE STRUCTURES

Denote by $S^1_{(p,q),(r,s)}$ the subgroup of G^1_N consisting of those elements

$$\partial^1_0 I_N(s^I_J d^1_0 I^J_N) \tag{4.1}$$

where (s^I_J) has the block form (2.3) and

$$\eta_{\alpha\beta} s^\alpha_\mu s^\beta_\nu = \eta_{\mu\nu}, \qquad \eta_{ab} s^a_c s^b_e = \eta_{ce}, \tag{4.2}$$

where $(\eta_{\alpha\beta})$ [respectively, (η_{ab})] is diagonal with $+1$ in the first p (respectively, r) positions and -1 in the remaining q (respectively, s) positions. $S^1_{(p,q),(r,s)}$ is a subgroup of $S^1_{n,m}$, where $p+q=n$ and $r+s=m$. If $q=0=s$, the subgroup will be denoted by $S^1_{(n),(m)}$. *A Galilean subspace structure* or $S^1_{(p,q),(r,s)}$-structure is defined by a cross section Σ of the associated bundle $S^1_{(p,q),(r,s)} \backslash \mathscr{H}^1{}^*(M)$ of $S^1_{(p,q),(r,s)}$ related N^1-coframes. Such a cross section may be conveniently represented by a family of local cross sections of $\mathscr{H}^1{}^*(M)$. For each local cross section $h: U \to H^1{}^*(U)$ belonging to the family, the N^1-coframe $h(p) \in \Sigma(p)$, the equivalence class of N^1-coframes determined by the $S^1_{(p,q),(r,s)}$-structure; moreover, if $\tilde{h}: \tilde{U} \to H^1{}^*(\tilde{U})$ is any other such local cross section and $U \cap \tilde{U} \neq \emptyset$, then h and $\tilde{h}$ are related by a local gauge transformation (2.10), where now $s(p) \in S^1_{(p,q),(r,s)}$. From (2.11) and the fact that in the present case $(s^\mu_\nu) \in O^1_{p,q}$ and $(s^a_b) \in O^1_{r,s}$, it is clear that a suitable standard representative for the N^1-coframes $\Sigma(p)$ is given by

$$\partial^1_0 I_N(\Sigma^I_J d^1_p x^J), \tag{4.3}$$

where

$$(\Sigma^I_J) = \begin{bmatrix} \Sigma^\mu_\nu & \Sigma^\mu_b \\ 0 & \Sigma^a_b \end{bmatrix} \tag{4.4}$$

in which (Σ^μ_ν) and (Σ^a_b) are upper triangular.

To prolong the $S^1_{(p,q),(r,s)}$-structure to an $S^2_{(p,q),(r,s)}$-structure, consider an arbitrary member of $\Sigma(p)$, namely,

$$\partial^1_0 I_N(s^I_R \Sigma^R_J d^1_p x^J) \tag{4.5}$$

and an arbitrary N^2-coframe which projects onto the N^1-coframe, namely,

$$\partial^2_0 I_N\left(s^I_R \Sigma^R_J d^2_p x^J + \frac{1}{2!} s^I_R \Gamma^R_{JK} d^2_p x^J d^2_p x^K\right). \tag{4.6}$$

This N^2-coframe determines the N^1-coframe

$$\partial^1_0 I_N(s^I_R(\Sigma^R_J + \Gamma^R_{JS} w^S) d^1_q x^J) \tag{4.7}$$

at q, where $w^I = x^I(q) - x^I(p)$. Next, bring (4.7) to standard form. First, consider

$$(\Sigma^I_J + \Gamma^I_{JS} w^S) = \begin{bmatrix} \Sigma^\mu_\nu + \Gamma^\mu_{\nu S} w^S & \Sigma^\mu_b + \Gamma^\mu_{bS} w^S \\ \Gamma^a_{\nu S} w^S & \Sigma^a_b + \Gamma^a_{bS} w^S \end{bmatrix}$$

$$= \begin{bmatrix} \delta^\mu_\nu & 0 \\ \Gamma^a_{\lambda S}(\Sigma^\lambda_\nu)^{-1} w^S & \delta^a_b \end{bmatrix} \begin{bmatrix} \Sigma^\mu_\nu + \Gamma^\mu_{\nu S} w^S & \Sigma^\mu_b + \Gamma^\mu_{bS} w^S \\ 0 & \Sigma^a_b + \Gamma^a_{bS} w^S - \Gamma^a_{\rho S}(\Sigma^\rho_\lambda)^{-1} \Sigma^\lambda_b w^S \end{bmatrix}. \tag{4.8}$$

Next, choose infinitesimal transformations $(\Lambda^\mu_\nu) \in O^1_{p,q}$ and $(\Lambda^a_b) \in O^1_{r,s}$, where

$$\Lambda^\mu_\nu = \delta^\mu_\nu + \lambda^\mu_{\nu S} w^S, \quad \Lambda^a_b = \delta^a_b + \lambda^a_{bS} w^S, \tag{4.9}$$

and

$$\eta_{\mu\rho} \lambda^\rho_{\nu S} = \lambda_{\mu\nu S} = -\lambda_{\nu\mu S}, \quad \eta_{ac} \lambda^c_{bS} = \lambda_{abS} = -\lambda_{baS} \tag{4.10}$$

such that

$$\begin{bmatrix} \Lambda^\mu_\nu & 0 \\ 0 & \Lambda^a_b \end{bmatrix} \begin{bmatrix} \Sigma^\mu_\nu + \Gamma^\mu_{\nu S} w^S & \Sigma^\mu_b + \Gamma^\mu_{bS} w^S \\ 0 & \Sigma^a_b + \Gamma^a_{bS} w^S - \Gamma^a_{\rho S}(\Sigma^\rho_\lambda)^{-1} \Sigma^\lambda_b w^S \end{bmatrix}$$

$$= \begin{bmatrix} \Sigma^\mu_\nu + \Gamma^\mu_{\nu S} w^S + \lambda^\mu_{\rho S} \Sigma^\rho_\nu w^S & \Sigma^\mu_b + \Gamma^\mu_{bS} w^S + \lambda^\mu_{\rho S} \Sigma^\rho_b w^S \\ 0 & \Sigma^a_b + \Gamma^a_{bS} w^S - \Gamma^a_{\rho s}(\Sigma^\rho_\lambda)^{-1} \Sigma^\lambda_b w^S + \lambda^a_{cS} \Sigma^c_b w^S \end{bmatrix}. \tag{4.11}$$

Since (Σ^μ_ν) and (Σ^a_b) are by definition upper triangular, the requirement that the diagonal elements of block matrix (4.11) be upper triangular yields the equations

$$\Gamma^\mu_{\nu S} + \lambda^\mu_{\rho S} \Sigma^\rho_\nu = 0 \quad \text{for } \mu > \nu,$$
$$\Gamma^a_{bS} - \Gamma^a_{\rho S}(\Sigma^\rho_\lambda)^{-1} \Sigma^\lambda_b + \lambda^a_{cS} \Sigma^c_b = 0 \quad \text{for } a > b. \tag{4.12}$$

In view of the skew symmetry (4.10), these equations may be solved for $\lambda^\mu_{\rho S}$ in terms of $\Gamma^\mu_{\nu S}$ and Σ^μ_ν and for λ^a_{bS} in terms of Γ^a_{bS}, $\Gamma^a_{\rho S}$, Σ^μ_ν, Σ^μ_b, and Σ^a_b. *In the following, it is assumed that this has been done.*

The $S^1_{(p,q),(r,s)}$-structure already specifies a standard N^1-

coframe at q; namely,

$$\partial_0^1 I_N(\Sigma^I_J(q) d^1_q x^J) = \partial_0^1 I_N [(\Sigma^I_J(p) + \Sigma^I_{J,S}(p) w^S) d^1_q x^J]. \tag{4.13}$$

In order that the prolonged structure be self-consistent, the matrix

$$\Sigma^I_J(q) = \begin{bmatrix} \Sigma^\mu_\nu + \Sigma^\mu_{\nu,S} w^S & \Sigma^\mu_b + \Sigma^\mu_{b,S} w^S \\ 0 & \Sigma^a_b + \Sigma^a_{b,S} w^S \end{bmatrix} \tag{4.14}$$

may differ from the standard form (4.11) by at most a matrix of the form (3.8), which satisfies

$$\begin{aligned} &B^\mu_{\nu S} = 0 \quad \text{for } \mu > \nu, \\ &B^a_{bS} = 0 \quad \text{for } a > b, \\ &B^a_{\nu S} = 0. \end{aligned} \tag{4.15}$$

Such a matrix has the explicit form

$$\begin{bmatrix} B^\mu_{\nu\lambda} w^\lambda + B^\mu_{\nu c} w^c & B^\mu_{b\lambda} w^\lambda + B^\mu_{bc} w^c \\ 0 & B^a_{bc} w^c \end{bmatrix}. \tag{4.16}$$

The compatibility conditions are

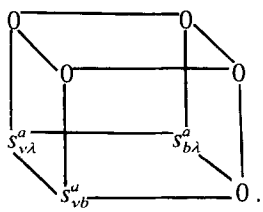
$$\begin{aligned} &\Sigma^\mu_{\nu,\lambda} + B^\mu_{\nu\lambda} = \Gamma^\mu_{\nu\lambda} + \lambda^\mu_{\rho\lambda} \Sigma^\rho_\nu, \\ &\Sigma^\mu_{\nu,c} + B^\mu_{\nu c} = \Gamma^\mu_{\nu c} + \lambda^\mu_{\rho c} \Sigma^\rho_\nu, \\ &\Sigma^\mu_{b,\lambda} + B^\mu_{b\lambda} = \Gamma^\mu_{b\lambda} + \lambda^\mu_{\rho\lambda} \Sigma^\rho_b, \\ &\Sigma^\mu_{b,c} + B^\mu_{bc} = \Gamma^\mu_{bc} + \lambda^\mu_{\rho c} \Sigma^\rho_b, \\ &\Sigma^a_{b,\lambda} = \Gamma^a_{b\lambda} - \Gamma^a_{\rho\lambda} (\Sigma^\rho_\sigma)^{-1} \Sigma^\sigma_b + \lambda^a_{e\lambda} \Sigma^e_b, \\ &\Sigma^a_{b,c} + B^a_{bc} = \Gamma^a_{bc} - \Gamma^a_{\rho c} (\Sigma^\rho_\sigma)^{-1} \Sigma^\sigma_b + \lambda^a_{ec} \Sigma^e_b. \end{aligned} \tag{4.17}$$

Equations (4.17) constitute a linear system for the unknowns Γ^I_{JK} and B^I_{JK}. The system is underdetermined and some of the variables may be chosen arbitrarily. The details of the analysis are presented in Appendix A. A description of the results is given here.

The general element of the prolonged group $S^2_{(p,q)(r,s)}$ is

$$\partial_0^2 I_N \left(s^I_J d^2_0 I^J_N + \frac{1}{2!} s^I_{JK} d^2_0 I^J_N d^2_0 I^K_N \right), \tag{4.18}$$

where s^I_{JK} has the block form



(4.19)

Moreover, if T^I_{JK} is defined by

$$s^I_{JK} = s^I_R T^R_{JK} \tag{4.20}$$

then the T^I_{JK} have the same block form as the s^I_{JK} and the $T^a_{b\lambda} = T^a_{\lambda b}$ satisfy the symmetry condition

$$T_{ab\lambda} = \eta_{ac} T^c_{b\lambda} = -T_{ba\lambda}. \tag{4.21}$$

If $\hat{s}$ and $\tilde{s}$ are any two elements of $S^2_{(p,q),(r,s)}$, their product s is explicitly given by

$$\begin{aligned} &s^\mu_\nu = \hat{s}^\mu_\lambda \tilde{s}^\lambda_\nu, \\ &s^a_\nu = \hat{s}^a_\lambda \tilde{s}^\lambda_\nu + \hat{s}^a_c \tilde{s}^c_\nu, \\ &s^a_b = \hat{s}^a_c \tilde{s}^c_b, \\ &s^a_{\nu\lambda} = \hat{s}^a_{\rho\sigma} \tilde{s}^\rho_\nu \tilde{s}^\sigma_\lambda + \hat{s}^a_{\rho e} \tilde{s}^\rho_\nu \tilde{s}^e_\lambda + \hat{s}^a_{e\rho} \tilde{s}^e_\nu \tilde{s}^\rho_\lambda + \hat{s}^a_e \tilde{s}^e_{\nu\lambda}, \\ &s^a_{b\lambda} = s^a_{\lambda b} = \hat{s}^a_e \tilde{s}^e_{b\lambda} + \hat{s}^a_{ef} \tilde{s}^e_b \tilde{s}^f_\lambda. \end{aligned} \tag{4.22}$$

From the last of these equations, one obtains

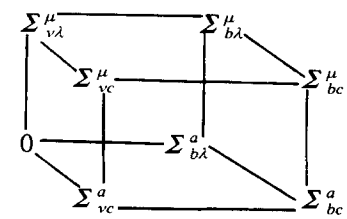
$$T^a_{b\lambda} = \tilde{T}^a_{b\lambda} + \tilde{s}_e^{-1a} \hat{T}^e_{fg} \tilde{s}^f_b \tilde{s}^g_\lambda. \tag{4.23}$$

By using the second of the relations (4.2), one may show that $T^a_{b\lambda}$ satisfies (4.10) provided that $\hat{T}^a_{b\lambda}$ and $\tilde{T}^a_{b\lambda}$ satisfy (4.10).

Denote the standard representative of the equivalence class of $S^2_{(p,q),(r,s)}$ related N^2-coframes by

$$\partial_0^2 I_N \left(\Sigma^I_J d^2_p x^J + \frac{1}{2!} \Sigma^I_{JK} d^2_p x^J d^2_p x^K \right). \tag{4.24}$$

Then Σ^I_{JK} has the block form



(4.25)

Also,

$$\begin{aligned} &\Sigma^\mu_{b\lambda} = \Sigma^\mu_{\lambda b}, \\ &\Sigma^a_{b\lambda} = \Sigma^a_{\lambda b}, \\ &\Sigma^a_{b\lambda} = 0 \text{ for } a > b. \end{aligned} \tag{4.26}$$

The Σ^I_{JK} are completely determined by the functions Σ^I_J which describe the first order structure. The explicit formulas are rather complicated and are given in Appendix A.

Finally, note that the N^2-coframe (4.6) is the composition of an $S^2_{(p,q),(r,s)}$ group element (4.18) and the standard N^2-coframe (4.13); consequently,

$$\Gamma^I_{JK} = \Sigma^I_{JK} + T^I_{RS} \Sigma^R_J \Sigma^S_K \tag{4.27}$$

or

$$\begin{aligned} &\Gamma^\mu_{\nu\lambda} = \Sigma^\mu_{\nu\lambda}, \\ &\Gamma^\mu_{b\lambda} = \Sigma^\mu_{b\lambda} = \Gamma^\mu_{\lambda b}, \\ &\Gamma^\mu_{bc} = \Sigma^\mu_{bc} \end{aligned} \tag{4.28}$$

and

$$\begin{aligned} &\Gamma^a_{\nu\lambda} = T^a_{\rho\sigma} \Sigma^\rho_\nu \Sigma^\sigma_\lambda, \\ &\Gamma^a_{b\lambda} = \Gamma^a_{\lambda b} = \Sigma^a_{b\lambda} + T^a_{\rho\sigma} \Sigma^\rho_b \Sigma^\sigma_\lambda + T^a_{e\sigma} \Sigma^e_b \Sigma^\sigma_\lambda, \\ &\Gamma^a_{bc} = \Sigma^a_{bc} + T^a_{\rho\sigma} \Sigma^\rho_b \Sigma^\sigma_c + T^a_{e\rho} \Sigma^e_c \Sigma^\rho_b + T^a_{e\rho} \Sigma^e_b \Sigma^\rho_c. \end{aligned} \tag{4.29}$$

5. THE GALILEAN METRIC FORMS

In Sec. 4, a Galilean subspace structure was defined as an $S^1_{(p,q),(r,s)}$-structure. However, it is customary to describe such a structure at least in part in terms of metrics naturally associated with such a structure. These metrics will now be discussed.

The standard N^1-coframe (4.3) defines a basis for the cotangent space at $p \in M$ consisting of the forms

$$\omega^\mu = \Sigma^\mu_\nu d_p x^\nu + \Sigma^\mu_b d_p x^b,$$
$$\omega^a = \Sigma^a_b d_p x^b. \tag{5.1}$$

The basis for the tangent space at $p \in M$ that is dual to the basis (5.1) is

$$\zeta_\mu = \Sigma^{-1\nu}_\mu \partial_p x_\nu,$$
$$\zeta_a = \Sigma^{-1b}_a \partial_p x_b - \Sigma^{-1\nu}_a \Sigma^a_e \Sigma^{-1e}_a \partial_p x_\nu, \tag{5.2}$$

or

$$\zeta_I = \Sigma^{-1J}_I \partial_p x_J.$$

Under a change of coordinate system defined by $X = x \circ \bar{x}^{-1}$, the *standard* N^1-coframes are related by

$$\bar{\Sigma}^I_J = s^I_A \Sigma^A_B X^B_J, \tag{5.3}$$

where the $(s^I_J) \in S^1_{(p,q),(r,s)}$ is uniquely determined by Σ^I_J and X^I_J. Thus, the forms (5.1) transform according to

$$\bar{\omega}^\mu = s^\mu_\nu \omega^\nu,$$
$$\bar{\omega}^a = s^a_\nu \omega^\nu + s^a_b \omega^b. \tag{5.4}$$

Clearly, for each $p \in M$, a subspace of the tangent space is invariantly defined which consists of all vectors V which satisfy

$$\omega^\mu(V) = 0. \tag{5.5}$$

Restricted to this subspace, the subspace metric

$$g_S = \eta_{ab} \omega^a \otimes \omega^b \tag{5.6}$$

is invariant. In addition, the invariant metric

$$g = \eta_{\mu\nu} \omega^\mu \otimes \omega^\nu \tag{5.7}$$

provides a measure of distance between subspaces.

The metric (5.7) and the metric (5.6) restricted to the appropriate subspace are also invariant under active microsymmetry transformations. Consider a diffeomorphism $f: M \to M$ such that $f(p) = p$, and set $F = x \circ f \circ x^{-1}$. Then the 1-jet

$$j^1_p f = \partial^1_p x (F^I_J d^{\,1}_p x^J) \tag{5.8}$$

is a microsymmetry iff any N^1-coframe belonging to the $S^1_{(p,q),(r,s)}$-structure at $p \in M$ is transformed into another such N^1-coframe. This condition is satisfied iff

$$F^I_J = \Sigma^{-1I}_A s^A_B \Sigma^B_J, \tag{5.9}$$

where the $(s^I_J) \in S^1_{(p,q),(r,s)}$ may be chosen arbitrarily. Under such a transformation the basis (5.1) will be transformed into another basis given by

$$\tilde{\omega}^\mu = s^\mu_\nu \omega^\nu,$$
$$\tilde{\omega}^a = s^a_\nu \omega^\nu + s^a_b \omega^b. \tag{5.10}$$

It is clear that the metric g, the subspace defined by (5.5) and the metric g_S restricted to this subspace are invariant under the active transformation (5.10). Note that the meaning of (5.4) is quite different from that of (5.10) despite the similar form.

6. THE GALILEAN SUBSPACE WORLD MODEL

Our geometric model for the unification of the spacetime metric and Yang–Mills fields is based on a C^∞ manifold M of dimension $4 + m$. This world manifold is equipped with a first order Galilean subspace structure determined by a cross section of the bundle $S^1_{(1,3),(m)} \backslash \mathscr{H}^1(M)$. In this model, the internal symmetry group is $O(M)$; however, the model may be adapted in the manner discussed below to permit a unitary internal symmetry group. The Galilean subspace structure determines a distribution on the world manifold M; that is, a subspace (of dimension m) of each tangent space is singled out in a smooth way. These distinguished subspaces play the role of tangent spaces of the internal symmetry submanifolds. There is therefore an *a priori* distinction between internal and spacetime dimensions.

For an arbitrary distribution, there will not in general exist submanifolds the tangent spaces of which are the subspaces distinguished by the distribution. As pointed out in Appendix B, in order that internal symmetry submanifolds exist, it is necessary and sufficient that the distribution is involutive.[4–6] In terms of the first order structure fields Σ^I_J, this condition may be expressed by the partial differential constraint equations (B1). For an involutive Galilean subspace structure, the metric g_S given by (5.6) and restricted to a given internal symmetry submanifold is a Riemann metric for that submanifold. In the neighborhood of any point $p \in M$, there exist adapted coordinate systems such that the internal symmetry submanifolds are determined in any such system by the equations

$$\bar{x}^\mu = 0. \tag{6.1}$$

In such a system, the metric g_S will take the form

$$g_S = \bar{g}_{Sab}(\bar{x}^\mu, \bar{x}^a) d\bar{x}^a \otimes d\bar{x}^b \tag{6.2}$$

and the curvature tensor $\bar{R}^{\,a}_{Sbcd}$ will be given by the usual expression with the $\bar{x}^\mu$ coordinates behaving as mere spectators. It should be emphasized that the above comments apply locally and not just at a point.

If desired, it is possible to compactify the internal symmetry submanifolds and to considerably reduce the number of dyamically interesting fields in the $S^1_{(1,3),(m)}$-structure by requiring that the internal symmetry submanifolds are spaces of constant positive curvature.[12] This requirement may be expressed as a system of second order partial differential constraint equations for $\bar{g}_{Sab}$; namely,

$$\bar{R}_{Sabcd} = \frac{\bar{R}_S}{n(n-1)} (\bar{g}_{Sac}\, \bar{g}_{Sbd} - \bar{g}_{Sad}\, \bar{g}_{Sbc}), \tag{6.3}$$

where the curvature scalar $\bar{R}_S$ may depend on the spacetime variable $\bar{x}^\mu$.

The metric g given by (5.7) is of course the spacetime metric. In the adapted coordinate system $\bar{\Sigma}^\mu_b = 0$ (locally not just at a point), and g takes the form

$$g = \bar{g}_{\mu\nu}(\bar{x}^\mu, \bar{x}^a) d\bar{x}^\mu \otimes d\bar{x}^\nu. \tag{6.4}$$

If the Galilean subspace structure is not only involutive but also first order flat then, as discussed in Appendix B, the first order structure fields Σ^I_J satisfy the condition (B4) as well as the condition (B1). It is easy to see that in the adapted coordi-

nate system $\overline{\Sigma}^{\mu}_{\nu,b} = 0$ locally; consequently, $\bar{g}_{\mu\nu}(\bar{x}^{\mu},\bar{x}^{b})$ is in fact *a function of the variable* $\bar{x}^{\mu}$ *only.*

In summary, for a theory based on a first order flat Galilean subspace structure with internal symmetry submanifolds which have constant positive curvature independent of the spacetime variables, the only field which is dynamically interesting in first order is the spacetime metric g which in a natural, locally adapted coordinate system is represented by a spacetime tensor field $\bar{g}_{\mu\nu}(\bar{x}^{\mu})$. Note that the coordinate transformations which relate adapted coordinate systems permit arbitrary spacetime coordinate transformations. Also, the special forms and functional dependence of the various fields are obtained as exact statements. No approximations are involved.

At this point, one might obtain a Kaluza–Klein model by a further reduction of the $S^{1}_{(1,3),(m)}$-structure. In this approach which will be discussed more fully in the next section, the first order structure of the world manifold is enriched to accomodate the Yang–Mills fields. A qualitatively different approach leads to a new model in which Yang–Mills fields are accomodated not as part of a first order G-structure on the world manifold but as part of a second order G-structure on the world manifold. The $S^{1}_{(1,3),(m)}$-structure determines by prolongation an $S^{2}_{(1,3),(m)}$-structure in the way explicated in Sec. 4 and Appendix A. Moreover, new gauge degrees of freedom appear in second order. The general element of the group $S^{2}_{(1,3),(m)}$ is given by (4.18)–(4.21). Define the subgroup ${}^{\dagger}S^{2}_{(1,3),(m)}$ by setting $T^{a}_{b\lambda} = 0$. Denote by $\mathscr{S}^{2*}_{(1,3),(m)}(M)$ the principal bundle of second order coframes defined by the $S^{2}_{(1,3),(m)}$-structure. The Yang–Mills fields are introduced by a reduction[13] of this principal bundle to the subgroup ${}^{\dagger}S^{2}_{(1,3),(m)}$. Such a reduction is defined by a cross section of the associated fiber bundle ${}^{\dagger}S^{2}_{(1,3),(m)} \backslash \mathscr{S}^{2*}_{(1,3),(m)}(M)$. Since an arbitrary element of $S^{2}_{(1,3),(m)}$ may be written as the product of an element ${}^{\dagger}S^{2}_{(1,3),(m)}$ and an element of G^{2}_{4+m} of the form $(\delta^{I}_{J}, A^{I}_{JK})$, where only $A^{a}_{b\lambda} = A^{a}_{\lambda b} \neq 0$ and $A^{a}_{b\lambda}$ satisfies (4.21), the reduction is defined locally by specifying the $A^{a}_{b\lambda}$ as smooth functions of $p \in U \subset M$. In this model the Yang–Mills fields are part of a connection on the world manifold. In contrast, the Yang–Mills fields in a Kaluza–Klein model are part of a subspace-metric structure on the world manifold which in *certain cases* may be regarded as the total space of a fiber bundle over a spacetime manifold of four dimensions in which cases the Yang–Mills fields may be interpreted as a connection over spacetime.

The analysis of the second order structure just defined is also greatly simplified by making use of those coordinate systems introduced above which are locally adapted to the involutive $S^{1}_{(1,3),(m)}$-structure. The simplifications that occur are briefly noted in Appendix C. The main purpose of Appendix C is to show that under a coordinate transformation (C1) relating any two locally adapted coordinate systems, $(\bar{U},\bar{x})$ and $(\hat{U},\hat{x})$, the fields $A^{a}_{b\lambda}$ transform for an infinitesimal transformation according to

$$\begin{aligned}\hat{A}^{a}_{b\lambda} = {} & \overline{A}^{a}_{b\lambda} + \hat{\omega}^{a}_{f}\overline{A}^{f}_{b\lambda} - \hat{\omega}^{e}_{b}\overline{A}^{a}_{e\lambda} \\ & - \hat{\omega}^{a}_{b,\rho}\overline{\Sigma}^{-1\rho}_{\lambda} - \hat{\omega}^{\rho}_{\lambda}\overline{A}^{a}_{b\rho} - \hat{\omega}^{f}_{\lambda}\overline{E}^{a}_{bf},\end{aligned} \tag{6.5}$$

where $\overline{\Sigma}^{a}_{b}$ and $\overline{\Sigma}^{a}_{bc}$ determine $\overline{E}^{a}_{bc}$ according to (C21). This transformation law justifies the identification of the fields $A^{a}_{b\lambda}$ as Yang–Mills fields.

Let $\overline{V}^{I}$ and $\overline{W}^{I}$ be the coordinates of two vectors relative to the orthonormal bases in one of the adapted coordinate systems. Then the Yang–Mills fields, regarded as part of a connection, yield the infinitesimal transformation

$$\begin{aligned}\delta\overline{V}^{\mu} &= 0, \\ \delta\overline{V}^{a} &= (A^{a}_{b\lambda}\overline{W}^{\lambda})\overline{V}^{b} + (A^{a}_{vc}\overline{W}^{c})\overline{V}^{v}\end{aligned} \tag{6.6}$$

for parallel transport of V along W. The two terms in the expression for $\delta\overline{V}^{a}$ represent an infinitesimal rotation and an infinitesimal special Galilean transformation, respectively. As for the other parts of the connection, $\overline{\Sigma}^{\mu}_{vc} = 0$, $\overline{\Sigma}^{\mu}_{bc} = 0$, $\overline{\Sigma}^{\mu}_{v\lambda}$, and $\overline{\Sigma}^{a}_{bc}$ have their customary interpretation, and there remains in second order a gauge freedom $s^{a}_{v\lambda}$.

The model may be adapted to accomodate U(r) as an internal symmetry group in the following way. Start with a $4 + 2r$ dimensional C^{∞} world manifold equipped with an involutive and first order flat $S^{1}_{(1,3),(2r)}$-structure. The group U(r) is a subgroup of O($2r$). Denote by $S^{1}_{(1,3),\langle r\rangle}$ the subgroup of $S^{1}_{(1,3),(2r)}$ obtained by restricting the $2r \times 2r$ diagonal block of the group elements to the group U(r). A cross section of the associated fiber bundle $S^{1}_{(1,3),\langle r\rangle} \backslash \mathscr{S}^{1*}_{(1,3),(2r)}(M)$ defines an $S^{1}_{(1,3),\langle r\rangle}$-structure on the world manifold where $\mathscr{S}^{1*}_{(1,3),(2r)}(M)$ denotes the principal bundle of $S^{1}_{(1,3),(2r)}$ related N^{1}-coframes. The $2r$ dimensional internal submanifolds are equipped with an almost Hermitian structure.[14] Clearly, one may compactify the internal symmetry submanifolds by imposing the condition of constant positive curvature.[15,16]

Although a considerable increase in the complexity of the algebraic details is to be expected, the procedure detailed in Sec. 4 and Appendix A may be used to prolong the $S^{1}_{(1,3),\langle r\rangle}$-structure to an $S^{2}_{(1,3),\langle r\rangle}$-structure. Again, one expects additional gauge freedoms $s^{a}_{v\lambda}$ and $s^{a}_{b\lambda}$ to appear; however, for each λ one expects that $T^{a}_{b\lambda}$ will be restricted to the Lie algebra of U(r) rather than just to the Lie algebra of O($2r$). By defining the group ${}^{\dagger}S^{2}_{(1,3),\langle r\rangle}$ to be the subgroup of $S^{2}_{(1,3),\langle r\rangle}$ consisting of those elements with $T^{a}_{b\lambda} = 0$, one may introduce the Yang–Mills fields $A^{a}_{b\lambda}$ by a reduction of the principal bundle $\mathscr{S}^{2*}_{(1,3),\langle r\rangle}(M)$ of second order $S^{2}_{(1,3),\langle r\rangle}$ related N^{2}-coframes to the group ${}^{\dagger}S^{2}_{(1,3),\langle r\rangle}$. The fields $A^{a}_{b\lambda}$ would in this case be skew Hermitian (expressed in real form) in the indices a and b.

7. COMPARISON WITH KALUZA–KLEIN MODELS

In order to relate the model discussed in the previous section to the Kaluza–Klein type of model, a brief description of the Kaluza–Klein models will be given from the G-structure viewpoint adopted in this paper. For simplicity, only those models for which the internal symmetry group is O(m) will be considered; however, U(r) can be accomodated as an internal symmetry group, and much of the comment at the end of Sec. 6 applies with equal force to the Kaluza–Klein case.

There are three approaches to the geometric structure that is characteristic of the Kaluza–Kelin type of model;

namely, (1) define an $S^2_{(1,3),(m)}$-structure on the world manifold, require it to be involutive and first order flat, and then reduce this structure to the subgroup $O^1_{1,3}\times O^1_m$; (2) define an $O^1_{1,3+m}$-structure on the world manifold, reduce this structure to the group $O^1_{1,3}\times O^1_m$, and require that the m-dimensional distribution so defined is involutive and first order flat (note that a four dimensional distribution is also defined); (3) define an $O^1_{1,3}\times O^1_m$-structure on the world manifold and require that the m-dimensional internal distribution is involutive and first order flat. From a purely geometric standpoint, all three approaches are equivalent. The third option is the most direct; however, either the first or the second option may be preferred depending on the nature of the underlying dynamical mechanism that is assumed. The paper by Cho[7] employs the theory of connections on a principal fiber bundle over spacetime which is a special case of option 1. On the other hand, option 2 is employed in the paper by Cho and Freund[9] in a dynamical context in which spontaneous symmetry breaking is used to generate in succession the $O^1_{1,3+m}$-structure and the $O^1_{1,3}\times O^1_m$-structure. For the purpose of comparing the Kaluza–Klein model with the Galilean subspace model, the first option is the most appropriate.

Two types of Kaluza–Klein models will be considered; namely, the model for which the internal symmetry submanifolds have the structure of the group $O(r)$ where $m = r(r-1)/2$, and the model for which the internal symmetry submanifolds have the structure of the sphere S^m. For the second model, the discussion in Sec. 6 up to and including the paragraph containing Eq. (6.4) applies without change to the Kaluza–Klein case. However, for the first model, condition (6.3) is not imposed. Instead, the internal submanifolds are compactified and given the structure of the group $O(r)$ by requiring that the forms $\overline{\omega}^a = \overline{\Sigma}^a_b d\bar{x}^b$ satisfy the Maurer–Cartan[17,18] equations for the group $O(r)$. This case corresponds to the model discussed in Cho[7] and Cho and Freund.[9]

In either case, the Yang–Mills fields are introduced by a reduction of the $S^1_{(1,3),(m)}$-structure to the subgroup $O^1_{1,3}\times O^1_m$. Such a reduction may be specified locally by smooth functions A^a_ν. The standard representative of the equivalence class of $O^1_{1,3}\times O^1_m$ related N^1-coframes is given by

$$\begin{bmatrix}\delta^\mu_\nu & 0\\ A^a_\nu & \delta^a_b\end{bmatrix}\begin{bmatrix}\Sigma^\mu_\nu & \Sigma^\mu_b\\ 0 & \Sigma^a_b\end{bmatrix}=\begin{bmatrix}\Sigma^\mu_\nu & \Sigma^\mu_b\\ A^a_\alpha\Sigma^\alpha_\nu & \Sigma^a_b + A^a_\alpha\Sigma^\alpha_b\end{bmatrix} \tag{7.1}$$

from which are obtained the forms

$$\begin{aligned}\omega^\mu &= \Sigma^\mu_\nu dx^\nu + \Sigma^\mu_b dx^b,\\ \omega^a &= \Sigma^a_b dx^b + A^a_\alpha\Sigma^\alpha_b dx^b + A^a_\alpha\Sigma^\alpha_\nu dx^\nu.\end{aligned} \tag{7.2}$$

The world manifold is equipped with a pseudo-Riemannian metric

$$g = \eta_{\mu\nu}\omega^\mu\otimes\omega^\nu + \eta_{ab}\omega^a\otimes\omega^b, \tag{7.3}$$

where $\eta_{\mu\nu}$ has signature (-2) and $\eta_{ab} = -\delta_{ab}$; consequently g has signature $(-2-m)$, a choice motivated by dynamical considerations.[19] In a coordinate system which is locally adapted to the involutive and first order flat $S^2_{(1,3),(m)}$-structure, the matrix of the metric (7.3) is given by (recall that $\Sigma^\mu_b = 0$)

$$g_{IJ} = \begin{bmatrix}\eta_{\alpha\beta}\overline{\Sigma}^\alpha_\mu\overline{\Sigma}^\beta_\nu + \eta_{ce}\overline{A}^c_\gamma\overline{\Sigma}^\gamma_\mu\overline{A}^e_\delta\overline{\Sigma}^\delta_\nu & \eta_{ce}\overline{A}^c_\gamma\overline{\Sigma}^\gamma_\mu\overline{\Sigma}^e_b\\ \eta_{ce}\overline{\Sigma}^c_a\overline{A}^e_\delta\overline{\Sigma}^\delta_\nu & \eta_{ce}\overline{\Sigma}^c_a\overline{\Sigma}^e_b\end{bmatrix}, \tag{7.4}$$

which evidently agrees, given suitable identifications, with Eq. (12) of Cho[7] and Eq. (4.2a) of Cho and Freund.[9]

For the model with internal submanifolds diffeomorphic to $O(m)$, the upper index on the field $\overline{A}^a_\nu$ is a Lie algebra index; consequently, these fields may be directly identified with the Yang–Mills fields. However, there is a problem in that these fields are functions not only of the spacetime variables $\bar{x}^\mu$ but also of the internal variables $\bar{x}^a$. There are two ways to circumvent this difficulty.[20,21] One way is to demand additional symmetry, basically invariance of the subspace structure under translations in the internal dimensions, in order that the fields A^a_ν will in fact be independent of the internal variables. The other way is to expand the fields in terms of harmonic functions defined on the group manifold and to argue on dynamical grounds that the zero order term dominates. It should be pointed out that a similar problem exists with the fields $A^a_{b\lambda}$ which play the role of the Yang–Mills fields in the Galilean subspace model described in Sec. 6. Note that in this case the pair of indices, a and b, constitutes a single Lie Algebra index.

For the Kaluza–Klein model having spheres for internal symmetry submanifolds,[22] the upper index on the fields $\overline{A}^a_\nu$ is not a Lie Algebra index; consequently, these fields cannot be directly interpreted as Yang–Mills fields. This type of model is related to the theory of connections on an associated fiber bundle rather than to the theory of connections on a principal fiber bundle. It is of course possible to work backwards to determine the symmetry conditions that must be imposed in order to recover the Yang–Mills fields from the fields $\overline{A}^a_\nu$. An analogous situation is that in which a linear connection on $T(M)$ determines a connection on $L(M)$.

In conclusion, at the geometric level, there exist two qualitatively distinct types of models in which Yang–Mills and gravitational fields can be unified in the context of a world manifold of higher dimension. In one of these, the Kaluza–Klein type of model, the Yang–Mills fields define a pair of mutually orthogonal subspace structures in a pseudo-Riemannian world manifold. In the other, the Yang–Mills fields are defined as part of a connection on the world manifold which has in first order only a Galilean subspace structure.

APPENDIX A: SOLVING THE GALILEAN PROLONGATION EQUATIONS

The system of linear equations (4.17), supplemented by Eqs. (4.12) which fix the $\lambda^\mu_{\nu S}$ and the λ^a_{bS}, determines the prolongation of an $S^1_{(p,q),(r,s)}$-structure to an $S^2_{(p,q),(r,s)}$-structure. The explicit solution of this system is derived in this appendix. The analysis of the general case will be presented; however, the reader will more readily obtain a grasp of the general strategy by making use of the fact that it is always

possible to choose a coordinate system which is adapted to the $S^1_{(p,q),(r,s)}$-structure at any *one* given point $p \in M$. With respect to such a system, $\hat{\Sigma}^{\mu}_{\nu} = \delta^{\mu}_{\nu}$, $\hat{\Sigma}^{\mu}_{b} = 0$, and $\hat{\Sigma}^{a}_{b} = \delta^{a}_{b}$ *at the point p* (note, however, that the derivatives of these functions are in general *not* zero), and Eqs. (4.12) and (4.17) are greatly simplified. However, since the transformation laws are rather complicated, it is easier to work out the general solution directly than to transform the solution of the simplified system.

The solution of (4.17a) is well known[23] since these equations arise in the prolongation of a pseudo-Riemannian or $O^1_{p,q}$-structure to an $O^2_{p,q}$-structure. The torsion $B^{\mu}_{\nu\lambda}$ is completely undetermined. The $\lambda^{\mu}_{\nu\lambda}$ are given by

$$\begin{aligned} 2\eta_{\mu\gamma}\lambda^{\gamma}_{\nu\beta}\Sigma^{-1\beta}_{\lambda} &= \eta_{\mu\gamma}(\Sigma^{\gamma}_{\alpha,\beta} - \Sigma^{\gamma}_{\beta,\alpha})\Sigma^{-1\alpha}_{\nu}\Sigma^{-1\beta}_{\lambda} \\ &+ 2\eta_{\mu\gamma}B^{\gamma}_{\alpha\beta}\Sigma^{-1\alpha}_{\nu}\Sigma^{-1\beta}_{\lambda} \\ &+ \eta_{\nu\gamma}(\Sigma^{\gamma}_{\alpha,\beta} - \Sigma^{\gamma}_{\beta,\alpha})\Sigma^{-1\alpha}_{\lambda}\Sigma^{-1\beta}_{\mu} \\ &+ 2\eta_{\nu\gamma}B^{\gamma}_{\alpha\beta}\Sigma^{-1\alpha}_{\lambda}\Sigma^{-1\beta}_{\mu} \\ &- \eta_{\lambda\gamma}(\Sigma^{\gamma}_{\alpha,\beta} - \Sigma^{\gamma}_{\beta,\alpha})\Sigma^{-1\alpha}_{\mu}\Sigma^{-1\beta}_{\nu} \\ &- 2\eta_{\lambda\gamma}B^{\gamma}_{\alpha\beta}\Sigma^{-1\alpha}_{\mu}\Sigma^{-1\beta}_{\nu}, \end{aligned} \tag{A1}$$

while the $\Gamma^{\mu}_{\nu\lambda}$ are given by

$$\begin{aligned} \Gamma^{\mu}_{\nu\lambda} &= \tfrac{1}{2}(\Sigma^{\mu}_{\nu,\lambda} + \Sigma^{\mu}_{\lambda,\nu}) + \tfrac{1}{2}\eta^{\mu\rho}\Sigma^{-1\gamma}_{\rho}\eta_{\alpha\beta}(\Sigma^{\alpha}_{\gamma,\lambda} - \Sigma^{\alpha}_{\lambda,\gamma})\Sigma^{\beta}_{\nu} \\ &+ \tfrac{1}{2}\eta^{\mu\rho}\Sigma^{-1\gamma}_{\rho}\eta_{\alpha\beta}(\Sigma^{\alpha}_{\gamma,\nu} - \Sigma^{\alpha}_{\nu,\gamma})\Sigma^{\beta}_{\lambda} \\ &+ \eta^{\mu\rho}\Sigma^{-1\gamma}_{\rho}\eta_{\alpha\beta}B^{\alpha}_{\gamma\lambda}\Sigma^{\beta}_{\nu} \\ &+ \eta^{\mu\rho}\Sigma^{-1\gamma}_{\rho}\eta_{\alpha\beta}B^{\alpha}_{\gamma\nu}\Sigma^{\beta}_{\lambda}. \end{aligned} \tag{A2}$$

Since the $\Gamma^{\mu}_{\nu\lambda}$ are fully determined by the Σ^{μ}_{ν} and the $B^{\mu}_{\nu\lambda}$, they form part of the standard N^2-coframe and may be renamed $\Sigma^{\mu}_{\nu\lambda}$.

From (4.17b) and (4.17c), one obtains

$$\eta_{\mu\alpha}\Sigma^{\alpha}_{\rho,c}\Sigma^{-1\rho}_{\nu} + \eta_{\mu\alpha}B^{\alpha}_{\rho c}\Sigma^{-1\rho}_{\nu} = \eta_{\mu\alpha}\Sigma^{\mu}_{\rho c}\Sigma^{-1\rho}_{\nu} + \lambda_{\mu\nu c} \tag{A3}$$

and

$$\begin{aligned} &\eta_{\mu\alpha}\Sigma^{\alpha}_{c,\rho}\Sigma^{-1\rho}_{\nu} - \eta_{\mu\alpha}B^{\alpha}_{\rho c}\Sigma^{-1\rho}_{\nu} \\ &\quad = \eta_{\mu\alpha}\Sigma^{\alpha}_{\rho c}\Sigma^{-1\rho}_{\nu} + \lambda_{\mu\rho\sigma}\Sigma^{\rho}_{c}\Sigma^{-1\sigma}_{\nu}, \end{aligned} \tag{A4}$$

respectively. From these equations, it follows that

$$\begin{aligned} \lambda_{\mu\nu c} &= \eta_{\mu\alpha}(\Sigma^{\alpha}_{\rho,c} - \Sigma^{\alpha}_{c,\rho})\Sigma^{-1\rho}_{\nu} \\ &+ 2\eta_{\mu\alpha}B^{\alpha}_{\rho c}\Sigma^{-1\rho}_{\nu} + \lambda_{\mu\rho\sigma}\Sigma^{\rho}_{c}\Sigma^{-1\sigma}_{\nu}. \end{aligned} \tag{A5}$$

Now $B^{\mu}_{\nu c} = 0$ and $\Sigma^{-1\mu}_{\nu} = 0$ unless $\mu < \nu$ (a consequence of the upper triangular gauge conditions). Thus $\eta_{\mu\alpha}B^{\alpha}_{\rho c}\Sigma^{-1\rho}_{\nu} = 0$ unless $\mu = \alpha < \rho < \nu$. Hence, for $\mu > \nu$

$$\lambda_{\mu\nu c} = \eta_{\mu\alpha}(\Sigma^{\alpha}_{\rho,c} - \Sigma^{\alpha}_{c,\rho})\Sigma^{-1\rho}_{\nu} + \lambda_{\mu\rho\sigma}\Sigma^{\rho}_{c}\Sigma^{-1\sigma}_{\nu}. \tag{A6}$$

For $\mu < \nu$, one may use $\lambda_{\mu\nu c} = -\lambda_{\nu\mu c}$. Also, note that $\eta_{\mu\alpha}\Sigma^{\alpha}_{\rho,c}\Sigma^{-1\rho}_{\nu} = 0$ for $\mu > \nu$. By adding and subtracting (4.17b) and (4.17c), one readily obtains

$$B^{\mu}_{\nu c} = -\tfrac{1}{2}(\Sigma^{\mu}_{\nu,c} - \Sigma^{\mu}_{c,\nu}) + \tfrac{1}{2}\lambda^{\mu}_{\rho c}\Sigma^{\rho}_{\nu} - \tfrac{1}{2}\lambda^{\mu}_{\rho\nu}\Sigma^{\rho}_{c} \tag{A7}$$

and

$$\Gamma^{\mu}_{\nu c} = \tfrac{1}{2}(\Sigma^{\mu}_{\nu,c} + \Sigma^{\mu}_{c,\nu}) - \tfrac{1}{2}\lambda^{\mu}_{\rho c}\Sigma^{\rho}_{\nu} - \tfrac{1}{2}\lambda^{\mu}_{\rho\nu}\Sigma^{\rho}_{c}. \tag{A8}$$

Again, $\Gamma^{\mu}_{\nu c} = \Sigma^{\mu}_{\nu c}$ because these components are fully determined by the first order structure.

Next, the skew and symmetric parts of (4.17d) yield

$$B^{\mu}_{bc} = -\tfrac{1}{2}(\Sigma^{\mu}_{b,c} - \Sigma^{\mu}_{c,b}) - \tfrac{1}{2}(\lambda^{\mu}_{\rho b}\Sigma^{\rho}_{c} - \lambda^{\mu}_{\rho c}\Sigma^{\rho}_{b}) \tag{A9}$$

and

$$\Sigma^{\mu}_{bc} \equiv \Gamma^{\mu}_{bc} = \tfrac{1}{2}(\Sigma^{\mu}_{b,c} + \Sigma^{\mu}_{c,b}) - \tfrac{1}{2}(\lambda^{\mu}_{\rho b}\Sigma^{\rho}_{c} + \lambda^{\mu}_{\rho c}\Sigma^{\rho}_{b}). \tag{A10}$$

Consider next Eq. (4.17e). The components $\Gamma^{a}_{\nu\lambda}$ may be chosen freely. This fact is indicated by the presence of the off diagonal submatrix Σ^{μ}_{b}, which vanishes in an adapted frame. It is more convenient to introduce as parameters for the second order gauge group the quantities

$$T^{a}_{\nu\lambda} = \Gamma^{a}_{\alpha\beta}\Sigma^{-1\alpha}_{\nu}\Sigma^{-1\beta}_{\lambda}. \tag{A11}$$

Define

$$\tilde{\Gamma}^{a}_{b\lambda} = \Gamma^{a}_{b\lambda} - T^{a}_{\alpha\beta}\Sigma^{\alpha}_{b}\Sigma^{\beta}_{\lambda}. \tag{A12}$$

Then (4.17e) becomes

$$\Sigma^{a}_{b,\lambda} = \tilde{\Gamma}^{a}_{b\lambda} + \lambda^{a}_{e\lambda}\Sigma^{e}_{b}, \tag{A13}$$

while the relevant part of (4.12b) becomes

$$\tilde{\Gamma}^{a}_{b\lambda} + \lambda^{a}_{e\lambda}\Sigma^{e}_{b} = 0 \quad \text{for } a > b, \tag{A14}$$

which is included in (A13) since $\Sigma^{a}_{b,\lambda} = 0$ for $a > b$. If $\tilde{\tilde{\Gamma}}^{a}_{b\lambda}$ is defined by

$$\tilde{\tilde{\Gamma}}^{a}_{b\lambda} = \tilde{\Gamma}^{a}_{b\lambda} - \Sigma^{a}_{b,\lambda}, \tag{A15}$$

then (A13) yields

$$\tilde{\tilde{\Gamma}}_{ae\lambda}\Sigma^{-1e}_{b} + \lambda_{ab\lambda} = 0. \tag{A16}$$

It follows that

$$\tilde{\tilde{\Gamma}}_{ae\lambda}\Sigma^{-1e}_{b} + \tilde{\tilde{\Gamma}}_{be\lambda}\Sigma^{-1e}_{a} = 0 \tag{A17}$$

while

$$-\lambda_{ab\lambda} = \tilde{\tilde{\Gamma}}_{ae\lambda}\Sigma^{-1e}_{b} - \tilde{\tilde{\Gamma}}_{be\lambda}\Sigma^{-1e}_{a} \tag{A18}$$

is undetermined. Define

$$T^{a}_{b\lambda} = \tilde{\tilde{\Gamma}}^{a}_{ep}\Sigma^{-1e}_{b}\Sigma^{-1\rho}_{\lambda}. \tag{A19}$$

Then $T^{a}_{b\lambda}$ satisfies (4.10) and

$$\Gamma^{a}_{b\lambda} = \Sigma^{a}_{b,\lambda} + T^{a}_{\alpha\beta}\Sigma^{\alpha}_{b}\Sigma^{\beta}_{\lambda} + T^{a}_{e\beta}\Sigma^{e}_{b}\Sigma^{\beta}_{\lambda}, \tag{A20}$$

from which it is clear that

$$\Sigma^{a}_{b\lambda} = \Sigma^{a}_{\lambda b} = \Sigma^{a}_{b,\lambda}. \tag{A21}$$

Finally, rewrite (4.17f) as

$$\Gamma^{a}_{bc} + \lambda^{a}_{ec}\Sigma^{e}_{b} = \Sigma^{a}_{b,c} + B^{a}_{bc} + \Gamma^{a}_{\alpha c}\Sigma^{-1\alpha}_{\beta}\Sigma^{\beta}_{b}, \tag{A22}$$

where all quantities on the right-hand side are regarded as known. This set of equations has the same structure as the set (4.17a) and may be solved in the same way. The result is

$$\begin{aligned} 2\eta_{ae}\lambda^{e}_{bf}\Sigma^{-1f}_{c} &= \eta_{ae}(\Sigma^{e}_{f,g} - \Sigma^{e}_{gf})\Sigma^{-1f}_{b}\Sigma^{-1g}_{c} \\ &+ 2\eta_{ae}B^{e}_{fg}\Sigma^{-1f}_{b}\Sigma^{-1g}_{c} \\ &+ \eta_{be}(\Sigma^{e}_{f,g} - \Sigma^{e}_{gf})\Sigma^{-1f}_{c}\Sigma^{-1g}_{a} \\ &+ 2\eta_{be}B^{e}_{fg}\Sigma^{-1f}_{c}\Sigma^{-1g}_{a} \\ &- \eta_{ce}(\Sigma^{e}_{f,g} - \Sigma^{e}_{gf})\Sigma^{-1f}_{a}\Sigma^{-1g}_{b} \\ &+ 2\eta_{ce}B^{e}_{fg}\Sigma^{-1f}_{a}\Sigma^{-1g}_{b} \\ &+ \eta_{ae}\Gamma^{e}_{f\alpha}\Sigma^{-1\alpha}_{\beta}\Sigma^{\beta}_{g} \\ &\times(\Sigma^{-1f}_{b}\Sigma^{-1g}_{c} - \Sigma^{-1f}_{c}\Sigma^{-1g}_{b}) \\ &+ \eta_{be}\Gamma^{e}_{f\alpha}\Sigma^{-1\alpha}_{\beta}\Sigma^{\beta}_{g} \\ &\times(\Sigma^{-1f}_{c}\Sigma^{-1g}_{a} - \Sigma^{-1f}_{a}\Sigma^{-1g}_{c}) \\ &- \eta_{ce}\Gamma^{e}_{f\alpha}\Sigma^{-1\alpha}_{\beta}\Sigma^{\beta}_{g} \\ &\times(\Sigma^{-1f}_{a}\Sigma^{-1g}_{b} - \Sigma^{-1f}_{b}\Sigma^{-1g}_{a}) \end{aligned} \tag{A23}$$

and

$$2\Gamma^{a}_{bc} = \Sigma^{a}_{b,c} + \Sigma^{a}_{c,b} + \eta^{ae}\Sigma_{e}^{-1f}\eta_{pq}(\Sigma^{p}_{f,b} - \Sigma^{p}_{b,f})\Sigma^{q}_{c}$$
$$+ \eta^{ae}\Sigma_{e}^{-1f}\eta_{pq}(\Sigma^{p}_{f,c} - \Sigma^{p}_{c,f})\Sigma^{q}_{b}$$
$$+ 2\eta^{ae}\Sigma_{e}^{-1f}\eta_{pq}(B^{p}_{fb}\Sigma^{q}_{c} + B^{p}_{fc}\Sigma^{q}_{b})$$
$$+ \eta^{ae}\Sigma_{e}^{-1f}\Sigma^{\alpha}_{f}\Sigma_{\alpha}^{-1\beta}\eta_{pq}(\Gamma^{p}_{\beta b}\Sigma^{q}_{c} + \Gamma^{p}_{\beta c}\Sigma^{q}_{b})$$
$$- \eta^{ae}\Sigma_{e}^{-1f}\eta_{pq}\Gamma^{p}_{f\alpha}\Sigma_{\beta}^{-1\alpha}(\Sigma^{\beta}_{b}\Sigma^{q}_{c} + \Sigma^{\beta}_{c}\Sigma^{q}_{b})$$
$$+ \Gamma^{a}_{b\alpha}\Sigma_{\beta}^{-1\alpha}\Sigma^{\beta}_{c} + \Gamma^{a}_{c\alpha}\Sigma_{\beta}^{-1\alpha}\Sigma^{\beta}_{b}. \quad \text{(A24)}$$

It is now straightforward albeit tedious to show by using (A20) that

$$\Gamma^{a}_{bc} = \Sigma^{a}_{bc} + T^{a}_{\alpha\beta}\Sigma^{\alpha}_{b}\Sigma^{\beta}_{c} + T^{a}_{e\beta}\Sigma^{e}_{b}\Sigma^{\beta}_{c} + T^{a}_{e\beta}\Sigma^{e}_{c}\Sigma^{\beta}_{b}, \quad \text{(A25)}$$

provided that Σ^{a}_{bc} is given by

$$2\Sigma^{a}_{bc} = \Sigma^{a}_{b,c} + \Sigma^{a}_{c,b} + \eta^{ae}\Sigma_{e}^{-1f}\eta_{pq}(\Sigma^{p}_{f,b} - \Sigma^{p}_{b,f})\Sigma^{q}_{c}$$
$$+ \eta^{ae}\Sigma_{e}^{-1f}\eta_{pq}(\Sigma^{p}_{f,c} - \Sigma^{p}_{c,f})\Sigma^{q}_{b}$$
$$+ \Sigma^{a}_{b\alpha}\Sigma_{\beta}^{-1\alpha}\Sigma^{\beta}_{c} + \Sigma^{a}_{c\alpha}\Sigma_{\beta}^{-1\alpha}\Sigma^{\beta}_{b}$$
$$+ \eta_{pq}(\Sigma^{p}_{b}\Sigma^{q}_{c\alpha} + \Sigma^{p}_{c}\Sigma^{q}_{b\alpha})\Sigma_{\beta}^{-1\alpha}\Sigma^{\beta}_{f}\Sigma_{e}^{-1f}\eta^{ea}$$
$$- \eta_{pq}\Sigma^{p}_{b}\Sigma^{q}_{f\alpha}\Sigma_{e}^{-1f}\eta^{ea}\Sigma_{\beta}^{-1\alpha}\Sigma^{\beta}_{c}$$
$$- \eta_{pq}\Sigma^{p}_{c}\Sigma^{q}_{f\alpha}\Sigma_{e}^{-1f}\eta^{ea}\Sigma_{\beta}^{-1\alpha}\Sigma^{\beta}_{b}$$
$$+ 2\eta^{ae}\Sigma_{e}^{-1f}\eta_{pq}(B^{p}_{fb}\Sigma^{q}_{c} + B^{p}_{fc}\Sigma^{q}_{b}). \quad \text{(A26)}$$

The fact that Eqs. (4.29) are just Eqs. (A11), (A20), and (A25) shows that the desired factorization of the general N^2-coframe (4.6) into a standard N^2-coframe (4.24) and an $S^{2}_{(p,q),(r,s)}$ transformation (4.29) occurs.

APPENDIX B: FIRST ORDER INTEGRABILITY CONDITIONS

As pointed out in Sec. 5, any subspace structure invariantly defines a differentiable distribution[4-6] on M; that is, for each $p\in M$, a subspace (of fixed dimension) of the tangent space is distinguished in such a way that for every local neighborhood $U\in M$, a set of differentiable local vector fields exist which provide a basis for the distinguished subspace for each $q\in U$. For the case of a Galilean subspace structure, the locally defined vector fields are the ζ_a given in (5.2).

It is natural to inquire under what conditions can the distinguished subspaces be pieced together to form maximal connected submanifolds of M in such a manner that each point $p\in M$ lies on one and only one such submanifold. The manifold M is then said to be *foliated* and the submanifolds are referred to as the *leaves* of the foliation, and $\forall p\in M$, the tangent space of the leaf through p is the subspace of the tangent space of M distinguished by the subspace structure on M. The answer to the question is provided by Frobenius's theorem, for a formal statement and proof of which the reader is referred to the text of Sternberg.[4] Briefly, the theorem states that a subspace structure is integrable in the sense that it determines a foliation iff it is involutive, that is, iff the commutator $[\zeta_a,\zeta_b]$ at each point belongs to the distinguished subspace at that point. The commutator may be expanded in terms of the basis ζ_μ, ζ_a at any point, and the criterion is equivalent to the requirement that the coefficient of ζ_μ vanish, which gives the condition

$$\Sigma^{\mu}_{a,b} - \Sigma^{\mu}_{b,a} + \Sigma^{\mu}_{\rho,a}\Sigma_{\sigma}^{-1\rho}\Sigma^{\sigma}_{b} - \Sigma^{\mu}_{\rho,b}\Sigma_{\sigma}^{-1\rho}\Sigma^{\sigma}_{a}$$
$$+ \Sigma^{\mu}_{\rho,\sigma}\Sigma_{\alpha}^{-1\rho}\Sigma_{\beta}^{-1\sigma}(\Sigma^{\alpha}_{a}\Sigma^{\beta}_{b} - \Sigma^{\beta}_{b}\Sigma^{\alpha}_{a})$$
$$- (\Sigma^{\mu}_{a,\rho}\Sigma_{\sigma}^{-1\rho}\Sigma^{\sigma}_{b} - \Sigma^{\mu}_{b,\rho}\Sigma_{\sigma}^{-1\rho}\Sigma^{\sigma}_{a}) = 0. \quad \text{(B1)}$$

For a simple subspace structure for which $\Sigma^{\mu}_{\nu} = \delta^{\mu}_{\nu}$ locally, the condition (B1) simplifies considerably to

$$\Sigma^{\mu}_{a,b} - \Sigma^{\mu}_{b,a} - (\Sigma^{\mu}_{a,\rho}\Sigma^{\rho}_{b} - \Sigma^{\mu}_{b,\rho}\Sigma^{\rho}_{a}) = 0. \quad \text{(B2)}$$

Note that each of the local vector fields ζ_a defines a local one parameter family of local diffeomorphisms of M, a local flow on M. If the subspace structure defines a foliation of M, then the flow lines of each flow will follow the leaves of the foliation; consequently, if a vector tangent to a leaf is intuitively pictured as an arrow joining two neighboring points of the leaf, it is clear that such a tangent vector should remain tangent to the leaf as the tail and tip flow along their respective flow lines for a given flow.

Finally, note that the criterion may also be stated in terms of the forms (5.1) as the requirement

$$d\omega^{\mu}(\zeta_a \wedge \zeta_b) = 0. \quad \text{(B3)}$$

There is also a somewhat stronger integrability condition that requires not only that the subspace structure determine a foliation on M but also that the leaves of this foliation flow into each other under the local flows on M generated by the local vector fields ζ_μ. If this stronger condition is satisfied, the subspace structure is said to be *first order flat*. A subspace structure is first order flat iff both of the commutators $[\zeta_a,\zeta_b]$ and $[\zeta_\mu,\zeta_b]$ belong to the distinguished subspace at each point $p\in M$. In addition to (B1), one obtains the condition

$$\Sigma^{\mu}_{\rho,\sigma}\Sigma_{\nu}^{-1\rho}\Sigma_{\beta}^{-1\sigma}\Sigma^{\beta}_{b} - \Sigma^{\mu}_{\rho,\sigma}\Sigma_{\beta}^{-1\rho}\Sigma^{\beta}_{b}\Sigma_{\nu}^{-1\sigma}$$
$$- \Sigma^{\mu}_{\rho,b}\Sigma_{\nu}^{-1\rho} + \Sigma^{\mu}_{b,\rho}\Sigma_{\nu}^{-1\rho} = 0. \quad \text{(B4)}$$

In combination with (B1), (B4) gives

$$\Sigma^{\mu}_{a,b} - \Sigma^{\mu}_{b,a} + \Sigma^{\mu}_{\rho,a}\Sigma_{\beta}^{-1\rho}\Sigma^{\beta}_{b} - \Sigma^{\mu}_{a,\rho}\Sigma_{\beta}^{-1\rho}\Sigma^{\beta}_{b} = 0. \quad \text{(B5)}$$

The condition (B4) also follows from

$$d\omega^{\mu}(\zeta_\mu \wedge \zeta_b) = 0. \quad \text{(B6)}$$

Finally, note that the condition (B1) may also be expressed in the form

$$B^{\mu}_{bc} + B^{\mu}_{\rho b}\Sigma_{\sigma}^{-1\rho}\Sigma^{\sigma}_{c}$$
$$- B^{\mu}_{\rho c}\Sigma_{\sigma}^{-1\rho}\Sigma^{\sigma}_{b} - B^{\mu}_{\alpha\beta}\Sigma_{\beta}^{-1\alpha}\Sigma^{\rho}_{b}\Sigma_{\sigma}^{-1\beta}\Sigma^{\sigma}_{c} = 0. \quad \text{(B7)}$$

APPENDIX C: THE YANG–MILLS GAUGE TRANSFORMATION

As pointed out in Sec. 6 [see (6.1)], an involutive $S^{1}_{(1,3),(m)}$-structure determines in a natural way a class of locally defined adapted coordinate systems. A coordinate transformation relating any two such systems has the form

$$\bar{x}^{\mu} = \bar{x}^{\mu}(\hat{x}^{\mu}), \quad \hat{x}^{\mu} = \hat{x}^{\mu}(\bar{x}^{\mu}),$$
$$\bar{x}^{a} = \bar{x}^{a}(\hat{x}^{\mu},\hat{x}^{a}), \quad \hat{x}^{a} = \hat{x}^{a}(\bar{x}^{\mu},\bar{x}^{a}). \quad \text{(C1)}$$

In this appendix, it will be shown that under such a transformation, the transformation relating $\hat{A}^{a}_{b\lambda}$ and $\bar{A}^{a}_{b\lambda}$ is essentially the usual Yang–Mills gauge transformation. For simplicity, only infinitesimal transformations will be considered.

In any of the special coordinate systems under consideration, $\bar{\Sigma}^{\mu}_{b}$, $\bar{\lambda}^{\mu}_{\nu c}$, $\bar{B}^{\mu}_{\nu c}$, $\bar{\Sigma}^{\mu}_{\nu c}$, $\bar{B}^{\mu}_{bc}$, and $\bar{\Sigma}^{\mu}_{bc}$ all vanish; moreover, $\bar{\Sigma}^{\mu}_{\nu\lambda}$ and $\bar{\Sigma}^{a}_{bc}$ are given by the usual formulas in terms of $\bar{\Sigma}^{\mu}_{\nu}$

and $\overline{\Sigma}^{a}_{b}$, respectively, with the variables $\bar{x}^{a}$ and $\bar{x}^{\mu}$, respectively, playing a spectator role. Since the torsions $\overline{B}^{\mu}_{\nu\lambda}$ and $\overline{B}^{a}_{bc}$ are completely undetermined, they may be chosen to be zero. If the $S^{1}_{(1,3),(m)}$-structure is first order flat, then $\overline{\Sigma}^{\mu}_{\nu}$ depends only on $\bar{x}^{\mu}$; consequently, that part of $\overline{\Sigma}^{\mu}_{\nu\lambda}$ which is independent of $\overline{B}^{\mu}_{\nu\lambda}$ depends only on $\bar{x}^{\mu}$. Thus, even if a theory involving spacetime torsion is desired, it would be natural to assume that $\overline{B}^{\mu}_{\nu\lambda}$ depends only on $\bar{x}^{\mu}$. For the following calculation, only those special results that follow from the existence of coordinate systems locally (not just at a point) adapted to an involutive Galilean subspace structure (in particular, the fact that the above mentioned quantities vanish) are required.

Let $(X^{I}_{J},X^{I}_{JK})=(\delta^{I}_{J}+\chi^{I}_{J},\chi^{I}_{JK})$ be the second degree approximation to an infinitesimal coordinate transformation of the type (C1) [we use here the notation: (X^{I}_{J},X^{I}_{JK}) $\equiv\partial^{2}_{p}\,x(X^{I}_{J}\,d^{2}_{p}\,x^{J}+(1/2!)X^{I}_{JK}\,d^{2}_{p}\,x^{J}\,d^{2}_{p}\,x^{K})]$. Then χ^{μ}_{b}, $\chi^{\mu}_{\nu c}=\chi^{\mu}_{c\nu}$, and χ^{μ}_{bc} are zero. An infinitesimal element of $S^{2}_{(1,3),(m)}$ is given by $(s^{I}_{J},s^{I}_{JK})=(\delta^{I}_{J}+\omega^{I}_{J},\omega^{I}_{JK})$, where $\omega^{\mu}_{b}=0$ and only $\omega^{a}_{\nu\lambda}\neq 0$ and $\omega^{a}_{b\lambda}=\omega^{a}_{\lambda b}\neq 0$. Note that $\omega_{ab\lambda}=-\omega_{ba\lambda}$. The transformation law for the structure fields $(\Sigma^{I}_{J},\Sigma^{I}_{JK})$ is determined by

$$(\hat{\Sigma}^{I}_{J},\hat{\Sigma}^{I}_{JK})=(\hat{s}^{I}_{J},\hat{s}^{I}_{JK})(\overline{\Sigma}^{I}_{J},\overline{\Sigma}^{I}_{JK})(\overline{X}^{I}_{J},\overline{X}^{I}_{JK}). \tag{C2}$$

To first order in the infinitesimal quantities, (C2) yields

$$\hat{\Sigma}^{I}_{J}=\overline{\Sigma}^{I}_{J}+\hat{\omega}^{I}_{R}\overline{\Sigma}^{R}_{J}+\overline{\Sigma}^{I}_{R}\bar{\chi}^{R}_{J} \tag{C3}$$

and

$$\hat{\Sigma}^{I}_{JK}=\overline{\Sigma}^{I}_{JK}+\hat{\omega}^{I}_{R}\overline{\Sigma}^{R}_{JK}+\overline{\Sigma}^{I}_{JR}\bar{\chi}^{R}_{K}+\overline{\Sigma}^{I}_{RK}\bar{\chi}^{R}_{J}+\overline{\Sigma}^{I}_{R}\bar{\chi}^{R}_{JK}+\hat{\omega}^{I}_{RS}\Sigma^{R}_{J}\Sigma^{S}_{K}. \tag{C4}$$

Consider the first order equations (C3). That the off diagonal blocks of $\hat{\Sigma}^{I}_{J}$ and $\overline{\Sigma}^{I}_{J}$ vanish while the diagonal blocks are upper triangular gives

$$\hat{\omega}^{\mu}_{\rho}\overline{\Sigma}^{\rho}_{\nu}+\overline{\Sigma}^{\mu}_{\rho}\bar{\chi}^{\rho}_{\nu}=0,\ \mu>\nu, \tag{C5a}$$

$$\hat{\omega}^{a}_{e}\overline{\Sigma}^{e}_{b}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{b}=0,\ a>b, \tag{C5b}$$

$$\hat{\omega}^{a}_{\rho}\overline{\Sigma}^{\rho}_{\nu}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{\nu}=0, \tag{C5c}$$

which equations determine $\hat{\omega}^{\mu}_{\nu}$, $\hat{\omega}^{a}_{b}$, and $\hat{\omega}^{a}_{\nu}$. Then Eqs. (C3) become

$$\hat{\Sigma}^{\mu}_{\nu}=\overline{\Sigma}^{\mu}_{\nu}+\hat{\omega}^{\mu}_{\rho}\overline{\Sigma}^{\rho}_{\nu}+\overline{\Sigma}^{\mu}_{\rho}\bar{\chi}^{\rho}_{\nu},$$

$$\hat{\Sigma}^{a}_{b}=\overline{\Sigma}^{a}_{b}+\hat{\omega}^{a}_{e}\overline{\Sigma}^{e}_{b}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{b}, \tag{C6}$$

from which follow (to first order)

$$\delta^{\mu}_{\nu}=\overline{\Sigma}^{\mu}_{\rho}\hat{\Sigma}^{-1\rho}_{\nu}+\hat{\omega}^{\mu}_{\nu}+\overline{\Sigma}^{\mu}_{\rho}\bar{\chi}^{\rho}_{\sigma}\overline{\Sigma}^{-1\sigma}_{\nu},$$

$$\delta^{a}_{b}=\overline{\Sigma}^{a}_{e}\hat{\Sigma}^{-1e}_{\nu}+\hat{\omega}^{a}_{b}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{f}\overline{\Sigma}^{-1f}_{b}. \tag{C7}$$

From the fact that $\hat{\Sigma}^{a}_{\nu\lambda}=0=\overline{\Sigma}^{a}_{\nu\lambda}$, it follows that

$$\overline{\Sigma}^{a}_{\nu e}\bar{\chi}^{e}_{\lambda}+\overline{\Sigma}^{a}_{e\lambda}\bar{\chi}^{e}_{\nu}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{\nu\lambda}+\hat{\omega}^{a}_{\rho\sigma}\overline{\Sigma}^{\rho}_{\nu}\overline{\Sigma}^{\sigma}_{\lambda}=0, \tag{C8}$$

which determines $\hat{\omega}^{a}_{\nu\lambda}$. The fact that $\hat{\Sigma}^{a}_{b\lambda}=0=\overline{\Sigma}^{a}_{b\lambda}$ for $a>b$ gives

$$\hat{\omega}^{a}_{e\rho}\overline{\Sigma}^{e}_{b}\overline{\Sigma}^{\rho}_{\lambda}+\hat{\omega}^{a}_{e}\overline{\Sigma}^{e}_{b\lambda}+\overline{\Sigma}^{a}_{be}\bar{\chi}^{e}_{\lambda}+\overline{\Sigma}^{a}_{e\lambda}\bar{\chi}^{e}_{b}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{b\lambda}=0,\quad a>b, \tag{C9}$$

from which $\hat{\omega}^{a}_{b\lambda}$ may be determined since $\hat{\omega}_{ab\lambda}=-\hat{\omega}_{ba\lambda}$. Then (C4) gives the transformation law

$$\hat{\Sigma}^{a}_{b\lambda}=\overline{\Sigma}^{a}_{b\lambda}+\hat{\omega}^{a}_{e}\overline{\Sigma}^{e}_{b\lambda}+\overline{\Sigma}^{a}_{be}\bar{\chi}^{e}_{\lambda}+\overline{\Sigma}^{a}_{b\rho}\bar{\chi}^{\rho}_{\lambda}+\overline{\Sigma}^{a}_{e\lambda}\bar{\chi}^{e}_{b}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{b\lambda}+\hat{\omega}^{a}_{e\rho}\overline{\Sigma}^{e}_{b}\overline{\Sigma}^{\rho}_{\lambda}. \tag{C10}$$

The Yang–Mills fields, $A^{a}_{b\lambda}$, define the reduction of the $S^{2}_{(1,3),(m)}$-structure to the $\dagger S^{2}_{(1,3),(m)}$-structure with structure fields $(\Sigma^{I}_{J},\dagger\Sigma^{I}_{JK})$, where

$$\dagger\Sigma^{I}_{JK}=\Sigma^{I}_{JK}+A^{I}_{RS}\Sigma^{R}_{J}\Sigma^{S}_{K}. \tag{C11}$$

Since only $A^{a}_{b\lambda}=A^{a}_{\lambda b}\neq 0$,

$$\dagger\Sigma^{\mu}_{JK}=\Sigma^{\mu}_{JK} \tag{C12}$$

while

$$\dagger\Sigma^{a}_{b\lambda}=\Sigma^{a}_{b\lambda}+A^{a}_{e\rho}\Sigma^{e}_{b}\Sigma^{\rho}_{\lambda} \tag{C13}$$

and

$$\dagger\Sigma^{a}_{bc}=\Sigma^{a}_{bc}+A^{a}_{e\rho}\Sigma^{e}_{b}\Sigma^{\rho}_{c}+A^{a}_{\rho e}\Sigma^{\rho}_{b}\Sigma^{e}_{c}. \tag{C14}$$

In an adapted coordinate system,

$$\dagger\overline{\Sigma}^{a}_{bc}=\overline{\Sigma}^{a}_{bc}. \tag{C15}$$

The transformation laws for the fields $(\overline{\Sigma}^{I}_{J},\dagger\Sigma^{I}_{JK})$ are determined by an equation similar to (C2) in which Σ^{I}_{JK}, $\overline{\Sigma}^{I}_{JK}$, and $\hat{s}^{I}_{JK}$ are replaced by $\dagger\hat{\Sigma}^{I}_{JK}$, $\dagger\overline{\Sigma}^{I}_{JK}$, and $\dagger\hat{s}^{I}_{JK}$, respectively. Note that the only nonzero component of $\dagger\hat{s}^{I}_{JK}$ is $\dagger\hat{s}^{a}_{\nu\lambda}$.

The first order results are unchanged. In second order, (C8) is replaced by

$$\dagger\overline{\Sigma}^{a}_{\nu e}\bar{\chi}^{e}_{\lambda}+\dagger\overline{\Sigma}^{a}_{e\lambda}\bar{\chi}^{e}_{\nu}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{\nu\lambda}+\dagger\hat{\omega}^{a}_{\rho\sigma}\overline{\Sigma}^{\rho}_{\nu}\overline{\Sigma}^{\sigma}_{\lambda}=0 \tag{C16}$$

and (C10) is replaced by

$$\dagger\hat{\Sigma}^{a}_{b\lambda}=\dagger\overline{\Sigma}^{a}_{b\lambda}+\hat{\omega}^{a}_{e}\dagger\overline{\Sigma}^{e}_{b\lambda}+\dagger\overline{\Sigma}^{a}_{be}\bar{\chi}^{e}_{\lambda}+\dagger\overline{\Sigma}^{a}_{b\rho}\bar{\chi}^{\rho}_{\lambda}+\dagger\overline{\Sigma}^{a}_{e\lambda}\bar{\chi}^{e}_{b}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{b\lambda}. \tag{C17}$$

From (C10), (C13), and (C17), it follows that

$$\hat{A}^{a}_{e\rho}\hat{\Sigma}^{e}_{b}\hat{\Sigma}^{\rho}_{\lambda}=\overline{A}^{a}_{e\rho}\overline{\Sigma}^{e}_{b}\overline{\Sigma}^{\rho}_{\lambda}+\hat{\omega}^{a}_{f}\overline{A}^{f}_{e\rho}\overline{\Sigma}^{e}_{b}\overline{\Sigma}^{\rho}_{\lambda}-\hat{\omega}^{a}_{e\rho}\overline{\Sigma}^{e}_{b}\overline{\Sigma}^{\rho}_{\lambda}+\overline{A}^{a}_{e\sigma}\overline{\Sigma}^{e}_{b}\overline{\Sigma}^{\sigma}_{\rho}\bar{\chi}^{\rho}_{\lambda}+\overline{A}^{a}_{f\rho}\overline{\Sigma}^{f}_{e}\bar{\chi}^{e}_{b}\overline{\Sigma}^{\rho}_{\lambda}. \tag{C18}$$

In order to relate $\hat{\omega}^{a}_{b\lambda}$ to $\hat{\omega}^{a}_{b,\lambda}$, differentiate the relation (C5b) to obtain (recall that the adapted coordinate systems are valid in an open neighborhood)

$$(\hat{\omega}^{a}_{e,\sigma}\overline{\Sigma}^{-1\sigma}_{\rho})\overline{\Sigma}^{e}_{b}\overline{\Sigma}^{\rho}_{\lambda}+\hat{\omega}^{a}_{e}\overline{\Sigma}^{e}_{b,\lambda}+\overline{\Sigma}^{a}_{e,\lambda}\bar{\chi}^{e}_{b}+\overline{\Sigma}^{a}_{e}\bar{\chi}^{e}_{b,\lambda}=0,\quad a>b. \tag{C19}$$

Since $\overline{\Sigma}^{a}_{b,\lambda}=\overline{\Sigma}^{a}_{b\lambda}$ and $\bar{\chi}^{a}_{b,\lambda}=\bar{\chi}^{a}_{b\lambda}$, (C9), (C19), and (C5c) give

$$(\hat{\omega}^{a}_{e\rho}-\hat{\omega}^{a}_{e,\sigma}\overline{\Sigma}^{-1\sigma}_{\rho})\overline{\Sigma}^{e}_{b}\overline{\Sigma}^{\rho}_{\lambda}=\overline{\Sigma}^{a}_{be}\overline{\Sigma}^{-1e}_{f}\hat{\omega}^{f}_{\rho}\overline{\Sigma}^{\rho}_{\lambda}. \tag{C20}$$

Let $\overline{E}^{a}_{bc}$ be the unique solution of

$$\overline{E}^{a}_{ec}\overline{\Sigma}^{e}_{b}=\overline{\Sigma}^{a}_{be}\overline{\Sigma}^{-1e}_{c} \tag{C21}$$

which satisfies $\overline{E}_{abc}=-\overline{E}_{bac}$. Then

$$\hat{\omega}^{a}_{b\lambda}-\hat{\omega}^{a}_{b,\sigma}\overline{\Sigma}^{-1\sigma}_{\lambda}=\hat{\omega}^{c}_{\lambda}\overline{E}^{a}_{be}. \tag{C22}$$

Finally, (C18) together with (C7) and (C22) yields the infinitesimal Yang–Mills gauge transformation

$$\hat{A}^{a}_{b\lambda}=\overline{A}^{a}_{b\lambda}+\hat{\omega}^{a}_{f}\overline{A}^{f}_{b\lambda}-\hat{\omega}^{e}_{b}\overline{A}^{a}_{e\lambda}-\omega^{a}_{b,\rho}\overline{\Sigma}^{-1\rho}_{\nu}-\hat{\omega}^{\rho}_{\lambda}\overline{A}^{a}_{b\rho}-\hat{\omega}^{f}_{\lambda}\overline{E}^{a}_{bf}. \tag{C23}$$

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Angular momentum operator in a nonabelian gauge field of an N-dimensional monopole and an SO(N) top operator

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(Received 5 June 1981; accepted for publication 21 August 1981)

This paper discusses the structure of the angular momentum operator in a nonabelian gauge field of an N-dimensional monopole. Besides the finite rotation operators with a general gauge group, infinitesimal operators in various moving frames are introduced. By using these the transformation of frames may be easily operated recursively, so the applied relation between the transitive and stationary parts in the top is displayed, and the explicit formulation of angular momentum operators including different gauge potential of a monopole are obtained quite conveniently. Hence the gauge potential of an N-dimensional monopole in the Schwinger gauge and the Wu-Yang overlapping gauge are given explicitly. In addition, we obtain also the result that the self-rotation operators (N th axis is stationary) in a fixed frame under geodesic gauge equal to the sum or difference of isospin and orbital momentum. Finally we have discussed the general gauge group of an N-dimensional monopole.

PACS numbers: 11.10.Np, 12.90. + b

I. INTRODUCTION

In the gauge field of a monopole, the space symmetry and unitary symmetry are closely connected. This gives a cue for analyzing the relation between the space freedom and isospin freedom. Since 1931 there have been a lot of papers discussing the angular momentum operator and its eigenfunctions in the field of a monopole, but all have adopted a definite gauge, so the theory contains explicitly only two rotation freedoms (θ and φ). In 1975, Wu–Yang[1] introduced a gauge with overlapping definition regions. In another paper[2] it was noticed that the gauge freedom and the freedom of rotation in space may be combined into the "body rotation" of a top, which has three freedoms in total and is gauge invariant. This paper provides generalization in N dimensions. This is contrary to the paper[2] in which we first analyzed the structure of N-dimensional top operator, and then obtain angular momentum operators including the gauge potential of an N-dimensional monopole. For the problem of many dimensions the situation becomes very complicated, and we do not know yet the applied expression of a general N-dimensional top operator (compare with Ref. 3). In order to analyze the problem penetratingly, we apply the method of moving frames. Thus in Sec. II, besides the finite SO(N) operators, infinitesimal operators in moving frames are introduced. By virtue of these the transformation of frames may be easily operated step by step, and the explicit expression of the top operator can be obtained. In Sec. III, the SO($N-1$) self-rotation group of the SO(N) top is replaced by the SO($N-1$) gauge group of an SO(N) monopole, from which the rotation operator including gauge potential can be conveniently obtained. By means of these we get the general expressions for the gauge potential of N-dimensional monopole under the Schwinger gauge and under the Wu–Yang overlapping gauge. For instance $N=5$, it is the SO(5) symmetry solution of the monopole obtained by Yang.[4] Yang had discovered that the self-rotation angular momentum of this solution equals the sum or difference of the isospin and orbital momentum.[5] In Sec. III, this relation is extended into N dimensions, and is related to the left–right symmetry of the finite rotation operator under the geodesic gauge. Simultaneously we obtain also the expression of an N-dimensional top operator in fixed frame. Finally we also discuss the general gauge group of an N-dimensional monopole.

II. SO(N) TOP OPERATOR

Let us first introduce the notation

$$R_{jk}(\theta)=\exp(\theta\hat{J}_{jk}), \tag{1}$$

which is a finite rotation operator in the (e_j-e_k) plane, where $\hat{J}_{jk}$ are the generators. For the sake of brevity we express $R_{k+1,k}(\theta)$ by $R_k(\theta)$. Any SO(N) finite rotation operator can be given in terms of $N(N-1)/2$ Euler anglers θ_j^k $(1\leqslant k\leqslant N-1,\ 1\leqslant j\leqslant k)$ as follows:

$$D^{[N]}=R^{[N-1]}\cdots R^{[1]}=R^{[N-1]}D^{[N-1]}, \tag{2}$$

in which

$$R^{[k]}=R_1(\theta_1^k)R_2(\theta_2^k)\cdots R_k(\theta_k^k), \tag{3}$$

namely, $D^{[N]}=D^{[N]}(\Omega)$, where $\Omega=\{\theta_j^k\}$ is the set of all Euler angles, which has the boundary condition

$$\begin{aligned}&0\leqslant\theta_1^k<2\pi,\\ &0\leqslant\theta_j^k<\pi\quad(j\neq 1).\end{aligned} \tag{4}$$

The wavefunction of the symmetry top is given by

$$\langle D^{[N]}(\Omega)\rangle=\langle e(\theta)|D^{[N]}(\Omega)|\bar{e}(\theta)\rangle, \tag{5}$$

 0022-2488/82/122488-06$02.50

where $|e(\theta)\rangle$ and $|\bar{e}(\theta)\rangle$ are the square integrable functions on the group manifold, and can be chosen as the bases of the unitary irreducible representation of SO(N). The differential operators corresponding to the second- and the first-parameter groups J_{jk} and $\bar{J}_{kj}$ are given as follows[6]:

$$\begin{aligned}\langle \hat{J}_{kj} D^{[N]}(\Omega)\rangle &= J_{kj}\langle D^{[N]}(\Omega)\rangle,\\ \langle D^{[N]}(\Omega)\hat{J}_{kj}\rangle &= \bar{J}_{kj}\langle D^{[N]}(\Omega)\rangle,\end{aligned} \tag{6}$$

J_{kj} or $\bar{J}_{kj}$ are the kj components of the top operator on the space fixed frame $\{e_k\}$ or in the final moving frame $\{\bar{e}_k\}$

$$\mathscr{J} = \sum_{jk} J_{jk} e_j \wedge e_k = \sum_{jk} \bar{J}_{jk} \bar{e}_j \wedge \bar{e}_k.$$

Furthermore we introduce the intermediary moving frames, for example, $\mathring{J}_{kj}$ is the components of the top operator on the natural bases $\{\mathring{e}_k\}$ (tangents of longitude and latitude), which are given by

$$\mathring{J}_{kj}\langle D^{[N]}\rangle = \langle R^{[N-1]}\hat{J}_{kj} D^{[N-1]}\rangle. \tag{7}$$

From (2), with respect to each θ_j^k, $D^{[N]}(\Omega)$ may be decomposed as

$$D^{[N]} = R^{[kj]}\cdot R_j(\theta_j^k)\cdot {}^{[kj]}R, \tag{8}$$

hence, in a similar way, we can introduce

$$\langle R^{[kj]}\hat{J}_{ih} R_j(\theta_j^k)\cdot {}^{[kj]}R\rangle = J_{ih}^{[kj]}\langle D^{[N]}\rangle. \tag{9}$$

The superscripts kj in $J_{ih}^{[kj]}$ mean that ih are tensor indices in the moving frame which is obtained from the fixed frame by the rotation $R^{[kj]}$ on the left of θ_j^k.

J_{kj}, $\bar{J}_{kj}$, $\mathring{J}_{kj}$ may be all expressed in terms of Euler angles and $P_j^k = -i\partial/\partial\theta_j^k$. Now, by using intermediary moving frames, the differential operator of a Euler angle P_j^k may be written as a component of $\mathscr{J}$ in the intermediary moving frame

$$P_j^k\langle D^{[N]}\rangle = -i\frac{\partial}{\partial\theta_j^k}\langle D^{[N]}\rangle = J_{j+1,j}^{[kj]}\langle D^{[N]}\rangle,$$

namely,

$$P_j^k = J_{j+1,j}^{[kj]}. \tag{10}$$

We project it on the natural frame, i.e., rotate it by the $(N-1-j)$ factor in $R^{[N-1]}$ on the right of $R_j(\theta_j^{N-1})$ step by step

$$\begin{aligned}P_j^{N-1} = J_{j+1,j}^{[N-1,j]} &= c_{j+1}^{N-1} J_{j+1,j}^{[N-1,j+1]} + s_{j+1}^{N-1} J_{j+2,j}^{[N-1,j+1]}\\ &= \sum_{l=j+1}^{N-1} A_l^{[N-1,j+1]}\mathring{J}_{l,j} + s_{j+1}^{N-1}s_{j+2}^{N-1}\cdots s_{N-1}^{N-1}\mathring{J}_{Nj},\end{aligned} \tag{11}$$

where

$$c_k^{N-1} = \cos\theta_k^{N-1}, \quad s_k^{N-1} = \sin\theta_k^{N-1}, \tag{12}$$

and

$$\begin{aligned}A_{j+1}^{[N-1,j+1]} &= c_{j+1}^{N-1},\\ A_l^{[N-1,j+1]} &= c_l^{N-1}s_l^{N-1}\cdots s_{j+1}^{N-1} \quad (j+1<l\leqslant N-1).\end{aligned} \tag{13}$$

The last term of (11) is the transitive part of the top operator which may be solved. Then we get

$$\begin{aligned}\mathring{J}_{N,N-1} &= P_{N-1}^{N-1},\\ \mathring{J}_{N,j} &= \left(P_j^{N-1} - \sum_{l=j+1}^{N-1} A_l^{[N-1,j+1]}\mathring{J}_{lj}\right)\Big/ s_{N-1}^{N-1}\cdots s_{j+1}^{N-1}\\ &\qquad (j<N-1).\end{aligned} \tag{14}$$

Because the latitudes are not geodesic lines, on the right-hand side of (14), besides the term of orbital part $P_j^{N-1}/s_{N-1}^{N-1}\cdots s_{j+1}^{N-1}$, there are also the terms of the stationary part $\mathring{J}_{lj}$. For example $N=3$,

$$D^{[3]} = R_1(\theta_1^2)R_2(\theta_2^2)R_1(\theta_1^1)\equiv R_1(\alpha)R_2(\beta)R_1(\gamma).$$

By virtue of (14) we get

$$\begin{aligned}J_{32} &= P_2^2 = -i\frac{\partial}{\partial\beta} = J_\varphi,\\ J_{31} &= (P_1^2 - c_2^2 J_{21})/s_2^2 = -i\frac{\partial}{\sin\beta\partial\alpha} + i\cot\beta\frac{\partial}{\partial\gamma}\\ &= -J_\theta,\end{aligned}$$

which are the well-known expressions for the three-dimensional top operator in the natural frame.

II. GAUGE POTENTIAL AND ANGULAR MOMENTUM OPERATOR IN FIELD OF AN N-DIMENSIONAL MONOPOLE

In a previous paper[7] the structure of the gauge field has been discussed and the potential of the point monopole in N dimensions has been given by $\mathscr{A}_i = \bar{T}_{ij}x^j/r^2$, where $\bar{T}_{ij}$ is the generator of SO(N) group. [For example: $N=2$, Dirac string; $N=3$, 'tHooft monopole; $N=4$, SO(4) meron and antimeron; $N=5$, SO(5) instanton and anti-instanton.]

The Euler freedom of the top can be divided into that of the stationary SO($N-1$) subgroup and that in coset space $S^{N-1}(\theta_k^{N-1})$

$$D^{[N]}(\Omega) = R^{[N-1]}(\omega)D^{[N-1]}(\Gamma),$$

where $\omega = \{\theta_k^{N-1}\}$ is the set of transitive angles along the surface $S^{N-1}(\theta_k^{N-1})$ and $\Gamma = \{\theta_i^j\}$ $(j\leqslant N-2)$ is the set of self-rotation angles in the stationary subgroup.

Let $S^{N-1}(\theta_k^{N-1})$ be synchronous with the space $S^{N-1}(\theta_k)$, the latter is described by θ_k as follows:

$$\begin{aligned}x_1 &= rs_{N-1}\cdots s_2 s_1,\\ x_2 &= rs_{N-1}\cdots s_2 c_1,\\ x_j &= rs_{N-1}\cdots s_j c_{j-1},\\ &\cdots\\ x_N &= rc_{N-1},\end{aligned} \tag{15}$$

namely,

$$\theta_k^{N-1} = \theta_k. \tag{16}$$

Noting that the gauge potential of a point monopole can be transformed into the explicit reduced form,[7,8] which contain only SO($N-1$) isospin, so that it may be replaced by the SO($N-1$) stationary subgroup of the SO(N) top. Simultaneously the symmetry top wavefunction is replaced by the gauge dependent wavefunction

$$\langle R^{[N-1]}(\omega)D_T^{[N-1]}(\Gamma)\rangle,$$

where the subscript T on $D_T^{[N-1]}(\Gamma)$ indicates that $\hat{J}_{kj}$ has been replaced by the isospin matrix $\hat{T}_{kj}$. Now the bases of the

representation become the direct product of $|e\rangle$ and $|\bar{i}\rangle$. Here $|e\rangle$ are square integrable functions on sphere S^{N-1}, $|\bar{i}\rangle$ are regular representations of SO($N-1$) isospin. As in the case of (6)–(9), we can write

$$\begin{aligned} J_{kj}\langle R^{[N-1]}D_T^{[N-1]}\rangle &= \langle R^{[N-1]}\hat{J}_{kj}D_T^{[N-1]}\rangle \\ &= \langle R^{[N-1]}\hat{T}_{kj}D_T^{[N-1]}\rangle \\ &= \mathring{T}_{kj}\langle R^{[N-1]}D_T^{[N-1]}\rangle, \end{aligned} \tag{17}$$

$$\langle R^{[N-1]}D_T^{[N-1]}\hat{T}_{kj}\rangle = \bar{T}_{kj}\langle R^{[N-1]}D_T^{[N-1]}\rangle, \tag{18}$$

$$P_i^j\langle R^{[N-1]}D_T^{[N-1]}\rangle = T^{[j,i]}_{i+1,i}\langle R^{[N-1]}D_T^{[N-1]}\rangle.$$

Since our gauge bases $|\bar{i}\rangle$ are eigenfunctions of $\hat{T}_{kj}$ in the final moving gauge frame, the gauge condition is fixed by choosing the dependence of local SO($N-1$) gauge rotation parameters $\{\theta_i^j\}$ on the coordinates θ_k

$$\theta_i^j = \theta_i^j(\{\theta_k\}) \quad (j<N-1). \tag{19}$$

Owing to (16), (19), we get

$$P_k = -i\frac{\partial}{\partial\theta_k} = P_k^{N-1} + \frac{\partial\theta_i^j}{\partial\theta_k}P_i^j. \tag{20}$$

Substituting (18), (20) into (14), expressing $\mathring{J}_{ji}$ by $\mathring{T}_{ji}$, projecting T_{ji}, $T^{[j,i]}_{i+1,i}$ to the right as in terms of $\bar{T}_{ji}$, we get

$$\mathring{J}_{Nj} = \mathring{L}_{Nj} - r\sum_{li}\mathscr{A}_j^{li}\bar{T}_{li}, \tag{21}$$

where

$$\begin{aligned} &L_{N,N-1} = P_{N-1}, \\ &\mathring{L}_{Nj} = P_j/s_{N-1}\cdots s_{j+1} \quad (\text{when } j<N-1), \end{aligned} \tag{22}$$

are components of the orbital momentum on the natural frame along the space, $\mathscr{A}_j^{li}$ are the li isospin and j-space components of the SO($N-1$) gauge potential of point monopole in N dimensions. For instance,

Schwinger gauge:

$$\theta_i^j = 0,$$

so

$$P_k = P_k^{N-1}, \quad \mathring{J}_{ji} = \mathring{T}_{ji} = \bar{T}_{ji}, \tag{23}$$

substitute these in (14), we get

$$\begin{aligned} &\mathring{J}_{Nj} = \left(P_j - \sum_{l=j+1}^{N-1} A_l^{[j+1]}\mathring{J}_{lj}\right)\Big/ s_{N-1}\cdots s_{j+1}, \\ &J_{N,N-1} = P_{N-1}, \end{aligned} \tag{24}$$

where coefficients $A_l^{[j+1]}$ are defined as (13), only that θ_k^{N-1} are replaced by θ_k. Comparing it with (21) we get

$$\mathscr{A}_j^{lj} = c_l/rs_{N-1}\cdots s_l \quad (N-1\geqslant l\geqslant j+1\geqslant 2), \tag{25}$$

all others are zero.

Wu-Yang gauge:

$$\begin{aligned} &\theta_{N-2}^{N-2} = \mp\theta_{N-2} \quad \left(\text{when } \theta_{N-1} \begin{matrix} <\pi-\epsilon \\ >0+\epsilon \end{matrix}\right), \\ &\theta_i^i = -\theta_i \quad (i\leqslant N-3), \\ &\theta_i^j = 0 \quad (i<j<N-1). \end{aligned} \tag{26}$$

Now

$$\begin{aligned} &P_{N-1} = P_{N-1}^{N-1}, \quad P_{N-2} = P_{N-2}^{N-1} \mp P_{N-2}^{N-2}, \\ &P_i = P^{N-1} - P_i^i \quad (i\leqslant N-3). \end{aligned} \tag{27}$$

Due to the gauge conditions (26) the rotation operator can be written as

$$\begin{aligned} R^{[N-1]}D_T^{[N-1]} = R_1(\theta_1)R_2(\theta_2)\cdots R_{N-2}(\theta_{N-2})R_{N-1}(\theta_{N-1}) \\ \times R_{N-2}^T(\mp\theta_{N-2})\cdots R_2^T(-\theta_2)R_1^T(-\theta_1). \end{aligned} \tag{28}$$

The left and right factors are nearly symmetrical. Hence the expression of $P_i^i = T^{[i,i]}_{i+1,i}$ by $\mathring{T}_{ji}$ is almost the same as that of P_j^{N-1} by $\mathring{J}_{ji}$ (except for one term and the sign of the last term).

$$\begin{aligned} &P_i^i = \sum_{l=i+1}^{N-2} A_l^{[i+1]}\mathring{T}_{li} \pm s_{N-2}\cdots s_{i+1}\mathring{T}_{N-1,i} \quad (i\leqslant N-3), \\ &P_{N-2}^{N-2} = \mathring{T}_{N-1,N-2}. \end{aligned} \tag{29}$$

By virtue of these, (14) becomes

$$\begin{aligned} \mathring{J}_{Nj} &= (P_j - c_{N-1}s_{N-2}\cdots s_{j+1}\mathring{T}_{N-1,j} \\ &\quad \pm s_{N-2}\cdots s_{j+1}\mathring{T}_{N-1,j})/s_{N-1}\cdots s_{j+1} \\ &= \mathring{L}_{Nj} + \frac{\pm 1 - c_{N-1}}{s_{N-1}}\mathring{T}_{N-1,j} \quad (j<N-1), \\ \mathring{J}_{N,N-1} &= P_{N-1} = \mathring{L}_{N,N-1}. \end{aligned} \tag{30}$$

Then we project $\mathring{T}_{N-1,j}$ on the right in terms of $\bar{T}_{ji}$. For simplicity we consider only in north region.

$$\begin{aligned} \mathring{T}_{N-1,N-2} &= T^{[N-2,N-2]}_{N-1,N-2} \\ &= T^{[N-3,N-3]}_{N-1,N-2} \\ &= c_{N-3}T^{[N-4,N-4]}_{N-1,N-2} + s_{N-3}T^{[N-4,N-4]}_{N-1,N-3} \\ &= \sum_{k=1}^{N-2} B_k^{[N-2]}\bar{T}_{N-1,k}, \end{aligned} \tag{31}$$

in which

$$\begin{aligned} &B_{N-2}^{[N-2]} = c_{N-3}, \\ &B_k^{[N-2]} = s_{N-3}\cdots s_k c_{k-1}, \end{aligned} \tag{32}$$

where, stipulating $c_0 = 1$, $s_0 = 0$, for $j<N-2$, we get

$$\begin{aligned} \mathring{T}_{N-1,j} &= T^{[N-2,N-2]}_{N-1,j} \\ &= c_{N-2}T^{[N-3,N-3]}_{N-1,j} + s_{N-2}T^{[N-3,N-3]}_{N-2,j} \\ &= \sum_{k=j+2}^{N-1} B_k^{[N-1]}T_{kj}^{[j,j]} + s_{N-2}\cdots s_{j+1}T_{j+1,j}^{[j,j]} \\ &= \sum_{k=j+2}^{N-1} B_k^{[N-1]}\left(c_j\sum_{l=1}^{j} B_l^{[j]}\bar{T}_{kl} - s_j\bar{T}_{k,j+1}\right) \\ &\quad + s_{N-2}\cdots s_{j+1}\sum_{l=1}^{j} B_l^{[j]}\bar{T}_{j+1,l}. \end{aligned} \tag{33}$$

Combining (31), (32), we can write

$$\mathring{T}_{N-1,j} = \sum_{k,l} B_{k,l}^{[N-1,j]}\bar{T}_{kl}, \tag{34}$$

where $B_{k,l}^{[N-1,j]}$ equal: (lower sign belongs to the south region)

$$\begin{aligned} &\mp s_{N-2}\cdots s_k c_{k-1}s_j && N-2\geqslant k>j+1=l\geqslant 2, \\ &-c_{k-1}s_j && N-1=k>j+1=l\geqslant 2, \\ &\pm s_{N-2}\cdots s_k c_{k-1}c_j c_{j-1} && N-2\geqslant k>j=l\geqslant 1, \end{aligned}$$

$$
\begin{cases}
c_{k-1}c_jc_{j-1} & N-1\geqslant k>j=l\geqslant 1,\\
\pm s_{N-2}\cdots s_k c_{k-1}c_j s_{j-1}\cdots s_l c_{l-1} & N-2\geqslant k>j>l\geqslant 1,\\
c_{k-1}c_j s_{j-1}\cdots s_l c_{l-1} & N-1=k>j>l\geqslant 1,
\end{cases}
\tag{35}
$$

all others are zero (when $k-1=j$, replace $c_{k-1}c_j$ by 1). Substituting (34) into (30), and compare with (21), we get

$$
\mathscr{A}_j^{kl}=\frac{\mp 1+c_{N-1}}{rs_{N-1}}B_{k,l}^{[N-1,j]}. \tag{36}
$$

For example $N=3$, it is the 'tHooft point monopole, from (25), Schwinger gauge potential

$$
\mathscr{A}_1^{21}=\frac{\cos\theta_2}{r\sin\theta_2},\quad \text{all others are zero;}
$$

from (36) and (35), Wu–Yang gauge potential

$$
\mathscr{A}_1^{21}=\frac{\mp 1+\cos\theta_2}{r\sin\theta_2},\quad \text{all others are zero.}
$$

These are well-known results.

Another example $N=5$, it is the SO(5) symmetry monopole, from (36) and (35), we get the Wu–Yang gauge potential [for simplicity, let $W=(\mp 1+c_{N-1})/rs_{N-1}$]:

$$
\begin{aligned}
&\mathscr{A}_1^{32}=\mp s_3c_2s_1W,\quad \mathscr{A}_1^{31}=\pm s_3c_2c_1W,\quad \mathscr{A}_1^{21}=\pm s_3s_2W,\\
&\mathscr{A}_1^{42}=-c_3s_1W,\quad \mathscr{A}_1^{41}=c_3c_1W,\\
&\mathscr{A}_2^{32}=\pm s_3c_1W,\quad \mathscr{A}_2^{31}=\pm s_3s_1W,\\
&\mathscr{A}_2^{43}=-c_3s_2W,\quad \mathscr{A}_2^{42}=c_3c_2c_1W,\quad \mathscr{A}_2^{41}=c_3c_2s_1W,\\
&\mathscr{A}_3^{43}=c_2W,\quad \mathscr{A}_3^{42}=s_2c_1W,\quad \mathscr{A}_3^{41}=s_2s_1W,
\end{aligned}
\tag{37}
$$

all other components are zero.

Furthermore, $\bar{T}_{j,k}$ may be decomposed into

$$
\bar{T}_i^{\pm}=\tfrac{1}{2}(\tfrac{1}{2}\epsilon_{ijk}\bar{T}_{jk}\pm\bar{T}_{i4}). \tag{38}
$$

Taking the representation with $\bar{T}^-=0$ (or $\bar{T}^+=0$), we get the SO(5) symmetrical self-dual (or anti-self-dual) monopole solution of the SU(2) gauge group, which components may expressed with the matrix as follows:

$$
(\mathscr{A}'^{[\alpha]})_i^j=W\begin{pmatrix}
\pm s_3c_2s_1+c_3c_1 & \pm s_3c_2c_1-c_3s_1 & \mp s_3s_2\\
\mp s_3c_1+c_3c_2s_1 & \pm s_3s_1+c_3c_2c_1 & -c_3s_2\\
s_2s_1 & s_2c_1 & c_2
\end{pmatrix},
$$

$$
(\mathscr{A}'^{[\beta]})_i^j=W\begin{pmatrix}
\pm s_3c_2s_1-c_3c_1 & \pm s_3c_2c_1+c_3s_1 & \mp s_3s_2\\
\mp s_3c_1-c_3c_2s_1 & \pm s_3s_1-c_3c_2c_1 & c_3s_2\\
-s_2s_1 & -s_2c_1 & -c_2
\end{pmatrix}.
$$

This is the solution obtained by Yang,[5] the gauge conditions are the same, only the space coordinate systems are different, the relations between coordinate systems $(r,\theta_1,\theta_2,\theta_3,\theta_4)$ [see (15)] and $(r,\theta,\xi_1,\xi_2,\xi_3)$ (Ref. 5) are as follows:

$$
\xi_1=\xi s_2s_1,\quad \xi_2=\xi s_2c_1,\quad \xi_3=c_2,\quad \xi=\tan(\theta_3/2). \tag{39}
$$

Thus the orientations of e_r and $e_\theta=e_{\theta_4}$ are unchanged, but its orthogonal three-dimensional subspace has to rotate the frame by $R=R_2(\theta_2)R_1(\theta_1)$, so

$$
(\mathscr{A}^{[\alpha]})_i^j=\begin{pmatrix}
c_1 & c_2s_1 & s_2s_1\\
-s_1 & c_2c_1 & s_2c_1\\
0 & -s_2 & c_2
\end{pmatrix}(\mathscr{A}'^{[\alpha]})_i^j,
$$

and we get

$$
\mathscr{A}_i^{[\alpha]j}=-W\left[\frac{1-\xi^2}{1+\xi^2}\delta_{ij}+\frac{2\xi_i\xi_j}{1+\xi^2}\mp\frac{2\epsilon_{ijk}\xi_k}{1+\xi^2}\right], \tag{40a}
$$

$$
\mathscr{A}_i^{[\beta]j}=W\left[\frac{1-\xi^2}{1+\xi^2}\delta_{ij}+\frac{2\xi_i\xi_j}{1+\xi^2}\pm\frac{2\epsilon_{ijk}\xi_k}{1+\xi^2}\right]. \tag{40b}
$$

The above formulas are just the same as in Ref. 5, but the way we have arrived at them is comparatively easier and simpler.

IV. TOP OPERATOR IN FIXED FRAME AND SELF-ROTATION ANGULAR MOMENTUM UNDER THE GEODESIC GAUGE

By virtue of moving frames the formulation of the top operator in a fixed frame can be easily obtained. Projecting $P_{k-1}^{N-1}=-i\partial/\partial\theta_{k-1}^{N-1}$ to the left in terms of J_{kj}, we obtain the result as follows (for simplicity of notation, except for the differential operator P_k^{N-1}, we omit the superscript $N-1$ on θ_k^{N-1}):

$$
P_{k-1}^{N-1}=J_{k,k-1}^{[k-1]}=\sum_{i=1}^{k-1}B_i^{[k-1]}J_{k,i}, \tag{41}
$$

where the coefficients $B_i^{[k-1]}$ are given by (32). Projecting $\mathring{J}_{k-1,j}$ $(j<k-1)$ to the left

$$
\mathring{J}_{k-1,j}=J_{k-1,j}^{[k]}=c_{k-1}J_{k-1,j}^{[k-1]}-s_{k-1}J_{k,j}^{[k-1]}, \tag{42}
$$

in which the first term can be reduced as in the case of (14), we get

$$
\begin{aligned}
&J_{k-1,j}^{[k-1]}=\left(P_j^{N-1}-\sum_{l=j+1}^{k-2}A_l^{[j+1]}J_{l,j}^{[k-1]}\right)\\
&s_{k-2}\cdots s_{j+1}\quad (j<k-2),\\
&J_{k-1,k-2}^{[k-1]}=P_{k-2}^{[N-1]}.
\end{aligned}
\tag{43}
$$

The second term of (42) can be reduced as follows:

$$
J_{k,j}^{[k-1]}=J_{kj}^{[j+1]}=c_j\sum_{i=1}^{j}B_i^{[j]}J_{k,i}-s_jJ_{k,j+1}. \tag{44}
$$

Substituting (43), (44) into (42) we get

$$
\begin{aligned}
\mathring{J}_{k-1,k-2}&=c_{k-1}P_{k-2}^{N-1}-s_{k-1}\\
&\left(c_{k-2}\sum_{i=1}^{k-2}B_i^{[k-2]}J_{k,i}-s_{k-2}J_{k,k-1}\right),
\end{aligned}
\tag{45a}
$$

$$
\begin{aligned}
\mathring{J}_{k-1,j}&=\frac{c_{k-1}}{s_{k-2}\cdots s_{j+1}}\left(P_j^{N-1}-\sum_{l=j+1}^{k-2}A_l^{[j+1]}\mathring{J}_{l,j}\right)\\
&\quad-s_{k-1}\left(c_j\sum_{i=1}^{j}B_i^{[j]}J_{ki}-s_jJ_{k,j+1}\right).
\end{aligned}
\tag{45b}
$$

When (41) and (45) are put together, for a certain k, we have $(k-1)$ equations, and the determinant of the coefficients of J_{ki} (when $i<k$, there are $k-1$ components also) is nonsingular, which is the transformation matrix between $J_{k,i}^{[k-1]}$ and $J_{k,i}$, so we can expressed J_{ki} in terms of P_j^{N-1} and $\mathring{J}_{lj}$ $(l,j\leqslant k-1)$. For instance, combining (41) with (45a), we get

$$
\begin{aligned}
J_{k,k-1}&=c_{k-2}P_{k-1}^{N-1}\\
&-\frac{c_{k-1}s_{k-2}}{s_{k-1}}P_{k-2}^{N-1}+\frac{s_{k-2}}{s_{k-1}}\mathring{J}_{k-1,k-2}\quad (N\geqslant k\geqslant 2).
\end{aligned}
\tag{46a}
$$

Furthermore, combining (41) with the expression of $\dot{J}_{k-1,k-3}$ (45b), we get

$$J_{k,k-2} = s_{k-2}c_{k-3}P^{N-1}_{k-1} + \frac{1}{s_{k-1}}(c_{k-1}c_{k-2}c_{k-3}P^{N-1}_{k-2} - c_{k-2}c_{k-3}\mathring{J}_{k-1,k-2} + s_{k-3}\dot{J}_{k-1,k-3}) - \frac{c_{k-1}s_{k-3}}{s_{k-1}s_{k-2}}(P^{N-1}_{k-3} - c_{k-2}\mathring{J}_{k-2,k-3})$$

$(N \geqslant k \geqslant 3)$. (46b)

By repeated application of these steps, we can obtain

$$J_{kj} = \sum_{l=j-1}^{k-1} D^{[kj]}_l P^{N-1}_l + \sum_{lh} C^{[kj]}_{lh}\mathring{J}_{lh}, \tag{47}$$

where we stipulate that the coefficients $D^{[kj]}_l$ equal

$$\begin{cases} c_{j-1} & k-1=l=j, \\ s_{k-2}\cdots s_j c_{j-1} & k-1=l>j, \\ c_{k-1}c_l c_{l-1}/s_{k-1}\cdots s_{l+1} & k-1>l=j, \\ c_{k-1}c_l s_{l-1}\cdots s_j c_{j-1}/s_{k-1}\cdots s_{l+1} & k-1>l>j, \\ -c_{k-1}s_l/s_{k-1}\cdots s_{l+1} & k-1>l=j-1, \end{cases} \tag{48}$$

and that the coefficient $c^{[kj]}_{lh}$ equal

$$\begin{cases} -c_{k-1}c_l c_h s_{h-1}\cdots s_j c_{j-1}/s_{k-1}\cdots s_l & k-1\geqslant l>h>j, \\ -c_{k-1}c_l c_h c_{h-1}/s_{k-1}\cdots s_l & k-1\geqslant l>h=j, \\ c_{k-1}c_l s_h/s_{k-1}\cdots s_l & k-1\geqslant l>h=j-1, \end{cases} \tag{49}$$

(when $l=k-1$, replace $c_{k-1}c_l$ by 1).

Yang[5] discovered that the self-rotation operator of O(5) symmetry monopole, which leaves the 5th axis unmoved, equals the sum or difference of the isospin and orbital momentum. This relation can be extended to any N dimensions. Noting that under the geodesic gauge the finite rotation operator has form like (28), with left and right factors nearly symmetrical, so as in the case of (41), we get

$$P^i_j = T^{[j,j]}_{j+1,j} = \sum_{i=1}^{j} B^{[j]}_i \bar{T}_{j+1,i} \quad (j<N-2).$$

Owing to the commutability of $R_{N-1}(\theta_{N-1})$ with $\mathring{T}_{ij}$ $(i,j<N-1)$, the expressions of $\mathring{T}_{ij}$ $(i,j<N-1)$ in the final moving frame are similar with $\mathring{J}_{ij}$ as in (45). In the case of (46), we obtained the expression of $\bar{T}_{kj}$, only P^{N-1}_j are replaced by P^i_j, and noting that in the south region the sign of θ_{N-2} is inverse, we get

$$\bar{T}_{kj} = \sum_{l=j-1}^{k-1} D^{[kj]}_l P^l_l + \sum_{lh} C^{[kj]}_{lh}\mathring{T}_{lh} \quad (j<k<N-1), \tag{50a}$$

$$\bar{T}_{N-1,j} = B^{[N-2]}_j P^{N-2}_{N-2} \pm \sum_{l=j-1}^{N-3} D^{[N-1,j]}_l P^l_l \pm \sum_{lh} C^{[N-1,j]}_{lh}\mathring{T}_{lh}. \tag{50b}$$

But by virtue of (15) the geodesic gauge condition

$$P_{N-2} = P^{N-1}_{N-2} \mp P^{N-2}_{N-2}, \quad P_j = P^{N-1}_j - P^j_j \quad (j<N-2), \tag{27}$$

$$\dot{J}_{ij} = \mathring{T}_{ij}, \tag{23}$$

and by virtue of (15) it may be easily proved that

$$\sum_{l=j-1}^{k-1} D^{[kj]}_l P_l = -i(x_k\partial_j - x_j\partial_k) = L_{kj}, \tag{51}$$

so we get

$$J_{kj} - \bar{T}_{kj} = L_{kj} \quad (k<N-1), \tag{52a}$$

and

$$J_{N-1,j} \mp \bar{T}_{N-1,j} = L_{N-1,j}. \tag{52b}$$

For example, $N=3$, $J_{12} = L_{12} \pm \bar{T}_{12}$,

$$\begin{aligned} N=4,\quad & J_{12} = L_{12} + \bar{T}_{12}, \\ & J_{32} = L_{32} \pm \bar{T}_{32},\ J_{31} = L_{31} \pm \bar{T}_{31}, \\ N=5,\quad & J_{12} = L_{12} + \bar{T}_{12}, \\ & J_{32} = L_{32} + \bar{T}_{32},\ J_{31} = L_{31} + \bar{T}_{31}, \\ & J_{41} = L_{41} \pm \bar{T}_{41}, \\ & J_{42} = L_{42} \pm \bar{T}_{42},\ J_{43} = L_{43} \pm \bar{T}_{43}. \end{aligned}$$

By virtue of (38), which may be decomposed into Yang's SU(2) result.

V. GENERAL GAUGE GROUP FOR N-DIMENSIONAL MONOPOLE AND GLOBAL SO(N) SYNCHRONOUS SYMMETRICAL GAUGE

For N-dimensional monopole, the reduced SO$(N-1)$ group H may be imbedded in group G. Here G may be any $G \supset T_H$, where T_H is equivalent to the matrix set on some representation space of H [e.g., when $N=5$, $H=$ SO(4) $=$ SO(3) $\otimes$ SO(3) T_H may be SO(3)]. But only when there exists a G', such as $G \supseteq G' \supset H$, $G'/H \sim S^{N-1}$, can we find a global gauge without overlapping region for the monopole potential (cf. Ref. 9). [e.g., there exists no such gauge when the T_H of $H=$ SO(2) corresponds to the λ_8 in $G=$ SU(3).]

Now we will discuss the global SO(N) synchronous symmetrical gauge, corresponding to the case of $G=G'=$ SO$(N) \supset H =$ SO$(N-1)$, which is frequently applied. Namely, choosing the gauge bases $|i\rangle = D^{[N]}_T(\Omega')^{-1}|\bar{i}\rangle$, the finite operator is given by

$$R^{[N-1]}(\omega)D^{[N-1]}_T(\Gamma)D^{[N]}_T(\Omega')^{-1}.$$

Let $\mathring{J}_{kj}$ and $\mathring{T}_{kj}$,

$$\theta^{N-1}_k = \theta_k, \quad \theta'^{N-1}_k = \theta_k, \quad \theta'^k_j = \theta^k_j(\{\theta_k\}) \quad (k<N-1), \tag{53}$$

so the finite rotation operator becomes

$$R^{[N-1]}(\omega)R^{[N-1]}_T(\omega)^{-1} = R_1(\theta_1)\cdots R_{N-2}(\theta_{N-2})R_{N-1}(\theta_{N-1})R^T_{N-1}(-\theta_{N-1})R^T_{N-2}(-\theta_{N-2})\cdots R_1(-\theta_1), \tag{54}$$

then

$$P_k = P_k^{N-1} = P_k'^{N-1}. \tag{55}$$

The formulation (54) is similar to (28), only with an additional factor $R_{N-1}^{T}(-\theta_{N-1})$, so a similar relation can be gotten easily. As in the case of (47) we get

$$T_{kj} = \sum_{l=j-1}^{k-1} D_l^{[kj]} P_l^l + \sum_{lh} C_{lh}^{[kj]} \mathring{T}_{lh}. \tag{56}$$

By virtue of (47), (49), (53), (55), (56), we get

$$J_{kj} = L_{kj} + T_{kj}. \tag{57}$$

It may be written in the gauge covariant form with the SO(N) potential and field as follows:

$$J_{kj} = x_k(-i\partial_j - \mathscr{A}_j) - x_j(-i\partial_k - \mathscr{A}_k) - \mathscr{F}_{kj} r^2, \tag{58}$$

where the field $\mathscr{F}_{kj} = \mathscr{F}_{kj}^{lh} T_{lh}$ given the synchronous rotation of both the space-self and the isospin SO($N-1$)-self-rotation, and the potential

$$\mathscr{A}_j = \mathscr{A}_j^{lh} T_{lh}, \tag{59}$$

where

$$\mathscr{A}_j^{lh} = -\frac{1}{r^2}(x^l \delta_j^h - x^h \delta_j^l).$$

Including this gauge potential, the covariant derivative gives the synchronous transition along the surface of a sphere.

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Scattering by slightly nonspherical particles in the high frequency limit. I. Impenetrable particles

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(Received 5 May 1981; accepted for publication 2 September 1981)

The scattering of a scalar plane wave by a slightly nonspherical impenetrable particle in the high frequency limit is investigated using a combination of boundary perturbation theory and the modified Watson transformation. Boundary perturbation theory is used to find the perturbed S-matrix for the problem. The modified Watson transformation is then used to sum the perturbed partial wave expansion in the short wavelength limit. This method is applied to backscattering by a slightly dilated sphere and a sphere whose shape is perturbed by making the radius a function of θ given by $r_p(\theta) = a[1 + \delta P_2(\cos\theta)]$, where P_2 is a Legendre function, a is the radius of the unperturbed sphere, and δ is the perturbation parameter. This method will be valid for $(ka)^{1/3} \gg 1$, where k is the wavenumber.

PACS numbers: 11.20.Dj

1. INTRODUCTION

The scattering of a plane scalar wave by a large impenetrable sphere was investigated by Nussenzveig.[1] In his paper he developed the modified Watson transformation which converts the slowly convergent partial wave series into an integral in the complex angular momentum plane. He approximated this integral, in the high frequency limit, by use of the saddle point method and the method of residues. The result was found to converge rapidly for short wavelengths.

In this paper the method used by Nussenzveig for the sphere will be extended to slightly nonspherical particles. This will be accomplished by combining the modified Watson transformation with boundary perturbation theory. Thus all the advantages gained by use of the Watson transformation for spheres will be extended to slightly nonspherical objects.

I will only consider impenetrable particles in this paper because this is the simplest case to treat and will allow the clearest presentation of the essentials of this method. In order to reduce the amount of algebra the examples treated will be limited to backward scattering by a particle with an axis of symmetry. The direction of the incoming beam will be parallel to this axis of symmetry.

The effects of slight distortions from a sphere should be much more interesting for transparent particles, especially when considering such phenomena as the glory.[2] The method presented here for impenetrable particles will be applied to the transparent case in a future paper.

In Sec. 2 the perturbed S matrix is derived using boundary perturbation theory. The conditions necessary for the application of the modified Watson transformation are considered in Sec. 3. Section 4 contains the results of using this method backscattering by a sphere whose radius is increased slightly. This result is equal to the exact solution to first order in the expansion parameter, thus demonstrating the validity of combining boundary perturbation theory with the modified Watson transformation, at least for the spherical case. In Sec. 5 the method is applied to backscattering by a sphere whose boundary is perturbed by adding $P_2(\cos\theta)$, where P_2 is a Legendre function.

Since this paper is mainly an extension of Nussenzveig's work I will try to follow the notation of Ref. 1 as closely as possible.

2. BOUNDARY PERTURBATION THEORY

I will use a perturbation method based on a Taylor series expansion of the boundary conditions similar to Yeh's,[3] except I will consider a scalar instead of a vector wave. The perturbation series will be worked out only to first order, generalization to higher orders being straight forward.

I begin by considering a surface defined by the points (r_p,θ,ϕ) in spherical coordinates, where

$$r_p(\theta) = a[1 + \delta\omega(\theta)], \tag{2.1}$$

a is the radius of the unperturbed sphere, δ is the perturbation parameter, and $\omega(\theta)$ is an arbitrary single valued, continuous function of θ. The wavefunction that is the solution for scattering by the perturbed sphere can be written

$$\psi(r) = \psi^{(0)} + \delta\psi^{(1)} + \delta^2\psi^{(2)} + \cdots, \tag{2.2}$$

where $\psi^{(0)}$ is the solution for the unperturbed problem given by

$$\psi^{(0)} = \sum_{l=0}^{\infty} \frac{(2l+1)}{2} i^l [h_l^{(2)}(kr) + S_l^{(0)}(\beta) h_l^{(1)}(kr)] P_l(\cos\theta), \tag{2.3}$$

where k is the wavenumber, $\beta = ka$, and $h^{(1)}$ and $h^{(2)}$ are spherical Hankel functions. $S_l^{(0)}(\beta)$ is the unperturbed scattering matrix determined by the unperturbed boundary condition $\psi^{(0)}(a,\theta) = 0$ yielding

$$S_l^{(0)}(\beta) = -h_l^{(2)}(\beta)/h_l^{(1)}(\beta). \tag{2.4}$$

Since $\psi^{(0)}$ is a solution of the wave equation and ψ is a solution for arbitary values of δ, $\psi^{(n)}$ must be a solution for $n \geqslant 1$. ψ must also meet the perturbed boundary condition, that is

$$\psi(r_p,\theta) = 0 \quad \text{for } 0 \leqslant \theta < \pi. \tag{2.5}$$

Expanding (2.5) to first order in δ gives

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$$\psi^{(0)}(a) + \delta a\omega(\theta)\frac{\partial\psi^{(0)}}{\partial r}\bigg|_{r=a} + \delta\psi^{(1)}(a) = 0. \tag{2.6}$$

But $\psi^{(0)}(a) = 0$ because $\psi^{(0)}$ satisfies the unperturbed boundary condition, so (2.6) becomes

$$\psi^{(1)}(a) = -a\omega(\theta)\frac{\partial\psi^{(0)}}{\partial r}\bigg|_{a}. \tag{2.7}$$

There is also a boundary condition on ψ as $r\to\infty$. This condition forces $\psi^{(1)}$to be a purely outgoing wave. Combining this with the fact that $\psi^{(1)}$ is a solution of the wave equation implies

$$\psi^{(1)}(r) = \sum_{l=0}^{\infty}\frac{(2l+1)}{2}i^l S_l^{(1)}(\beta)h_l^{(1)}(kr)P_l(\cos\theta), \tag{2.8}$$

where the $S_l^{(1)}(\beta)$ are coefficients that are left to be determined. Combining (2.7) and (2.8), and utilizing the orthogonality of the Legendre functions, yields

$$\begin{aligned} S_l^{(1)}(\beta) &= -\frac{a}{i^l h_l^{(1)}(\beta)}\int_{-1}^{1}\frac{\partial\psi^{(0)}}{\partial r}\bigg|_{a}\omega(\theta)P_l(\cos\theta)d\cos\theta \\ &= \frac{2i}{\beta}\frac{1}{h_l^{(1)}(\beta)}\sum_{n=0}^{\infty}\frac{(2n+1)}{2}i^{(n-l)}\frac{\omega_{ln}}{h_n^{(1)}(\beta)}, \end{aligned} \tag{2.9}$$

where

$$\omega_{ln} = \int_{-1}^{1}P_l(\cos\theta)\omega(\theta)P_n(\cos\theta)d\cos\theta. \tag{2.10}$$

The Wronskian relation,

$$W\{h_n^{(1)}(\beta), h_n^{(2)}(\beta)\} = 2/i\beta^2, \tag{2.11}$$

has been used in deriving (2.9). Finally $\omega(r)$ to first order in δ is

$$\begin{aligned} \psi(r) \cong \sum_{l=0}^{\infty}\frac{(2l+1)}{2}i^l\,&[h_l^{(2)}(kr) \\ &+ (S_l^{(0)}(\beta) + \delta S_l^{(1)}(\beta))h_l^{(1)}(kr)]P_l(\cos\theta). \end{aligned} \tag{2.12}$$

Let $f(\theta)$ be the scattering amplitude. This quantity can be extracted from $\psi(r)$ in the usual way to get

$$f(\theta) \cong f^{(0)}(\theta) + \delta f^{(1)}(\theta). \tag{2.13}$$

$$f^{(0)}(\theta) = \sum_{l=0}^{\infty}\frac{(2l+1)}{2ik}[S_l^{(0)}(\beta) - 1]P_l(\cos\theta), \tag{2.14}$$

$$f^{(1)}(\theta) = \sum_{l=0}^{\infty}\frac{(2l+1)}{2ik}S_l^{(1)}(\beta)P_l(\cos\theta). \tag{2.15}$$

Nussenzveig applied his modified Watson transformation to $f^{(0)}(\theta)$. I will now analyze $f^{(1)}(\theta)$ using the same method.

3. NECESSARY CONDITIONS FOR APPLICATION OF THE MODIFIED WATSON TRANSFORMATION

Equation (2.9) may be used to compute $S_l^{(1)}(\beta)$ only for integer values of l. Before the modified Watson transformation can be applied to $f^{(1)}(\theta)$ a continuation, to complex l, of $S_l^{(1)}(\beta)$ must be chosen. This continuation must satisfy three conditions. First, $(2l+1)S_l^{(1)}(\beta)$ can have no poles on the real l-axis so that Poisson's sum formula can be utilized. Second, $S_l^{(1)}(\beta)$ should have a simple reflection property as l goes to $-l-1$. Third, $S_l^{(1)}(\beta)$ should have the proper asymptotic behavior in the complex l plane so certain integrals can be reduced to sums over residues. I will now define a continuation of $S_l^{(1)}(\beta)$ and show that it satisfies each of these conditions.

A. The continuation of $S_l^{(1)}(\beta)$

Before continuing $S_l^{(1)}(\beta)$ into the complex l plane a specific function must be chosen for $\omega(\theta)$. In order that ω_{ln} be a simple function of l the obvious choice for $\omega(\theta)$ is a Legendre function,

$$\omega(\theta) = P_m(\cos\theta). \tag{3.1}$$

An arbitrary $\omega(\theta)$ can then be represented by a linear combination of Legendre functions. With the choice (3.1), (2.10) can be easily evaluated in terms of Clebsch–Gordan coefficients to get

$$\omega_{ln} = \frac{2}{(2m+1)}|\langle ln00|lnm0\rangle|^2, \tag{3.2}$$

where $\langle ln00|lnm0\rangle$ is a Clebsch–Gordan coefficient. Substituting this in (2.9), using the selection rules for Clebsch-Gordan coefficients, and shifting the sum to make it symmetric around zero yields

$$\begin{aligned} &S_l^{(1)}(\beta) \\ &= \frac{4i}{(2m+1)}\frac{1}{\beta}\frac{1}{h_l^{(1)}(\beta)}{\sum_{n=-m}^{m}}'\left(\frac{2l+2n+1}{2}\right)i^n\frac{1}{h_{l+n}^{(1)}(\beta)} \\ &\quad\times|\langle l+nl00|l+nlm0\rangle|^2. \end{aligned} \tag{3.3}$$

The notation

$${\sum_{n=-m}^{m}}'$$

means summation over $n = -m, -m+2, -m+4,\ldots, m-2, m$. I now continue $S_l^{(1)}(\beta)$ into the complex l plane by using the same continuation of the spherical Hankel functions as Nussenzveig did in Ref. 1. I also choose the following continuation for the Clebsch–Gordan coefficient[4]:

$$\begin{aligned} &|\langle l+nl00|l+nlm0\rangle|^2 \\ &= \left(\frac{2m+1}{2\pi}\right)\frac{\Gamma\left(\frac{m-n+1}{2}\right)}{\Gamma\left(\frac{m-n+2}{2}\right)}\frac{\Gamma\left(\frac{m+n+1}{2}\right)}{\Gamma\left(\frac{m+n+2}{2}\right)} \\ &\quad\times\frac{\Gamma\left(\frac{2l+n-m+1}{2}\right)}{\Gamma\left(\frac{2l+n-m+2}{2}\right)}\frac{\Gamma\left(\frac{2l+n+m+2}{2}\right)}{\Gamma\left(\frac{2l+n+m+3}{2}\right)} \end{aligned} \tag{3.4}$$

This function has simple poles at

$$l = \frac{-(n+m+1)}{2}, \frac{-(n+m-1)}{2},\ldots, \frac{-(n-m+1)}{2}, \tag{3.5}$$

so it seems that my continuation of $S_l^{(1)}(\beta)$ has poles on the real l axis. This is not the case, however, as will be shown in the next section.

B. No poles on the real l axis

Since $h_l^{(1)}(\beta)$ has no zeroes for real l, Eq. (3.3) implies that any poles on the real l axis must come from the Clebsch–Gordan coefficient. I will now show that the continuation

given in Eq. (3.4) contributes no real poles to $S_l^{(1)}(\beta)$. It will be simpler to work in the complex λ plane, where

$$\lambda = l + \tfrac{1}{2}. \tag{3.6}$$

Then what must be proven is that

$$\text{residue}\,\{\lambda S^{(1)}(\lambda,\beta)\}_{\lambda=p} = 0, \tag{3.7}$$

where

$$\begin{aligned} S^{(1)}(\lambda,\beta) &= S^{(1)}_{\lambda-1/2}(\beta) \\ &= \frac{8i}{\pi^2}\frac{1}{H^{(1)}_{\lambda}(\beta)}\sum_{n=-m}^{m}{}' (\lambda+n) i^n \frac{1}{H^{(1)}_{\lambda+n}(\beta)} \\ &\quad\times \frac{\Gamma\left(\frac{m-n+1}{2}\right)}{\Gamma\left(\frac{m-n+2}{2}\right)}\frac{\Gamma\left(\frac{m+n+1}{2}\right)}{\Gamma\left(\frac{m+n+2}{2}\right)} \\ &\quad\times \frac{\Gamma\left(\frac{2\lambda+n-m}{2}\right)}{\Gamma\left(\frac{2\lambda+n-m+1}{2}\right)}\frac{\Gamma\left(\frac{2\lambda+n+m+1}{2}\right)}{\Gamma\left(\frac{2\lambda+n+m+2}{2}\right)}, \end{aligned} \tag{3.8}$$

and

$$p = -m, -m+1, \ldots, m-1, m. \tag{3.9}$$

I have used in (3.8),

$$h_l^{(1)}(\beta) = \left(\frac{\pi}{2\beta}\right)^{1/2} H^{(1)}_{l+1/2}(\beta). \tag{3.10}$$

All the real poles of $\lambda S^{(1)}(\lambda,\beta)$ are contained in the $\Gamma((2\lambda + n - m)/2)$ term of (3.8). First consider the residues of the poles at $p \geqslant 0$. The fact that

$$\begin{aligned} &\text{residue}\left\{\Gamma\left(\frac{2\lambda+n-m}{2}\right)\right\}_{\lambda=p} \\ &= \begin{cases} 0 & \text{for } n > m-2p \\ \dfrac{(-1)^{(m-n-2p)/2}}{\Gamma\left(\dfrac{m-n-2p+2}{2}\right)} & \text{for } n \leqslant m-2p \end{cases} \end{aligned} \tag{3.11}$$

implies

$$\begin{aligned} &\text{residue}\,\{\lambda S^{(1)}(\lambda,\beta)\}_{\lambda=p} \\ &= \frac{8i}{\pi^2}\frac{p}{H^{(1)}_p(\beta)}\sum_{n=-m+p}^{m-p}{}' n i^{(m-2p)}\frac{1}{H^{(1)}_n(\beta)} \\ &\quad\times \frac{\Gamma\left(\frac{p+m+1+n}{2}\right)}{\Gamma\left(\frac{p+m+2+n}{2}\right)}\frac{\Gamma\left(\frac{p+m+1-n}{2}\right)}{\Gamma\left(\frac{p+m+2-n}{2}\right)} \\ &\quad\times \frac{1}{\Gamma\left(\frac{m-p+2+n}{2}\right)}\frac{1}{\Gamma\left(\frac{m-p+2-n}{2}\right)} \\ &\quad\times \left(\frac{n+p-m+1}{2}\right)\left(\frac{n+p-m+3}{2}\right)\cdots \\ &\quad\times \left(\frac{n+m-p-3}{2}\right)\left(\frac{n+m-p-1}{2}\right). \end{aligned} \tag{3.12}$$

In deriving (3.12) the summation has again been shifted to make it symmetric around zero. Using the facts that the sum is only over $n + m + p$ even and that

$$H^{(1)}_{\lambda}(\beta) = e^{-i\pi\lambda} H^{(1)}_{-\lambda}(\beta), \tag{3.13}$$

it is easy to see that the summand of (3.12) is an odd function of n. Therefore that sum is zero and (3.7) is true. The same proof can be used to show that the residues equal zero for $p \leqslant 0$. So $\lambda S^{(1)}(\lambda,\beta)$ has no poles on the real λ axis.

C. Reflection property for $S^{(1)}(\lambda,\beta)$

I will now show that the behavior of $S^{(1)}(\lambda,\beta)$ under reflection is

$$S^{(1)}(-\lambda,\beta) = e^{-2i\pi\lambda} S^{(1)}(\lambda,\beta). \tag{3.14}$$

Using Eqs. (3.8) and (3.13), and changing the summation variable from n to $-n$ gives

$$\begin{aligned} S^{(1)}(-\lambda,\beta) = {} & -\frac{8i}{\pi^2}\frac{e^{-2i\pi\lambda}}{H^{(1)}_{\lambda}(\beta)}\sum_{n=-m}^{m}{}' (\lambda+n) i^{-n}\frac{e^{-i\pi n}}{H^{(1)}_{\lambda+n}(\beta)}\frac{\Gamma\left(\frac{m-n+1}{2}\right)\Gamma\left(\frac{m+n+1}{2}\right)}{\Gamma\left(\frac{m-n+2}{2}\right)\Gamma\left(\frac{m+n+2}{2}\right)} \\ & \times \frac{\left(-\frac{2\lambda-n+m-1}{2}\right)\left(\frac{-2\lambda-n+m-3}{2}\right)\cdots\left(\frac{-2\lambda-n-m+1}{2}\right)}{\left(\frac{-2\lambda-n+m}{2}\right)\left(\frac{-2\lambda-n+m-2}{2}\right)\cdots\left(\frac{-2\lambda-n-m}{2}\right)} \end{aligned} \tag{3.15}$$

$$= \frac{8i}{\pi^2}\frac{e^{-2i\pi\lambda}}{H_\lambda^{(1)}(\beta)}\sum_{n=-m}^{m}{}' (\lambda+n)i^n \frac{1}{H_{\lambda+n}^{(1)}(\beta)} \frac{\Gamma\left(\frac{m-n+1}{2}\right)\Gamma\left(\frac{m+n+1}{2}\right)}{\Gamma\left(\frac{m-n+2}{2}\right)\Gamma\left(\frac{m+n+2}{2}\right)}$$

$$\times \frac{\Gamma\left(\frac{2\lambda+n-m}{2}\right)\Gamma\left(\frac{2\lambda+n+m+1}{2}\right)}{\Gamma\left(\frac{2\lambda+n-m+1}{2}\right)\Gamma\left(\frac{2\lambda+n+m+2}{2}\right)} \tag{3.16}$$

$$= e^{-2i\pi\lambda} S^{(1)}(\lambda,\beta). \tag{3.17}$$

So (3.14) is true.

D. Behavior $S^{(1)}(\lambda,\beta)$ as $|\lambda|\to\infty$.

Appendix A contains the asympototic behavior of $H_\lambda^{(1)}(\beta)$ in the complex λ plane. These formulas will now be used to get the behavior of $S^{(1)}(\lambda,\beta)$ as $|\lambda|\to\infty$.

Using the fact that

$$\lim_{|\lambda|\to\infty} (\lambda+n)\frac{\Gamma\left(\frac{2\lambda+n-m}{2}\right)}{\Gamma\left(\frac{2\lambda+n-m+1}{2}\right)}\frac{\Gamma\left(\frac{2\lambda+n+m+1}{2}\right)}{\Gamma\left(\frac{2\lambda+n+m+2}{2}\right)} = 1, \tag{3.18}$$

and Eq. (3.8) gives the following asymptotic behavior $S^{(1)}(\lambda,\beta)$:

$$S^{(1)}(\lambda,\beta) \to \frac{8i}{\pi^2}\sum_{n=-m}^{m}{}' i^n \frac{\Gamma\left(\frac{m-n+1}{2}\right)}{\Gamma\left(\frac{m-n+2}{2}\right)}\frac{\Gamma\left(\frac{m+n+1}{2}\right)}{\Gamma\left(\frac{m+n+2}{2}\right)} \times \frac{1}{H_\lambda^{(1)}(\beta)}\frac{1}{H_{\lambda+n}^{(1)}(\beta)}. \tag{3.19}$$

The asymptotic behavior of

$$\frac{1}{H_\lambda^{(1)}(\beta)}\frac{1}{H_{\lambda+n}^{(1)}(\beta)}$$

can be obtained from Appendix A and is displayed in Fig. 1.

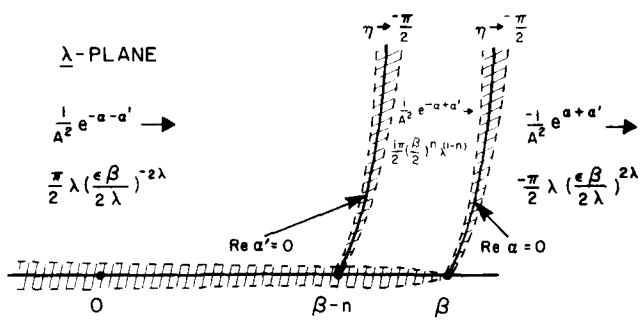

FIG. 1. Asympotic behavior of $[H_\lambda^{(1)}(\beta)H_{\lambda+n}^{(1)}(\beta)]^{-1}$ for $n\geq 0$. The notation is as in Appendix A. A similar figure will hold for $n<0$.

In the following sections it will be seen that this behavior for $S^{(1)}(\lambda,\beta)$ is sufficient to allow application of the modified Watson transformation.

4. SOLUTION FOR BACKSCATTERING BY A SLIGHTLY DILATED SPHERE

To obtain $f^{(1)}(\pi)$ for a slightly dilated sphere $\omega(\theta)$ must be

$$\omega(\theta) = P_0(\cos\theta) = 1, \tag{4.1}$$

giving

$$r_p = a(1+\delta). \tag{4.2}$$

This choice implies $n=0$ in (3.3) so that

$$S_l^{(1)}(\beta) = \frac{2i}{\beta}[h_l^{(1)}(\beta)]^{-2}. \tag{4.3}$$

Evaluation of Eq. (2.15) using the modified Watson transformation is very similar to the procedure used by Nussenzveig in Sec. IX.D of Ref. 1. First the Watson transformation,

$$\sum_{l=0}^{\infty} g(l+\tfrac{1}{2}) = \frac{1}{2}\int_C g(\lambda)e^{-i\pi\lambda}\frac{d\lambda}{\cos\pi\lambda}, \tag{4.4}$$

is applied to Eq. (2.15). The contour C is displayed in Fig. 2. This gives

$$f^{(1)}(\pi) = -\frac{1}{2k}\int_C S^{(1)}(\lambda,\beta)\frac{\lambda d\lambda}{\cos\pi\lambda}, \tag{4.5}$$

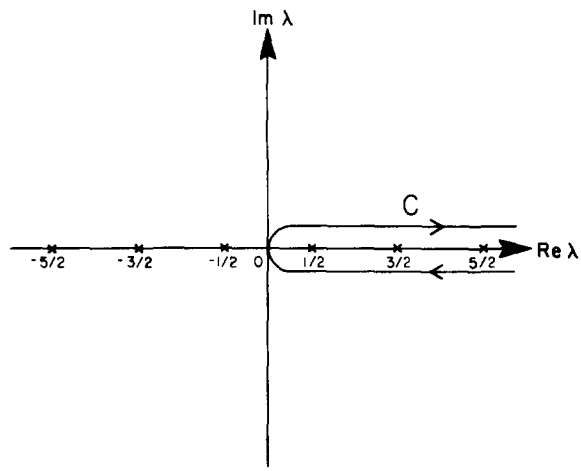

FIG. 2. Contour of integration C.

where $P_l(\cos\pi)$ has been continued to complex l using $P_l(-1)\equiv e^{i\pi(\lambda-1/2)}$. In Eq. (4.5)

$$S^{(1)}(\lambda,\beta)=\frac{4i}{\pi}\left[H_\lambda^{(1)}(\beta)\right]^{-2}. \tag{4.6}$$

By changing λ to $-\lambda$ in the integral over the lower half of C and using Eq. (3.14), Eq. (4.5) becomes

$$f^{(1)}(\pi)=\frac{1}{2k}\int_{C'}S^{(1)}(\lambda,\beta)e^{-2i\pi\lambda}\frac{\lambda d\lambda}{\cos\pi\lambda} - \frac{1}{2k}\int_{C''}S^{(1)}(\lambda,\beta)\frac{\lambda d\lambda}{\cos\pi\lambda}, \tag{4.7}$$

where the contour C'' is the upper half of C and the contour C' is displayed in Fig. 3. Using the fact that

$$e^{-2i\pi\lambda}=-2ie^{-i\pi\lambda}\sin(\pi\lambda)+1, \tag{4.8}$$

Eq. (4.7) can be rewritten

$$f^{(1)}(\pi)=f_s^{(1)}(\pi)+f_{\rm res}^{(1)}(\pi), \tag{4.9}$$

$$f^{(1)}(\pi)=-\frac{i}{k}\int_{C'}S^{(1)}(\lambda,\beta)e^{-i\pi\lambda}\tan(\pi\lambda)\lambda d\lambda, \tag{4.10}$$

$$f_{\rm res}^{(1)}(\pi)=-\frac{1}{2k}\int_{-\infty+i\alpha}^{\infty+i\alpha}S^{(1)}(\lambda,\beta)\frac{\lambda d\lambda}{\cos\pi\lambda}, \tag{4.11}$$

where $\alpha>0$. The integrand of Eq. (4.11) can be simplified by utilizing

$$\frac{1}{\cos\pi\lambda}=2\sum_{m=0}^{\infty}(-1)^m\exp[i(2m+1)\pi\lambda], \tag{4.12}$$

to get

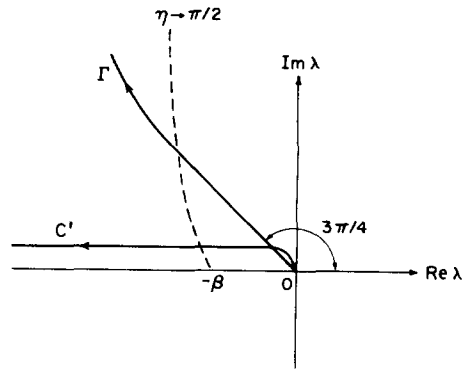

FIG. 3. Contours of integration C' and Γ. The notation for the curve $\eta\to\pi/2$ is in Appendix A.

$$f_{\rm res}^{(1)}(\pi)=-\frac{1}{k}\sum_{m=0}^{\infty}(-1)^m\times\int_{-\infty}^{\infty}S^{(1)}(\lambda,\beta)e^{i(2m+1)\pi\lambda}\lambda d\lambda. \tag{4.13}$$

The saddle point method can now be used to evaluate $f_s^{(1)}(\pi)$. The integrand of (4.10) goes to zero at least exponentially as $|\lambda|\to\infty$ in the upper half-plane to the left of the curve $\eta\to\pi/2$ in Fig. 3, thus the contour C' can be shifted to the contour Γ. The main contribution to the integral is from the region $|\lambda|\lesssim\beta^{1/2}$. Expanding $e^{-i\pi\lambda}S^{(1)}(\lambda,\beta)$ to order $1/\beta$ in this region using (A9) yields

$$e^{-i\pi\lambda}S^{(1)}(\lambda,\beta)=-2\beta e^{-2i\beta}e^{-i\lambda^2/\beta}\times\left[1+\frac{i}{4\beta}-\frac{\lambda^2}{2\beta^2}-\frac{i\lambda^4}{12\beta^3}+O(\beta^{-2})\right] \quad \text{for } |\lambda|\lesssim\beta^{1/2}. \tag{4.14}$$

This gives

$$f_s^{(1)}(\pi)=2iae^{-2i\beta}\int_\Gamma e^{-i\lambda^2/\beta}\left[1+\frac{i}{4\beta}-\frac{\lambda^2}{2\beta^2}-\frac{i\lambda^4}{12\beta^3}+O(\beta^{-2})\right]\tan(\pi\lambda)\lambda d\lambda \tag{4.15}$$

$$=2\beta ae^{-2i\beta}\int_0^\infty e^{-x^2}\left[1+\frac{i}{4\beta}+\frac{ix^2}{2\beta}+\frac{ix^4}{12\beta}+O(\beta^{-2})\right]\tan(\pi\alpha x)x dx \tag{4.16}$$

where

$$\lambda=e^{3i\pi/4}\beta^{1/2}x=\alpha x. \tag{4.17}$$

This integral can be evaluated by the method set forth in Appendix B to yield

$$f_s^{(1)}(\pi)=i\beta ae^{-2i\beta}[1+i/\beta+O(\beta^{-2})]. \tag{4.18}$$

The residue method can be used to evaluate $f_{\rm res}^{(1)}(\pi)$ if a series of paths C_n, shown in Fig. 4, can be found such that

$$\lim_{n\to\infty}\int_{C_n}S^{(1)}(\lambda,\beta)e^{i(2m+1)\pi\lambda}\lambda d\lambda=0. \tag{4.19}$$

The contours C_n must avoid the poles of $S^{(1)}(\lambda,\beta)$ located along the curve h_1. I choose C_n to be of radius R_n passing halfway between consecutive poles λ_n of $S^{(1)}(\lambda,\beta)$, then

$$R_n\ln\left(\frac{2R_n}{e\beta}\right)=n\pi+\frac{\pi}{4} \quad \text{for } |\lambda_n|\gg\beta^2. \tag{4.20}$$

It can be seen from Fig. 4 that the integrand of (4.19) goes to zero at least exponentially as $|\lambda|\to\infty$ in the upper half-plane, except possibly near the curve h_1. Near h_1 $S^{(1)}(\lambda,\beta)$ takes the form

$$S^{(1)}(\lambda,\beta)=\frac{\pi}{2}\left[\sinh\left(\lambda\ln\left(\frac{e\beta}{2\lambda}\right)-i\frac{\pi}{4}\right)\right]^{-2}\lambda^2. \tag{4.21}$$

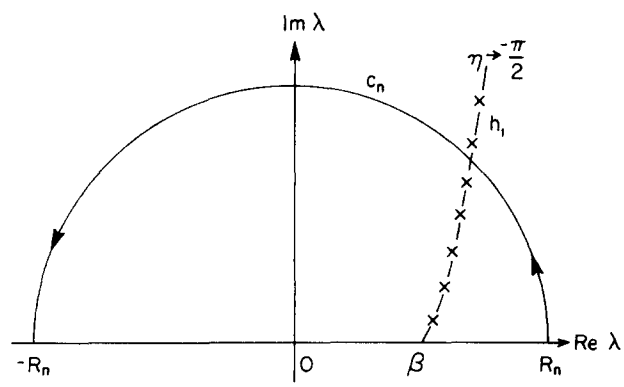

FIG. 4. Contour of integration C_n. The x's are the poles of $S^{(1)}(\lambda,\beta)$ for the dilated sphere.

On C_n, and h_1, $\lambda = R_n \exp[i(\pi/2 - \epsilon)]$, so the absolute value of (4.21) becomes

$$|S^{(1)}(\lambda,\beta)e^{i(2m+1)\pi\lambda}\lambda| = \frac{\pi}{2} e^{-(2m+1)\pi R_n} R_n^{\frac{2}{n}} \left|\sinh\left[R_n \epsilon \ln\left(\frac{2R_n}{e\beta}\right) - \frac{\pi}{2}R_n + i\left(n\pi + \frac{\pi}{2}\right)\right]\right|^{-2}, \tag{4.22}$$

where (4.20) has been used. Using the fact that

$$|\sinh(a+ib)| = (\sinh^2 a \cos^2 b + \cosh^2 a \sin^2 b)^{1/2} \geqslant \cosh a |\sin b| \tag{4.23}$$

and Eq. (4.22) gives

$$|S^{(1)}(\lambda,\beta)e^{i(2m+1)\pi\lambda}\lambda| \leqslant \pi e^{-(2m+1)\pi R_n} R_n^{\frac{2}{n}} \left[\cosh\left(R_n \epsilon \ln\left(\frac{2R_n}{e\beta}\right) - \frac{\pi}{2}R_n\right)\right]^{-2}. \tag{4.24}$$

So the integrand of Eq. (4.19) goes to zero at least exponentially along C_n as $n \to \infty$. Thus (4.19) is true, and (4.13) is reduced to the residue series,

$$f_{\text{res}}^{(1)}(\pi) = -\frac{2\pi i}{k} \sum_{m=0}^{\infty} (-1)^m \sum_n \text{residue}[S^{(1)}(\lambda,\beta)e^{i(2m+1)\pi\lambda}\lambda]_{\lambda=\lambda_n}, \tag{4.25}$$

where λ_n are the poles of $S^{(1)}(\lambda,\beta)$. These poles are of the second order. If only the highest order in β is kept and λ_n is near β then using (A10)

$$\text{residue}[S^{(1)}(\lambda,\beta)\lambda e^{i(2m+1)\pi\lambda}]_{\lambda_n}$$

$$= \frac{e^{i\pi/3}(2m+1)\beta^2}{2\gamma[Ai'(-x_n)]^2} e^{i(2m+1)\pi\lambda_n} + \text{lower order}, \tag{4.26}$$

where

$$\gamma = (2/\beta)^{1/3}, \tag{4.27}$$

Ai(x) is the Airy function, and $-x_n$ is its n^{th} zero. Only the poles λ_n near β will contribute significantly to (4.25) because of the $e^{i(2m+1)\pi\lambda_n}$ term in (4.26). So combining (4.25) and (4.26) gives

$$f_{\text{res}}^{(1)}(\pi) = -e^{i\pi/3}\frac{a}{\gamma} \sum_{m=0}^{\infty} (-1)^m \sum_n \{i\pi(2m+1) \times \beta [\text{Ai}'(-x_n)]^{-2} e^{i(2m+1)\pi\lambda_n} + \text{lower order}\}. \tag{4.28}$$

Finally, combining (4.9), (4.18), and (4.28) gives

$$f^{(1)}(\pi) = i\beta a e^{-2i\beta}\left[1 + \frac{i}{\beta} + O(\beta^{-2})\right] - e^{i\pi/3}\frac{a}{\gamma} \sum_{m=0}^{\infty} (-1)^m \times \sum_n \{i\pi(2m+1)\beta [\text{Ai}'(-x_n)]^{-2} \times e^{i(2m+1)\pi\lambda_n} + \text{lower order}\}. \tag{4.29}$$

The unperturbed solution $f^{(0)}(\pi)$ can be obtained from Eq. (9.54) of Ref. 1 and is

$$f^{(0)}(\pi) = -\frac{a}{2} e^{-2i\beta}\left(1 + \frac{i}{2\beta}\right) - e^{i\pi/3}\frac{a}{\gamma} \sum_{m=0}^{\infty} (-1)^m \times \sum_n [\text{Ai}'(-x_n)]^{-2} e^{i(2m+1)\pi\lambda_n}. \tag{4.30}$$

Of course (4.30) could have been used to find the solution for the dilated sphere by letting a go to $a(1+\delta)$ and β go to $\beta(1+\delta)$. Then

$$f(\pi) = -\frac{a(1+\delta)}{2} e^{-2i\beta(1+\delta)}\left[1 + \frac{i}{2\beta(1+\delta)} + O(\beta^{-2})\right] - e^{i\pi/3}\frac{a}{\gamma}(1+\delta)^{4/3} \sum_{m=0}^{\infty} (-1)^m \sum_n \{[\text{Ai}'(-x_n)]^{-2} \times e^{i(2m+1)\pi\lambda_n'} + \text{lower order}\}, \tag{4.31}$$

where λ_n' are the poles of $1/H_\lambda^{(1)}(\beta(1+\delta))$. Equation (A11) implies

$$\lambda_n' = \lambda_n + \beta\delta + \text{lower order}. \tag{4.32}$$

Expanding (4.31) to first order in δ gives

$$f(\pi) = f^{(0)}(\pi) + \delta\left[i\beta a e^{-2i\beta}(1 + i/\beta + O(\beta^{-2})) - e^{i\pi/3}\frac{a}{\gamma} \sum_{m=0}^{\infty} (-1)^m \sum_n \{i\pi(2m+1)\beta [\text{Ai}'(-x_n)]^{-2} \times e^{i(2m+1)\pi\lambda_n} + \text{lower order}\}\right] = f^{(0)}(\pi) + \delta f^{(1)}(\pi). \tag{4.33}$$

This is the same answer as obtained by combining boundary perturbation theory and the modified Watson transformation. This proves the validity of the combination of these methods at least for the case of the dilated sphere.

5. SOLUTION FOR BACKSCATTERING BY A P_2 CONDUCTING PARTICLE

In this section I will consider the scattering by a particle with its surface defined by

$$r_p = a[1 + \delta P_2(\cos\theta)]. \tag{5.1}$$

This choice of $\omega(\theta)$ implies $m = 2$ in (3.8), which gives

$$S^{(1)}(\lambda,\beta) = -\frac{i}{2\pi}\frac{1}{H_\lambda^{(1)}(\beta)}\left[\frac{3}{H_{\lambda-2}^{(1)}(\beta)}\frac{(\lambda-\frac{3}{2})(\lambda-\frac{1}{2})}{(\lambda-1)(\lambda)} - \frac{2}{H_\lambda^{(1)}(\beta)}\frac{(\lambda^2-\frac{1}{4})}{(\lambda^2-1)} + \frac{3}{H_{\lambda+2}^{(1)}(\beta)}\frac{(\lambda+\frac{1}{2})(\lambda+\frac{3}{2})}{(\lambda)(\lambda+1)}\right]. \tag{5.2}$$

Evaluation of $f^{(1)}(\pi)$ for this case proceeds almost the same as for the dilated sphere. Equations (4.9)–(4.13) are still valid for the P_2 particle since they were derived using only the general properties of $S^{(1)}(\lambda,\beta)$ discussed in Sec. 3.

Evaluation of $f_s^{(1)}(\pi)$ is about the same as in Sec. 4 except that now instead of Eq. (4.21) the following is used:

$$e^{-i\pi\lambda}S^{(1)}(\lambda,\beta) = 2\beta e^{-2i\beta}e^{-i\lambda^2/\beta} \times\left[1 - \frac{11i}{4\beta} - \frac{2\lambda^2}{\beta^2} - \frac{i\lambda^4}{12\beta^3} + O(\beta^{-2})\right]. \tag{5.3}$$

The integral in (4.19) can be evaluated using the same method as Eq. (4.22)–(4.25) to get

$$\begin{aligned} f_s^{(1)}(\pi) &= -2a\beta e^{-2i\beta}\int_0^\infty e^{-x^2}\left[1 - \frac{11i}{4\beta} + \frac{2ix^2}{\beta} + \frac{ix^4}{12\beta} + O(\beta^{-2})\right]\tan(\pi\alpha x)x\,dx \\ &= -ia\beta e^{-2i\beta}[1 - i/2\beta + O(\beta^{-2})]. \end{aligned} \tag{5.4}$$

The residue method can be used to evaluate $f_{\text{res}}^{(1)}(\pi)$ just as in Sec. 4. The paths C_n that ensure that (4.19) is true are shown in Fig. 5, so $f_{\text{res}}^{(1)}(\pi)$ is reduced to the residue series

$$f_{\text{res}}^{(1)}(\pi) = \frac{-2\pi i}{k}\sum_{m=0}^{\infty}(-1)^m\sum_n \text{residues}\,[S^{(1)}(\lambda,\beta)e^{i(2m+1)\pi\lambda}]_{\lambda_n,\lambda_n\pm 2}. \tag{5.5}$$

If only the results to highest order in β are retained in the residue series, then the only poles that contribute to (5.5) are the second order poles at λ_n. The result is

$$\begin{aligned} &\text{residue}\left[\frac{i}{\pi}[H_\lambda^{(1)}(\beta)]^{-2}\frac{(\lambda^2-\frac{1}{4})}{(\lambda^2-1)}\lambda e^{i(2m+1)\pi\lambda}\right]_{\lambda_n} \\ &= e^{i\pi/3}\frac{\beta^2(2m+1)}{8\gamma}[\text{Ai}'(-x_n)]^{-2}e^{i(2m+1)\pi\lambda_n} \\ &\quad + \text{lower order}. \end{aligned} \tag{5.6}$$

So finally,

$$\begin{aligned} f_{\text{res}}^{(1)}(\pi) = &-e^{i\pi/3}\frac{a}{4\gamma}\sum_{m=0}^{\infty}(-1)^m\sum_n\{i\pi(2m+1) \\ &\times\beta\,\text{Ai}'(-x_n)]^{-2}e^{i(2m+1)\pi\lambda_n} + \text{lower order}\}. \end{aligned} \tag{5.7}$$

This gives

$$\begin{aligned} f^{(1)}(\pi) &= -ia\beta e^{-2i\beta}[1 - i/2\beta + O(\beta^{-2})] - e^{i\pi/3}\frac{a}{4\gamma}\sum_{m=0}^{\infty}(-1)^m \\ &\quad\times\sum_n\{i\pi(2m+1)\beta\,[\text{Ai}'(-x_n)]^{-2}e^{i(2m+1)\pi\lambda_n} \\ &\quad + \text{lower order}\}. \end{aligned} \tag{5.8}$$

6. CONCLUSION

I have shown, in this paper, that it is possible to extend the modified Watson transformation method of Nussenzveig to slightly nonspherical impenetrable particles. This was accomplished by combining the modified Watson transformation with boundary perturbation theory. The method was applied to the cases of backscattering by a dilated sphere and a sphere perturbed by adding $P_2(\cos\theta)$. The results for the dilated sphere were found to be consistent with the exact result.

The examples in this paper can be easily extended to the entire angular domain of θ by using the same methods as in Ref. 1. Higher order solutions in δ can be obtained by using methods similar to those presented here. It should also be possible to treat particles without an axis of symmetry by letting $\omega(\theta)$ be a function of ϕ and substituting spherical harmonics for the Legendre functions in (2.12).

In a future paper I will discuss the problem of a slightly nonspherical transparent particle. The groundwork for the transparent problem is contained in this paper and in Ref. 2.

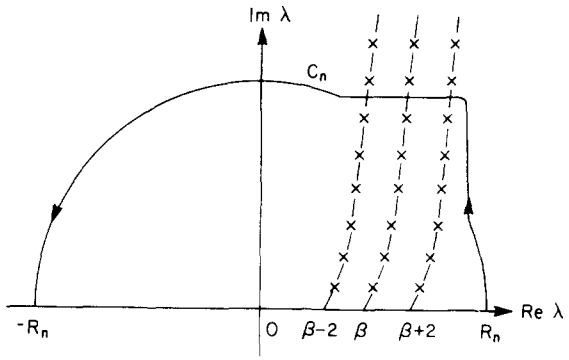

FIG. 5. Contour of integration C_n. The x's are the poles of $S^{(1)}(\lambda,\beta)$ for the sphere perturbed by $P_2(\cos\theta)$.

ACKNOWLEDGMENTS

I would like to thank B. Durand, L. Durand, and J. Weinman for bringing this problem to my attention and for many helpful conversations.

This research was supported in part by the University of Wisconsin Research Committee with funds granted by the Wisconsin Alumni Research Foundation, and in part by the Department of Energy under Contract No. DOE-ER-00881, COO-881-191, and by the National Oceanic and Atmospheric Administration, NOAA-MO-A-01-78-00-4320.

APPENDIX A. ASYMPTOTIC BEHAVIOR OF $H_\lambda^{(1)}(\beta)$

The asymptotic behavior of the cylindrical function $H_\lambda^{(1)}(\beta)$, $\beta>0$, in the complex λ plane is graphically presented in Fig. 6.[5] The notation is as follows:

$$A(\lambda,\beta) = (2/\pi)^{1/2}(\lambda^2-\beta^2)^{-1/4}, \tag{A1}$$

$$\alpha(\lambda,\beta)^{1/2} = (\lambda^2-\beta^2)^{1/2} - \lambda\ln\left[\frac{\lambda}{\beta} + \frac{(\lambda^2-\beta^2)^{1/2}}{\beta}\right], \tag{A2}$$

where the branch of $(\lambda^2-\beta^2)^{1/2}$ to be taken is specified by

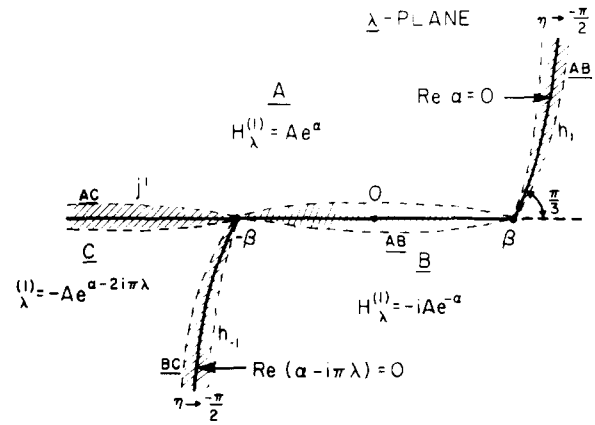

FIG. 6. Asymptotic behavior of $H_\lambda^{(1)}(\beta)$.

the condition

$$(\lambda^2-\beta^2)^{1/2}\to\lambda=|\lambda|\exp(i\phi)\,(-\pi<\phi<\pi)\quad\text{for }|\lambda|\to\infty. \tag{A3}$$

Thus,

$$A\to\left(\frac{2}{\pi\lambda}\right)^{1/2},\quad e^{\alpha}\to\left(\frac{e\beta}{2\lambda}\right)^{\lambda}\quad\text{for }|\lambda|\to\infty. \tag{A4}$$

The asymptotic behavior of $H_\lambda^{(1)}(\beta)$ changes (Stokes' phenomenon) across certain branch lines, shown as thick lines in Fig. 6. For $H_\lambda^{(1)}(\beta)$ the curves are h_1 ($\mathrm{Re}\,\alpha=0$, $\mathrm{Im}\,\lambda>0$) and h_{-1} [$\mathrm{Re}(\alpha-i\pi\lambda)=0$, $\mathrm{Im}\,\lambda<0$]. These curves are symmetrical with respect to the origin and the zeros of $H_\lambda^{(1)}(\beta)$ are asymptotically located on them. The curve h_1 cuts the real axis as $\lambda=\beta$ at an angle of $\pi/3$. The tangent to this curve tends to the vertical direction for $|\lambda|\to\infty$. Asymptotically, the curve approaches $\lambda=\sigma|\lambda|$, $\eta\to-\pi/2$, where σ and η are defined by

$$\sigma=\exp[i(\pi/2+\epsilon)],\quad \eta=\epsilon\ln|2\lambda/e\beta|. \tag{A5}$$

These results have to be modified in the neighborhood of each of the branch lines, when the two representations for the same function become comparable in order of magnitude. Then the functions must be taken to be the sum of the two representations. This is indicated by the shaded regions of Fig. 6. Thus,

$$H_\lambda^{(1)}(\beta)\approx 2Ae^{i\pi/4}\sinh(\alpha-i\pi/4)\quad\text{in } AB, \tag{A6}$$

$$H_\lambda^{(1)}(\beta)\approx -2Ae^{-i\pi\lambda}e^{-i\pi/4}\sinh(\alpha-i\pi\lambda+i\pi/4)\quad\text{in } BC. \tag{A7}$$

The angular widths of the shaded regions are

$$\Delta\epsilon=2C/|\lambda|\ln\left|\frac{2\lambda}{e\beta}\right|, \tag{A8}$$

where C is a constant such that $e^{2C}\gg 1$. The corresponding arc length $|\lambda|\Delta\epsilon$ tends to zero like $(\ln|\lambda|)^{-1}$.

It must be noted that, due to the choice of phase (A3), A goes to $-A$ and the phase of α changes by $2i\pi\lambda$ on crossing the line j' so that, in spite of appearances to the contrary, the representation of $H_\lambda^{(1)}(\beta)$ given in Fig. 6 is continuous across j'.

The asymptotic expansions of Fig. 6 should be employed for $|\lambda|\gg\beta$. For smaller values of $|\lambda|$ additional results are required. In region AB, in the neighborhood of the real axis, the Debye asymptotic expansion may be employed,

$$H_\lambda^{(1)}(\beta)=\left(\frac{2}{\pi}\right)^{1/2}(\beta^2-\lambda^2)^{-1/4}\times\exp\left\{i\left[(\beta^2-\lambda^2)^{1/2}-\lambda\cos^{-1}\frac{\lambda}{\beta}-\frac{\pi}{4}\right]\right\}\times\left[1-\frac{i}{8(\beta^2-\lambda^2)^{1/2}}+\cdots\right], \tag{A9}$$

where $(\beta^2-\lambda^2)^{-1/4}>0$, $0<\cos^{-1}(\lambda/\beta)<\pi/2$ for $-\beta<\lambda<\beta$. These expansions fail in the neighborhood of $\lambda=\pm\beta$. If $|\lambda-\beta|$ becomes comparable with $|\lambda|^{1/3}$ use the expansion

$$H_\lambda^{(1)}(\beta)=2e^{-i\pi/3}\left(\frac{2}{\lambda}\right)^{1/3}\mathrm{Ai}\left[e^{2i\pi/3}\left(\frac{2}{\lambda}\right)^{1/3}(\lambda-\beta)\right]+O(\lambda^{-1}), \tag{A10}$$

where $\mathrm{Ai}(z)$ denotes the Airy function. From (A10) it can be seen that the poles λ_n of $1/H_\lambda^{(1)}(\beta)$ are

$$\lambda_n=\beta+(\beta/2)^{1/3}x_n e^{i\pi/3}+O(\beta^{-1/3}) \tag{A11}$$

when λ_n is near β. In (A11) $-x_n$ is the nth zero of $\mathrm{Ai}(z)$.

APPENDIX B. EVALUATION OF $\int_0^\infty e^{-x^2}\tan(\pi\alpha x)x^n dx$

To evaluate $\int_0^\infty e^{-x^2}\tan(\pi\alpha x)x\,dx$,[5] employ the expansion

$$\tan(\pi\alpha x)=i+2i\sum_{n=1}^{\infty}(-1)^n\exp(2in\pi\alpha x), \tag{B1}$$

which gives

$$\int_0^\infty e^{-x^2}\tan(\pi\alpha x)x\,dx=i\int_0^\infty e^{-x^2}x\,dx+2i\sum_{n=1}^{\infty}(-1)^n\int_0^\infty\exp(-x^2+2in\pi\alpha x)x\,dx. \tag{B2}$$

By partial integration

$$\int_0^\infty\exp(-x^2+2in\pi\alpha x)x\,dx=-\frac{1}{(2n\pi\alpha)^2}+O(\beta^{-2}) \tag{B3}$$

so that, finally,

$$\int_0^\infty e^{-x^2}\tan(\pi\alpha x)x\,dx=\frac{i}{2}+\frac{i}{24\alpha^2}+O(\beta^{-2}), \tag{B4}$$

where the formula

$$\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^2}=\frac{\pi^2}{12} \tag{B5}$$

has been employed.

It is clear from the above calculation that, since terms of order β^{-2} are being neglected, $\tan(\pi\alpha x)$ may be replaced by i in all the remaining integrals of (4.23). Thus the rest of the integrals are simple to compute.

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[2] H. M. Nussenzveig, J. Math. Phys. **10**, 82 (1969); **10**, 125 (1969).
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[4] D. M. Brink and G. R. Satchler, *Angular Momentum* (Oxford University, Oxford, England, 1968), p. 34, Eq. (2.35).
[5] Appendices A and B of this paper have been taken, more or less, directly from Appendices A and F, respectively, of Ref. 1.

Scattering by slightly nonspherical particles in the high frequency limit. II. Transparent particles

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(Received 5 May 1981; accepted for publication 2 September 1981)

The scattering of a scalar plane wave by a slightly nonspherical transparent particle is investigated using a combination of boundary perturbation theory, the Debye expansion, and the modified Watson transformation. Boundary perturbation theory is used to find the perturbed scattering matrix for the problem. The Debye expansion is then substituted into the perturbed S matrix and the modified Watson transformation is used to sum the resulting partial wave expansion in the short wavelength limit. This method is applied to backscattering by a sphere whose shape is perturbed by making the radius a function of θ given by $r_p(\theta) = a[1 + \delta P_2(\cos\theta)]$, where a is the radius of the unperturbed sphere, δ is the perturbation parameter, and P_2 is a Legendre function. This method will be valid when both $(ka)^{1/3} \gg 1$ and $|N-1|^{1/2}(ka)^{1/3} \gg 1$, where k is the wavenumber and N is the index of refraction of the particle.

PACS numbers: 11.20.Dj

I. INTRODUCTION

In a previous paper[1] I investigated the scattering of plane scalar waves by slightly nonspherical impenetrable particles in the high frequency limit, using boundary perturbation theory and the modified Watson transformation developed by Nussenzveig.[2] In this paper I will consider the same problem except that now I will work with transparent instead of impenetrable particles. I will again use a combination of boundary perturbation theory and the modified Watson transformation to get an expansion for the scattering amplitude in the high frequency limit.

The main difference between this analysis and the analysis for the impenetrable particle is that the modified Watson transformation can no longer be applied directly to the perturbed partial wave expansion, because direct application results in a residue series that does not converge. Instead, the perturbed scattering matrix must first be expanded in a form similar to the Debye expansion given in Ref. 3. The modified Watson transformation can then be applied to the resulting partial wave expansion.

This method will be valid when both $(ka)^{1/3} \gg 1$ and $|N-1|^{1/2}(ka)^{1/3} \gg 1$, where k is the wavenumber, a is the radius of the unperturbed sphere, and N is the index of refraction of the particle. In order to simplify the problem I will only consider real N such that $1 < N < \sqrt{2}$, which includes $N = 1.33$, the index of refraction of water. Also, in order to reduce the amount of algebra, I will only treat the example of backscattering by a particle with an axis of symmetry. The direction of the incoming beam will be parallel to this axis of symmetry.

In Sec. 2 the perturbed S matrix is derived using boundary perturbation theory. The Debye expansion for the perturbed S matrix is formulated in Sec. 3. The conditions necessary for the application of the modified Watson transformation are considered in Sec. 4. In Sec. 5 the method is applied to the problem of backscattering by a sphere whose boundary is perturbed by adding a term $\delta a P_2(\cos\theta)$ to the radius, where P_2 is a Legendre function.

Since this paper is mainly an extension of Nussenzveig's work I will try to follow the notation of Refs. 3 and 4 as closely as possible.

II. BOUNDARY PERTURBATION THEORY

I will work out the perturbation series for the transparent particle using the same method as was used in Paper I for the impenetrable particle. The series will be evaluated only to first order in the perturbation parameter, generalization to higher orders being straightforward.

The wavefunction that is the solution for scattering by the unperturbed sphere is given in three parts: the incoming wave

$$\psi_i = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta), \tag{2.1}$$

the transmitted wave inside the sphere,

$$\psi_t^{(0)} = \sum_{l=0}^{\infty} (2l+1) i^l T_l^{(0)}(\beta) j_l(Nkr) P_l(\cos\theta), \tag{2.2}$$

and the scattered wave outside the sphere,

$$\psi_s^{(0)} = \sum_{l=0}^{\infty} \frac{(2l+1)}{2} i^l [S_l^{(0)}(\beta) - 1] h_l^{(1)}(kr) P_l(\cos\theta), \tag{2.3}$$

where the superscript (0) indicates the solution to the unperturbed problem. The notation in the above is as follows:

$$T_l^{(0)}(\beta) = \frac{h_l^{(2)}(\beta)}{2 j_l(\alpha)} \left[\frac{\langle 1\beta\rangle - \langle 2\beta\rangle}{\langle 1\beta\rangle - N\langle\alpha\rangle} \right], \tag{2.4}$$

$$S_l^{(0)}(\beta) = -\frac{h_l^{(2)}(\beta)}{h_l^{(1)}(\beta)} \left[\frac{\langle 2\beta\rangle - N\langle\alpha\rangle}{\langle 1\beta\rangle - N\langle\alpha\rangle} \right], \tag{2.5}$$

$$\langle x\rangle = \frac{1}{j_l(x)} \frac{\partial j_l(x)}{\partial x}, \tag{2.6}$$

$$\langle 1x\rangle = \frac{1}{h_l^{(1)}(x)} \frac{h_l^{(1)}(x)}{\partial x}, \tag{2.7}$$

$$\langle 2x\rangle = \frac{1}{h_l^{(2)}(x)} \frac{h_l^{(2)}(x)}{\partial x}, \tag{2.8}$$

$$\alpha = Nka = N\beta. \tag{2.9}$$

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In the above j_l and $h_l^{(1,2)}$ are spherical Bessel and Hankel functions, respectively.

To solve the perturbed problem I begin by considering the surface defined by $r_p(\theta) = a[1 + \delta\omega(\theta)]$. The wavefunction that is a solution for scattering by this particle can be written as a Taylor series in δ,

$$\psi_s = \psi_s^{(0)} + \delta\psi_s^{(1)} + \cdots \tag{2.10}$$

for the scattered wave outside the particle and

$$\psi_t = \psi_t^{(0)} + \delta\psi_t^{(1)} + \cdots \tag{2.11}$$

for the transmitted wave inside the particle. In order to find the perturbed scattering matrix, $\psi_s^{(1)}$ must be determined in terms of the unperturbed wavefunction. The method used to accomplish this is the same as was used in Sec. 2 of Paper I, except that now the boundary conditions are different. Two of these conditions are that $\psi_s^{(1)}$ be a purely outgoing wave as $r \to \infty$ and that $\psi_t^{(1)}$ be finite at the origin. There are also two boundary conditions at the surface of the particle

$$\psi_i(r_p,\theta) + \psi_s(r_p,\theta) - \psi_t(r_p,\theta) = 0 \quad \text{for } 0 \leqslant \theta < \pi, \tag{2.12}$$

$$\hat{n}_p \cdot \nabla[\psi_i(r,\theta) + \psi_s(r,\theta) - \psi_t(r,\theta)]_{r=r_p} \quad \text{for } 0 \leqslant \theta < \pi. \tag{2.13}$$

The unit vector $\hat{n}_p$ is normal to the surface so using Eq. (2.1) of Paper I

$$\hat{n}_P \cdot \nabla = \frac{\partial}{\partial r} - \frac{\delta}{r}\frac{d\omega(\theta)}{d\theta}\frac{\partial}{\partial\theta} + O(\delta^2). \tag{2.14}$$

By writing out these boundary conditions in terms of partial wave expansions for ψ_i, ψ_s, and ψ_t, utilizing the orthogonality of the Legendre functions, and extracting the scattering amplitude from ψ the following is obtained:

$$f(\theta) = f^{(0)}(\theta) + \delta f^{(1)}(\theta) + \cdots, \tag{2.15}$$

$$f^{(0)}(\theta) = \sum_{l=0}^{\infty} \frac{(2l+1)}{2ik}[S_l^{(0)}(\beta) - 1]P_l(\cos\theta), \tag{2.16}$$

$$f^{(1)}(\theta) = \sum_{l=0}^{\infty} \frac{(2l+1)}{2ik} S_l^{(1)}(\beta) P_l(\cos\theta), \tag{2.17}$$

where

$$S_l^{(1)}(\beta) = \frac{i\beta^3(N^2-1)}{2}[h_l^{(2)}(\beta) + h_l^{(1)}(\beta)S_l^{(0)}(\beta)] \times \sum_{n=0}^{\infty} \frac{(2n+1)}{2} i^{n-l}\omega_{ln}[h_n^{(2)}(\beta) + h_n^{(1)}(\beta)S_n^{(0)}(\beta)], \tag{2.18}$$

$$\omega_{ln} = \int_{-1}^{1} P_l(\cos\theta)\omega(\theta)P_n(\cos\theta)\, d\cos\theta. \tag{2.19}$$

In simplifying $S_l^{(1)}(\beta)$ to the form given in Eq. (2.18) both the Wronskian relation and the differential equation for the spherical Hankel functions were utilized.

Just as in Paper I, $\omega(\theta)$ must be specified before the modified Watson transformation can be applied to Eq. (2.17). I will again choose $\omega(\theta)$ to be a Legendre function

$$\omega(\theta) = P_m(\cos\theta); \tag{2.20}$$

then ω_{ln} can be computed in terms of Clebsch–Gordan coefficients to get

$$\omega_{ln} = \frac{2}{(2m+1)}|\langle l\, n\, 0\, 0 \mid l\, n\, m\, 0\rangle|^2. \tag{2.21}$$

Equation (2.18) is only useful for computing $S_l^{(1)}(\beta)$ for integer l. I will continue $S_l^{(1)}(\beta)$ to complex l by using the same continuation of the spherical Bessel and Hankel functions that were used in Paper I. The Clebsch–Gordan coefficients in ω_{ln} will be continued to complex l as was done in Eq. (3.4) of Paper I. Writing out this continuation of $S_l^{(1)}(\beta)$ in terms of λ, where $\lambda = l + \frac{1}{2}$,

$$S^{(1)}(\lambda,\beta) = S^{(1)}_{\lambda-1/2}(\beta) = \frac{i\pi\beta^2(N^2-1)}{4}[H_\lambda^{(2)}(\beta) + H_\lambda^{(1)}(\beta)S^{(0)}(\lambda,\beta)] \times \sum_{n=-m}^{m}{}' c_n(\lambda)[H_{\lambda+n}^{(2)}(\beta) + H_{\lambda+n}^{(1)}(\beta)S^{(0)}(\lambda+n,\beta)]. \tag{2.22}$$

In Eq. (2.21) I have made use of the selection rules for Clebsch–Gordan coefficients, $H^{(1,2)}(\beta)$ are cylindrical Hankel functions,

$$S^{(0)}(\lambda,\beta) = S^{(0)}_{\lambda-1/2}(\beta) = -\frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)}\left[\frac{[2\beta] - N[\alpha]}{[1\beta] - N[\alpha]}\right], \tag{2.23}$$

$$c_n(\lambda) = (\lambda+n)i^n\omega_{\lambda+n-1/2,\,n} = \frac{(\lambda+n)}{\pi} i^n \frac{\Gamma\left(\frac{m-n+1}{2}\right)}{\Gamma\left(\frac{m-n+2}{2}\right)} \frac{\Gamma\left(\frac{m+n+1}{2}\right)}{\Gamma\left(\frac{m+n+2}{2}\right)} \times \frac{\Gamma\left(\frac{2\lambda+n-m}{2}\right)}{\Gamma\left(\frac{2\lambda+n-m+1}{2}\right)} \frac{\Gamma\left(\frac{2\lambda+n+m+1}{2}\right)}{\Gamma\left(\frac{2\lambda+n+m+2}{2}\right)}. \tag{2.24}$$

The notation in Eq. (2.23) is

$$[x] = \frac{1}{J_\lambda(x)}\frac{\partial J_\lambda(x)}{\partial x}, \tag{2.25}$$

$$[1x] = \frac{1}{H_\lambda^{(1)}(x)}\frac{\partial H_\lambda^{(1)}(x)}{\partial x}, \tag{2.26}$$

$$[2x] = \frac{1}{H_\lambda^{(2)}(x)}\frac{\partial H_\lambda^{(2)}(x)}{\partial x}, \tag{2.27}$$

where J_λ and $H_\lambda^{(1,2)}$ are cyclindrical Bessel and Hankel function. Also the notation $\sum_{n=-m}^{m}{}'$ means sum over $n = -m, -m+2, \ldots, m-2, m$.

In Sec. 4 I will show that this choice of continuation of $S_l^{(1)}(\beta)$ to complex l is the right choice for use in the modified Watson transformation.

3. THE DEBYE EXPANSION FOR $S^{(1)}(\lambda, \beta)$

In Ref. 3 Nussenzveig has shown that the modified Watson transformation cannot be applied directly to Eq. (2.16) because $S^{(0)}(\lambda,\beta)$ has an infinite number of poles near the real λ axis, as can be seen in Fig. 1. These poles contribute a residue series which does not converge, unlike the residue series for the impenetrable sphere. Nussenzveig "cured" this difficulty by using the Debye expansion for $S^{(0)}(\lambda,\beta)$.

The Debye expansion for $S^{(0)}(\lambda,\beta)$ is

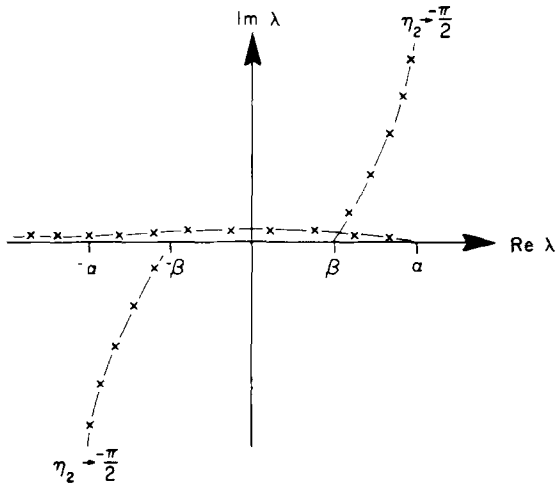

FIG. 1. The poles of $S^{(0)}(\lambda,\beta)$ for $\alpha \gg \beta \gg 1$. The x's mark the location of the poles. The Appendix contains the definition for η_2.

$$S^{(0)}(\lambda,\beta) = \sum_{p=0}^{\infty} S_p^{(0)}(\lambda,\beta), \tag{3.1}$$

where

$$S_0^{(0)}(\lambda,\beta) = \frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)} R_{22}(\lambda,\beta), \tag{3.2}$$

$$S_p^{(0)}(\lambda,\beta) = U(\lambda,\beta)[\rho(\lambda,\beta)]^{p-1} \quad \text{for } p \geqslant 1, \tag{3.3}$$

$$U(\lambda,\beta) = \frac{H_\lambda^{(2)}(\beta)}{H_\lambda^{(1)}(\beta)} T_{21}(\lambda,\beta)\, T_{12}(\lambda,\beta) \frac{H_\lambda^{(1)}(\alpha)}{H_\lambda^{(2)}(\alpha)}, \tag{3.4}$$

$$\rho(\lambda,\beta) = \frac{H_\lambda^{(1)}(\alpha)}{H_\lambda^{(2)}(\alpha)} R_{11}(\lambda,\beta). \tag{3.5}$$

R_{11} and R_{22} are external and internal spherical reflection coefficients, respectively. T_{21} and T_{12} are spherical transmission coefficients. These coefficients are given by

$$R_{11}(\lambda,\beta) = -\frac{[1\beta] - N[1\alpha]}{[1\beta] - N[2\alpha]}, \tag{3.6}$$

$$R_{22}(\lambda,\beta) = -\frac{[2\beta] - N[2\alpha]}{[1\beta] - N[2\alpha]}, \tag{3.7}$$

$$T_{21}(\lambda,\beta) = 1 + R_{22}(\lambda,\beta), \tag{3.8}$$

$$T_{12}(\lambda,\beta) = 1 + R_{11}(\lambda,\beta). \tag{3.9}$$

The Debye expansion solves the nonconvergent residue series problem because R_{11}, R_{22}, T_{21}, and T_{12} do not have a large number of poles lying near the real λ axis, as can be seen in Fig. 2. Of course this advantage is gained at the expense of introducing another summation into the solution which may or may not converge quickly, depending on the values of N and θ.

It can be seen from Eq. (2.22) that $S^{(0)}(\lambda,\beta)$ will also have an infinite number of poles near the real λ axis because $S^{(0)}(\lambda,\beta)$ contains $S^{(0)}(\lambda,\beta)$ in it. The obvious solution to this difficulty is to substitute the Debye expansion for $S^{(0)}(\lambda,\beta)$ into $S^{(1)}(\lambda,\beta)$.

The Debye expansion for $S^{(1)}(\lambda,\beta)$ can be written

$$S^{(1)}(\lambda,\beta) = \sum_{p=0}^{\infty} S_p^{(1)}(\lambda,\beta), \tag{3.10}$$

where

$$S_p^{(1)}(\lambda,\beta) = i\frac{\pi}{4}\beta^2(N^2-1)\sum_{q=0}^{p}\Big\{[H_\lambda^{(2)}(\beta)\delta_{q,0} + H_\lambda^{(1)}(\beta)S_q^{(0)}(\lambda,\beta)] \times \sum_{n=-m}^{n}{}' c_n(\lambda)[H_{\lambda+n}^{(2)}(\beta)\delta_{p-q,0} + H_{\lambda+n}^{(1)}(\beta)S_{p-q}^{(0)}(\lambda+n,\beta)]\Big\}, \tag{3.11}$$

and $\delta_{a,b}$ is the Kronecker delta. I have chosen the Debye expansion for $S^{(1)}(\lambda,\beta)$ so that corresponding terms of the Debye expansions for $S^{(0)}(\lambda,\beta)$ and $S^{(1)}(\lambda,\beta)$ have the same reflection properties as λ goes to $-\lambda$. These are

$$S_p^{(0)}(-\lambda,\beta) = e^{2i\pi(p-1)\lambda} S_p^{(0)}(\lambda,\beta), \tag{3.12}$$

$$S_p^{(1)}(-\lambda,\beta) = e^{2i\pi(p-1)\lambda} S_p^{(1)}(\lambda,\beta). \tag{3.13}$$

The identity (3.12) can be proved using

$$H_{-\lambda}^{(1)}(\beta) = e^{i\pi\lambda} H_\lambda^{(1)}(\beta), \tag{3.14}$$

$$H_{-\lambda}^{(2)}(\beta) = e^{-i\pi\lambda} H_\lambda^{(2)}(\beta). \tag{3.15}$$

Equation (3.13) can then be proved using the same method as was used in Sec. 3C of Paper I.

4. NECESSARY CONDITIONS FOR APPLICATION OF THE MODIFIED WATSON TRANSFORMATION

I will now show that the continuation $S^{(1)}(\lambda,\beta)$ given in Eq. (2.21) meets the conditions that are necessary for application of the modified Watson transformation. These conditions are that $\lambda S^{(1)}(\lambda,\beta)$ have no poles on the real λ axis, so

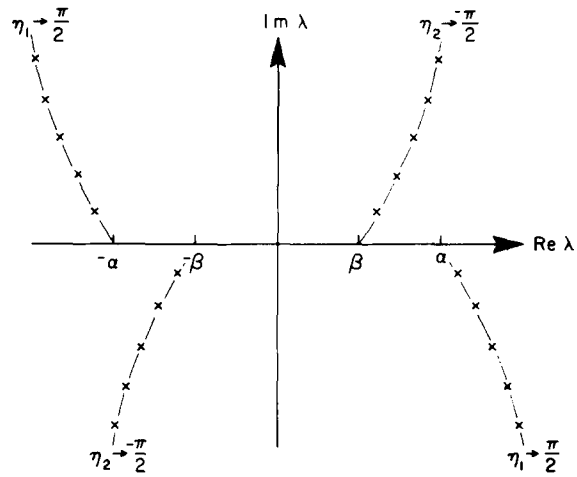

FIG. 2. The poles of $S_p^{(0)}(\lambda,\beta)$ for any value of p and $\alpha \gg \beta \gg 1$. The x's mark the location of the poles. The Appendix contains the definitions for η_1 and η_2.

that Poisson's sum formula can be used, and that $S^{(1)}(\lambda,\beta)$ have the proper behavior as $|\lambda|\to\infty$, so that certain contours of integration can be deformed. Actually these conditions must be met by each term of the Debye expansion for $S^{(1)}(\lambda,\beta)$ since the modified Watson transformation will be applied to each term separately.

A. No poles on the real λ axis

It can seen from Eq. (3.11) that the only place where poles on the real λ axis could come from is the $c_n(\lambda)$ term. The $c_n(\lambda)$ term does have poles on the real λ axis, but these poles cancel when the summation over n is performed in Eq. (3.11).

This can be proved in the same way it was shown for the impenetrable particle in Sec. 3B of Paper I. The main ingredient of that proof was that $H^{(1)}_{-n}(\beta)=(-1)^n H^{(1)}_n(\beta)$, for integer n, so that the summand of Eq. (3.12) of Paper I is an odd function of the summation variable and therefore the sum is zero. The same sum will hold here, for the transparent case, except the $[H^{(1)}_n(\beta)]^{-1}$ is replaced by $[H^{(2)}_n(\beta)\delta_{p0}+H^{(1)}_n(\beta)S^{(0)}_p(n,\beta)]$. It is easy to see that this factor has the same reflection property, when n goes to $-n$ as $H^{(1)}_n(\beta)$ has. Therefore the same proof as was used in Sec. 3B of Paper I will work here, so $H^{(1)}_p(\lambda,\beta)$ has no poles on the real λ axis.

B. Behavior of $S^{(1)}_p(\lambda,\beta)$ as $|\lambda|\to\infty$

The asymptotic behavior of $S^{(1)}_p(\lambda,\beta)$ can be derived in the same way as for the impenetrable particle in Sec. 3D of Paper I. Again $c_n(\lambda)$ approaches a finite constant as $|\lambda|\to\infty$ so the asymptotic behavior of $S^{(1)}_p(\lambda,\beta)$ is given by

$$S_p(\lambda,\beta)\to i\frac{\pi}{4}\beta^2(N^2-1)\sum_{n=-m}^{m}{}' c_n\sum_{q=0}^{p}\times[H^{(2)}_\lambda(\beta)\delta_{q,0}+H^{(1)}_\lambda(\beta)S^{(0)}_q(\lambda,\beta)]\times[H^{(2)}_{\lambda+n}(\beta)\delta_{p-q,0}\,H^{(1)}_{\lambda+n}(\beta)S^{(0)}_{p-q}(\lambda+n,\beta)], \tag{4.1}$$

where

$$c_n=\lim_{\lambda\to\infty}c_n(\lambda). \tag{4.2}$$

The asymptotic behavior of the summand can be derived from the formulas given in the Appendix. In Sec. 5 it will be seen that this is sufficient for application of the modified Watson transformation.

5. SOLUTION FOR BACKSCATTERING BY A TRANSPARENT P_2 PARTICLE

In this section I will evaluate the amplitude for backscattering by a particle with its surface defined by

$$r_p(\theta)=a[1+\delta P_2(\cos\theta)]. \tag{5.1}$$

This choice of $\omega(\theta)$ implies $m=2$ in Eq. (3.11) and $c_n(\lambda)$ is given by

$$c_0(\lambda)=\frac{1}{4}\frac{(\lambda^2-\frac{1}{4})}{(\lambda^2-1)}, \tag{5.2}$$

$$c_{\pm 2}(\lambda)=-\frac{3}{8}\frac{(\lambda^2\pm\frac{3}{2})(\lambda\pm\frac{1}{2})}{\lambda(\lambda\pm 1)}. \tag{5.3}$$

I will now evaluate the first three terms of the Debye expansion for $f^{(1)}(\pi)$ using modified Watson transformation. Higher terms in the Debye expansion are calculated using similar methods.

A. The first term of the Debye expansion

The first term of the Debye expansion for $f^{(1)}(\pi)$ is

$$f^{(1)}_0(\pi)=\sum_{l=0}^{\infty}\frac{(2l+1)}{2ik}S^{(1)}_{0,l}(\beta)P_l(-1), \tag{5.4}$$

where

$$S^{(1)}_{0,l}(\beta)=S^{(1)}_0(l+\tfrac{1}{2},\beta). \tag{5.5}$$

Using the Watson transformation,

$$\sum_{l=0}^{\infty}g(l+\tfrac{1}{2})=\frac{1}{2}\int_C g(\lambda)e^{-i\pi\lambda}\frac{d\lambda}{\cos\pi\lambda}, \tag{5.6}$$

$f^{(1)}_0(\pi)$ can be written

$$f^{(1)}_0(\pi)=-\frac{1}{2k}\int_C S^{(1)}_0(\lambda,\beta)\frac{\lambda\,d\lambda}{\cos\pi\lambda}, \tag{5.7}$$

where $P_l(-1)$ has been continued to complex l using $P_l(-1)\equiv e^{i\pi(\lambda-1/2)}$. The contour of integration C is displayed in Fig. 3. It can be seen from the Appendix that the lower half of the contour C can be deformed to the lower half of the contour Γ, shown in Fig. 4, and the upper half of C can be deformed to the upper half of Γ.[5] These deformations give rise to residue series contributions from the poles λ_n, $\lambda_n\pm 2$ and λ'_n and $\lambda'_n\pm 2$, where λ_n and λ'_n are given in Appendix A of Ref. 3. So $f^{(1)}_0(\pi)$ can now be written

$$f^{(1)}_0(\pi)=f^{(1)}_{0,s}(\pi)+f^{(1)}_{0,s}(\pi)+f'^{(1)}_{0,r}(\pi), \tag{5.8}$$

$$f^{(1)}_{0,s}(\pi)=-\frac{1}{2k}\int_\Gamma S^{(1)}_0(\lambda,\beta)\frac{\lambda\,d\lambda}{\cos\pi\lambda}, \tag{5.9}$$

$$f^{(1)}_{0,r}(\pi)=-\frac{\pi i}{k}\sum_n\text{residues}\left[S^{(1)}_0(\lambda,\beta)\frac{\lambda}{\cos\pi\lambda}\right]_{\lambda_n,\lambda_n\pm 2}, \tag{5.10}$$

$$f'^{(1)}_{0,r}(\pi)=-\frac{\pi i}{k}\sum_n\text{residues}\left[S^{(1)}_0(\lambda,\beta)\frac{\lambda}{\cos\pi\lambda}\right]_{\lambda'_n,\lambda'_n\pm 2}. \tag{5.11}$$

The integral $f^{(1)}_{0,s}(\pi)$ can be simplified by letting λ go to $-\lambda$ on the lower half of Γ and using Eq. (3.13) to get

$$f^{(1)}_{0,s}(\pi)=\frac{i}{k}\int_{\Gamma'}S^{(1)}_0(\lambda,\beta)e^{-i\pi\lambda}\tan(\pi\lambda)\lambda\,d\lambda, \tag{5.12}$$

where Γ' is the upper half of Γ. The main contribution to this integral is from $|\lambda|\lesssim\beta^{1/2}$. Expanding $e^{-i\pi\lambda}S^{(1)}_0(\lambda,\beta)$ to order $1/\beta$ in this region yields

$$e^{-i\pi\lambda}S^{(1)}_0(\lambda,\beta)=2\beta\left(\frac{N-1}{N+1}\right)e^{-2i\beta}e^{-i\lambda^2/\beta}\times\left[1-\frac{11}{4}\frac{i}{\beta}-\left(\frac{2N-1}{N}\right)\frac{\lambda^2}{\beta^2}-\frac{i}{12}\frac{\lambda^4}{\beta^3}+O(\beta^{-2})\right]\quad\text{for }|\lambda|\lesssim\beta^{1/2}. \tag{5.13}$$

Substituting this into Eq. (5.12) and changing variables to

$$\lambda = e^{3i\pi/4}\beta^{1/2}x = \alpha x \tag{5.14}$$

gives

$$f^{(1)}_{0,s}(\pi) = 2a\beta\left(\frac{N-1}{N+1}\right)e^{-2i\beta}\int_0^\infty e^{-x^2} \times\left[1 - \frac{11}{4}\frac{i}{\beta} + \left(\frac{2N-1}{N}\right)i\frac{x^2}{\beta} + \frac{i}{12}\frac{x^4}{\beta} + O(\beta^{-2})\right]\tan(\pi\alpha x)\,x\,dx. \tag{5.15}$$

This integral can be evaluated using the method given in Appendix B of Paper I to get

$$f^{(1)}_{0,s}(\pi) = -ia\beta\left(\frac{N-1}{N+1}\right)e^{-2i\beta}\left[1 - \left(\frac{N-2}{2N}\right)\frac{i}{\beta} + O(\beta^{-2})\right]. \tag{5.16}$$

In evaluating $f^{(1)}_{0,r}(\pi)$ it is useful to employ the expansion

$$\frac{1}{\cos\pi\lambda} = 2\sum_{m=0}^{\infty}(-1)^m\exp[i(2m+1)\pi\lambda\,]. \tag{5.17}$$

Substituting this in Eq. (5.10) yields

$$f^{(1)}_{0,r}(\pi) = -\frac{2\pi i}{k}\sum_{m=0}^{\infty}(-1)^m\sum_n \text{residues}\,[S^{(1)}_0(\lambda,\beta)\,e^{i(2m+1)\pi\lambda}\,\lambda\,]_{\lambda_n,\lambda_n\pm 2}. \tag{5.18}$$

If only the highest order in β is kept in the residue series then only the second order pole at λ_n will contribute to $f^{(1)}_{0,r}(\pi)$. These residues can be computed using Appendix A of Ref. 3 to get

$$f^{(1)}_{0,r}(\pi) = -e^{i\pi/3}\frac{a\beta}{4\gamma}\sum_{m=0}^{\infty}(-1)^m\sum_n\{i\pi(2m+1) \times[\mathrm{Ai}'(-x_n)]^{-2}e^{i(2m+1)\pi\lambda_n} + \text{lower order}\}, \tag{5.19}$$

where $\gamma = (2/\beta)^{1/3}$, $\mathrm{Ai}(x)$ is the Airy function, and $-x_n$ is its nth zero. It should be noted that the sums in Eq. (5.19) converge very quickly due to the $e^{i(2m+1)\pi\lambda_n}$ term.

In evaluating $f'^{(1)}_{0,r}(\pi)$ it is useful to employ the expansion

$$\frac{1}{\cos\pi\lambda} = 2\sum_{m=0}^{\infty}(-1)^m\exp[-i(2m+1)\pi\lambda\,]. \tag{5.20}$$

Substituting this in Eq. (5.11) yields

$$f'^{(1)}_{0,r}(\pi) = -\frac{2\pi i}{k}\sum_{m=0}^{\infty}(-1)^m\sum_n \text{residues}\,[S^{(1)}_0(\lambda,\beta)\,e^{-i(2m+1)\pi\lambda}\,\lambda\,]_{\lambda'_n,\lambda'_n\pm 2}. \tag{5.21}$$

Again if only the highest-order term in β is kept in the residue series then only the second order poles at λ'_n will contribute to $f'^{(1)}_{0,r}(\pi)$. These residues can be computed using Appendix A of Ref. 2 and Appendix A of Ref. 3 to get

$$f'^{(1)}_{0,r}(\pi) = e^{i\pi/3}\frac{\pi\beta a}{M}e^{-2\beta[N\cosh^{-1}N - M]}\sum_{m=0}^{\infty}(-1)^m \times\sum_n[i(2m+1)\pi + 2\cosh^{-1}N + 2iMN\,]\,e^{-i(2m+1)\pi\lambda'_n} \times\exp\left[-2\beta\cosh^{-1}N\frac{e^{i\pi/3}x_n}{N^{1/3}\gamma}\right], \tag{5.22}$$

where $M = (N^2-1)^{1/2}$. It should be noted that the sums in Eq. (5.22) converge quickly due to the $e^{-i(2m+1)\pi\lambda'_n}$ term. Also, for the range of values of N being considered here, $f'^{(1)}_{0,r}(\pi)$ is negligible when compared with $f^{(1)}_{0,r}(\pi)$.

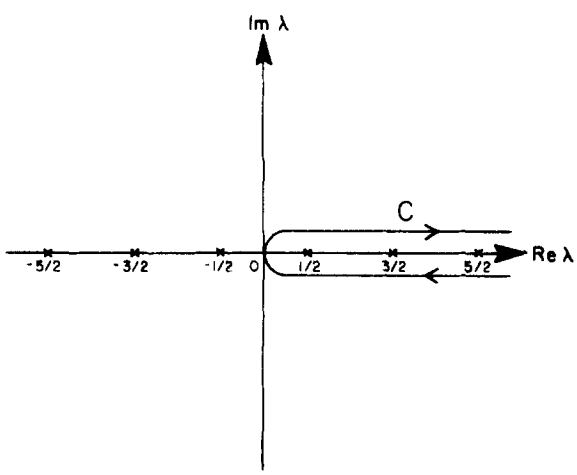

FIG. 3. The contour C.

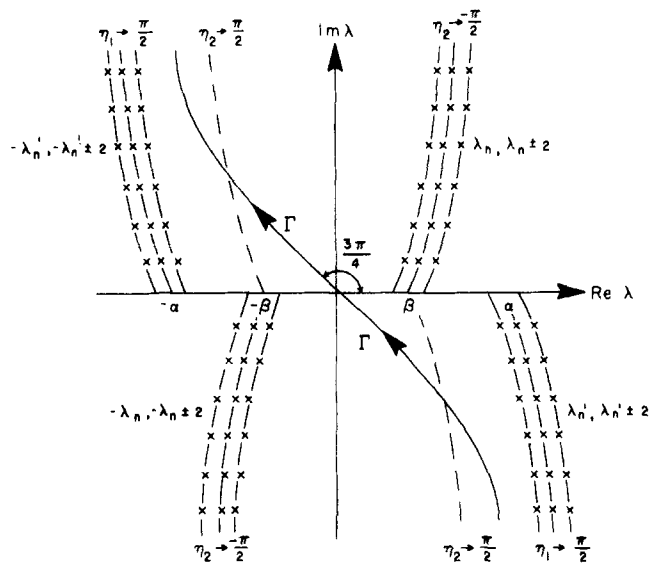

FIG. 4. The contour Γ. The x's are the poles of $S^{(1)}_p(\lambda,\beta)$ for any p.

B. The second term of the Debye expansion

The second term of the Debye expansion for $f^{(1)}(\pi)$ is

$$f_1^{(1)}(\pi) = \sum_{l=0}^{\infty} \frac{(2l+1)}{2ik} S_{1,l}^{(1)}(\beta) P_l(-1), \tag{5.23}$$

where

$$S_{1,l}^{(1)}(\beta) = S_1^{(1)}(l+\tfrac{1}{2}, \beta). \tag{5.24}$$

Using the Poisson sum formula

$$\sum_{l=0}^{\infty} g(l+\tfrac{1}{2}) = \sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} g(\lambda) e^{2im\pi\lambda} d\lambda, \tag{5.25}$$

$f_1^{(1)}(\pi)$ can be written

$$f_1^{(1)}(\pi) = -\frac{1}{k} \sum_{m=-\infty}^{\infty} (-1)^m \int_0^{\infty} S_1^{(1)}(\lambda, \beta)\, e^{i(2m+1)\pi\lambda}\, \lambda\, d\lambda, \tag{5.26}$$

where $P_l(-1)$ has been continued to complex l using $P_l(-1) \equiv e^{-i\pi(\lambda - 1/2)}$. Changing λ to $-\lambda$ in the sum from $m = -1$ to $-\infty$ and using Eq. (3.13) gives

$$f_1^{(1)}(\pi) = -\frac{1}{k} \sum_{m=0}^{\infty} (-1)^m \int_{-\infty}^{\infty} S_1^{(1)}(\lambda, \beta)\, e^{i(2m+1)\pi\lambda}\, \lambda\, d\lambda. \tag{5.27}$$

It can be seen from the Appendix that this integral can be reduced to a pure residue series by closing the path of integration at infinity in the upper half-plane.[5] This residue series is

$$f_1^{(1)}(\pi) = f_{1,r}^{(1)}(\pi) + f'^{(1)}_{1,r}(\pi), \tag{5.28}$$

$$f_{1,r}^{(1)}(\pi) = \frac{-2\pi i}{k} \sum_{m=0}^{\infty} (-1)^m \sum_n \text{residues}\left[S_1^{(1)}(\lambda, \beta)\, e^{i(2m+1)\pi\lambda}\, \lambda\right]_{\lambda_n,\, \lambda_n \pm 2}, \tag{5.29}$$

$$f'^{(1)}_{1,r}(\pi) = -\frac{2\pi i}{k} \sum_{m=0}^{\infty} (-1)^m \sum_n \text{residues}\left[S_1^{(1)}(\lambda, \beta)\, e^{i(2m+1)\pi\lambda}\, \lambda\right]_{-\lambda'_n,\, -\lambda'_n \pm 2}. \tag{5.30}$$

These residues can be computed using Appendix A of Ref. 3 to get

$$f_{1,r}^{(1)}(\pi) = -e^{-i\pi/6} \frac{\beta a}{2\pi M\gamma} e^{2iM\beta} \sum_{m=0}^{\infty} (-1)^m \sum_n [Ai'(-x_n)]^{-2} \times e^{i\theta_m \lambda_n} \left\{ \frac{3i}{4} [\cos(2\theta_t) + 2M \sin(2\theta_t)] + \frac{i}{4} [\theta_m^2 + 2M\theta_m - 2M^2] + \text{lower order} \right\}, \tag{5.31}$$

where

$$\cos\frac{\theta_t}{2} = \frac{1}{N}, \tag{5.32}$$

$$\theta_m = [(2m+1)\pi - \theta_t]. \tag{5.33}$$

The sums in Eq. (5.31) converge quickly, for the range of N values being considered here, due to the $e^{i\theta_m \lambda_n}$ term. The contribution from $f'^{(1)}_{1,r}(\pi)$ is negligible when compared with $f_{1,r}^{(1)}(\pi)$ for the range of values of N being considered here, so I will not write it out here.

C. The third term of the Debye expansion

The third term of the Debye expansion for $f^{(1)}(\pi)$ is

$$f_2^{(1)}(\pi) = \sum_{l=0}^{\infty} \frac{(2l+1)}{2ik} S_{2,l}^{(1)}(\beta) P_l(-1), \tag{5.34}$$

where

$$S_{2,l}^{(1)}(\beta) = S_2^{(1)}(l+\tfrac{1}{2}, \beta). \tag{5.35}$$

Applying the Watson transformation, given in Eq. (5.6), to Eq. (5.34) yields

$$f_2^{(1)}(\pi) = -\frac{1}{2k} \int_C S_2^{(1)}(\lambda, \beta) \frac{\lambda\, d\lambda}{\cos \pi\lambda}, \tag{5.36}$$

where $P_l(-1)$ has been continued to complex l using $P_l(-1) \equiv e^{i\pi(\lambda - 1/2)}$. Changing λ to $-\lambda$ in the integral over the lower half of C and utilizing Eq. (3.13) gives

$$f_2^{(1)}(\pi) = -\frac{1}{2k} \int_0^{\infty + i\alpha} S_2^{(1)}(\lambda, \beta) \frac{\lambda\, d\lambda}{\cos \pi\lambda} - \frac{1}{2k} \int_{-\infty + i\alpha}^{0} S_2^{(1)}(\lambda, \beta) e^{2i\pi\lambda} \frac{\lambda\, d\lambda}{\cos \pi\lambda}. \tag{5.37}$$

Using the fact that

$$1 = e^{2i\pi\lambda} - 2ie^{i\pi\lambda} \sin(\pi\lambda), \tag{5.38}$$

Eq. (5.37) can be rewritten

$$f_2^{(1)}(\pi) = f_{2,s}^{(1)}(\pi) + f_{2,\text{res}}^{(1)}(\pi), \tag{5.39}$$

$$f_{2,s}^{(1)}(\pi) = \frac{i}{k} \int_0^{\infty + i\alpha} S_2^{(1)}(\lambda, \beta) e^{i\pi\lambda} \tan(\pi\lambda)\, \lambda\, d\lambda, \tag{5.40}$$

$$f_{2,\text{res}}^{(1)}(\pi) = -\frac{1}{2k} \int_{-\infty + i\alpha}^{\infty + i\alpha} S_2^{(1)}(\lambda, \beta) e^{2i\pi\lambda} \frac{\lambda\, d\lambda}{\cos \pi\lambda}. \tag{5.41}$$

The integral for $f_{2,s}^{(1)}(\pi)$ can be evaluated using the sad-

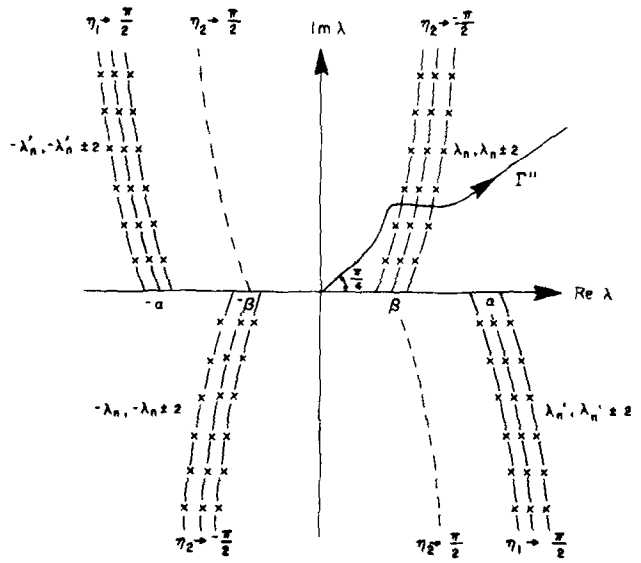

FIG. 5. The contour Γ''. The x's are the poles of $S_2^{(1)}(\lambda, \beta)$.

dle point method. It can be seen, from the appendix, that the path of integration can be shifted to the contour Γ'' shown in Fig. 5. This deformation gives rise to a residue series from the poles at λ_n and $\lambda_n \pm 2$. The number of poles that contribute to this residue series depends on the shape of Γ'' in the region near the poles λ_n. However, since the poles far from the real axis give negligible contribution, I will add all the residues from λ_n and $\lambda_n \pm 2$ to the residue series to give

$$f^{(1)}_{2,s}(\pi) = \frac{i}{k}\int_{\Gamma''} S^{(1)}_2(\lambda,\beta)e^{i\pi\lambda}\tan(\pi\lambda)\lambda\, d\lambda - \frac{2\pi}{k}\sum_n \text{residues}\,[S^{(1)}_2(\lambda,\beta)e^{i\pi\lambda}\tan(\pi\lambda)\lambda\,]_{\lambda_n,\lambda_n\pm 2}. \quad (5.42)$$

Along the contour Γ'' the main contribution to the integral in Eq. (5.42) is from $|\lambda| \lesssim \beta^{1/2}$. Expanding $e^{i\pi\lambda}S^{(1)}_2(\lambda,\beta)$ about $\lambda = 0$ gives

$$e^{i\pi\lambda}S^{(1)}_2(\lambda,\beta) = -8\beta\frac{N(N-1)}{(N+1)^3}e^{2i(2N-1)\beta}\exp\left[-i\frac{(N-2)}{N}\frac{\lambda^2}{\beta}\right] \times\left[1 - \frac{11i}{4\beta}\frac{(N-2)}{N} - \frac{1}{2}\frac{(5N^2-28N+25)}{N^2}\frac{\lambda^2}{\beta^2} - \frac{i}{12}\frac{(N^3-2)}{N^3}\frac{\lambda^4}{\beta^3} + O\left(\frac{1}{\beta^2}\right)\right] \quad \text{for } |\lambda| \lesssim \beta^{1/2}. \quad (5.43)$$

Substituting this into the integral in Eq. (5.42), changing variables to

$$\lambda = e^{i\pi/4}\left(\frac{N\beta}{2-N}\right)^{1/2}x, \quad (5.44)$$

and performing the resulting integral as in Appendix B of Paper I gives

$$f^{(1)}_{2,s}(\pi) = -4ia\beta\frac{N^2(N-1)}{(N-2)(N+1)^3}e^{2i(2N-1)\beta}\left[1 + \frac{1}{12\beta}\times\left(\frac{N^3+30N^2-42N+40}{N(N-2)^2}\right) + O(-\beta^{-2})\right] - \frac{2\pi}{k}\times\sum_n \text{residues}\,[S^{(1)}(\lambda,\beta)e^{i\pi\lambda}\tan(\pi\lambda)\lambda\,]_{\lambda_n,\lambda_n\pm 2}. \quad (5.45)$$

The residue series in Eq. (5.45) can be simplified by using

$$\tan(\pi\lambda) = i - 2i\sum_{m=0}^{\infty}(-1)^m e^{i(2m+2)\pi\lambda} \quad (5.46)$$

to get

$$f^{(1)}_{2,s}(\pi) = -4ia\beta\frac{N^2(N-1)}{(N-2)(N+1)^3}e^{2i(2N-1)\beta}\times\left[1 + \frac{1}{12}\frac{(N^3+30N^2-42N+40)}{N(N-2)^2} + O(\beta^{-2})\right] - \frac{2\pi i}{k}\sum_n \text{residues}\,[S^{(1)}(\lambda,\beta)e^{i\pi\lambda}\lambda\,]_{\lambda_n,\lambda_n\pm 2} + \frac{4\pi i}{k}\sum_{m=0}^{\infty}(-1)^m\sum_n \text{residues}\,[S^{(1)}_2(\lambda,\beta)e^{i(2m+3)\pi\lambda}\lambda\,]_{\lambda_n,\lambda_n\pm 2}. \quad (5.47)$$

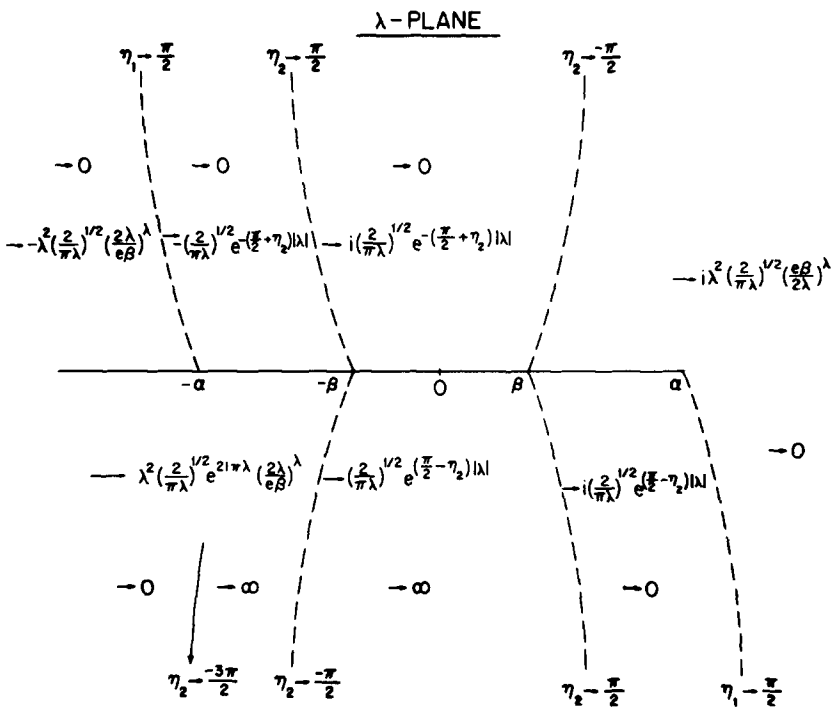

FIG. 6. The asymptotic behavior of $H^{(2)}_\lambda(\beta) + H^{(1)}_\lambda(\beta)S^{(0)}_o(\lambda,\beta) = H^{(2)}(\beta)T_{21}(\lambda,\beta)$.

Equation (5.41) can be simplified by utilizing Eq. (5.17) to get

$$f^{(1)}_{2,\mathrm{res}}(\pi) = -\frac{1}{k}\sum_{m=0}^{\infty}(-1)^m\int_{-\infty}^{\infty} S^{(1)}_2(\lambda,\beta)\, e^{i(2m+3)\pi\lambda}\lambda\, d\lambda. \tag{5.48}$$

It can now be seen from the Appendix that $f^{(1)}_{2,\mathrm{res}}(\pi)$ can be reduced to a pure residue series by completing the contour of integration in the upper half-plane[5] to get

$$f^{(1)}_{2,\mathrm{res}}(\pi) = f^{(1)}_{2,r}(\pi) + f'^{(1)}_{2,r}(\pi), \tag{5.49}$$

$$f^{(1)}_{2,r}(\pi) = \frac{-2\pi i}{k}\sum_{m=0}^{\infty}(-1)^m\sum_n \mathrm{residues}\left[S^{(1)}_2(\lambda,\beta)\, e^{i(2m+3)\pi\lambda}\lambda\right]_{\lambda_n,\,\lambda_n\pm 2}, \tag{5.50}$$

$$f'^{(1)}_{2,r}(\pi) = \frac{-2\pi i}{k}\sum_{m=0}^{\infty}(-1)^m\sum_n \mathrm{residues}\left[S^{(1)}_2(\lambda,\beta)\, e^{i(2m+3)\pi\lambda}\lambda\right]_{-\lambda'_n,\,-\lambda'_n\pm 2}. \tag{5.51}$$

Finally, combining Eqs. (5.47), (5.50), and (5.51),

$$\begin{aligned} f^{(1)}_2(\pi) = {} & -4ia\beta\frac{N^2(N-1)}{(N-2)(N+1)^3}e^{2i(2N-1)\beta}\left[1+\frac{1}{12\beta}\frac{(N^3+30N^2-42N+40)}{N(N-2)^2}+O(\beta^{-2})\right] \\ & -\frac{2\pi i}{k}\sum_{m=0}^{\infty}(-1)^m\sum_n \mathrm{residues}\left[S^{(1)}_2(\lambda,\beta)\, e^{i(2m+1)\pi\lambda}\lambda\right]_{\lambda_n,\,\lambda_n\pm 2} \\ & -\frac{2\pi i}{k}\sum_{m=0}^{\infty}(-1)^m\sum_n \mathrm{residues}\left[S^{(1)}_2(\lambda,\beta)\, e^{i(2m+3)\pi\lambda}\lambda\right]_{-\lambda'_n,\,-\lambda_n\pm 2}. \end{aligned} \tag{5.52}$$

I will not write out the expression for the residues here since it is complicated. As was the case for the first and second terms of the Debye expansion, the contribution from the poles at $-\lambda'_n$ and $-\lambda'_n \pm 2$ is negligible in comparison with the contribution from λ_n and $\lambda_n \pm 2$.

6. CONCLUSION

I have shown in this paper that it is possible to extend the modified Watson transformation for spherical transparent particles to slightly nonspherical transparent particles. This was accomplished by combining boundary perturbation theory, the Debye expansion, and the modified Watson transformation. This method yields for the scattering amplitude

$$f(\theta) = f^{(0)}(\theta) + \delta f^{(1)}(\theta) + \cdots, \tag{6.1}$$

where $f^{(0)}(\theta)$ is the scattering amplitude for the unperturbed sphere. The function $f^{(1)}(\theta)$ is given by an expansion similar to the Debye expansion for $f^{(0)}(\theta)$,

$$f^{(1)}(\theta) = \sum_{p=0}^{\infty} f^{(1)}_p(\theta). \tag{6.2}$$

The functions $f^{(1)}_p(\theta)$, which are obtained using the Debye expansion for $S^{(1)}(\lambda,\beta)$ given in Eq. (3.11), are evaluated using the modified Watson transformation. This method was applied to the problem of backscattering by a sphere with its shape perturbed by adding $\delta a P_2(\cos\theta)$ to the radius.

The example in this paper can be easily extended to the entire angular domain of θ and to any value of N which satisfied $|N-1|^{1/2}(ka)^{1/3} \gg 1$, by using the same methods as were used in Refs. 3 and 4. Higher-order solutions in δ can be obtained using methods similar to those presented here.

In the example treated in Sec. 5, I have only calculated the first three terms of the Debye expansion. Higher-order terms can be calculated using methods similar to the ones used in Sec. 5. The contribution from these higher-order terms may not be negligible, depending on the value of N.

It should be possible to treat particles without an axis of symmetry by letting $\omega(\theta)$ be a function of ϕ and substituting spherical harmonics for the Legendre functions in the partial wave expansion. This case should be more interesting than the particle with an axis of symmetry, especially when considering the glory. The reason for this is that the glory occurs

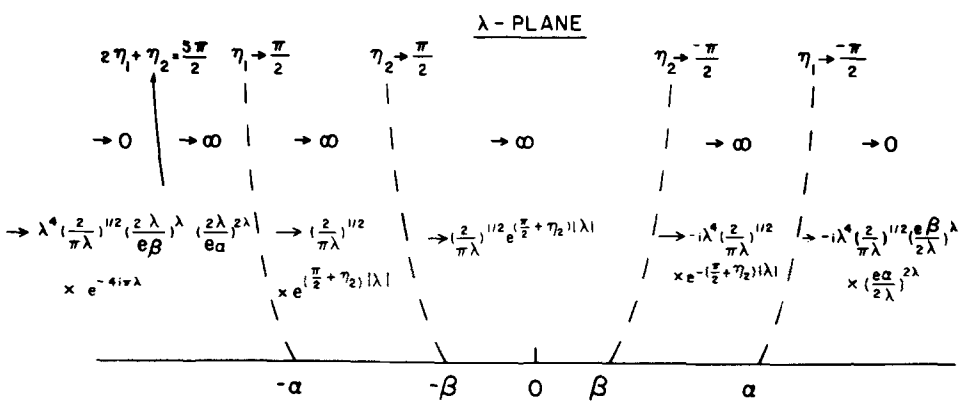

FIG. 7. The asymptotic behavior of $H^{(1)}_\lambda(\beta)S^{(0)}_1(\lambda,\beta) = H^{(1)}_\lambda(\beta)U(\lambda,\beta)$.

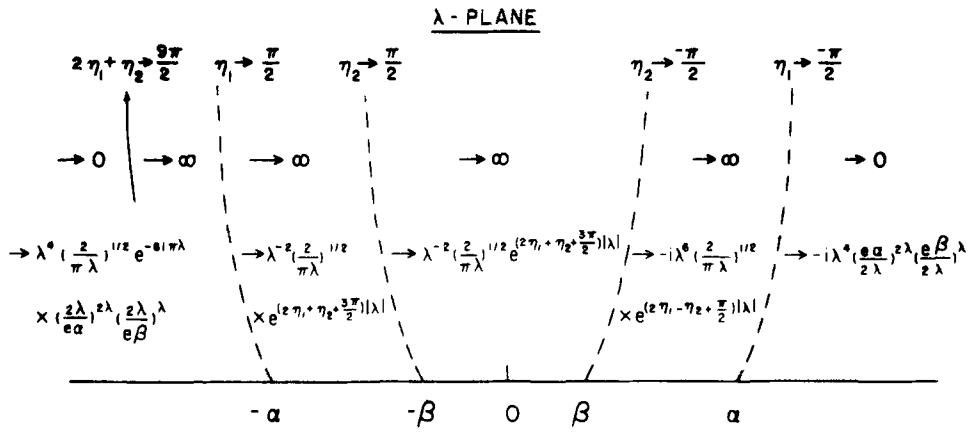

FIG. 8. The asymptotic behavior of $H_{\lambda}^{(1)}(\beta)S^{(0)}(\lambda,\beta)=H_{\lambda}^{(1)}(\beta)U(l,\beta)\rho(\lambda,\beta)$.

partly because surface waves, after traveling around a sphere, add up in phase in backward direction. This would no longer be the case for a particle without an axis of symmetry; therefore the glory should be strongly affected.

In a future paper I will use the solutions generated in Paper I and in this paper to investigate the effects of particle shape on scattering cross sections. I will also look at the rate of convergence of the Debye expansion for $f^{(1)}(\pi)$.

ACKNOWLEDGMENTS

I would like to thank B. Durand, L. Durand, and J. Weinman for bringing this problem to my attention and for many helpful conversations.

This research was supported, in part, by the University of Wisconsin Research Committee with funds granted by the Wisconsin Alumni Research Foundation and, in part, by the Department of Energy under Contract No.DOE-ER-00881, and by the National Oceanic and Atmospheric Administration, NOAA-MO-A-01-00-4320.

APPENDIX: ASYMPTOTIC BEHAVIOR OF $S_p^{(1)}(\lambda,\beta)$

The asymptotic behavior of $S_p^{(1)}(\lambda,\beta)$ can be derived from the asymptotic behavior of $H_{\lambda}^{(1,2)}(\beta)$ and $S_p^{(0)}(\lambda,\beta)$ given in Refs. 2–4. The results are displayed in Figs. 6–8.

The notation is the same as in Appendix B of Ref. 2. For $|\lambda|\to\infty$ along directions approaching the positive or negative imaginary axis the notation is

$$\lambda=\pm\sigma|\lambda|, \tag{A1}$$

$$\sigma=\exp[i(\pi/2+\epsilon)], \tag{A2}$$

$$\eta_1=\epsilon\ln|2\lambda/e\alpha|, \tag{A3}$$

$$\eta_2=\epsilon\ln|2\lambda/e\beta|. \tag{A4}$$

The results given here are all for $N>1$.

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[4] H. M. Nussenzveig, J. Math. Phys. **10**, 125 (1969).
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Large momentum behavior of the Feynman amplitudes in the ϕ_4^4-theory

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(Received 29 October 1981; accepted for publication 19 March 1982)

The complete asymptotic expansion of the Feynman amplitudes for large values of the scale parameter is derived in the ϕ_4^4-theory for Euclidean and Minkowski metrics.

PACS numbers: 11.20.Dj, 11.10.Jj, 11.10.Gh

I. INTRODUCTION

The large-momentum behavior of Feynman amplitudes has attracted attention since the early days of renormalization theory.[1] Weinberg's power counting theorem,[2] proved for convergent graphs and Euclidean metrics, found innumerable applications in Lagrangian field theory. In 1968, Fink[3] obtained more detailed information concerning the logarithms which accompany the leading power of the scale parameter Λ. In 1973, Slavnov[4] showed that every (inverse) power of the overall scale parameter Λ in the asymptotic expansion of the Feynman amplitude is accompanied by a polynomial in $\ln \Lambda$—and nothing else. In 1974, Bergère and Lam[5] determined all the coefficients going along with the leading power of Λ.

In the context of local gauge theories and chiral dynamics the transition from massive to massless propagators is of interest. On the other hand, the behavior of a Feynman amplitude when all masses in the propagators shrink to zero, the mass ratios (and the external momenta) being kept fixed, is intimately related to that of the same Feynman amplitude when all (external) momenta are rescaled by a common factor Λ tending to infinity, the masses in the propagators being kept fixed. Hence, there is additional motivation for the analysis of the large-momentum behavior of individual Feynman amplitudes. In particular, our analysis includes Feynman amplitudes of massless theories.

The present work gives the complete large-momentum (and small mass) behavior of Feynman amplitudes for individual vertex graphs and thereby for arbitrary individual graphs in the ϕ_4^4-theory to which we restrict ourselves for the sake of transparency.

It should be pointed out here that no restrictions are imposed on the momenta carried by the external lines of the graph in question, either linear ones (of the kind of vanishing partial sums of the momenta) or quadratic ones (mass shell conditions). Restrictions of this or a similar kind require special consideration because we view the asymptotic expansion in the context of distributions and not for every configuration of the external momenta separately. This distribution-theoretical formulation of the problem turns out to be both adequate and helpful for Minkowski metrics.

The appropriate frame for the derivation of the asymptotic expansion of the Feynman amplitudes appears to be the analytic renormalization scheme[6–8] (and possibly the renormalization formalism which is based on dimensional regularization[9]). In this scheme integrations over contours in the complex plane achieving analytic continuation take the place of the cumbersome Taylor operator in the Bogoliubov–Parasiuk–Hepp–Zimmermann renormalization formalism (cf., e.g., Ref. 5). Also, the concept of labeled (singularity-) s-families $(\mathbb{E},\sigma)$ in the analytic renormalization scheme[7] corresponding to the resolution of the ultraviolet singularities of the Feynman integrand[10] lends itself in a natural way to a generalization: the concept of labeled s_∞-families $(\mathbb{E}_\infty,\sigma_\infty)$ (explained below in Sec. IV) corresponding to the resolution of the combined ultraviolet and infrared singularities. In order to derive the complete asymptotic expansion for the scale parameter Λ tending to plus infinity, the degeneracies of the quadratic form of the external momenta entering the Feynman integrand need to be extracted completely. This is achieved by diagonalization of the quadratic form (Sec. III), subdivision of the integration domain of the Feynman parameters (Sec. IV), and parametrization of the resulting subdomains (Sec. V). Section VI recalls the analytic renormalization procedure. In Sec. VII the asymptotic expansion is derived and stated in a form which allows one to read off the error committed when it is truncated after a finite number of terms.

Actually, if one is interested only in the first few terms of the asymptotic expansion and the error committed when truncating the asymptotic expansion already after those, a partial diagonalization of the quadratic form and a less detailed subdivision of the integration domain of the Feynman parameters will be sufficient.

For the convenience of the reader some basic notations and definitions of the theory of Feynman graphs—so far as they are relevant in the present context—are collected in Sec. II. The material is taken from Refs. 11 and 12.

The present article reports work done in 1974.[13] This work has not been published up to now with the exception of a short introduction to the problem and an announcement of the results.[14] Nevertheless, meanwhile the basic ideas and methods have been applied in the literature (cf., e.g., Ref. 15). The actual presentation differs from the original one by the incorporation of Trute's graphical rules for the diagonalization of the relevant quadratic form, very appealing and efficient rules, indeed, which replace the author's own less elegant diagonalization techniques.

Since August 1974, several articles[16–19] appeared dealing with the (pointwise) asymptotic behavior of Feynman amplitudes. On the one hand, they carried the analysis of the asymptotic behavior beyond the limitations of the present paper establishing, e.g., the (pointwise) asymptotics when an arbitrary subset of the invariant momenta is scaled[17,18] or the Regge pole behavior of the four body scattering amplitude

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for the ϕ_4^3-theory.[19] On the other hand, the procedure described there for constructing a required number of terms of the asymptotic expansion and for determining the error committed by truncation is in general much more time consuming than the algorithm presented here, where the coefficients of the asymptotic expansion are expressed in terms of subgraphs and reduced graphs; only the minimal amount of partial ordering of the Feynman parameters is employed and the dimension of the multiple Mellin transformation is independent of the order of perturbation theory. Moreover, the analysis of Refs. 16–19 requires Euclidean metrics. It applies to Minkowski metrics only in special situations.

It is recommended that the reader look up Ref. 14 for a general orientation before going through the following detailed analysis.

II. BASIC GRAPH-THEORETICAL NOTATIONS AND DEFINITIONS

A *graph* G is a triplet consisting of a (finite) collection $\nu(G)$ of $|\nu(G)|$ vertices v, a (finite) collection $\mathcal{L}(G)$ of $|\mathcal{L}(G)|$ (internal) lines l and a mapping $\phi_G: \mathcal{L}(G) \to \nu(G) \times \nu(G)$, $l \overset{\phi_G}{\to} (\phi_i(l), \phi_f(l))$, where $\phi_i(l)$, $\phi_f(l)$ are the initial and final vertices of the line l.

$$G = (\nu(G), \mathcal{L}(G), \phi_G).$$

The *union* G of two graphs G_1 and G_2: $G = G_1 \cup G_2$ defined by $\nu(G) = \nu(G_1) \cup \nu(G_2)$, $\mathcal{L}(G) = \mathcal{L}(G_1) \cup \mathcal{L}(G_2)$,

$$\phi_G(l) = \begin{cases} \phi_{G_1}(l) & \text{if } l \in \mathcal{L}(G_1), \\ \phi_{G_2}(l) & \text{if } l \in \mathcal{L}(G_2), \end{cases}$$

provided $\phi_{G_1}(l) = \phi_{G_2}(l)$ for every $l \in \mathcal{L}(G_1) \cap \mathcal{L}(G_2)$ is again a graph.

A *subgraph* H of a graph G is a graph $(\nu(H), \mathcal{L}(H), \phi_H)$ such that $\nu(H) \subset \nu(G)$, $\mathcal{L}(H) \subset \mathcal{L}(G)$, $\phi_H = \phi_G | \mathcal{L}(H)$ [in words, ϕ_G restricted to $\mathcal{L}(H)$].

A subgraph F of a subgraph H of a graph G is a subgraph of G.

If H is a subgraph of G we shall write $H \subset G$.

Let v be an element of $\nu(G)$. We define sets of lines $\mathcal{S}(v)$ and $\mathcal{L}(v)$ according to

$$\mathcal{S}(v) = \{ l \in \mathcal{L}(G) / \phi_i(l) = v \quad \text{or} \quad \phi_f(l) = v \},$$
$$\mathcal{L}(v) = \{ l \in \mathcal{L}(G) / \phi_i(l) = v = \phi_f(l) \}.$$

Two distinct vertices v and v' are called *adjacent* if $\mathcal{S}(v) \cap \mathcal{S}(v') \neq \emptyset$. Two vertices v and v' are *connected* if there is a sequence of vertices $v = v_0, v_1, \ldots, v_k = v'$ such that v_j and v_{j+1} $(j = 0,1,\ldots,k-1)$ are adjacent.

A graph G is said to be *connected* if any two of its vertices are connected. Otherwise, G is said to be *disconnected*.

A graph G can uniquely be decomposed into a union of connected subgraphs H_i of G $i = 1,2,\ldots, p(G)$:

$$G = \bigcup_{i=1}^{p(G)} H_i.$$

The H_i's $i = 1,2,\ldots, p(G)$ are called the *connected components* of G.

For any subset $\mathcal{I}$ of $\mathcal{L}(G)$ we define the subgraph $G - \mathcal{I}$ of the graph G according to

$$G - \mathcal{I} = (\nu(G), \quad \mathcal{L}(G) \setminus \mathcal{I}, \phi_G | \mathcal{L}(G) \setminus \mathcal{I}).$$

For an arbitrary line $l_0 \in \mathcal{L}(G)$ consider the subgraph $G - \{l_0\}$ obtained from G by deleting the line l_0. The line l_0 is said to be a *cut-line* if $p(G - \{l_0\}) > p(G)$.

A graph G is called *one-line-irreducible* (or strongly connected) if it is connected and if it does not contain a cut-line. Otherwise, G is called *one-line-reducible*.

Any connected component H_i of a graph G can be decomposed uniquely into $c(H_i)$ one-line-irreducible components joined by $(c(H_i) - 1)$ cut-lines.

A vertex $v \in \nu(G)$ is said to be a *cut-vertex* of the graph G if a connected component H of G has two subgraphs F_1 and F_2 such that $\mathcal{L}(F_1) \neq \emptyset$, $\mathcal{L}(F_2) \neq \emptyset$, $\mathcal{L}(F_1) \cap \mathcal{L}(F_2) = \emptyset$, $\mathcal{L}(F_1) \cup \mathcal{L}(F_2) = \mathcal{L}(H)$, and $\nu(F_1) \cap \nu(F_2) = \{v\}$.

A graph G is said to be *one-vertex-irreducible* if $\nu(G)$ contains no cut-vertex. Otherwise, G is said to be *one-vertex-reducible*.

Any connected component H_i of G can be decomposed uniquely into $k(H_i)$ one-vertex-irreducible components joined by $(k(H_i) - 1)$ or fewer cut-vertices.

A graph G is said to be *irreducible* if it is both one-line-irreducible and one-vertex-irreducible. Otherwise, G is said to be *reducible*.

Let $\mathcal{K}$ be a subset of $\nu(G)$ containing more than one element. We define $G(\mathcal{K})$ to be the graph $((\nu(G) \setminus \mathcal{K}) \cup \{[\mathcal{K}]\}, \mathcal{L}(G), \phi_{G(\mathcal{K})})$ obtained by identifying the vertices in $\mathcal{K}$

$$\phi_{G(\mathcal{K})}(l) = \begin{cases} (\phi_i(l), \phi_f(l)) & \text{if } \phi_i(l), \phi_f(l) \in \nu(G) \setminus \mathcal{K}, \\ (\phi_i(l), [\mathcal{K}]) & \text{if } \phi_i(l) \in \nu(G) \setminus \mathcal{K}, \ \phi_f(l) \in \mathcal{K}, \\ ([\mathcal{K}], \phi_f(l)) & \text{if } \phi_i(l) \in \mathcal{K}, \phi_f(l) \in \nu(G) \setminus \mathcal{K}, \\ ([\mathcal{K}], [\mathcal{K}]) & \text{if } \phi_i(l), \phi_f(l) \in \mathcal{K}. \end{cases}$$

If $v \in \nu(G)$, then $v^{\mathcal{K}}$ will denote the corresponding vertex in $G(\mathcal{K})$.

Let $\mathcal{K}' = \{v_1, \ldots, v_{|\mathcal{K}'|}\}$ be a subset of $\nu(G)$ such that $|\{v_1^{\mathcal{K}}, \ldots, v_{|\mathcal{K}'|}^{\mathcal{K}}\}| \geq 2$. Then the symbol $G(\mathcal{K}|\mathcal{K}')$ denotes the graph

$$(G(\mathcal{K}))(\{v_1^{\mathcal{K}}, \ldots, v_{|\mathcal{K}'|}^{\mathcal{K}}\}),$$

obtained from the graph $G(\mathcal{K})$ by identifying the vertices $v_1^{\mathcal{K}}, \ldots, v_{|\mathcal{K}'|}^{\mathcal{K}}$. We define similarly $G(\mathcal{K}|\mathcal{K}'|\mathcal{K}'')$, and so on.

Let $H \subset G$ be a subgraph of G. For any $v \in \nu(G)$ define a number

$$D(v,H) = |\mathcal{S}(v) \cap \mathcal{L}(H)| + |\mathcal{L}(v) \cap \mathcal{L}(H)|.$$

A *path* P between two distinct vertices v_1 and v_2 is a minimal connected subgraph of G such that for any $v \in \nu(G)$

$$D(v,P) = \begin{cases} 0 \quad \text{or} \quad 2 & \text{if } v \neq v_1, v_2, \\ 1 & \text{if } v = v_1 \text{ or } v = v_2. \end{cases}$$

A *loop* C is a minimal connected nonempty subgraph of G such that for any $v \in \nu(G)$

$$D(v,C) = 0 \quad \text{or} \quad 2.$$

Let G be a graph. The *number of independent loops* of G will be denoted by $N(G)$. The numbers $|\nu(G)|$, $|\mathcal{L}(G)|$, $p(G)$, and $N(G)$ are related by the equation

$$N(G) = |\mathcal{L}(G)| + p(G) - |\nu(G)|.$$

From now on, the graph G will always denote a connected graph.

A subgraph $T_1 = T$ of G is called a 1-tree or a *tree* of G if $\nu(T) = \nu(G)$, $|\mathscr{L}(T)| = |\nu(G)| - 1$, $p(T) = 1$; i.e., if T connects all vertices of G to each other, and if $\mathscr{L}(T)$ does not form loops ($N(T) = 0$).

The set of all trees of G will be denoted by $\mathbb{T}_G$.

A subgraph T_r of G is called an *r-tree* of G if $\nu(T_r) = \nu(G)$, $|\mathscr{L}(T_r)| = |\nu(T_r)| - r, p(T_r) = r$, i.e., if T_r effects a partition of the vertices of G into r mutually disjoint sets any two vertices of the same set being connected in T_r, and if $\mathscr{L}(T_r)$ does not form loops.

The set of all 2-trees of G effecting a partition of the disjoint subsets $\mathcal{h}_1, \mathcal{h}_2$ of $\nu(G)$ from each other will be denoted by $\mathbb{T}_G(\mathcal{h}_1|\mathcal{h}_2)$.

A subgraph T_r' of G, related to some r-tree T_r of G as follows:

$$\begin{aligned}\nu(T_r') = \{v/v = \phi_i(l) \text{ or } v = \phi_f(l) \text{ for some } \\ l \in \mathscr{L}(G)\setminus\mathscr{L}(T_r)\},\\ \mathscr{L}(T_r') = \mathscr{L}(G)\setminus\mathscr{L}(T_r),\\ \phi_{T_r'} = \phi_{G/\mathscr{L}(T_r')},\end{aligned}$$

is called a *co-r-tree* of G. Among the various subsets of $\nu(G)$ we distinguish *the set $\mathcal{g}_G$ of all $|\mathcal{g}_G|$ external vertices*. If $\mathcal{h}_\varphi$ is a subset of $\mathcal{g}_G$, $\mathcal{h}_\varphi'$ will denote the complementary subset $\mathcal{g}_G \setminus \mathcal{h}_\varphi$ of $\mathcal{g}_G$.

Next, following Trute,[12] we introduce the concept of an *m-family* of subsets of $\mathcal{g}_G$ (the latter m stands for "momentum"):

A collection $\mathbb{H}_G$ of subsets $\mathcal{h}$ of $\mathcal{g}_G$ is called an m- family if it meets the following requirements:

(α) If $\mathcal{h}_1, \mathcal{h}_2 \in \mathbb{H}_G$, then either $\mathcal{h}_1 \subset \mathcal{h}_2$ or $\mathcal{h}_2 \subset \mathcal{h}_1$ or $\mathcal{h}_1 \cap \mathcal{h}_2 = \emptyset$;

(β) $\emptyset \notin \mathbb{H}_G$. If $\mathbf{F} \subset \mathbb{H}_G$, then $\mathcal{g}_G \setminus \bigcup_{\mathcal{h}\in\mathbf{F}} \mathcal{h} \notin \mathbb{H}_G$;

(γ) If $\mathcal{h} \in \mathbb{H}_G$, then $|\mathcal{h}| = |\bigcup_{\mathcal{h}_1 \in \mathbb{H}_G,\ \mathcal{h}_1 \subsetneq \mathcal{h}} \mathcal{h}_1| + 1$;

(δ) $\mathbb{H}_G$ is maximal.

Given an m-family $\mathbb{H}_G$, then the following statements are true:

(i) $|\mathbb{H}_G| = |\mathcal{g}_G|$;

(ii) $\mathcal{g}_G \in \mathbb{H}_G$;

(iii) Each $\mathcal{h} \in \mathbb{H}_G$ can be labeled by the unique vertex $v_\mathcal{h} \in \mathcal{g}_G$, which is contained in $\mathcal{h}$ and is not contained in any of its proper subsets from $\mathbb{H}_G$.

(iv) Each $v = v_\mathcal{h}$, $\mathcal{h} \in \mathbb{H}_G$, $\mathcal{h} \neq \mathcal{g}_G$ possesses a unique predecessor $v_{\hat{\mathcal{h}}}$ such that

$\mathcal{h} \subsetneq \hat{\mathcal{h}} \in \mathbb{H}_G$, $\hat{\mathcal{h}}$ is minimal.

III. DIAGONALIZATION OF THE RELEVANT QUADRATIC FORMS

The integrand of the Feynman-parametric integral corresponding to the (connected) Feynman graph G involves the external momenta by means of the quadratic form

$$V_G = U_G^{-1} \times \sum_{\{\mathcal{h},\mathcal{h}'\} = \mathcal{g}_G} W_G^{(\mathcal{h}|\mathcal{h}')} \times \left(\sum_{v\in\mathcal{h}} p_v\right)^2, \quad p_v \in \mathbb{R}^4,$$

$$\sum_{v\in\mathcal{g}_G} p_v = 0.$$

Here the quantities U_G and $W_G^{(\mathcal{h}|\mathcal{h}')}$ are defined by

$$U_G = \sum_{\mathbf{T}_1\in\mathbb{T}_G} \prod_{l\in T_1'} \alpha_l, \quad W_G^{(\mathcal{h}|\mathcal{h}')} = \sum_{T_2\in\mathbb{T}_G(\mathcal{h}|\mathcal{h}')} \prod_{l\in\mathbf{T}_2'} \alpha_l.$$

The quadratic form V_G can be diagonalized. In this context, Trute[12] derived the following important statement.

Let $\mathbb{H}_G$ be an arbitrary m-family of G. Let the elements of $\mathbb{H}_G$; $\mathcal{h}_i$, $i = 1,\ldots, |\mathcal{g}_G|$; $\mathcal{h}_{|\mathcal{g}_G|} = \mathcal{g}_G$ be ordered (in some arbitrary fashion) according to the index i. Define $G(v_{\mathcal{h}_0} v_{\hat{\mathcal{h}}_0})$ to be the graph G, denote the vertices of $G(v_{\mathcal{h}_1} v_{\hat{\mathcal{h}}_1} \ldots v_{\mathcal{h}_{i-1}} v_{\hat{\mathcal{h}}_{i-1}})$ by $v^{\mathcal{h}_1\cdots\mathcal{h}_{i-1}}$ and let W_{ij} stand for the following function (in the definition of $W^{(\ldots|\ldots)}_{G(\ldots|\ldots)}$ the sum extends over all 2-trees separating the indicated sets of external vertices)

$$W^{(v^{\mathcal{h}_1\cdots\mathcal{h}_i}, v^{\mathcal{h}_1\cdots\mathcal{h}_j}|v^{\mathcal{h}_1\cdots\mathcal{h}_i}, v^{\mathcal{h}_1\cdots\mathcal{h}_j})}_{G(v_{\mathcal{h}_1} v_{\hat{\mathcal{h}}_1}|\cdots|v_{\mathcal{h}_{i-1}} v_{\hat{\mathcal{h}}_{i-1}})} - W^{(v^{\mathcal{h}_1\cdots\mathcal{h}_i}, v^{\mathcal{h}_1\cdots\mathcal{h}_j}|v^{\mathcal{h}_1\cdots\mathcal{h}_j}, v^{\mathcal{h}_1\cdots\mathcal{h}_i})}_{G(v_{\mathcal{h}_1} v_{\hat{\mathcal{h}}_1}|\cdots|v_{\mathcal{h}_{i-1}} v_{\hat{\mathcal{h}}_{i-1}})}.$$

Then the following formula is valid:

$$V_G = \sum_{i=1}^{|\mathcal{g}_G|-1} \frac{U_{G(v_{\mathcal{h}_1} v_{\hat{\mathcal{h}}_1}|\cdots|v_{\mathcal{h}_i} v_{\hat{\mathcal{h}}_i})}}{U_{G(v_{\mathcal{h}_1} v_{\hat{\mathcal{h}}_1}|\cdots|v_{\mathcal{h}_{i-1}} v_{\hat{\mathcal{h}}_{i-1}})}} q_{\mathcal{h}_i}^2$$

with

$$q_{\mathcal{h}_i} = \sum_{v\in\mathcal{h}_i} p_v + \sum_{j>i}^{|\mathcal{g}_G|-1} \frac{W_{ij}}{U_{G(v_{\mathcal{h}_1} v_{\hat{\mathcal{h}}_1}|\cdots|v_{\mathcal{h}_i} v_{\hat{\mathcal{h}}_i})}} \sum_{v\in\mathcal{h}_j} p_v.$$

The transformation

$$\{p_1,\ldots p_{|\mathcal{g}_G|}\}/\sum_{v\in\mathcal{g}_G} p_v = 0 \to \{q_{\mathcal{h}_i}\}_{i=1,\ldots,|\mathcal{g}_G|-1}$$

is a nonsingular linear mapping of $\mathbb{R}^{4|\mathcal{g}_G|-4}$ onto $\mathbb{R}^{4|\mathcal{g}_G|-4}$ depending smoothly (C^∞), on the Feynman parameters α in the range $\alpha_l > 0$ for all $l \in \mathscr{L}(G)$.

In the preceding, we have employed a shorthand notation by writing, for instance, $G(v_{\mathcal{h}_1} v_{\hat{\mathcal{h}}_1}|\cdots|v_{\mathcal{h}_i} v_{\hat{\mathcal{h}}_i})$ instead of $G(\{v_{\mathcal{h}_1}, v_{\hat{\mathcal{h}}_1}\}|\cdots|\{v_{\mathcal{h}_i}, v_{\hat{\mathcal{h}}_i}\})$. In the sequel we shall continue to use this shorthand notation.

IV. SUBDIVISION OF THE INTEGRATION DOMAIN OF THE FEYNMAN PARAMETERS

Given a (connected) graph of G, $|\mathcal{g}_G| \neq 0$. Along with G consider the graph $G(\mathcal{g}_G)$

$$G(\mathcal{g}_G) = (\nu(G)\setminus\mathcal{g}_G \cup \{[\mathcal{g}_G]\}, \quad \mathscr{L}(G), \ \phi_{G(\mathcal{g}_G)}),$$

obtained from G by identifying all external vertices. We shall write

$$v_\infty = [\mathcal{g}_G].$$

Consider also the graphs $G(\mathcal{g}_G\setminus\{v\})$, $v \in \mathcal{g}_G$,

$$G(\mathcal{g}_G\setminus\{v\}) = (\nu(G)\setminus(\mathcal{g}_G\setminus\{v\}) \cup \{[\mathcal{g}_G\setminus\{v\}]\}, \mathscr{L}(G), \ \phi_{G(\mathcal{g}_G\setminus\{v\})}),$$

obtained from G by identifying all external vertices but one: v. We shall write

$$[\mathcal{g}_G\setminus\{v\}] = v_\infty(v) \quad \text{if} \quad \mathcal{g}_G\setminus\{v\} \neq \emptyset.$$

A subgraph H of G is said to be irreducible "in view of infinity" (I_∞) if the subgraphs $H(\varphi_G)$ and $H(\varphi_G \setminus \{v\})$ ($v \in \varphi_G \cap \nu(H)$) of $G(\varphi_G)$ and $G(\varphi_G \setminus \{v\})$ ($v \in \varphi_G \cap \nu(H)$), respectively satisfy

$$\nu(H(\varphi_G)) = \begin{cases} \nu(H) \setminus (\varphi_G \cap \nu(H)) \cap \{v_\infty\} & \text{if } \varphi_G \cap \nu(H) \neq \emptyset, \\ \nu(H) & \text{if } \varphi_G \cap \nu(H) = \emptyset, \end{cases}$$

and

$$\mathscr{L}(H(\varphi_G)) = \mathscr{L}(H), \quad \phi_{H(\varphi_G)} = \phi_{G(\varphi_G)|\mathscr{L}(H)},$$

and

$$\nu(H(\varphi_G \setminus \{v\})) = \begin{cases} \nu(H) \setminus ((\varphi_G \setminus \{v\}) \cap \nu(H)) \cup \{v_\infty(v)\}, & \text{if } (\varphi_G \setminus \{v\}) \cap \nu(H) \neq \emptyset, \\ \nu(H), & \text{if } (\varphi_G \setminus \{v\}) \cap \nu(H) = \emptyset, \end{cases}$$

and

$$\mathscr{L}(H(\varphi_G \setminus \{v\})) = \mathscr{L}(H), \phi_{H(\varphi_G \setminus \{v\})} = \phi_{G(\varphi_G \setminus \{v\})|\mathscr{L}(H)}$$

have the following properties:

(i) $H(\varphi_G)$ is one-line-irreducible,

(ii) none of the vertices contained in $\nu(H(\varphi_G)) \setminus \{v_\infty\}$ a cut-vertex of $H(\varphi_G)$,

(iii) $H(\varphi_G \setminus \{v\})$, $v \in \varphi_G \cap \nu(H)$ is connected, and

(iv) no vertex $v \in \varphi_G \cap \nu(H)$ is a cut-vertex of $H(\varphi_G \setminus \{v\})$.

Otherwise, H is called *reducible "in spite of infinity"* (R_∞). Next, we define an s_∞ *-family* $\mathbb{E}_\infty$ for G as a maximal collection of I_∞ -subgraphs H of G with the following properties (cf. Ref. 13):

($S_\infty - 0$) $\mathscr{L}(H) \neq \emptyset$.

($S_\infty - 1$) If $H, H' \in \mathbb{E}_\infty$, then either $H \subset H'$, $H' \subset H$, or $\mathscr{L}(H) \cap \mathscr{L}(H') = \emptyset$.

($S_\infty - 2$) If $H_1, \ldots, H_r \in \mathbb{E}_\infty$ and $\mathscr{L}(H_i) \cap \mathscr{L}(H_j) = \emptyset$ for any $i \neq j$, then $\cup_{i=1}^r H_i$ is R_∞.

Moreover, we define a labeled s_∞ -family for G to be a pair $(\mathbb{E}_\infty, \sigma_\infty)$ where $\mathbb{E}_\infty$ is an s_∞ -family for G and σ_∞ a mapping $\sigma_\infty : \mathbb{E}_\infty \to \mathscr{L}(G)$ satisfying

($S_\infty - 3$) $\sigma_\infty(H) \in \mathscr{L}(H)$.

($S_\infty - 4$) If $H' \in \mathbb{E}_\infty$ is a proper subset of $H \in \mathbb{E}_\infty$, then $\sigma_\infty(H) \notin \mathscr{L}(H')$.

The following statements can be proved along the lines of Ref. 20.

(i) For every $H \in \mathbb{E}_\infty$ there exists a line $l \in \mathscr{L}(H)$ not contained in $\mathscr{L}(H')$ for any $H' \in \mathbb{E}_\infty$, $H' \subsetneq H$.

(ii) $|\{H' \in \mathbb{E}_\infty / H' \subset H\}| = N(H(\varphi_G))$.

(iii) Every s_∞ -family $\mathbb{E}_\infty$ for a (connected graph G may be labeled, i.e., there exists a mapping $\sigma_\infty : \mathbb{E}_\infty \to \mathscr{L}(G)$ such that $(\mathbb{E}_\infty, \sigma_\infty)$ is a labeled s_∞ -family for G.

(iv) If $(\mathbb{E}_\infty, \sigma_\infty)$ is a labeled s_∞ -family for G, then $T_{|\varphi_G|} = T_{|\varphi_G|}(\mathbb{E}_\infty, \sigma_\infty); \{\nu(G), \mathscr{L}(G) \setminus \{\sigma_\infty(\mathbb{E}_\infty)\}, \phi_{G/\mathscr{L}(G) \setminus \{\sigma_\infty(\mathbb{E}_\infty)\}}\}$ is a $|\varphi_G|$-tree of G, each of the $|\varphi_G|$ connected components of $T_{|\varphi_G|}$ containing exactly one external vertex. Consequently $T = T(\mathbb{E}_\infty, \sigma_\infty) = (\nu(G) \setminus \varphi_G \cup \{v_\infty\}, \mathscr{L}(G) \setminus \{\sigma_\infty(\mathbb{E}_\infty)\}, \phi_{G(\varphi_G)/\mathscr{L}(G) \setminus \{\sigma_\infty(\mathbb{E}_\infty)\}})$ is a 1-tree of $G(\varphi_G)$.

(v) Consider the domain of integration of the Feynman parameters α_l, $l \in \mathscr{L}(G)$: $\{\underline{\alpha} = (\alpha_1, \ldots, \alpha_{|\mathscr{L}(G)|})/\alpha_l \geqslant 0$ for all $l \in \mathscr{L}(G)\}$.

If $(\mathbb{E}_\infty, \sigma_\infty)$ is a labeled s_∞ -family for G we define $\mathscr{D}_\infty = \mathscr{D}_\infty(\mathbb{E}_\infty, \sigma_\infty)$ to be the subset of the above integration domain given by $\mathscr{D}_\infty = \{\underline{\alpha}/\alpha_l \geqslant 0$ for all $l \in \mathscr{L}(G)$, $\alpha_l \leqslant \alpha_{\sigma_\infty}(H)$ for all $l \in \mathscr{L}(H)$, $H \in \mathbb{E}_\infty\}$.

Then it is true that:

(a) $\cup \mathscr{D}_\infty = \cup \mathscr{D}_\infty(\mathbb{E}_\infty, \sigma_\infty) = \{\alpha/\alpha_l \geqslant 0$ for all $l \in \mathscr{L}(G)\}$, where the union extends over all labeled s_∞ -families for G.

(b) $\mathscr{D}_\infty(\mathbb{E}_\infty, \sigma_\infty) \cap \mathscr{D}_\infty(\mathbb{E}'_\infty, \sigma'_\infty)$ has Lebesgue measure zero for any two distinct labeled s_∞ -families for G: $(\mathbb{E}_\infty, \sigma_\infty)$ and $(\mathbb{E}'_\infty, \sigma'_\infty)$.

(vi) Set $\mathbb{H}_\infty = \{H / H \in \mathbb{E}_\infty, N(H) = N(H - \{\sigma_\infty(H)\})$ and $N(H(\varphi_G)) = N(H(\varphi_G) - \{\sigma_\infty(H)\}) + 1\}$. There exists a mapping τ: $H \in \mathbb{H}_\infty \overset{\tau}{\underset{\tau^{-1}}{\leftrightarrow}} \aleph \in \mathbb{H}_G \setminus \{\varphi_G\}$ for some m-family $\mathbb{H}_G$ such that the partial sum of external momenta that flow through the line $\sigma_\infty(H)$ in the tree $(\nu(G), \mathscr{L}(G) \setminus \{\sigma_\infty(\mathbb{E}_\infty \setminus \mathbb{H}_\infty)\}, \phi_{G/\ldots})$ can be written as $\Sigma_{v \in \aleph} p_v$. The elements of $\mathbb{H}_G$ are totally ordered $\aleph_i$ $i = 1, \ldots, |\varphi_G| - 1$, $\aleph_{|\varphi_G|} = \varphi_G$: $j > i$ if $H_j = \tau^{-1}(\aleph_j) \supseteq H_i = \tau^{-1}(\aleph_i)$.

V. PARAMETRIZATION OF THE SUBDOMAINS OF α-INTEGRATION

For any line $l \in \mathscr{L}(G)$ we define H_l to be the minimal element of $\mathbb{E}_\infty$ containing the line l. With this notation the subset $\mathscr{D}_\infty$ of the domain of α-integration can be parametrized as follows:

$$\alpha_l = \begin{cases} \prod_{H' : \mathbb{E}_\infty \ni H' \supset H_l} t_{H'} & \text{if } l = \sigma_\infty(H) \text{ for some } H \in \mathbb{E}_\infty, \\ \beta_l \prod_{H' : \mathbb{E}_\infty \ni H' \supset H_l} t_{H'} & \text{if } l \neq \sigma_\infty(H) \text{ for any } H \in \mathbb{E}_\infty, \end{cases}$$

where $0 \leqslant t_G < \infty$, $0 \leqslant t_H \leqslant 1$ for any $H \in \mathbb{E}_\infty$, $H \neq G$, $0 \leqslant \beta_l \leqslant 1$, $l \neq \sigma_\infty(H)$ for any $H \in \mathbb{E}_\infty$ or, writing the symbol $\underline{t}$ for $(t_H)_{H \in \mathbb{E}_\infty, H \neq G}$ and the symbol $\underline{\beta}$ for $(\beta_l)_{l \neq \sigma_\infty(H), \forall H \in \mathbb{E}_\infty}$ $0 \leqslant t_G < \infty$, $(\underline{t}, \underline{\beta}) \in I^{|\mathscr{L}(G)| - 1}$ with $I = [0,1]$.

Now, arguing along the lines of Ref. 20, one finds in $\mathscr{D}_\infty$,

(i) $$U_G = \prod_{H \in \mathbb{E}_\infty} t^{N(H)} d^{(\mathbb{E}_\infty, \sigma_\infty)}_{G,0}(\underline{t}, \underline{\beta}),$$

$$\frac{U_{G(v_{\aleph_1} v_{\bar{\aleph}_1} | \cdots | v_{\aleph_{l-1}} v_{\bar{\aleph}_{l-1}})}}{U_{G(v_{\aleph_1} v_{\bar{\aleph}_1} | \cdots | v_{\aleph_l} v_{\bar{\aleph}_l})}} = \frac{U_{G(\{v_{\aleph_1}, \ldots, v_{\aleph_{l-1}}\})}}{U_{G(\{v_{\aleph_1}, \ldots, v_{\aleph_l}\})}} = \left(\prod_{\substack{H' \in \mathbb{E}_\infty \\ H' \supset H_l}} t_{H'} \right) e_{H_l}(\underline{t}, \underline{\beta}),$$

where

$$e_{H_l}(\underline{t}, \underline{\beta}) = \frac{d^{(\mathbb{E}_\infty, \sigma_\infty)}_{G,l}(\underline{t}, \underline{\beta})}{d^{(\mathbb{E}_\infty, \sigma_\infty)}_{G,l-1}(\underline{t}, \underline{\beta})}$$

and where

$$d^{(\mathbb{E}_\infty,\sigma_\infty)}_{G,i}(\underline{t},\underline{\beta}) = d^{(\mathbb{E}_\infty,\sigma_\infty)}_{G(\{v_{\lambda_1},\ldots,v_{\lambda_i}\})}(\underline{t},\underline{\beta}), \quad i = 0,\ldots,|\mathcal{P}_G| - 1$$

are polynomials in $\underline{t},\underline{\beta}$ larger than or equal to one for $(\underline{t},\underline{\beta}) \in I^{|\mathcal{L}(G)|-1}$;

(ii) the transformation

$$\{p_1,\ldots,p_{|\mathcal{P}_G|}\} / \sum_{v\in\mathcal{P}_G} p_v = 0 \to \{q_H = q_H(\underline{t},\underline{\beta})\}_{H\in\mathbb{H}_\infty} = \underline{q}(\underline{t},\underline{\beta}) = \underline{q},$$

$q_H = q_\lambda$ where $\lambda = \tau(H)$, $H\in\mathbb{H}_\infty$ is a nonsingular linear mapping of $\mathbb{R}^{4|\mathcal{P}_G|-4}$ onto $\mathbb{R}^{4|\mathcal{P}_G|-4}$ depending smoothly (i.e., in an infinite differential manner) on the parameters $\underline{t},\underline{\beta}$ for $(\underline{t},\underline{\beta})$ for $(t,\beta)\in I^{|\mathcal{L}(G)|-1}$.

Thus the quadratic form V_G in $\mathcal{D}_\infty$ is

$$V_G = -t_G E_{\underline{t},\underline{\beta}}(\underline{q}(\underline{t},\underline{\beta}),\underline{q}(\underline{t},\underline{\beta})),$$

$$E_{\underline{t},\underline{\beta}}(\underline{q},\underline{q}) = +\sum_{H\in\mathbb{H}_\infty}\left(\prod_{\substack{H'\in\mathbb{E}_\infty\setminus\{G\}\\ H'\supset H}} t_{H'}\right) e_H(\underline{t},\underline{\beta})(-q_H^2).$$

VI. ANALYTICALLY RENORMALIZED FEYNMAN AMPLITUDES

For the sake of simplicity and definiteness, we shall restrict our discussion to Feynman amplitudes occurring in the perturbation expansion of a $P(\phi)_4$ Lagrangian field theory describing a polynomial self-interaction of one sort of neutral scalar massive (m) particles in one time and three space dimensions. The generalization to theories involving massive particles with spin and derivative coupling in one time and arbitrarily many space dimensions is straightforward (cf., e.g., Ref. 12).

Consider a vertex graph G. Without loss of generality it may be assumed that G is irreducible. Set

$$v(G) = v,\ \mathcal{P}_G = \mathcal{P},\ \mathcal{L}(G) = \mathcal{L},\ N(G) = N.$$

With Speer[6] we associate with every line l of the vertex graph G a complex variable λ_l, $\underline{\lambda} = (\lambda_l)_{l\in\mathcal{L}}$, and modify the propagators according to

$$\frac{i}{(2\pi)^2}\frac{1}{k^2 - m^2 + i0} \to \frac{e^{i\pi\lambda}\Gamma(\lambda)}{i(2\pi)^2}[k^2 - m^2 + i0]^{-\lambda},$$

$$\Delta_F(x_{i(l)} - x_{f(l)};m) \to \Delta_F^{\lambda_l}(x_{i(l)} - x_{f(l)};m) = \mathcal{F}_k\left\{\frac{e^{i\pi\lambda_l}\Gamma(\lambda_l)}{i(2\pi)^2}[k^2 - m^2 + i0]^{-\lambda_l}\right\} \times (x_{i(l)} - x_{f(l)}).$$

This modification of the propagators results in the replacement of the amplitude

$$i^{|v|-1}\frac{(4\pi^2)^{|\mathcal{L}|+|\mathcal{P}|}4^N}{(4\pi^2)^{|v|+1}}\int\cdots\int\prod_{v\in v\setminus\mathcal{P}} d^4x_v \prod_{l\in\mathcal{L}}\Delta_F(x_{i(l)} - x_{f(l)};m),$$

which in general is ill-defined, by the analytically regularized amplitude

$$\mathcal{T}_{\underline{\lambda}}((x_v)_{v\in\mathcal{P}};m) = i^{|v|-1}\frac{(4\pi^2)^{|\mathcal{L}|+|\mathcal{P}|}4^N}{(4\pi^2)^{|v|+1}} \times\int\cdots\int\prod_{v\in v\setminus\mathcal{P}} d^4x_v\prod_{l\in\mathcal{L}}\Delta_F^{\lambda_l}(x_{i(l)} - x_{f(l)};m)$$

which is well-defined for $\underline{\lambda}\in\Omega_2 = \{\underline{\lambda}\,/\,\mathcal{R}e\lambda_l > 2 \text{ for all } l\in\mathcal{L}\}$.

In Ω_2 the Fourier transform of $\mathcal{T}_{\underline{\lambda}}$ can be expressed with the help of the parameters $\underline{t}$ and $\underline{\beta}$ as follows (cf. Ref. 7)

$$\tilde{\mathcal{T}}_{\underline{\lambda}}(\underline{p};m) = \sum\tilde{\mathcal{T}}^{\mathcal{D}}_{\underline{\lambda}^*}(\underline{p};m),$$

where

$$\tilde{\mathcal{T}}^{\mathcal{D}}_{\underline{\lambda}^*}(\underline{p};m) = \delta\left(\sum_{v\in\mathcal{P}} p_v\right)\prod_{l\in\mathcal{L}\setminus\{\sigma_\infty(\mathbb{E}_\infty)\}}\left[\int_0^1 d\beta_l\beta_l^{\lambda_l-1}\right] \times\prod_{H\in\mathbb{E}_\infty\setminus\{G\}}\left[\int_0^1 dt_H t_H^{\nu(H)-1}\right] \times\frac{\Gamma(\nu)}{[d(\underline{t},\underline{\beta})]^2}[E_{\underline{t},\underline{\beta}}(\underline{q}(\underline{t},\underline{\beta}),\underline{q}(\underline{t},\underline{\beta})) + m^2\sum_{l\in\mathcal{L}}(\alpha_l/\alpha_{\sigma_\infty(G)}) - i0]^{-\nu},$$

$\nu(H) = \Sigma_{l\in\mathcal{L}(H)}(\lambda_l - 1) + n(H)$, $n(H) = |\mathcal{L}(H)| - 2N(H)$, $\nu = \nu(G)$, $n = n(G)$ and where the sum extends over all labeled s_∞-families $(\mathbb{E}_\infty,\sigma_\infty)$ for G.

Using the fact that $[E_{\underline{t},\underline{\beta}}(\underline{q}(\underline{t},\underline{\beta}),\underline{q}(\underline{t},\underline{\beta})) + m^2\Sigma_{l\in\mathcal{L}}(\alpha_l/\alpha_{\sigma_\infty(G)}) - i0]^{-\nu}$ is an infinitely differentiable distribution-valued function of $\underline{t}$ and $\underline{\beta}$ as long as m is larger than zero, we may convince ourselves that

$$\prod_{H\in\mathbb{E}_\infty}\Gamma(\nu(H))^{-1}\tilde{\mathcal{T}}^{\mathcal{D}}_{\underline{\lambda}^*}(\underline{p};m)$$

is an entire distribution-valued function of $\underline{\lambda}$ for every labeled s_∞-family. Hence the distribution-valued function of $\underline{\lambda}$

$$\prod_H\Gamma\left(\sum_{l\in\mathcal{L}(H)}(\lambda_l - 1) + n(H)\right)^{-1}\tilde{\mathcal{T}}_{\underline{\lambda}}(\underline{p};m)$$

is an entire distribution-valued function of $\underline{\lambda}$ for every labeled s_∞-family. Hence the distribution-valued function of $\underline{\lambda}$

Speer's generalized evaluator $\mathcal{W} = \{\mathcal{W}_L / L = 1,2,\ldots\}$ is applicable to the amplitudes $\tilde{\mathcal{T}}_{\underline{\lambda}}(\underline{p};m)$. The result of the application $\mathcal{W}_{|\mathcal{L}|}\tilde{\mathcal{T}}_{\underline{\lambda}}(\underline{p};m)$ is the analytically renormalized Feynman amplitude of the vertex graph G contributing in $|v|$th order perturbation theory to the vertex function of the momenta carried by the "external lines" of G.

VII. ASYMPTOTIC EXPANSION OF ANALYTICALLY RENORMALIZED FEYNMAN AMPLITUDES

Now we are in the position to determine the complete asymptotic expansion of the (Λ-) parameter dependent distribution

$$\tilde{\mathcal{Z}}_\Lambda(\underline{p};m) = \mathcal{W}_{|\mathcal{L}|}\tilde{\mathcal{T}}_{\underline{\lambda}}(\Lambda\underline{p};m)$$

for Λ tending to plus infinity. By contrast to other authors having contributed to this subject, we do not discuss the asymptotic behavior in Λ of $\tilde{\mathcal{Z}}_\Lambda(\underline{p};m)$ pointwise, i.e., for a fixed configuration of the external momenta $(p_v)_{v\in\mathcal{P}}$. Instead, we establish the asymptotic behavior of the complex-valued function of Λ

$$\langle\tilde{\mathcal{Z}}_\Lambda,\tilde{\varphi}\rangle = \int d^{4|\mathcal{P}|}p\tilde{\varphi}(\underline{p})\tilde{\mathcal{Z}}_\Lambda(\underline{p};m)$$

for any $\tilde{\varphi}\in\mathcal{S}(\mathbb{R}^{4|\mathcal{P}|})$. At the first sight, this seems to complicate matters unnecessarily. For Minkowski metrics, however, the latter formulation of the problem turns out to be both adequate and helpful.

In order to establish the asymptotic expansion of the parameter-dependent distribution $\mathscr{F}_{\Lambda}(\underline{p};m)$ for Λ tending to plus infinity, it suffices to determine the asymptotic behavior of

$$[\Lambda^2]^{n+2}\mathscr{F}^{\mathscr{G}}_{\Lambda^\infty}(\underline{p};m) = [\Lambda^2]^{n+2}\mathscr{W}_{|\mathscr{L}|}\mathscr{T}^{\mathscr{G}}_{\underline{\lambda}^\infty}(\Lambda\underline{p};m) = \mathscr{W}_{\Lambda,|\mathscr{L}|}\mathscr{T}^{\mathscr{G}}_{\underline{\lambda}^\infty}(\underline{p};m/\Lambda) = \delta\Big(\sum_{v\in g} p_v\Big)\mathscr{W}_{|\mathscr{L}|}$$
$$\times\Bigg\{[\Lambda^2]^{-\sum_{l\in\mathscr{L}}(\lambda_l-1)}\Gamma(\nu)\prod_{l\in\mathscr{L}\setminus\{\sigma_\infty(\mathbb{E}_\infty)\}}\Big[\int_0^1 d\beta_l\beta_l^{\lambda_l-1}\Big]\prod_{H\in\mathbb{E}^-_\infty(G)}\Big[\int_0^1 dt_H t_H^{\nu(H)-1}\Big]$$
$$\times[E_{\underline{t},\underline{\beta}}(\underline{q}(\underline{t},\underline{\beta}),\underline{q}(\underline{t},\underline{\beta})) + e(\underline{t},\underline{\beta})m^2/\Lambda^2 - i0]^{-\nu}/[d(\underline{t},\underline{\beta})]^2\Bigg\}$$

for every labeled s_∞-family where we have set

$$e(\underline{t},\underline{\beta}) = e^{(\mathbb{E}_\infty,\sigma_\infty)}(\underline{t},\underline{\beta}) = \sum_{l\in\mathscr{L}}(\alpha_l/\alpha_{\sigma_\infty(G)})\geqslant 1$$

and

$$\mathscr{W}_{\Lambda,|\mathscr{L}|} = \mathscr{W}_{|\mathscr{L}|}[\Lambda^2]^{-\sum_{l\in\mathscr{L}}(\lambda_l-1)}.$$

Without loss of generality we may assume that $|\mathscr{L}|$ is larger than or equal to two.

The limit $\Lambda\to+\infty$ corresponds formally to the transition from the Feynman amplitude with massive lines to the Feynman amplitude (for the same vertex graph G) with massless lines. In the zero mass case, however, we are dealing with a complex power of a homogeneous quadratic form: $[E_{\underline{t},\underline{\beta}}(\underline{q}(\underline{t},\underline{\beta}),\underline{q}(\underline{t},\underline{\beta})) - i0]^{-\nu}$ which fails to be an infinitely differentiable function of $\underline{t}$ whenever and wherever the quadratic form $E_{\underline{t},\underline{\beta}}(\underline{q},\underline{q})$ degenerates. It is this lack of infinite differentiability which prevents us from finding the answer to our problem right away, and, moreover, forces us to introduce the subsets of α-space $\mathscr{D}_\infty = \mathscr{D}_\infty(\mathbb{E}_\infty,\sigma_\infty)$ instead of $\mathscr{D}(\mathbb{E},\sigma)$ (cf. Ref. 7).

In order to control the formation of the singularity under consideration, we convert the additive occurrence of $-q^2_H$ and m^2/Λ^2 in

$$\Bigg[+\sum_{H\in\mathbb{H}_\infty}\Bigg(\prod_{\substack{H'\in\mathbb{E}^\infty_+\setminus|G|\\H'\supset H}} t_{H'}\Bigg)e_H(\underline{t},\underline{\beta})(-q_H^2) + e(\underline{t},\underline{\beta})m^2/\Lambda^2 - i0\Bigg]^{-\nu}$$

into a multiplicative occurrence with the help of Mellin transforms. The result is

$$\Gamma(\nu)^{-1}\Big[\frac{\Lambda^2}{m^2e(\underline{t},\underline{\beta})}\Big]^{\nu}\prod_{H\in\mathbb{H}_\infty}\Bigg[\frac{1}{2\pi i}\int_{-\gamma_H+i\infty}^{-\gamma_H+i\infty}ds_H\Gamma(-s_H)\Bigg(\frac{e_H(\underline{t},\underline{\beta})\Lambda^2}{e(\underline{t},\underline{\beta})m^2}\prod_{H'\in\mathbb{E}^\infty_+(H)\setminus|G|}t_{H'}\Bigg)^{s_H}(-q_H^2-i0)^{s_H}\Bigg]\Gamma\Big(\nu+\sum_{H\in\mathbb{H}_\infty}s_H\Big),$$

where the γ_H's, $H\in\mathbb{H}_\infty$ are real numbers between zero and two.

Moreover, we have partly employed the following notation:
Let $\mathbb{G}_\infty$ be an arbitrary family of subgraphs of G. Then for a subgraph H of G we define

$$\mathbb{G}^+_\infty(H) = \{F/F\in\mathbb{G}_\infty, F\subset H\},$$
$$\mathbb{G}^-_\infty(H) = \{F/F\in\mathbb{G}_\infty, F\subsetneq H\},$$
$$\mathbb{G}^\infty_+(H) = \{F/F\in\mathbb{G}_\infty, F\supset H\},$$
$$\mathbb{G}^\infty_-(H) = \{F/F\in\mathbb{G}_\infty, F\supsetneq H\}.$$

For $\underline{\lambda}$ contained in a compact subset of $\Omega_{2(|\mathscr{L}|-1)} = \{\lambda/\mathscr{R}e\lambda_l > 2(|\mathscr{L}|-1)$ for all $l\in\mathscr{L}\}$ and for $(\underline{t},\underline{\beta})$ contained in $I^{|\mathscr{L}|-1}$, the integrations over s_H converge uniformly. In order to prove the uniform convergence, we note the identity

$$(-q^2-i0)^s = \frac{(-q^2-i0)^{s+j}}{[(s+1)\cdots(s+j+1)][(s+2)\cdots(s+j)]}\Big(-\frac{\Box_q}{4}\Big)^j$$

for any $j = 0,1,\ldots$. In view of this identity and the above Mellin representation we obtain

$$\Big(\prod_{H\in\mathbb{E}^-_\infty(G)}t_H^{\nu(H)-1}\Big)[E_{\underline{t},\underline{\beta}}(\underline{q},\underline{q}) + e(\underline{t},\underline{\beta})m^2/\Lambda^2 - i0]^{-\nu}$$
$$= \prod_{H\in\mathbb{H}_\infty}\Bigg[\frac{1}{2\pi i}\int_{-\gamma_H-i\infty}^{-\gamma_H+i\infty}ds_H\frac{\Gamma(-s_H-j_H-1)}{(s_H+2)\cdots(s_H+j_H)}\Bigg(\frac{\Lambda^2e_H(\underline{t},\underline{\beta})}{m^2e(\underline{t},\underline{\beta})}\prod_{H'\in\mathbb{E}^-_\infty(G)\cap\mathbb{E}^\infty_+(H)}t_{H'}\Bigg)^{s_H}(-q_H^2-i0)^{s_H+j_H}\Bigg]$$
$$\times\Gamma\Big(\nu+\sum_{H\in\mathbb{H}_\infty}s_H\Big)\Big(\prod_{F\in\mathbb{E}^-_\infty(G)}t_F^{\nu(F)-1}\Big)\frac{(-1)^{|\mathscr{L}|-1}}{\Gamma(\nu)}\Big[\frac{\Lambda^2}{m^2e(\underline{t},\underline{\beta})}\Big]^{\nu}\prod_{H\in\mathbb{H}_\infty}\Big(\frac{\Box_{q_H}}{4}\Big)^{j_H},$$

where the following estimate for $\gamma_H\neq-1, j_H\geqslant 2$, $H\in\mathbb{H}_\infty$ can be used

$$\left|\prod_{H\in\mathbb{H}_\cdot}\left[\frac{\Gamma(-s_H-j_H-1)}{(s_H+2)\cdots(s_H+j_H)}\left(\frac{\Lambda^2 e_H(\underline{t},\underline{\beta})}{m^2 e(\underline{t},\underline{\beta})}\prod_{H'\in\mathbb{E}_+^\infty(H)\cap\mathbb{E}_\infty^-(G)}t_{H'}\right)^{s_H}(-q_H^2-i0)^{s_H+j_H}\right]\Gamma\left(\nu+\sum_{H\in\mathbb{H}_\infty}s_H\right)\right|\prod_{F\in\mathbb{E}_\infty^-(G)}t_F^{\mathscr{R}e\,\nu(F)-1}$$

$$<\text{const}\times\left[1+\left|\sum_{H\in\mathbb{H}_\cdot}\eta_H\right|\right]^{\mathscr{R}e\,\nu-\Sigma\gamma_H-1/2}\prod_{H\in\mathbb{H}_\cdot}\frac{[1+\|q_H\|^2]^{j_H}}{[1+|\eta_H|]^{1/2-\gamma_H+2j_H}}$$

for $s_H=-\gamma_H+i\eta_H$.

In the pointwise discussion for Minkowski metrics, on the other hand, even in the case that *all* $q_H^2>0$, $H\in\mathbb{H}_\infty$, the corresponding s-integrations would not converge uniformly in $\underline{\lambda}$, $\underline{t}$, and $\underline{\beta}$ provided that $\mathscr{R}e\,\nu$ is larger than or equal to zero.

For $\underline{\lambda}\in\Omega_{2(|\varphi|-1)}$ we have shown the following representation to be valid

$$\tilde{\mathscr{T}}_{\underline{\lambda}}^{\mathscr{L}\cdot}(\Lambda\underline{p};m)=\delta\left(\sum_{v\in\varphi}p_v\right)\prod_{H\in\mathbb{H}_\cdot}\left[\frac{1}{2\pi i}\int_{-\gamma_H-i\infty}^{-\gamma_H+i\infty}ds_H\Gamma(-s_H)\Gamma(s_H+2)\right][\Lambda^2]^{\sum_{H\in\mathbb{E}_\cdot}s_H-2}g_{\underline{\lambda};\underline{s}}(\underline{p};\underline{m}),$$

where

$$g_{\underline{\lambda};\underline{s}}(\underline{p};m)=g_{\underline{\lambda};\underline{s}}^{(\mathbb{E}_\cdot,\sigma_\cdot)}(\underline{p};m)=\prod_{H\in\mathbb{E}_\cdot}\left[\Gamma(\nu(H)+\sum_{H'\in\mathbb{H}_\infty^-(H)}s_H)\right]h_{\underline{\lambda};\underline{s}}(\underline{p};m)$$

with the entire function of $\underline{\lambda}$ and $\underline{s}$

$$h_{\underline{\lambda};\underline{s}}(\underline{p};m)=h_{\underline{\lambda};\underline{s}}^{(\mathbb{E}_\cdot,\sigma_\cdot)}(\underline{p};m)=\prod_{l\in\mathscr{L}\setminus\{\sigma_\infty(\mathbb{E}_\infty)\}}\left[\int_0^1 d\beta_l\beta_l^{\lambda_l-1}\right]$$

$$\times\prod_{F\in\mathbb{E}_\infty^-(G)}\left[\Gamma\left(\nu(F)+\sum_{F'\in\mathbb{H}_\infty^-(F)}s_{F'}\right)^{-1}\int_0^1 dt_F t_F^{\{\nu(F)+\sum_{F'\in\mathbb{H}_\infty^-(F)}s_{F'}-1\}}\right][d(\underline{t},\underline{\beta})]^{-2}$$

$$\times[m^2e(\underline{t},\underline{\beta})]^{-\nu}\prod_{H\in\mathbb{H}_\cdot}\left[\left(\frac{e_H(\underline{t},\underline{\beta})}{m^2e(\underline{t},\underline{\beta})}\right)^{s_H}\Gamma(2+s_H)^{-1}(-q_H(\underline{t},\underline{\beta})^2-i0)^{s_H}\right]$$

and where the s-integrations converge uniformly for $\underline{\lambda}$ contained in any compact subset of $\Omega_{2(|\varphi|-1)}$. We define $K=K(\mathbb{E}_\infty,\sigma_\infty)$ to be the minimal element of $\mathbb{H}_\infty$ with the property $n(H)>0$ for every $H\in\mathbb{E}_+^\infty(K)$. Specializing to the quartic self-interaction and to vertex graphs "with more than two external lines" we notice that $n(H)$ is larger than or equal to zero for all $H\in\mathbb{E}_+^\infty(F)$, $F\in\mathbb{H}_\infty$. We shift some of the s-contours to the right and obtain

$$\prod_{H\in\mathbb{E}_\cdot}\left[\Gamma\left(\sum_{l\in\mathscr{L}(H)}(\lambda_l-1)+n(H)\right)^{-1}\right]\tilde{\mathscr{T}}_{\underline{\lambda}}^{\mathscr{L}\cdot}(\Lambda\underline{p};m)$$

$$=\sum_{F\in\mathbb{H}_\infty^+(K)}\delta\left(\sum_{v\in\varphi}p_v\right)\prod_{H\in\mathbb{H}_\infty^\infty(F)}\left[\frac{1}{2\pi i}\int_{-\gamma_H-i\infty}^{-\gamma_H+i\infty}ds_H\Gamma(-s_H)\Gamma(2+s_H)\right]\frac{1}{2\pi i}\int_{S_F-i\infty}^{S_F+i\infty}ds_F\Gamma(-s_F)\Gamma(2+s_F)$$

$$\times[\Lambda^2]^{\sum_{H\in\mathbb{H}_\infty^\infty(F)}s_H-2}\left\{\prod_{H'\in\mathbb{E}_\cdot}\left[\Gamma\left(\sum_{l\in\mathscr{L}(H')}(\lambda_l-1)+n(H')\right)^{-1}\right]g_{\underline{\lambda};\underline{s}}(\underline{p};m)\right\}_{/s_H=0,H\in\mathbb{H}_\infty^-(F)},$$

where $0<\gamma_H<1$, $0<\Sigma_{H\in\mathbb{H}^\infty(F)}\gamma_H<S_F<1$ for $F\in\mathbb{H}_\infty^-(K)$ and $0<\Sigma_{H\in\mathbb{H}^\infty(K)}\gamma_H-S_K<-S_K<1$. The s-integrations converge uniformly not only when $\underline{\lambda}$ varies over any compact subset of $\Omega_{2(|\varphi|-1)}$ but also after analytic continuation of the integrand when $\underline{\lambda}$ varies over any compact subset of $\Omega_{1-\epsilon}=\{\underline{\lambda}/\mathscr{R}e\,\lambda_l>1-\epsilon\text{ for all }l\in\mathscr{L}\}$. Thus, for the quartic self-interaction and vertex graphs "with more than two external lines"—we shall restrict the subsequent discussion to this case—we may continue $\tilde{\mathscr{T}}_{\underline{\lambda}}^{\mathscr{L}\cdot}(\Lambda\underline{p};m)$ analytically from $\Omega_{2(|\varphi|-1)}$ to a neighborhood of $\lambda_l=1$, $l\in\mathscr{L}$. Again in view of the uniform convergence of the above s-integrations, the generalized evaluator $\mathscr{W}_{|\mathscr{L}|}$ operates directly on the integrand:

$$\mathscr{W}_{|\mathscr{L}|}\tilde{\mathscr{T}}_{\underline{\lambda}}^{\mathscr{L}\cdot}(\Lambda\underline{p};m)=\sum_{F\in\mathbb{H}_\infty^+(K)}\tilde{\mathscr{T}}_{F;\mathscr{W}}^{\mathscr{L}\cdot}(\Lambda\underline{p};m).$$

The terms $\tilde{\mathscr{T}}_{F;\mathscr{W}}^{\mathscr{L}\cdot}(\Lambda\underline{p};m)$ stand for

$$\delta\left(\sum_{v\in\varphi}p_v\right)\frac{1}{2\pi i}\int_{\rho_{o(F)}-i\infty}^{\rho_{o(F)}+i\infty}dz_{o(F)}\cdots\frac{1}{2\pi i}\int_{\rho_2-i\infty}^{\rho_2+i\infty}dz_2\frac{1}{2\pi i}\int_{\rho_1-i\infty}^{\rho_1+i\infty}dz_1$$

$$\times\prod_{j=1}^{o(F)-1}[\Gamma(z_{j+1}-z_j)$$

$$\times\Gamma(2+z_j-z_{j+1})]\Gamma(-z_{o(F)})\Gamma(2+z_{o(F)})[\Lambda^2]^{z_1-2}$$

$$\times f_{z_1,\ldots,z_{o(F)}}^{(\mathscr{W})}(\underline{p};m)$$

with $o(F)=|\mathbb{H}_+^\infty(F)|$ and, further, with $1>\rho_{o(F)}>\cdots>\rho_2>\rho_1>0$ for $F\in\mathbb{H}_\infty^-(K)$ and $0>\rho_{0(K)}>\cdots>\rho_2>\rho_1>-1$ for $F=K$. We replaced the integration variables s_H and s_F by the new variables z_j, $1\leqslant j\leqslant o(F)$, defined by

$$z_j=\sum_{i=j}^{o(F)}s_{H_i}$$

after having enumerated the elements of $\mathbb{H}_\infty$ according to

the inverted previously introduced order, i.e.,

$$H_1 = \text{maximal element of } \mathbb{H}_\infty,$$

$$H_j = \text{maximal element of } \mathbb{H}_\infty^-(H_{j-1}) \quad j = 2,\ldots o(F).$$

Finally, $f^{(\mathscr{W})}_{z_1,\ldots,z_{o(F)}}(\underline{p};m)$ stands for

$$\mathscr{W}_{|\mathscr{L}|}\{g_{\underline{\lambda};s}(\underline{p};m)/_{s_H=0, H\in\mathbb{H}_\infty^-(F)}\},$$

a distribution-valued meromorphic function of z_j, $1\leqslant j\leqslant o(F)$, with poles at $z_j = -n_j, -n_j-1, -n_j-2,\ldots$, $n_j = n_j(\mathbb{E}_\infty,\sigma_\infty) = \min\{n(H)/H\in\mathbb{E}_j^\infty\}$ $j = 1,2,\ldots o(F)$ and

$$\mathbb{E}_j^\infty = \begin{cases} \mathbb{E}_+^\infty(H_j)\cap\mathbb{E}_\infty^-(H_{j-1}) & \text{for } j = 2,\ldots,o(F), \\ \mathbb{E}_+^\infty(H_1) & \text{for } j = 1. \end{cases}$$

The order of the pole at $z_j = -\mu_j, \mu_j = n_j, n_j+1, n_j+2,\ldots$, for every j separately, is at most equal to

$$|\mathbb{E}^\infty_{j,\mu_j}| + |\{H'/H'\in\mathbb{E}_\infty^-(H)\setminus\mathbb{E}_+^\infty(F)$$

for some

$$H\in\mathbb{E}^\infty_{j,\mu_j}, n(H')\leqslant 0\}|,$$

where

$$\mathbb{E}_{j,\mu_j} = \{H/H\in\mathbb{E}_j^\infty,\ n(H)\leqslant\mu_j\}.$$

We move the z_1-contour to the left and obtain

$$\tilde{\mathscr{T}}^{\mathscr{L}}_{F;\mathscr{H}}(\underline{\Lambda p};m)$$

$$= \sum_{\mu=\mu_0(F)}^{M}\frac{1}{2\pi i}\oint_{|z_1+\mu|=\epsilon} dz_1[\Lambda^2]^{z_1-2}\tilde{\mathscr{T}}^{\mathscr{L}}_{F;\mathscr{H}}{}^{;z_1}(\underline{p};m)$$

$$+\frac{1}{2\pi i}\int_{\rho-i\infty}^{\rho+i\infty} dz_1[\Lambda^2]^{z_1-2}\tilde{\mathscr{T}}^{\mathscr{L}}_{F;\mathscr{H}}{}^{z_1}(\underline{p};m)$$

for $F\in\mathbb{H}_\infty^+(K)$, any integer $M\geqslant\mu_0(F)$, $-(M+1)<\rho<-M$, $\epsilon>0$ sufficiently small. Here, for every $F\in\mathbb{H}_\infty^+(K)$, $\tilde{\mathscr{T}}^{\mathscr{L}}_{F;\mathscr{H}}{}^{;z_1}(\underline{p};m)$ is a distribution-valued meromorphic function of z_1 with poles at $z_1 = -\mu, \mu = -\mu_0(F), -\mu_0(F)-1, -\mu_0(F)-2,\ldots$.

$$\mu_0(F) = \mu_0(\mathbb{E}_\infty,\sigma_\infty;F) = \min_{1\leqslant j\leqslant o(F)}\{n_j + 2(j-1)\}$$

of order $m_\mu(F)$

$$m_\mu(F) = m_\mu(\mathbb{E}_\infty,\sigma_\infty;F) = \Big|\bigcup_{j=1}^{o(F)}\mathbb{E}^\infty_{j,\mu_j-2(j-1)}\Big|$$

for some $\quad + |\{H'/H'\in\mathbb{E}_\infty^-(H)\setminus\mathbb{E}_+^\infty(F)$

$$H\in\bigcup_{j=1}^{o(F)}\mathbb{E}^\infty_{j,\mu_j-2(j-1)}, n(H')\leqslant 0\}|$$

$$+\begin{cases} 1 & \text{if } \mu\geqslant 2(o(F)-1) \quad \text{for } F\in\mathbb{H}_\infty^-(K), \\ 1 & \text{if } \mu\geqslant 2o(K) \quad \text{for } F = K, \\ 0 & \text{otherwise.} \end{cases}$$

For $-\mu > \mathscr{R}ez_1 > -(\mu+1)$, $\tilde{\mathscr{T}}^{\mathscr{L}}_{F;\mathscr{H}}{}^{;z_1}(\underline{p};m)$ is given by

$$\delta\Big(\sum_{v\in\mathscr{V}}p_v\Big)\sum_{r=1}^{o(F)}\sum_{\mu_2=2}^{\mu-\theta(2)}(-1)^{\mu_2}(\mu_2-1)\cdots\sum_{\mu_r=2}^{\mu-\theta(r)-[\mu_2+\cdots+\mu_{r-1}]}(-1)^{\mu_r}$$

$$\times(\mu_r-1)!\frac{1}{2\pi i}\int_{\rho_{r-1}-i\infty}^{\rho_{r-1}+i\infty}dz_{r+1}\cdots\frac{1}{2\pi i}\int_{\rho_{o(F)}-i\infty}^{\rho_{o(F)}+i\infty}dz_{o(F)}$$

$$\times\Gamma([2+\mu_2+\cdots+\mu_r+z_1]-z_{r+1})$$

$$\times\Gamma(z_{r+1}-[\mu_2+\cdots+\mu_r+z_1])$$

$$\times\prod_{j=r+1}^{o(F)-1}[\Gamma(2+z_j-z_{j+1})\Gamma(z_{j+1}-z_j)]$$

$$\times\Gamma(2+z_{o(F)})\Gamma(-z_{o(F)})f^{(\mathscr{W})}_{z_1,\ldots,z_{o(F)}}(\underline{p};m)/_{\substack{z_2=\mu_2+z_1\\ \vdots\\ z_r=\mu_2+\cdots+\mu_r+z_1}}$$

with

$$\theta(j) = \begin{cases} 1 \text{ if } j\leqslant o(K) \\ 0 \text{ otherwise} \end{cases}$$

and

$$0<\theta(r+1)+\rho_{r+1}<1+\mu+\mathscr{R}ez_1,$$

$$0<\theta(r+1)+\rho_{r+1}<\cdots<\theta(o(F))+\rho_{o(F)}<+1.$$

This formula may be proved by induction on μ. As to the possible values of $\mu_0(F)$ we note the inequality

$$p(H)\leqslant j \quad \text{for} \quad H\in\mathbb{E}_j^\infty$$

and take into account the following relation valid for the ϕ_4^4-theory

$$n(H) = \frac{1}{2}\sum_{i=1}^{p(H)}\{\#[\text{external lines of } H_i] - 4\},$$

where the H_i's denote the connected components of H. From this we infer for the ϕ_4^4-theory

$$n_1 = n, \quad n_j\geqslant n+2-j, \quad j = 2,3,\ldots,o(F).$$

Actually, these relations are true for all monomial interactions apart from the cubic one. Hence $\mu_0(F) = \mu_0(\mathbb{E}_\infty,\sigma_\infty;F)$ is equal to n for all $F\in\mathbb{H}_\infty^+(K)$ and all labeled s_∞-families $(\mathbb{E}_\infty,\sigma_\infty)$ for G. Moreover, the order of the poles at $z_1 = -\mu = -n, -n-1, -n-2,\ldots$ of

(i) $\sum_{F\in\mathbb{H}_\infty^+(K)}\tilde{\mathscr{T}}^{\mathscr{L}}_{F;\mathscr{H}}{}^{;z_1}(\underline{p};m)$ is equal to $m_\mu(\mathbb{E}_\infty,\sigma_\infty)$

$$= \operatorname{Max}_{F\in\mathbb{H}_\infty^+(K)} m_\mu(\mathbb{E}_\infty,\sigma_\infty;F)$$

(ii) $\sum_{(\mathbb{E}_\infty,\sigma_\infty)}\sum_{F\in\mathbb{H}_\infty^+(K)}\tilde{\mathscr{T}}^{\mathscr{L}}_{F;\mathscr{H}}{}^{;z_1}(\underline{p};m) = \tilde{\mathscr{T}}^{z_1}_{\mathscr{H}}(\underline{p};m)$ is equal to

$$m_\mu = \operatorname{Max}_{(\mathbb{E}_\infty,\sigma_\infty)} m_\mu(\mathbb{E}_\infty,\sigma_\infty).$$

Now, we have all the necessary information at hand to write down the asymptotic expansion for the analytically renormalized Feynman amplitude $\mathscr{W}_{|\mathscr{L}|}\tilde{\mathscr{T}}_{\underline{\lambda}}(\underline{\Lambda p};m)$ of the vertex graph G:

$$\sum_{\mu=n}^{M}\sum_{\kappa=0}^{m_\mu-1}[\Lambda^2]^{-\mu-2}[\ln\Lambda^2]^\kappa\tilde{\mathscr{T}}^{(\mathscr{H})}_{\mu,\kappa}(\underline{p};m) + \mathscr{R}_m$$

with

$$\tilde{\mathscr{T}}^{(\mathscr{H})}_{\mu,\kappa}(\underline{p};m) = \frac{1}{\kappa!}\frac{1}{2\pi i}\oint_{|z_1+\mu|=\epsilon}dz_1(z_1+\mu)^\kappa\tilde{\mathscr{T}}^{z_1}_{\mathscr{H}}(\underline{p};m)$$

and

$$\mathscr{R}_M = \frac{1}{2\pi i}\int_{\rho-i\infty}^{\rho+i\infty}dz_1[\Lambda^2]^{z_1-2}\tilde{\mathscr{T}}^{z_1}_{\mathscr{H}}(\underline{p};m),$$

where $-(M+1)<\rho<-M$.

If the number of "external lines" is equal to two (and $|\mathscr{P}| = 2$) we adopt the same procedure as before with the only difference that in the beginning we push the s-contour further to the right. In this way we obtain

$$\mathscr{W}\tilde{\mathscr{T}}_{\underline{\lambda}}(\underline{\Lambda p};m) = [\Lambda^2]^{-1}\delta(p_1+p_2)$$

$$\times\frac{1}{2\pi i}\oint_{|s-1|=\epsilon}ds\frac{\pi(s+1)}{\sin\pi(s-1)}$$

$$\{[\Lambda^2]^{s-1}\mathscr{W}_{g\underline{\lambda};s}(\underline{p};m) - \mathscr{W}g_{\underline{\lambda};1}(p;m)\} - [\Lambda^2]^{-2}$$

$$\times\delta(p_1+p_2).$$

$$\frac{1}{2\pi i}\oint_{|s|=\epsilon} ds \frac{\pi(s+1)}{\sin \pi s}\{[\Lambda^2]^s \mathscr{W} g_{\underline{\lambda};s}(\underline{p};m) - \mathscr{W} g_{\underline{\lambda};o}(\underline{p};m)\}$$
$$+ \sum_{\mu=1}^{M} \delta(p_1+p_2)\frac{1}{2\pi i}\oint_{|s+\mu|=\epsilon} ds\, \Gamma(2+s)\Gamma(-s)[\Lambda^2]^{s-2}$$
$$\times \mathscr{W} g_{\underline{\lambda};s}(\underline{p};m)$$
$$+ \delta(p_1+p_2)\frac{1}{2\pi i}\int_{\rho-i\infty}^{\rho+i\infty} ds \Gamma(2+s)\Gamma(-s)[\Lambda^2]^{s-2}$$
$$\times \mathscr{W} g_{\underline{\lambda};s}(\underline{p};m)$$

for any positive integer M, $-(M+1)<\rho<-M$ and $\epsilon>0$ sufficiently small,

$$\mathscr{W} \equiv \mathscr{W}_{|\mathscr{L}|}.$$

The order of the pole of the integrand at $s=-\mu$, $\mu=-1,0,1,2,\ldots$ is equal to

$$1-\delta_{\mu,1} + |\{H/H\in\mathbb{E}_\infty, \mathscr{G}\subset\mathscr{C}(H),\ n(H)\leqslant\mu\}|$$
$$+ |\{H/H\in\mathbb{E}_\infty, \mathscr{G}\not\subset\mathscr{C}(H),\ n(H)\leqslant 0\}|.$$

Now, the asymptotic expansion in powers of Λ^{-2} and $\ln\Lambda^2$ of the Feynman amplitude corresponding to G which contributes in $|\mathscr{C}|$th order perturbation theory to the two point vertex function can be read off easily.

An arbitrary number j of mass insertions can be incorporated into the above scheme by partitioning j in all possible ways into a sum of $|\mathscr{L}|$ non-negative integers $j_1,\ldots,j_{|\mathscr{L}|}$ replacing the propagator of the line l in the amplitude $\mathscr{T}_{\underline{\lambda}}(\Lambda\underline{p};m)$

$$\frac{e^{i\pi\lambda_l}\Gamma(\lambda_l)}{i(2\pi)^2}[k_l^2-m^2+i0]^{-\lambda_l}$$

by

$$(m^2)^{j_l}\frac{\exp(i\pi\Sigma_{\nu=1}^{j_l+1}\lambda_{l,\nu})\Pi_{\nu=1}^{j_l+1}\Gamma(\lambda_{l,\nu})}{[i(2\pi)^2]^{j_l+1}}$$
$$\times[k_l^2-m^2+i0]^{-\Sigma_{\nu=1}^{j_l+1}\lambda_{l,\nu}}$$

multiplying subsequently by the combinatorial factor $j!/j_1!\cdots j_l!$, summing over all different partitions and applying finally an appropriate generalized evaluator $\mathscr{W}_{|\mathscr{L}|+j}$.

ACKNOWLEDGMENT

The author profited from numerous discussions with the late Dr. H. Trute.

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Representation of the active Lorentz transformation for particle dynamics

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(Received 9 December 1981; accepted for publication 23 July 1982)

The rank-2 tensor representation of a passive Lorentz transformation constructed by Krause solely from the four-velocities of two inertial observers is shown to lack sufficient generality to describe unambiguously the active Lorentz transformation completely specifying the dynamic change of a classical particle from an initial state to a later state. This lack of uniqueness is traced to an arbitrary three-parameter little group transformation. For states described both by their four-vector momentum and polarization, we construct a rank-2 tensor representation of the active Lorentz transformation, connecting initial and later states, which is constructed solely from initial and later momenta and polarizations. This representation now contains a single arbitrary parameter. A unique active Lorentz transformation is achieved by further specification of an additional four-vector associated with the initial and later states.

PACS numbers: 11.30.Cp

I. INTRODUCTION

Recently, Krause[1] has displayed a proper orthochronous Lorentz transformation connecting an initial four-vector velocity p_μ with a final four-vector velocity P_μ, such transformation being a rank-2 tensor constructed solely from these four-vectors themselves. The Krause transformation, which satisfies $L_{\mu\nu}(P,p)\,p^\nu = P_\mu$, may be written

$$L_{\mu\nu}(P,p) = g_{\mu\nu} - [1+(pP)]^{-1} \times\{p_\mu p_\nu + P_\mu P_\nu + p_\mu P_\nu - [1+2(pP)]P_\mu p_\nu\}, \tag{1}$$

where the metric $g_{\mu\nu}$ has a signature (-2), the notation (pP) signifies $p_\pi P^\pi$ where Greek indices run over the range 0–3, and $(pp) = (PP) = 1$. Krause further went on to show that his transformation could be factorized into two Lorentz space-time reflections,

$$L_{\mu\nu}(P,p) = R_\mu{}^\pi(p\leftrightarrow P)\mathscr{R}_{\pi\nu}(P),$$

where

$$\mathscr{R}_{\pi\nu}(P) = g_{\pi\nu} - 2[1-(pP)^2]^{-1} \times [P_\pi - (pP)p_\pi]\,[P_\nu - (pP)p_\nu], \tag{2}$$

so that $\mathscr{R}_{\pi\nu}(P)p^\nu = p_\pi$ and

$$R_{\mu\pi}(p\leftrightarrow P) = g_{\mu\pi} - [1-(pP)]^{-1} \times (p_\mu - P_\mu)(p_\pi - P_\pi), \tag{3}$$

so that $R_{\mu\pi}(p\leftrightarrow P)\,P^\pi = p_\mu$.

For particle dynamics, instead of considering p,P as four-velocities of different inertial observers, one may take p as the particle's initial dimensionless four-vector energy/momentum (hereafter called simply the four-vector momentum) and P (possibly space-time dependent) as the particle's later dimensionless four-vector momentum. In this case, one might be tempted to interpret the Krause transformation as the active local Lorentz transformation which contains all the relevant dynamic information. However, the change in a single timelike four-vector, $p\to P$ does not uniquely specify a Lorentz transformation, so the Krause transformation is too restrictive to play the role of the required active dynamic transformation. In this paper, we investigate forms of rank-2 tensors that may serve as the active dynamic transformation.

II. LITTLE GROUP TRANSFORMATION

Before describing dynamical changes of momentum four-vectors in terms of the associated Lorentz transformation operator, we will briefly discuss those proper Lorentz transformation operators $\mathscr{O}^{\mu\nu}$, known as the "little group" operators,[2] that leave the four-vector momentum invariant:

$$\mathscr{O}^\mu{}_\nu\, p^\nu = p^\mu. \tag{4}$$

As is well known, such operators are just the compounded result of an initial Lorentz transformation without rotation to the rest system (accomplished with a relative velocity $\vec{\beta} = -\vec{p}/p^0$ between the lab and rest frames of reference), followed by a pure spatial rotation about some axis $\hat{W}_{\rm rest}$ in the rest system, after which another Lorentz transformation without rotation is performed that is the inverse of the initial one. This procedure yields the result

$$\mathscr{O}^{\mu\nu}(W,\omega;p) = g^{\mu\nu} + (1-\cos\omega)(p^\mu p^\nu - W^\mu W^\nu - g^{\mu\nu}) + (\sin\omega)\epsilon^{\mu\nu\lambda\pi}p_\lambda W_\pi. \tag{5}$$

The four-vector W^μ is the lab four-vector whose rest-system representation is $(0;\hat{W}_{\rm rest})$ and whose significance is that $\hat{W}_{\rm rest}$ is the axis of the spatial rotation. The parameter ω is the angle of rotation about that axis in the rest system, and $\epsilon^{\mu\nu\lambda\pi}$ is the completely antisymmetric tensor with $\epsilon_{0213}\equiv 1$ satisfying the relation

$$\epsilon_{\mu\lambda\xi\eta}\epsilon^{\nu\pi\alpha\beta} = -\det\begin{pmatrix} g_\mu{}^\nu & g_\mu{}^\pi & g_\mu{}^\alpha & g_\mu{}^\beta \\ g_\lambda{}^\nu & g_\lambda{}^\pi & g_\lambda{}^\alpha & g_\lambda{}^\beta \\ g_\xi{}^\nu & g_\xi{}^\pi & g_\xi{}^\alpha & g_\xi{}^\beta \\ g_\eta{}^\nu & g_\eta{}^\pi & g_\eta{}^\alpha & g_\eta{}^\beta \end{pmatrix}. \tag{6}$$

From its definition, the "rotation axis" four-vector W^μ is spacelike and orthogonal to the four-vector momentum,

$$W^\mu W_\mu = -1, \quad W^\mu p_\mu = 0, \tag{7}$$

and is also an eigenvector of the little group operator

$$\mathscr{O}^\mu{}_\nu W^\nu = W^\mu. \tag{8}$$

 0022-2488/82/122520-04$02.50

[Here, we have suppressed the functional dependence of $\mathcal{O}^{\mu}{}_{\nu}$].

For completeness we present the additional two eigenvectors of the little group operator. Defining the unnormalizing nonidentically 0 four-vectors

$$\begin{aligned} X^{\lambda} &\equiv \epsilon^{\lambda\pi\xi\eta} d_{\pi} p_{\xi} W_{\eta}, \\ Y^{\lambda} &\equiv d^{\lambda} + W^{\lambda}(Wd) - p^{\lambda}(pd), \end{aligned} \tag{9}$$

where d_{π} is some four-vector that is not a linear combination of p_{π} and W_{π} (so $X^{\lambda} \neq 0$) but is otherwise arbitrary, it follows that these together with p_{π} and W_{π} constitute an orthogonal vierbein

$$\begin{aligned} &p_{\lambda} X^{\lambda} = W_{\lambda} X^{\lambda} = 0, \\ &P_{\lambda} Y^{\lambda} = W_{\lambda} Y^{\lambda} = 0, \quad X_{\lambda} Y^{\lambda} = 0. \end{aligned} \tag{10}$$

It is easily shown that

$$\begin{aligned} &\epsilon^{\mu\nu\alpha\beta} p_{\nu} W_{\alpha} X_{\beta} = -Y^{\mu}, \\ &\epsilon^{\mu\nu\alpha\beta} p_{\nu} W_{\alpha} Y_{\beta} = X^{\mu}, \\ &\epsilon^{\mu\nu\alpha\beta} p_{\nu} X_{\alpha} Y_{\beta} = \delta W^{\mu}, \\ &\epsilon^{\mu\nu\alpha\beta} W_{\nu} X_{\alpha} Y_{\beta} = \delta p^{\mu}, \end{aligned} \tag{11}$$

where

$$\delta \equiv (dd) + (Wd)^2 - (pd)^2 = X^{\lambda} X_{\lambda} = Y^{\lambda} Y_{\lambda}. \tag{12}$$

The linear combinations, $X^{\lambda} \pm iY^{\mu}$, which are null-vectors, are the other two eigenvectors of the little group operator,

$$\mathcal{O}^{\mu}{}_{\nu}(X^{\nu} \pm iY^{\nu}) = e^{\pm i\omega}(X^{\mu} \pm iY^{\mu}). \tag{13}$$

Finally, we note that instead of using the "rotation axis" four-vector W^{μ}, the little group operator may be parameterized in terms of the antisymmetric tensor[3]

$$N^{\alpha\beta} \equiv \epsilon^{\alpha\beta\mu\lambda} W_{\mu} p_{\lambda}. \tag{14}$$

The little group operator becomes simply

$$\mathcal{O}^{\mu\nu} = g^{\mu\nu} + (1 - \cos\omega) N^{\mu\lambda} N_{\lambda}{}^{\nu} - (\sin\omega) N^{\mu\nu}. \tag{15}$$

It can be directly established that $N^{\alpha\beta}$ satisfies the following relations

$$\begin{aligned} &N^{\mu\nu} W_{\nu} = 0 = N^{\mu\nu} p_{\nu}, \\ &\epsilon_{\mu\nu\lambda\pi} N^{\mu\nu} N^{\lambda\xi} = 0, \\ &N^{\lambda\mu} N_{\mu\nu} N^{\nu\pi} = -N^{\lambda\pi}, \\ &N^{\alpha\beta} N_{\alpha\beta} = 2. \end{aligned} \tag{16}$$

The most general proper orthochronous Lorentz transformation $\Lambda_{\mu\nu}$ that carries $p \to P$ may be constructed by compounding the Krause transformation with the little group operator

$$\Lambda_{\mu\nu} = L_{\mu}{}^{\pi}(P,p) \mathcal{O}_{\pi\nu}(W,\omega;p), \tag{17}$$

since it is obvious that $\Lambda_{\mu\nu} p^{\nu} = P_{\mu}$. This transformation contains three additional parameters: the two independent parameters of W_{μ} (note the constraints $W_{\mu} W^{\mu} = -1$, $W_{\mu} p^{\mu} = 0$), and the rotation angle ω.

In the next section, for nonzero spin particles, we construct an alternative active Lorentz transformation that carries the particle from some initial state to a later state.

III. LORENTZ TRANSFORMATION CONNECTING INITIAL AND LATER MOMENTUM AND POLARIZATION STATES

Consider a particle whose initial state is characterized by a four-vector momentum p_{μ} and a four-vector polarization[4] s_{μ}, which satisfy constraints

$$(pp) = -(ss) = 1, \quad (sp) = 0. \tag{18}$$

[Note: It is the little group transformation $\mathcal{O}_{\mu\nu}(W,\omega;p)$ that in general changes the four-vector polarization leaving the four-vector momentum invariant]. Now, suppose at some latter time the four-vector momentum and polarization are P_{μ} and S_{μ}, respectively, where

$$(PP) = -(SS) = 1, \quad (SP) = 0. \tag{19}$$

Using just the four-vectors p, s, P, and S, we will now attempt to construct a rank-two tensor that represent an active Lorentz transformation connecting initial and final states. In formulating this tensor, we will assume that these four-vectors are linearly independent. [Upon obtaining our results, this condition may be relaxed by a suitable limiting process.] Thus, we take

$$\epsilon_{\mu\nu\rho\pi} s^{\mu} P^{\nu} S^{\rho} P^{\pi} \equiv k \neq 0. \tag{20}$$

Using the product algebra of two uncontracted epsilons, this linear independence condition may alternatively be written

$$\begin{aligned} k^2 = {} & (sS)^2 + (pP)^2 - (sP)^2 - (pS)^2 - 1 \\ & - [(pS)(sP) - (pP)(sS)]^2 > 0. \end{aligned} \tag{21}$$

We now take the desired Lorentz transformation to be of the form

$$\begin{aligned} L_{\mu\nu} = \{ & g_{\mu\nu} + A_1 p_{\mu} p_{\nu} + A_2 P_{\mu} P_{\nu} + A_3 s_{\mu} s_{\nu} + A_4 S_{\mu} S_{\nu} \\ & + A_5 p_{\mu} P_{\nu} + A_6 p_{\mu} s_{\nu} + A_7 p_{\mu} S_{\nu} + A_8 P_{\mu} p_{\nu} \\ & + A_9 P_{\mu} s_{\nu} + A_{10} P_{\mu} S_{\nu} + A_{11} s_{\mu} p_{\nu} + A_{12} s_{\mu} P_{\nu} \\ & + A_{13} s_{\mu} S_{\nu} + A_{14} S_{\mu} p_{\nu} + A_{15} S_{\mu} P_{\nu} + A_{16} S_{\mu} s_{\nu} \}, \end{aligned} \tag{22}$$

where the sixteen A coefficients are to be determined. For convenience, a factor of $g_{\mu\nu}$ has been explicitly written, although it could be subsumed into a redefinition of the A coefficient since it may be shown that

$$\begin{aligned} g_{\mu\nu} = k^{-2} \{ & [(sS)^2 - (sP)^2 - 1] p_{\mu} p_{\nu} \\ & + [(sS)^2 - (pS)^2 - 1] P_{\mu} P_{\nu} \\ & + [1 + (pS)^2 - (pP)^2] s_{\mu} s_{\nu} \\ & + [1 + (sP)^2 - (pP)^2] S_{\mu} S_{\nu} \\ & + [(pP) + \Delta(sS)](p_{\mu} P_{\nu} + P_{\mu} p_{\nu}) \\ & + [(sP)(pP) - (sS)(pS)](p_{\mu} s_{\nu} + s_{\mu} p_{\nu}) \\ & - [(pS) + \Delta(sP)](p_{\mu} S_{\nu} + S_{\mu} p_{\nu}) \\ & - [(sP) + \Delta(pS)](P_{\mu} s_{\nu} + s_{\mu} P_{\nu}) \\ & + [(pS)(pP) - (sS)(sP)](P_{\mu} S_{\nu} + S_{\mu} P_{\nu}) \\ & + [(sS) + \Delta(pP)](s_{\mu} S_{\nu} + S_{\mu} s_{\nu}) \}, \end{aligned} \tag{23}$$

where

$$\Delta \equiv (pS)(sP) - (pP)(sS). \tag{24}$$

Substituting Eq. (22) into the necessary relations

$$L^{\mu}{}_{\nu} P^{\nu} = P^{\mu}, \quad L^{\mu}{}_{\nu} s^{\nu} = S^{\mu}, \tag{25}$$

as well as into the inverse relations

$$L^{\mu}{}_{\nu}\, P_{\mu} = p_{\nu}, \quad L^{\mu}{}_{\nu} S_{\mu} = s_{\nu}\,, \tag{26}$$

and equating the coefficients of the independent basis vectors to 0, after considerable algebraic manipulation these sixteen equations yield ten independent linear relations among the A coefficients:

$$\begin{aligned}
A_1 &= -1 - (pP)A_5 - (pS)A_7\,,\\
A_2 &= -1 - (pP)A_5 - (sP)A_{12},\\
A_3 &= 1 + (sP)A_{12} + (sS)A_{13}\,,\\
A_4 &= 1 + (pS)A_7 + (sS)A_{13},\\
A_6 &= (sP)A_5 + (sS)A_7,\\
A_8 &= \{1 + (pP)[1 + (pP)A_5 + (sP)A_{12}]\\
&\quad + (pS)[(pP)A_7 + (sP)A_{13}]\},\\
A_9 &= \{-(sP)[1 + (pP)A_5 + (sP)A_{12}]\\
&\quad - (sS)[(pP)A_7 + (sP)A_{13}]\}\,,\\
A_{10} &= -(pP)A_7 - (sP)A_{13},\\
A_{11} &= -(pP)A_{12} - (pS)A_{13},\\
A_{14} &= \{-(pS)[1 + (pP)A_5 + (pS)A_7]\\
&\quad - (sS)[(pP)A_{12} + (pS)A_{13}]\},\\
A_{15} &= (pS)A_5 + (sS)A_{12}\,,\\
A_{16} &= \{-1 + (sS)[1 + (sP)A_{12} + (sS)A_{13}]\\
&\quad + (pS)[(sP)A_5 + (sS)A_7]\}\,.
\end{aligned} \tag{27}$$

From these relations, all the A coefficients are given in terms of the four coefficients A_5, A_7, A_{12}, and A_{13}. Additional quadratic relationships are derivable from the quadratic condition $g_{\nu\pi} = L^{\mu}{}_{\nu} L_{\mu\pi}$ which is symmetric in its free indices. Substituting Eq. (22) into this quadratic condition, and equating the coefficients of the independent tensor basis (which are direct products of the four-vectors p, s, P, and S), we obtain ten additional quadratic relations among the A's. Upon substitution of the linear equations given in Eq. (27), one finds after much algebra that the ten quadratic equations yield just three independent quadratic relations among the coefficients A_5, A_7, A_{12} and A_{13}. These independent quadratic relations are

$$\begin{aligned}
&\{[(pS)A_5 + (sS)A_{12}]^2 - [(pP)A_5 + (sP)A_{12} + 1]^2\\
&\quad + (A_5)^2 - (A_{12})^2\} = 0,\\
&\{[(pS)A_7 + (sS)A_{13} + 1]^2 - [(pP)A_7 + (sP)A_{13}]^2\\
&\quad + (A_7)^2 - (A_{13})^2\} = 0\,,\\
&\{[(pS)A_5 + (sS)A_{12}][(pS)A_7 + (sS)A_{13} + 1]\\
&\quad - [(pP)A_7 + (sP)A_{13}][(pP)A_5 + (sP)A_{12} + 1]\\
&\quad + A_5A_7 - A_{12}A_{13}\} = 0.
\end{aligned} \tag{28}$$

Thus, we see that the requirement that the Lorentz transformation connect the initial four-vector momentum and four-vector polarization with later specification of these quantities [Eq. (25] does not uniquely determine the coefficients of the Lorentz transformation, but leaves one parameter still to be chosen. This nonuniqueness of the Lorentz transformation will be discussed in the next section.

We now display one relatively simple set of coefficients that are consistent with Eqs. (27) and (28) and involve the choice of an additional relationship. This special set is

$$\begin{aligned}
&A_5 = A_8 = -A_1 = -A_2 = [1 + (sS)]/D,\\
&A_3 = A_4 = -A_{13} = -A_{16} = [1 - (pP)]/D,\\
&A_6 = A_{10} = -A_7 = -A_9 = (sP)/D,\\
&A_{11} = A_{15} = -A_{12} = -A_{14} = (pS)/D\,,
\end{aligned} \tag{29}$$

where

$$D \equiv 1 - (pP) + (sS) + \Delta\,, \tag{30}$$

in which Δ has the same definition given in Eq. (24). Via Eq. (22), the Lorentz transformation involving this special set of coefficients is

$$\begin{aligned}
L_{\mu\nu} = g_{\mu\nu} &- D^{-1}[1 + (sS)](p_{\mu} - P_{\mu})(p_{\nu} - P_{\nu})\\
&+ D^{-1}[1 - (pP)](s_{\mu} - S_{\mu})(s_{\nu} - S_{\nu})\\
&+ D^{-1}(sP)(p_{\mu} - P_{\mu})(s_{\nu} - S_{\nu})\\
&+ D^{-1}(pS)(s_{\mu} - S_{\mu})(p_{\nu} - P_{\nu})\,.
\end{aligned} \tag{31}$$

One may explicitly verify that this indeed is a proper transformation (det = 1), by showing that $\epsilon_{\mu\nu\rho\pi} L^{\mu 0} L^{\nu 1} L^{\rho 2} L^{\pi 3} = \epsilon^{0123}$.

The Lorentz transformation displayed in Eq. (31) leaves invariant the four-vector

$$[1 + (sS)](P^{\mu} + p^{\mu}) - (sP)S^{\mu} - (pS)s^{\mu}\,, \tag{32}$$

as well as the four-vector

$$(pS)P^{\mu} + (sP)p^{\mu} + [1 - (pP)](S^{\mu} + s^{\mu})\,. \tag{33}$$

Thus, this Lorentz transformation represents a "rotation" in the two-flat orthogonal to these four-vectors.

It will now be shown that $L_{\mu\nu}$ [Eq. (31)] reduces to $g_{\mu\nu}$ in an appropriate limiting process as $P_{\mu} \to p_{\mu}$ and $S_{\mu} \to s_{\mu}$. If we write

$$\begin{aligned}
P_{\mu} &= p_{\mu} + \epsilon q_{\mu} + \epsilon^2 r_{\mu},\\
S_{\mu} &= s_{\mu} + \lambda t_{\mu} + \lambda^2 w_{\mu},
\end{aligned} \tag{34}$$

where ϵ, λ are infinitesimals, and q_{μ}, r_{μ}, t_{μ}, w_{μ} are finite, then the constraints $(PP) = 1 = -(SS)$, $(PS) = 0$, imply the relationships

$$\begin{aligned}
&(pq) = 0, \quad (st) = 0,\\
&2(pr) + (qq) = 0, \quad 2(sw) + (tt) = 0,\\
&\lambda(pt) + \epsilon(sq) = 0, \quad \epsilon\lambda(qt) + \lambda^2(pw) + \epsilon^2(rs) = 0\,.
\end{aligned} \tag{35}$$

Thus, it follows that

$$\begin{aligned}
&[1 - (pP)] = -\epsilon^2(pr)\,,\\
&[1 + (sS)] = \lambda^2(sw),\\
&(sP) = \epsilon(sq) + \epsilon^2(sr),\\
&(pS) = \lambda(pt) + \lambda^2(pw)\,,\\
&D = -\epsilon^2\lambda^2(pr)(sw) + \epsilon\lambda[(sq) + \epsilon(sr)][(pt) + \lambda(pw)]\,.
\end{aligned} \tag{36}$$

We see that if $(sq) \neq 0$ [so that also $(pt) \neq 0$], then D is second order in infinitesimals, but the numerator for $L_{\mu\nu} - g_{\mu\nu}$ is either third order [(sP) and (pS) terms] or fourth order [the other terms], hence as $\epsilon \to 0$, $\lambda \to 0$, $L_{\mu\nu} \to g_{\mu\nu}$.

IV. FREE PARAMETER DESCRIPTION AND SPECIFICATION

As already mentioned, the Lorentz transformation $L_{\mu\nu}$ [Eq. (31)] involving the special set of coefficients is not the most general one connecting initial and later momentum and polarization states. The most general transformation effecting this connection involves an additional free parameter. A simple way of introducing such a parameter is by employing the little group operator $\mathscr{O}^{\mu\nu}(W,\omega;p)$ displayed in Eq. (5). If, consistent with the constraints $(WW) = -1$, $(pW) = 0$, one takes the initial polarization s as W itself, then adopting the notation $\mathscr{O}^{\mu\nu}(s,\omega;p) \equiv \mathscr{O}^{\mu\nu}(\omega)$ in which the initial state specification is suppressed, it trivally follows that

$$\mathscr{O}^{\mu\nu}(\omega)p_\nu = p^\mu, \quad \mathscr{O}^{\mu\nu}(\omega)s_\nu = s^\mu . \tag{37}$$

Thus

$$\begin{aligned} &\{L_{\mu\pi}\,\mathscr{O}^{\pi}{}_{\nu}(\omega)\}\,p^\nu = P_\mu , \\ &\{L_{\mu\pi}\,\mathscr{O}^{\pi}{}_{\nu}(\omega)\}s^\nu = S_\mu , \end{aligned} \tag{38}$$

where (in this section) L refers to the transformation displayed in Eq. (31). Hence, by the group property of Lorentz transformation, the product $\{L_{\mu\pi}\,\mathscr{O}^{\pi}{}_{\nu}(\omega)\}$, involving both a free parameter ω and tensor products of the initial and later four-momentum and four-polarization components, produces an active Lorentz transformation that connects initial and later momentum and polarization states.

One may tie down the parameters ω by requiring that the active transformation connects an independent initial four-vector b to its later state B, i.e.,

$$\{L_{\mu\pi}\,\mathscr{O}^{\pi}{}_{\nu}(\omega)\}b^\nu = B_\mu , \tag{39}$$

or equivalently,

$$\mathscr{O}_{\lambda\nu}(\omega)b^\nu = B^\mu L_{\mu\lambda} . \tag{40}$$

For convenience, we take

$$(bb) = 1, \quad (pb) = (sb) = 0, \tag{41}$$

so that

$$(BB) = 1, \quad (PB) = (SB) = 0 . \tag{42}$$

Then, substitution of the explicit forms of $\mathscr{O}_{\lambda\nu}(\omega)$ and $L_{\mu\nu}$ into Eq. (40) yields the relation

$$\begin{aligned} &[(\cos\omega)b_\lambda + (\sin\omega)f_\lambda] \\ &\quad = \{B_\lambda - D^{-1}[1 + (sS)](pB)[p_\lambda - P_\lambda] \\ &\qquad + D^{-1}[1 - (pP)](sB)[s_\lambda - S_\lambda] \\ &\qquad + D^{-1}(sP)(pB)[s_\lambda - S_\lambda] \\ &\qquad + D^{-1}(pS)(sB)[p_\lambda - P_\lambda]\} , \end{aligned} \tag{43}$$

where

$$f_\lambda \equiv \epsilon_{\lambda\nu\alpha\beta}b^\nu p^\alpha s^\beta \tag{44}$$

and D has been defined in Eq. (30). Invoking the basis $p_\lambda, s_\lambda, b_\lambda, f_\lambda$, we may write

$$\begin{aligned} B_\lambda &= (pB)p_\lambda - (sB)s_\lambda + (bB)b_\lambda + (fB)f_\lambda , \\ P_\lambda &= (pP)p_\lambda - (sP)s_\lambda + (bP)b_\lambda + (fP)f_\lambda , \\ S_\lambda &= (pS)p_\lambda - (sS)s_\lambda + (bS)b_\lambda + (fS)f_\lambda . \end{aligned} \tag{45}$$

Substituting this into Eq. (43), we may verify that the coefficients of the basis components p_λ, s_λ vanish on the right-hand side, and the parameter ω is given via the expressions

$$\begin{aligned} (\cos\omega) &= (B_\alpha\, T^{\alpha\beta}b_\beta) , \\ (\sin\omega) &= (B_\alpha\, T^{\alpha\beta}f_\beta) . \end{aligned} \tag{46}$$

In the preceding, the tensor $T^{\alpha\beta}$ is defined by

$$\begin{aligned} T^{\alpha\beta} \equiv{}& g^{\alpha\beta} + D^{-1}p^\alpha\{[1 + (sS)]P^\beta - (sP)S^\beta\} \\ &- D^{-1}s^\alpha\{[1 - (pP)]S^\beta + (pS)P^\beta\} . \end{aligned} \tag{47}$$

Alternatively, we may write the results in the form

$$\begin{aligned} (\cos\omega) &= 1 + D^{-1}\epsilon_{\lambda\nu\alpha\beta}(B^\nu - b^\nu) \\ &\quad \times (P^\alpha - p^\alpha)(S^\beta - s^\beta)f^\lambda , \\ (\sin\omega) &= -D^{-1}\epsilon_{\lambda\nu\alpha\beta}(B^\nu - b^\nu) \\ &\quad \times (P^\alpha - p^\alpha)(S^\beta - s^\beta)b^\lambda . \end{aligned} \tag{48}$$

It is straightforward, but tedious, to verify that these expressions satisfy the necessary condition $(\sin\omega)^2 + (\cos\omega)^2 = 1$.

In conclusion, we see that the active Lorentz transformation connecting the initial and later states is uniquely specified if the transformation of an additional four-vector attribute, besides the four-vector momentum and polarization, is given.

ACKNOWLEDGMENT

This work was supported by the U. S. Department of Energy, Division of Chemical Sciences, under Contract No. DE-AC02-80ER10669.

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What happens to the position, spin, and parity when the mass goes to zero

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(Received 16 March 1982; accepted for publication 30 July 1982)

The unitary transformation to the helicity form and the limit of zero mass are examined in terms of the position, spin, parity and time-reversal operators for an irreducible unitary representation of the Poincaré group for positive mass. The position, spin, parity and time-reversal operators do not change as the mass goes to zero, but if the space of particle states becomes smaller as the Poincaré group is reduced to a separate representation for each helicity, the position and spin operators, which are not reduced, will no longer be defined on the particle states. Since the parity operator connects states of opposite helicity, it will be defined on the particle states if they have paired plus and minus helicities.

PACS numbers: 11.30.Cp, 11.30.Er

1. INTRODUCTION

The way we describe a particle changes as we move from classical mechanics and nonrelativistic quantum mechanics to relativistic quantum mechanics, and the change is most evident when we get to particles with zero mass. In nonrelativistic quantum mechanics, the position variable still plays a central role, in the wave functions and in defining operators such as the orbital angular momentum, the corresponding spin part of the angular momentum, and the parity operator. In relativistic quantum mechanics, the Newton–Wigner position[1–3] can be made to play a similar role for particles with positive mass, but for particles with zero mass there is no Newton–Wigner position operator,[1,2,4,5] no spin operator,[6–8] and the parity operator hardly resembles reflection of the position variable in a wave function.[9]

To see how this happens, we examine two equivalent descriptions of a particle with positive mass in relativistic quantum mechanics. In the form developed by Foldy,[10] an irreducible unitary representation of the Poincaré group for positive mass consists of operators on wave functions of the Newton–Wigner position variable and spin. The position, spin, parity and time-reversal operators are all the same as in nonrelativistic quantum mechanics. The nonrelativistic limit is directly available. We call this the position form.

We examine in some detail the unitary transformation from the position form to the helicity form developed by Moses,[11] focusing on the transformation of the position, spin, parity and time-reversal operators. From the helicity form we can see immediately what happens in the limit of zero mass.

The position, spin, parity and time-reversal operators are not changed as the mass goes to zero. In the generators for the Poincaré group, there is no change in the momentum or angular momentum, and only the obvious change in the Hamiltonian, but there is one important change in the Lorentz generator which causes the representation of the Poincaré group to be reduced to a separate representation for each helicity. If the space of particle states is then a smaller space corresponding to fewer helicity values, the position and spin operators will no longer be defined on the space of particle states, because they are not reduced to separate operators on any such subspace. Thus, what is needed for a particle with zero mass to have position and spin operators the same as for a particle with positive mass is simply that the particle states include the same helicities for zero mass as for positive mass: for example, for spin 1, helicities $1, 0, -1$; for spin $1/2$, helicities $1/2, -1/2$. That this is not so for the particles with zero mass found in nature suggests that position and spin are not as important as earlier ways of describing particles have made them appear.

The situation is similar for parity. The parity operator connects states for opposite helicities, so what is needed for the parity operator to be defined on the space of particle states is simply that the particle states have paired plus and minus helicity values.

2. POSITION FORM

We consider an irreducible unitary representation of the Poincaré group with positive mass m, spin s, and positive energy.[6] We use units such that c and $\hbar$ are 1.

Let $\vec{P}$ denote the generator for space translations. The generator for time translations is

$$H = (\vec{P}^2 + m^2)^{1/2}. \tag{2.1}$$

In the position form developed by Foldy[10] the generators for rotations and Lorentz transformations are

$$\vec{J} = \vec{Q} \times \vec{P} + \vec{S}, \tag{2.2}$$

$$\vec{K} = (1/2)(H\vec{Q} + \vec{Q}H) + (H + m)^{-1}\vec{P} \times \vec{S}. \tag{2.3}$$

We use wave functions $\psi(\vec{x})$ with $2s + 1$ components on which $\vec{P}$ and $\vec{Q}$ act as $-i\nabla$ and multiplication by $\vec{x}$ and S_1, S_2, S_3 are the usual $(2s + 1) \times (2s + 1)$ irreducible spin matrices for spin s. The $2s + 1$ components $\psi_\lambda(\vec{x})$ of $\psi(\vec{x})$ are labeled by the eigenvalues $\lambda = -s, -s + 1, \ldots s$ of the diagonal matrix S_3. The inner product is

$$(\psi, \phi) = \sum_{\lambda=-s}^{s} \int d^3\vec{x}\, \psi_\lambda(\vec{x})^* \phi_\lambda(\vec{x}). \tag{2.4}$$

The parity and time-reversal operators are given by

$$(P\psi)(\vec{x}) = \eta\psi(-\vec{x}), \tag{2.5}$$

$$(T\psi)(\vec{x}) = e^{i\pi S_2}\psi(\vec{x})^*, \tag{2.6}$$

where the "intrinsic parity" η is a phase factor (that is a complex number such that $|\eta|$ is 1). These operators are

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unique to within phase factors because, to fit in with the transformations of the Poincaré group, P must be linear, commute with H and $\vec{J}$, and anticommute with $\vec{P}$ and $\vec{K}$, and T must be antilinear (anticommute with i), commute with H and $\vec{K}$, and anticommute with $\vec{P}$ and $\vec{J}$.[12]

The Newton–Wigner position operator[1–3] is $\vec{Q}$. It is the unique Hermitian operator with commuting components that transforms as a position operator should for space translations and rotations and time reversal and allows Lorentz transformations that are at least not completely wrong in the nonrelativistic limit.[3]

With this form for the generators of the Poincaré group, the position, spin, parity and time-reversal operators are the same as in nonrelativistic quantum mechanics. The nonrelativistic limit yields rather directly[3] the generators of the Galilei group used in nonrelativistic quantum mechanics. The relativistic Hamiltonian (2.1) becomes the nonrelativistic Hamiltonian

$$H = m + \vec{P}^2/2m, \tag{2.7}$$

and the Lorentz generator (2.3) becomes the Galilei generator

$$\vec{G} = m\vec{Q}. \tag{2.8}$$

Everything else remains unchanged.

We use the Fourier decomposition

$$\psi(\vec{x}) = \sum_{\lambda=-s}^{s} \int d^3\vec{p}\, f_\lambda(\vec{p})(2\pi)^{-3/2} e^{i\vec{p}\cdot\vec{x}} |\lambda\rangle\,, \tag{2.9}$$

where $f_\lambda(\vec{p})$ is a complex function representing ψ and the $|\lambda\rangle$ are the orthonormal eigenvectors of S_3 that are the basis vectors for the spin matrices, specifically

$$|-s\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix},\quad |-s+1\rangle = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ 0 \end{pmatrix},\quad \cdots |s\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

We write $|\vec{p},\lambda\rangle$ for $(2\pi)^{-3/2}e^{i\vec{p}\cdot\vec{x}}|\lambda\rangle$, and

$$\vec{P}\,|\vec{p},\lambda\rangle = \vec{p}\,|\vec{p},\lambda\rangle, \tag{2.10}$$

$$S_3|\vec{p},\lambda\rangle = \lambda\,|\vec{p},\lambda\rangle. \tag{2.11}$$

In terms of these we have

$$P\,|\vec{p},\lambda\rangle = \eta|-\vec{p},\lambda\rangle, \tag{2.12}$$

$$T\,|\vec{p},\lambda\rangle = e^{i\pi S_2}|-\vec{p},\lambda\rangle = (-1)^{\lambda+s}|-\vec{p},-\lambda\rangle. \tag{2.13}$$

3. HELICITY FORM

By making a unitary transformation, which we will discuss in more detail later, we can change each operator from the position form to the helicity form developed by Moses.[11] The unitary transformation commutes with $\vec{P}$, so the translation generator $\vec{P}$ and the Hamiltonian H given by (2.1) are not changed. The generators for rotations and Lorentz transformations are changed to

$$U^\dagger\vec{J}U = \vec{Q}\times\vec{P} + \vec{M}S_3, \tag{3.1}$$

$$U^\dagger\vec{K}U = (1/2)(H\vec{Q} + \vec{Q}H) + H|\vec{P}|^{-1}\vec{N}S_3 - m|\vec{P}|^{-1}(\vec{E}_2S_1 - \vec{E}_1S_2), \tag{3.2}$$

where

$$\vec{M} = (P_1/[|\vec{P}| + P_3], P_2/[|\vec{P}| + P_3], 1) = (|\vec{P}|\hat{z} + \vec{P})/[|\vec{P}| + \vec{P}\cdot\hat{z}], \tag{3.3}$$

$$\vec{N} = (P_2/[|\vec{P}| + P_3], -P_1/[|\vec{P}| + P_3], 0) = \vec{P}\times\hat{z}/[|\vec{P}| + \vec{P}\cdot\hat{z}], \tag{3.4}$$

$$\vec{E}_1 = (P_1P_2/|\vec{P}|[|\vec{P}| + P_3], -P_1^2/|\vec{P}|[|\vec{P}| + P_3] - P_3/|\vec{P}|, P_2/|\vec{P}|), \tag{3.5}$$

$$\vec{E}_2 = (P_2^2/|\vec{P}|[|\vec{P}| + P_3] + P_3/|\vec{P}|, -P_1P_2/|\vec{P}|[|\vec{P}| + P_3], -P_1/|\vec{P}|). \tag{3.6}$$

The vectors $\vec{E}_1$, $\vec{E}_2$ and $\hat{P} = \vec{P}/|\vec{P}|$ are orthonormal and $\hat{P}\times\vec{E}_1$ is $\vec{E}_2$, etc. Since

$$\vec{P}\cdot\vec{M} = |\vec{P}|\,, \tag{3.7}$$

we have

$$U^\dagger\hat{P}\cdot\vec{J}U = \hat{P}\cdot U^\dagger\vec{J}U = S_3\,. \tag{3.8}$$

The unitary transformation diagonalizes the helicity by changing it to the diagonal matrix S_3.

The position is changed to

$$U^\dagger\vec{Q}U = \vec{Q} + |\vec{P}|^{-1}\vec{N}S_3 - |\vec{P}|^{-1}(\vec{E}_2S_1 - \vec{E}_1S_2). \tag{3.9}$$

This is the Newton–Wigner position operator in the helicity form. The spin is changed to

$$U^\dagger\vec{S}U = \vec{E}_1S_1 + \vec{E}_2S_2 + \hat{P}S_3. \tag{3.10}$$

Since the generators $\vec{J}$ and $\vec{K}$ are the functions (2.2) and (2.3) of $\vec{Q}$, $\vec{P}$, H and $\vec{S}$, the transformations (3.1) and (3.2) of $\vec{J}$ and $\vec{K}$ can be calculated from the transformations (3.9) and (3.10) of $\vec{Q}$ and $\vec{S}$ and the fact that $\vec{P}$ and H are not changed. For this it is helpful to use

$$\vec{N}\times\hat{P} = \vec{M} - \hat{P} \tag{3.11}$$

together with the properties of $\vec{E}_1,\vec{E}_2,\hat{P}$ already mentioned. Conversely, $\vec{Q}$ and $\vec{S}$ can be written as functions of the generators $\vec{P},H,\vec{J},\vec{K}$ and the unitary transformations of $\vec{Q}$ and $\vec{S}$ can be calculated from the transformations of the generators.[3]

For the parity and time-reversal operators we get

$$U^\dagger PU\,|\vec{p},\lambda\rangle = \eta(-1)^{\lambda-s}e^{i\pi\lambda}e^{i2\phi(\hat{p})\lambda}\,|-\vec{p},-\lambda\rangle, \tag{3.12}$$

$$U^\dagger TU\,|\vec{p},\lambda\rangle = e^{-i\pi\lambda}e^{-i2\phi(\hat{p})\lambda}\,|-\vec{p},\lambda\rangle, \tag{3.13}$$

where

$$\phi(\hat{p}) = \tan^{-1}(p_y/p_x) \tag{3.14}$$

is the usual cylindrical angle of $\vec{p}$.

4. ZERO MASS

The limit as the mass m goes to zero is easily obtained from the helicity form. The Hamiltonian (2.1) becomes

$$H = (\vec{P}^2)^{1/2} = |\vec{P}|.$$

The last term in the formula (3.2) for $U^\dagger\vec{K}U$ goes to zero. There are no other changes in the operators we have written in the helicity form.

The representation of the Poincaré group is reduced to a separate representation for each helicity λ. None of the generators $\vec{P},H,U^\dagger\vec{J}U,U^\dagger\vec{K}U$ connects states with different he-

licities. They are all diagonal as far as the helicity is concerned because they depend only on the diagonal matrix S_3 and not on the nondiagonal matrices S_1 and S_2. The same is true for the time-reversal operator $U^\dagger TU$.

The parity operator $U^\dagger PU$ connects states with opposite helicities $\lambda = \pm|\lambda|$. If parity is important, as it evidently is for photons, the space of particle states includes two irreducible unitary representations of the Poincaré group for opposite helicities so the parity operator is defined on the space of particle states. If parity is not important, as is evidently the case for neutrinos, the space of particle states may include just one irreducible unitary representation of the Poincaré group for just one value of helicity so there is no parity operator on the space of particle states.

The position and spin operators $U^\dagger\vec{Q}U$ and $U^\dagger\vec{S}U$ are not reduced at all. They depend on the nondiagonal matrices S_1 and S_2. They connect states will all the different helicities $\lambda = -s, -s+1, \ldots s$. The irreducible unitary representations of the Poincaré group for all these helicities have to be included in the space of particle states to have the position and spin operators defined on the space of particle states.

This would be true in a trivial way if s were zero. A particle with zero mass and zero helicity would have a Newton–Wigner position operator the same as for a particle with positive mass. This is the only possibility for a particle with zero mass to have a Newton–Wigner position operator when the space of particle states includes just one irreducible unitary representation of the Poincaré group for just one helicity value.

There is another unique possibility when s is 1/2. If both helicities $\lambda = \pm 1/2$ are included in the particle states, the position and spin operators are defined on the space of particle states. A particle with zero mass and spin 1/2 would have position and spin operators the same as for a particle with positive mass if it had both plus and minus helicity. This is the only possibility for a particle with zero mass to have a Newton–Wigner position operator when the space of particle states includes just two irreducible unitary representations of the Poincaré group for two opposite helicities.[1,2,5]

For every kind of particle with zero mass that has been found in nature, the particle states evidently do not include all the helicities $\lambda = -s, -s+1, \ldots s$ so the position and spin operators are not defined on the space of particle states. Mathematically, there are possibilities for particles with zero mass to have position variables the same as for particles with positive mass, but these possibilities are not realized in nature. This may be an indication that position variables are not as important in nature as they have been in our concept of a particle.

What happens to the position, spin, and parity operators when the mass goes to zero? Nothing. They are not changed at all. But the space of particle states is pulled out from under them and reduced to a smaller space that is sometimes too small for the parity operator and evidently always too small for the position and spin operators.

5. UNITARY TRANSFORMATION

The transformation from the position form to the helicity form is made by the unitary operator[13]

$$U = e^{-i\theta(\hat{P})\hat{z}\wedge\hat{P}\cdot\vec{S}}e^{i(\pi/2)S_3}, \tag{5.1}$$

where

$$\theta(\hat{P}) = \cos^{-1}(P_3/|\vec{P}|), \tag{5.2}$$

is the usual spherical coordinate of $\vec{P}$ and $\hat{z}\wedge\hat{P}$ is the unit vector in the direction of $\hat{z}\times\hat{P}$.

We can see that U commutes with $\vec{P}$, so $\vec{P}$ and H are not changed by the unitary transformation.

Let $R(\hat{P})$ be the rotation through the angle $\theta(\hat{P})$ around the axis $\hat{z}\wedge\hat{P}$, so that

$$R(\hat{P})\hat{z} = \hat{P}. \tag{5.3}$$

We will use the fact that

$$\begin{aligned} R(\hat{P})\hat{x} &= \vec{E}_2(\hat{P}), \\ R(\hat{P})\hat{y} &= -\vec{E}_1(\hat{P}). \end{aligned} \tag{5.4}$$

This is easy to verify. We know, or can easily check, that $\vec{E}_1$ and $\vec{E}_2$ are orthogonal unit vectors perpendicular to $\hat{P}$, with

$$\vec{E}_1\times\vec{E}_2 = \hat{P}. \tag{5.5}$$

The same is true for $R(\hat{P})\hat{x}$ and $R(\hat{P})\hat{y}$. Therefore $R(\hat{P})\hat{x}$ and $R(\hat{P})\hat{y}$ can differ from $\vec{E}_2$ and $-\vec{E}_1$ only by rotation around $\hat{P}$. They are the same if they have the same components in the $\hat{z}\times\vec{P}$ direction. Using

$$\hat{z}\times\vec{P} = (-P_2, P_1, 0), \tag{5.6}$$

we can check that in fact

$$\begin{aligned} \vec{E}_2\cdot\hat{z}\times\vec{P} &= -P_2 = \hat{x}\cdot\hat{z}\times\vec{P} = R(\hat{P})\hat{x}\cdot\hat{z}\times\vec{P}, \\ -\vec{E}_1\cdot\hat{z}\times\vec{P} &= P_1 = \hat{y}\cdot\hat{z}\times\vec{P} = R(\hat{P})\hat{y}\cdot\hat{z}\times\vec{P}. \end{aligned} \tag{5.7}$$

For the transformation of the spin operator we get

$$\begin{aligned} e^{i\theta(\hat{P})\hat{z}\wedge\hat{P}\cdot\vec{S}}\vec{S}e^{-i\theta(\hat{P})\hat{z}\wedge\hat{P}\cdot\vec{S}} &= R(\hat{P})\vec{S} \\ &= R(\hat{P})\hat{x}S_1 + R(\hat{P})\hat{y}S_2 + R(\hat{P})\hat{z}S_3 \\ &= \vec{E}_2S_1 - \vec{E}_1S_2 + \hat{P}S_3, \end{aligned} \tag{5.8}$$

$$e^{-i(\pi/2)S_3}(S_1, S_2, S_3)e^{i(\pi/2)S_3} = (S_2, -S_1, S_3), \tag{5.9}$$

$$U^\dagger\vec{S}U = \vec{E}_1S_1 + \vec{E}_2S_2 + \hat{P}S_3. \tag{5.10}$$

In the last step of the transformation, the factor $e^{i(\pi/2)S_3}$ of U just rotates (S_1, S_2) as a two-dimensional vector. This rotation by $-\pi/2$ corresponds to a convention for the x-y axes in the helicity form. For a different choice of x-y axes we would rotate through a different angle.

One can calculate the result (3.9) for $U^\dagger\vec{Q}U$ directly. However, it is more instructive to get the result (3.1) for $U^\dagger\vec{J}U$. Then we get $U^\dagger\vec{Q}U$ from

$$\vec{Q} = \hat{P}\times(\vec{Q}\times\hat{P}) + (\hat{P}\cdot\vec{Q})\hat{P} \tag{5.11}$$

as follows. From (2.2), (3.1), (5.10) and (3.11) we have

$$\begin{aligned} U^\dagger\vec{Q}\times\vec{P}U &= U^\dagger\vec{J}U - U^\dagger\vec{S}U \\ &= \vec{Q}\times\vec{P} + \vec{M}S_3 - \vec{E}_1S_1 - \vec{E}_2S_2 - \hat{P}S_3 \\ &= \vec{Q}\times\vec{P} + \vec{N}\times\hat{P}S_3 - \vec{E}_1S_1 - \vec{E}_2S_2. \end{aligned} \tag{5.12}$$

For a function f of $\vec{P}$

$$\begin{aligned} [\vec{Q}\cdot\vec{P}, f(\vec{P})] &= i\vec{P}\cdot\nabla f(\vec{P}) \\ &= i|\vec{P}|\partial f(\vec{P})/\partial|\vec{P}|. \end{aligned} \tag{5.13}$$

From this we see that $\vec{Q}\cdot\vec{P}$ commutes with U so $\hat{P}\cdot\vec{Q}$ commutes with U and is not changed by the transformation. Thus from (5.11) and (5.12) we get

$$U^{\dagger}\vec{Q}U = \hat{P}\times(U^{\dagger}\vec{Q}\times\hat{P}U) + (\hat{P}\cdot\vec{Q})\hat{P}$$
$$= \hat{P}\times(\vec{Q}\times\hat{P}) + |\vec{P}|^{-1}\hat{P}\times(\vec{N}\times\hat{P}S_3 - \vec{E}_1S_1 - \vec{E}_2S_2) + (\hat{P}\cdot\vec{Q})\hat{P}$$
$$= \vec{Q} + |\vec{P}|^{-1}\vec{N}S_3 - |\vec{P}|^{-1}(\vec{E}_2S_1 - \vec{E}_1S_2), \quad (5.14)$$

because $\vec{P}\cdot\vec{N}$ is zero, $\hat{P}\times\vec{E}_1$ is $\vec{E}_2$, and $\hat{P}\times\vec{E}_2$ is $-\vec{E}_1$.

Let R denote the rotation through the angle $|\vec{\theta}|$ around the axis in the direction of $\vec{\theta}$. For the unitary operator that represents this rotation in the position form we have

$$(e^{-i\vec{\theta}\cdot\vec{J}}\psi)(\vec{x}) = ((e^{-i\vec{\theta}\cdot\vec{S}}e^{-i\vec{\theta}\cdot\vec{Q}\times\vec{P}}\psi)(\vec{x})$$
$$= e^{i\vec{\theta}\cdot\vec{S}}\ \psi(R^{-1}\vec{x}), \quad (5.15)$$

which corresponds to

$$e^{-i\vec{\theta}\cdot\vec{J}}|\vec{p},\lambda\rangle = e^{-i\vec{\theta}\cdot\vec{S}}e^{-i\vec{\theta}\cdot\vec{Q}\times\vec{P}}|\vec{p},\lambda\rangle$$
$$= e^{-i\vec{\theta}\cdot\vec{S}}|R\vec{p},\lambda\rangle. \quad (5.16)$$

For the unitary transform of this operator, which represents the rotation in the helicity form, we get

$$e^{-i(\pi/2)S_3}e^{i\theta(\hat{P})\hat{z}\wedge\hat{P}\cdot\vec{S}}e^{-i\vec{\theta}\cdot\vec{J}}e^{-i\theta(\hat{P})\hat{z}\wedge\hat{P}\cdot\vec{S}}e^{i(\pi/2)S_3}|\vec{p},\lambda\rangle$$
$$= e^{-i(\pi/2)S_3}e^{i\theta(\hat{P})\hat{z}\wedge\hat{P}\cdot\vec{S}}e^{-i\vec{\theta}\cdot\vec{S}}e^{-i\vec{\theta}\cdot\vec{Q}\times\vec{P}} \times e^{-i\theta(\hat{p})\hat{z}\wedge\hat{p}\cdot\vec{S}}e^{i(\pi/2)\lambda}|\vec{p},\lambda\rangle$$
$$= e^{i(\pi/2)\lambda}e^{-i(\pi/2)S_3}e^{i\theta(R\hat{p})\hat{z}\wedge R\hat{p}\cdot\vec{S}}e^{-i\vec{\theta}\cdot\vec{S}} \times e^{-i\theta(\hat{p})\hat{z}\wedge\hat{p}\cdot\vec{S}}|R\vec{p},\lambda\rangle$$
$$= e^{i(\pi/2)\lambda}e^{-i(\pi/2)S_3}e^{-i\delta S_3}|R\vec{p},\lambda\rangle$$
$$= e^{-i\delta S_3}e^{-i\vec{\theta}\cdot\vec{Q}\times\hat{P}}|\vec{p},\lambda\rangle, \quad (5.17)$$

where δ is the angle of

$$R^{-1}(R\hat{p})RR(\hat{p}), \quad (5.18)$$

which is a rotation around the z axis since

$$R^{-1}(R\hat{p})RR(\hat{p})\hat{z} = R^{-1}(R\hat{p})R\hat{p} = \hat{z}. \quad (5.19)$$

For an infinitesimal rotation R of a vector $\vec{x}$ we have

$$R\vec{x} = \vec{x} + \vec{\theta}\times\vec{x}, \quad (5.20)$$

to first order in $\vec{\theta}$. We can calculate δ from

$$R^{-1}(R\hat{p})RR(\hat{p})(\hat{z}\times\hat{p}) = \hat{z}\times\hat{p} + \delta\hat{z}\times(\hat{z}\times\hat{p}), \quad (5.21)$$

by taking the dot product of both sides with $\hat{z}\times(\hat{z}\times R\hat{p})$ to first order. From the left side, after rotating the vectors in the dot product first by $R(R\hat{p})$ and then by R^{-1} and recognizing $\hat{z}\times\hat{p}$ and $\hat{z}\times R\hat{p}$ as the axes of $R(\hat{p})$ and $R(R\hat{p})$, we get

$$\hat{z}\times(\hat{z}\times R\hat{p})\cdot R^{-1}(R\hat{p})RR(\hat{p})(\hat{z}\times\hat{p})$$
$$= R\hat{p}\times(\hat{z}\times R\hat{p})\cdot R(\hat{z}\times\hat{p})$$
$$= \hat{p}\times(R^{-1}\hat{z}\times\hat{p})\cdot\hat{z}\times\hat{p}$$
$$= ((\vec{\theta}\times\hat{z})\times\hat{p})\times\hat{p}\cdot\hat{z}\times\vec{p}$$
$$= \vec{\theta}\cdot\hat{p} - (\vec{\theta}\cdot\hat{z})(\hat{p}\cdot\hat{z}). \quad (5.22)$$

From the right side we get

$$\hat{z}\times(\hat{z}\times R\hat{p})\cdot[\hat{z}\times\hat{p} + \delta\hat{z}\times(\hat{z}\times\hat{p})]$$
$$= \delta|\hat{z}\times(\hat{z}\times\hat{p})|^2 + \hat{z}\times(\hat{z}\times(\vec{\theta}\times\hat{p}))\cdot\hat{z}\times\hat{p}$$
$$= \delta[1 - (\hat{p}\cdot\hat{z})^2] - \vec{\theta}\cdot\hat{z} + (\vec{\theta}\cdot\hat{p})(\hat{p}\cdot\hat{z}). \quad (5.23)$$

Equating the two results (5.22) and 5.23) yields

$$\delta = (\vec{\theta}\cdot\hat{p} + \vec{\theta}\cdot\hat{z})(1 - \hat{p}\cdot\hat{z})/[1 - (\hat{p}\cdot\hat{z})^2]. \quad (5.24)$$

Then from (5.17) we have

$$U^{\dagger}e^{-i\vec{\theta}\cdot\vec{J}}U = e^{-i\vec{\theta}\cdot\vec{Q}\times\vec{P}}e^{-i\vec{\theta}\cdot(\hat{P}+\hat{z})(1+\hat{P}\cdot\hat{z})^{-1}S_3}, \quad (5.25)$$

to first order in $\vec{\theta}$, or

$$U^{\dagger}\vec{J}U = \vec{Q}\times\vec{P} + (\hat{P}+\hat{z})(1+\hat{P}\cdot\hat{z})^{-1}S_3, \quad (5.26)$$

which is the same as the formulas (3.1) and (3.3) that we have used for $U^{\dagger}\vec{J}U$ in the helicity form.

As we already mentioned, the result (3.2) for $U^{\dagger}\vec{K}U$ can be easily calculated from (2.3), (5.10) and (5.14), using (3.11).

From the formula (2.12) for the parity operator P in the position form, and the facts that P commutes with $\vec{S}$, and

$$e^{-i\pi S_2}|\vec{p},\lambda\rangle = (-1)^{\lambda-s}|\vec{p},-\lambda\rangle, \quad (5.27)$$

we get

$$U^{\dagger}PU|\vec{p},\lambda\rangle$$
$$= e^{-i(\pi/2)S_3}e^{i\theta(\hat{P})\hat{z}\wedge\hat{P}\cdot\vec{S}}Pe^{-i\theta(\hat{p})\hat{z}\wedge\hat{p}\cdot\vec{S}}e^{i(\pi/2)\lambda}|\vec{p},\lambda\rangle$$
$$= e^{i(\pi/2)\lambda}e^{-i(\pi/2)S_3}e^{i\theta(\hat{P})\hat{z}\wedge\hat{P}\cdot\vec{S}}e^{-i\theta(\hat{p})\hat{z}\wedge\hat{p}\cdot\vec{S}}\eta|-\vec{p},\lambda\rangle$$
$$= \eta e^{i(\pi/2)\lambda}e^{-i(\pi/2)S_3}e^{i\theta(-\hat{p})\hat{z}\wedge(-\hat{p})\cdot\vec{S}} \times e^{-i\theta(\hat{p})\hat{z}\wedge\hat{p}\cdot\vec{S}}e^{i\pi S_2}(-1)^{\lambda-s}|-\vec{p},-\lambda\rangle$$
$$= \eta(-1)^{\lambda-s}e^{i(\pi/2)\lambda}e^{-i(\pi/2)S_3}e^{-i2\phi(\hat{p})S_3}|-\vec{p},-\lambda\rangle$$
$$= \eta(-1)^{\lambda-s}e^{i\pi\lambda}e^{i2\phi(\hat{p})\lambda}|-\vec{p},-\lambda\rangle, \quad (5.28)$$

with $2\phi(\hat{p})$ the angle of

$$R^{-1}(-\hat{p})R(\hat{p})R_y(-\pi), \quad (5.29)$$

where $R_y(-\pi)$ is the rotation through the angle $-\pi$ around the y axis. We can see that the combination of rotations (5.29) is around the z axis because

$$R^{-1}(-\hat{p})R(\hat{p})R_y(-\pi)\hat{z} = R^{-1}(-\hat{p})R(\hat{p})(-\hat{z})$$
$$= R^{-1}(-\hat{p})(-\hat{p}) = \hat{z}. \quad (5.30)$$

Thus we obtain the formula (3.12) for the parity operator $U^{\dagger}PU$ in the helicity form, only with a different definition of $\phi(\hat{p})$. A similar calculation produces the formula (3.13) for the time-reversal operator $U^{\dagger}TU$ in the helicity form from the formula (2.13) for T in the position form and the facts that T is antilinear (anticommutes with i) and commutes with $i\vec{S}$. The factors $e^{\pm i\pi\lambda}$ come from the factor $e^{i(\pi/2)S_3}$ of U which corresponds to a convention for x-y axes in the helicity form.

It remains only to show that the two definitions of $\phi(\hat{p})$ are equivalent. Let $\phi(\hat{p})$ be the cylindrical angle (3.14) of $\hat{p}$. We shall show that $2\phi(\hat{p})$ is the angle of the combination of rotations (5.29). For this we can use the two-dimensional faithful representation of the rotation group generated by the Pauli matrices $\sigma_1,\sigma_2,\sigma_3$. Since $R^{-1}(-\hat{p})R(\hat{p})$ is the rotation by π around $\hat{z}\wedge\hat{p}$, and

$$\hat{z}\wedge\hat{p} = -\hat{x}\sin\phi(\hat{p}) + \hat{y}\cos\phi(\hat{p}), \quad (5.31)$$

the matrix representing $R^{-1}(-\hat{p})R(\hat{p})$ is

$$e^{-i\pi\hat{z}\wedge\hat{p}\cdot\vec{\sigma}/2} = i\sigma_1\sin\phi(\hat{p}) - i\sigma_2\cos\phi(\hat{p}). \quad (5.32)$$

The matrix representing $R_y(-\pi)$ is

$$e^{i\pi\sigma_2/2} = i\sigma_2, \quad (5.33)$$

so the matrix representing the combination of rotations (5.29) is

$$-i\sigma_3\sin\phi(\hat{p}) + \cos\phi(\hat{p}) = e^{-i2\phi(\hat{p})\sigma_3/2}, \quad (5.34)$$

which represents the rotation by 2ϕ ($\hat{p}$) around the z axis. The full range of 2ϕ ($\hat{p}$) from zero to 4π is used in the formulas (3.12) and (3.13) for $U^{\dagger}PU$ and $U^{\dagger}TU$ for half-integer spin.

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Anomaly-free complex representations in SU(*N*)

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(Received 13 January 1982; accepted for publication 16 April 1982)

We have found all irreducible, anomaly-free and complex representations of SU(N) up to dimension 4×10^9 and SU(16). None of these representations are asymptotically free. For each SU(N), we have given a complete list of complex reducible representations which satisfy both asymptotic and anomaly freedom. Applications of such solutions are briefly discussed.

PACS numbers: 11.30.Ly

I. INTRODUCTION

To construct a gauge model unifying the strong, electromagnetic, and weak interactions, one needs several constraints to be satisfied by the representation. Georgi and Glashow,[1] Georgi,[2] and Gell-Mann, Ramond, and Slansky[3] have suggested the existence of complex representations as a criterion for grand unified theories. Complex representations can be found in gauge groups SU(N), SO($4N+2$), and E_6.

Renormalizability of gauge theories necessitates use of anomaly-free representations.[4] Among the groups with complex representations, SO($4N+2$) and E_6 are free of anomaly. For SU(N) one usually needs to combine several representations to cancel anomalies with each other. Actually there are two different ways of getting anomaly-free and complex representations in SU(N). One method is to find anomaly-free, irreducible, and complex representations (AFICR), and the other is to form anomaly-free combinations with several complex representations.

The highly reducible nature of the fermion representations is cited[5] as one of the least attractive features of the SU(N) models. For this reason, it may be interesting to find AFICR in the SU(N) group. Okubo[6] and Cox[7] have already observed that none is known with dimensionality below $D=3\times 10^5$ for SU(N) with $N\leqslant 6$.

On the other hand, recent developments of grand unified theories[8] and preon dynamics[9] require comprehensive list of the anomaly-free, reducible, and complex representations (AFRCR) for model building.

In this paper, AFICR and AFRCR are presented. A thorough search for AFICR has been carried out with dimensions less than $D=4\times 10^9$ in SU(N) for N less than 17. The smallest AFICR occurs in SU(6) with $D=374\,556$. The next lowest AFICR is in SU(5) with $D=1\,357\,824$. Altogether, 28 AFICR are presented in Sec. II. These representations are only of mathematical curiosity and do not have any practical use due to their awesome dimensionality. In addition, they usually contain color exotics, i.e., those representations other than $\underline{1}$, $\underline{3}$, and $\underline{3}^*$ of the color group SU(3). Furthermore, a close examination of the branching rules contained in Sec. III reveals that the SU(6) representation with $D=374\,556$ can accomodate only one generation of quarks and leptons, along with many exotic particles.

In Sec. IV, we obtain for every SU(N) all AFRCR which also satisfy the asymptotic freedom condition. The requirement of asymptotic freedom is needed here to limit the number of dimensions of reducible representations.

TABLE I. Anomaly free irreducible complex representations in SU(N). Weight is given by $(\lambda_1,\lambda_2,\ldots,\lambda_{N-1})$, where λ_i equals the number of Young tableau with i boxes. This notation agrees with the Cartan labels for the highest weight of an irreducible representation.

SU(N)	Weight	Dimension
5	0 7 3 3	1357824
5	1 8 1 5	3048474
5	7 7 15 1	1390411776
6	0 5 0 0 4	374556
6	0 5 3 2 3	192615423
6	0 6 0 3 3	28514304
6	0 10 0 0 8	108645537
6	0 10 0 2 7	1000276992
6	1 5 5 0 5	832637988
6	1 6 1 1 5	128035908
6	2 7 1 0 7	303771468
7	0 0 6 3 0 2	1189284096
7	0 1 6 0 2 2	1540923584
7	0 2 4 2 0 5	1747519488
7	0 3 3 1 1 5	1911816192
7	0 4 2 0 2 5	823550528
7	1 3 4 0 0 5	1941877958
7	1 5 1 0 1 5	1207195704
8	0 0 4 0 0 1 2	37981044
8	0 1 3 0 0 0 5	12960348
8	0 4 1 0 0 2 5	1646701056
8	1 5 0 0 0 1 5	1207195704
10	0 0 0 3 0 0 0 0 2	19423464
10	0 3 0 1 0 0 0 1 5	308056320[illegible]
10	1 3 1 0 0 0 0 0 5	2615590692
12	0 2 0 0 1 0 0 0 0 0 3	266982144
14	0 0 1 0 0 1 0 0 0 0 0 0 2	72813512
16	0 0 1 1 0 0 0 0 0 0 0 0 0 0 3	37180416[illegible]

a) Alfred P. Sloan Foundation Fellow.
b) Supported in part by the U.S. Department of Energy under Contract DE-AC02-76ER03130.A007-Task A.
c) Senior Fulbright Fellow.

 0022-2488/82/122529-08$02.50

TABLE II. Branching of the smallest anomaly-free complex representation (4 0 0 5 0) of SU(6) into SU(5)×U^a(1). SU(5) weight is given by $(\lambda_1,\ldots,\lambda_4)$ in Cartan labels.

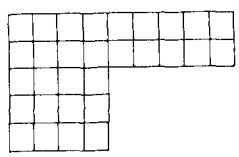
SU(5) weight	dimension	anomaly in SU(5)	Y^a
0 0 5 0	1176	-1050	-30
1 0 3 0	1410	-5559	-24
2 0 3 0	20280	4851	-18
3 0 3 0	21560	1232	-12
1 0 3 0	38220	30303	-6
0 1 4 1	1470	-1525	-24
1 0 4 1	5600	-4320	-18
2 0 4 1	13860	-6655	-12
3 0 4 1	26460	209	-6
4 0 4 1	30030	35750	0
0 0 3 2	1260	-1287	-18
1 0 3 2	4900	-4445	-12
2 0 3 2	12320	-7852	-6
3 0 3 2	25200	-4500	0
4 0 3 2	45500	22425	6
0 0 2 3	840	-1032	-12
1 0 2 3	3360	-3816	-6
2 0 2 3	8624	-7700	0
3 0 2 3	17920	-8448	6
4 0 2 3	32760	5148	12
0 0 1 4	420	-627	-6
1 0 1 4	1750	-2500	0
2 0 1 4	5120	-5645	6
3 0 1 4	9800	-8260	12
4 0 1 4	18200	-4810	18
0 0 0 5	126	-225	0
1 0 0 5	560	-984	6
2 0 0 5	1540	-2465	12
3 0 0 5	3360	-4248	18
4 0 0 5	6370	-4752	24

II. ANOMALY-FREE IRREDUCIBLE COMPLEX REPRESENTATIONS (AFICR)

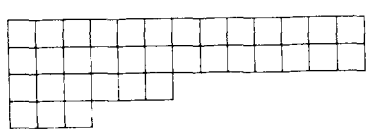
Irreducible representations of SU(N) will be specified by a set of integers $(\lambda_1,\lambda_2,\ldots,\lambda_{N-1})$, where λ_i equals the number of columns of the Young tableau with i boxes.[10] This notation agrees with the Cartan labels for the highest weight of an irreducible representation.

Complex representations in SU(N) satisfy $(\lambda_1,\lambda_2,\ldots,\lambda_{N-1})\neq(\lambda_{N-1},\ldots,\lambda_1)$. Only very few of them are anomaly-free and irreducible. There are no complex representations in SU(2). For SU(3) and SU(4), no AFICR exist below $D=4\times10^9$. Table I summarizes all AFICR in SU(N) with dimensionality up to $D=4\times10^9$ and $N\leqslant16$. Conjugate representations are not repeated in Table I.

The smallest AFICR mentioned before corresponds to (0,5,0,0,4) of SU(6) in the Cartan labels. The next lowest AFICR is (0,7,3,3) of SU(5). For clarity, we show the corresponding Young tableaux in Fig. 1.



(a)



(b)

FIG. 1. (a) (0,5,0,0,4) of SU(6) with $D=374\,556$; (b) (0,7,3,3) of SU(5) with $D=1\,357\,824$. These are the two lowest dimensional AFICR.

III. BRANCHING RULES

To study the branching rules of the smallest AFICR (0,5,0,0,4) of SU(6), we follow the method of elementary multiplets suggested by Patera and Sharp.[11]

For SU(6)→SU(5)×U(1), there are ten elementary multiplets. We use the notation $(\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5;\alpha_1\alpha_2\alpha_3\alpha_4,Y^a)$, where λ_i and α_i are the Cartan labels for SU(6) and SU(5) respectively, and Y^a is the hypercharge of U^a(1) label.

They are

$$A^1_1=(10\,000;0000,-5, \tag{1}$$

$$A^1_2=(10\,000;1000,\ \ 1), \tag{2}$$

$$A^2_1=(01\,000;1000,-4), \tag{3}$$

$$A^2_2=(01\,000;0100,\ \ 2), \tag{4}$$

$$A^3_1=(00\,100;0100,-3), \tag{5}$$

$$A^3_2=(00\,100;0010,\ \ 3), \tag{6}$$

$$A^4_1=(00\,010;0010,-2), \tag{7}$$

$$A^4_2=(00\,010;0001,\ \ 4), \tag{8}$$

$$A^5_1=(00\,001;0001,-1), \tag{9}$$

$$A^5_2=(00\,001;0000,\ \ 5). \tag{10}$$

Table II shows the branching rules of SU(6) to SU(5) with dimensions, anomaly in SU(5), and U^a(1) hypercharge. The anomaly and hypercharge in Table II add up zero as expected.

To reduce SU(5) further into SU(3)×SU(2)×U^b(1), there are ten elementary multiplets [the notation is $(\lambda_1\lambda_2\lambda_3\lambda_4;\alpha_1\alpha_2,\alpha,Y^b)$, where $\lambda_i\alpha_i$ and α are the Cartan labels for SU(5), SU(3), and SU(2), respectively; Y^b is the hypercharge of U^b(1) normalized to have integer value]:

$$A^1_1=(10000;10,0,2), \tag{11}$$

$$A^1_2=(1000;00,1,-3), \tag{12}$$

$$A^2_1=(0100;01,0,4), \tag{13}$$

$$A^2_2=(0100;10,1,-1), \tag{14}$$

$$A^2_3=(0100;00,0,-6), \tag{15}$$

$$A^3_1=(0010;00,0,6), \tag{16}$$

$$A^3_2=(0010;01,1,1), \tag{17}$$

$$A^3_3=(0010;10,0,-4), \tag{18}$$

$$A^4_2=(0001;00,1,3), \tag{19}$$

$$A^4_3=(0001;01,0,-2). \tag{20}$$

In addition to those listed above, three more composite elementary factors are necessary and they are

$$A^{13}=(1010;01,0,-2), \tag{21}$$

$$A^{14}=(1001;00,0,0), \tag{22}$$

$$A^{24}=(0101;10,0,2). \tag{23}$$

TABLE III. The nine irreducible and complex representations of SU(N) which satisfy the asymptotic freedom constraint. The first and the second columns define the representations and the corresponding Young tableaux. The dimension of the representation, the second index (T_2), the value of the quadratic Casimir operator (C_2), and the anomaly (A) are given in the next four columns. The final column gives the maximum allowed value for N consistent with asymptotic freedom.

Representation	Young Tableau	Dimension	T_2	C_2	A	N_{max}
R_1		$\frac{N(N-1)(N-2)(N-3)}{24}$	$\frac{(N-2)(N-3)(N-4)}{12}$	$\frac{2}{N}(N-4)(N+1)$	$\frac{(N-8)(N-3)(N-4)}{6}$	12
R_2		$\frac{1}{12}N^2(N^2-1)$	$\frac{N(N^2-4)}{6}$	$\frac{2}{N}(N^2-4)$	$\frac{N(N^2-16)}{3}$	6
R_3		$\frac{1}{6}N(N-1)(N-2)$	$\frac{(N-2)(N-3)}{4}$	$\frac{3(N-3)(N+1)}{2N}$	$\frac{(N-3)(N-6)}{2}$	26
R_4	N-1 	$\frac{1}{2}N(N-1)(N+2)$	$\frac{(N+2)(3N-1)}{4}$	$\frac{(3N-1)(N+1)}{2N}$	$\frac{(N^2+7N-2)}{2}$	5
R_5	N-2 	$\frac{1}{2}N(N+1)(N-2)$	$\frac{(N-2)(3N+1)}{4}$	$\frac{(3N+1)(N-1)}{2N}$	$\frac{(-N^2+7N+2)}{2}$	9
R_6		$\frac{1}{3}N(N^2-1)$	$\frac{N^2-3}{2}$	$\frac{3}{2}(\frac{N^2-3}{N})$	(N^2-9)	11
R_7		$\frac{N(N+1)}{2}$	$\frac{N+2}{2}$	$\frac{(N-1)(N+2)}{N}$	$N+4$	None
R_8		$\frac{N(N-1)}{2}$	$\frac{N-2}{2}$	$\frac{(N+1)(N-2)}{N}$	$N-4$	None
R_9		N	$\frac{1}{2}$	$\frac{N^2-1}{2N}$	1	None

The following pairs of elementary factors are incompatible[11]: A^{13} with $A^{\frac{2}{2}}$ or A^{24}; A^{14} with $A^{\frac{2}{2}}$ or $A^{\frac{3}{2}}$; and A^{24} with $A^{\frac{3}{2}}$ or A^{13}.

The electric charge generator[12] can generally be a linear combination of T_3, Y^a, and Y^b:

$$Q = T_3 + AY^a + BY^b, \tag{24}$$

where A and B are to be determined to give correct charge assignment. An exhaustive search was made for possible values of A and B which give correct charges for 15 chiral fields $(ud)_L, u^c{}_L, d^c{}_L, (ve)_L e, {}^c{}_L$. Correct charge assignment for one generation can be made with nine different choices of A and B in Eq. (24), but there are huge numbers of exotic states.

IV. ANOMALY-FREE REDUCIBLE COMPLEX REPRESENTATIONS (AFRCR)

All of the AFICR in Table I are of enormous dimensions and therefore are only of mathematical interest. In physically interesting theories, the dimensions of representations can be limited by the constraint of asymptotic freedom.[13] This condition gives the following group theoretical constraint[14]:

$$\sum_{R_i} T_2(R_i) \leqslant \tfrac{11}{2} C_2(G), \tag{25}$$

where R_i is the irreducible representation of fermions; C_2 is the quadratic Casimir operator; G is the adjoint representation; and T_2 is defined by

$$T_2(R)\dim(G) \equiv C_2(R)\dim(R). \tag{26}$$

There are nine irreducible and complex representations of SU(N), $R_1, R_2, \ldots, R_9$, which satisfy the asymptotic freedom. They are defined in Table III along with the associated properties of the representation such as the dimension, T_2, the value of the Casimir operator C_2, the anomaly A, and the maximum allowed value of N for asymptotic freedom.

Among simple groups, the only complex irreducible representations, which are both anomaly-free and asymptotic-free, are the following: 16-, 126-, 144-dimensional representations of SO(10); the lowest-dimensional spinorial representations of SO(14) and SO(18); and 27-dimensional representation of E_6. The maximum multiplicities of these representations bounded by the asymptotic freedom are: 22, 1, 1; 8, 2; and 22 respectively. There are no complex irreducible representations which are both anomaly-free and asymptotic-free in SU(N).

Relaxing the condition of irreducibility,[15] we have considered reducible complex representations $\Sigma\, n_i R_i, n_i$ being integers, which are both anomaly-free and asymptotic-free. Anomaly-free complex representations which satisfy asymptotic freedom are greatly constrained, and a complete list of such representations in SU(N) is reported here. We give a separate list of AFRCR with asymptotic freedom that contain tensor representations of rank at most 2 for the obvious reason of simplicity.

Tables IV and V show all anomaly-free and asymptotic-free combinations of the following form:

$$n_7 R_7 \oplus n_8 R_8 \oplus \bar{n}_9 R_9^*, \tag{27}$$

where n_7, n_8, and $\bar{n}_9$ are integers, whose magnitudes are constrained by asymptotic freedom as[16]

$$|n_7|(N+2) + |n_8|(N-2) + |\bar{n}_9| \leqslant 11N. \tag{28}$$

Negative values of n_i are to be interpreted as the appearance of n_i times of the associated complex conjugate representations. Table IV contains all AFRCR with asymptotic freedom for arbitrarily large values of N, whereas Table V includes only those for finite range of N.

Except for the solutions in Tables IV and V, all other anomaly-free and asymptotic-free representations contain at

TABLE IV. Complex representations of SU(N) of the form of Eq. (26) which satisfy the constraints of anomaly cancellation and asymptotic freedom for arbitrary large N. The representations R_7, R_8, and R_9 are defined in Table III. In a given row, the representation $n_7R_7 + n_8R_8 + \bar{n}_9R_9^*$ is denoted by the integer n_7, n_8, and $\bar{n}_9$. If $n_i < 0$, n_iR_i is to be interpreted as $|n_i|R_i^*$. β gives twice the sum of the $T_2(R)$ for given anomaly-free combinations. The last column gives the maximum multiplicity of the representation (denoted by l) consistent with the constraint of asymptotic freedom and its dependence on N. Except for the first row, N is greater than or equal to 5.

n_7	n_8	$\bar{n}_9$	β	l
1	0	N+4	2(N+3)	l=2 (N=3), l=3 (4≤N≤7), l=4 (8≤N≤29), l=5 (N=30)
0	1	N-4	2(N-3)	l=13 (N=5), l=11 (N=6), l=9 (N=7), l=8 (8≤N≤9), l=7 (10≤N≤14), l=6 (15≤N≤36) l=5 (N≥37)
1	1	2N	4N	l=2
1	2	3N-4	6N-6	l=2 (N≥12), l=1 (N≥13)
1	3	4N-8	8N-12	l=1
1	4	5N-12	10N-18	l=1
1	-1	8	2N+8	l=3 (5≤N≤10), l=4 (11≤N≤39) l=5 (N≥40)
1	-2	-N+12	3N-2+|N-12|	l=2 (N=5, N≥43) l=3 (6≤N≤42)
1	-3	-2(N-8)	4N-4+2|N-8|	l=2 (N≤7), l=3 (N=8) l=2 (9≤N≤40), l=1 (N≥41)
1	-4	-3N+20	5N-6+|3N-20|	l=2 (N≤10), l=1 (N≥11)
1	-5	-4(N-6)	6N-8+4|N-6|	l=2 (N≤7), l=1 (N≥8)
2	1	3N+4	6N+6	l=1
2	3	5N-4	10N-6	l=1
2	-1	N+12	4N+14	l=1 (N≤9), l=2 (N≥10)
2	-3	-N+20	5N-2+|N-20	l=1 (5≤N≤11, N≥45) l=2 (12≤N≤44)
2	-5	-3N+28	7N-6+|3N-28|	l=1
3	1	4N+8	8N+12	l=1
3	2	5N+4	10N+6	l=1 (N≥6)
3	-1	2N+16	6N+20	l=1
3	-2	N+20	6N+22	l=1
3	-4	-N+28	7N-2+|N-28|	l=1 (N≥6)
3	-5	-2N+32	8N-4+2|N-16|	l=1 (N≥6)
4	1	5N+12	10N+18	l=1 (N≥18)
4	-1	3N+20	8N+26	l=1 (N≥9)
4	-3	N+28	8N+30	l=1 (N≥10)
4	-5	-N+36	9N-2+|N-36|	l=1 (N≥12)
5	-1	4N+24	10N+32	l=1 (N≥32)
5	-2	3N+28	10N+34	l=1 (N≥34)
5	-3	2N+32	10N+36	l=1 (N≥36)
5	-4	N+36	10N+38	l=1 (N≥38)

TABLE V. Complex representations of SU(N) of the form $n_7R_7 \oplus n_8R_8 \oplus \bar{n}_9R_9^*$ which satisfy Eq. (25) but only for a finite range of N. The notations for the first three columns are the same as in Table IV. Column 4 gives the range of N for which an asymptotic-free solution exists. The maximum multiplicity of each of these solutions is $l = 1$. N is greater than or equal to 5.

n_7	n_8	$\bar{n}_9$	N
1	5	6N-16	N ≥ 24
1	6	7N-20	N ≥ 10
1	7	8N-24	N ≥ 7
1	8	9N-28	N ≥ 6
1	9	10N-32	N ≥ 5
1	-6	-5N+28	N ≤ 58
1	-7	-6N+32	N ≤ 14
1	-8	-7N+36	N ≤ 10
1	-9	-8N+40	N ≤ 8
1	-10	-9N+44	N ≤ 6
1	-11	-10N+48	N ≤ 6
1	-12	-11N+52	N ≤ 7
1	-13	-12N+56	N ≤ 5
1	-14	-13N+60	N ≤ 5
2	5	7N-12	N ≥ 6
2	-7	-5N+36	N ≤ 15
2	-9	-7N+44	N ≤ 8
2	-11	-9N+52	N ≤ 6
3	-7	-4N+40	7 ≤ N ≤ 16
3	-8	-5N+44	7 ≤ N ≤ 10
4	-7	-5N+44	13 ≤ N ≤ 16
5	-6	-5N+44	42 ≤ N ≤ 46

least one term whose tensor representation has the rank greater than 2. Such solutions, however, exist, only for $N \leqslant 17$, and are listed in Table IV for $3 \leqslant N \leqslant 7$, in Table VII for $8 \leqslant N \leqslant 10$, and in Table VIII for $11 \leqslant N \leqslant 17$. Again the negative n_i's in these tables represent the occurrence of the associated complex conjugate representation.

It is to be emphasized that all anomaly-free and asymptotic-free complex representations for $N \geqslant 18$ are only of the type listed in Tables IV and V.

Since there are a number of representations which differ only in the number of occurrence of R_8 and R_9, we group these different possibilities collectively by P. The variable P takes integer values between finite limits as shown in the last column of Tables VI, VII, and VIII. The l appearing in the tenth column of these tables is the maximum magnitude of the multiplicities of the associated representation consistent with the asymptotic freedom.

V. COMMENTS ON RESULTS

We have found both irreducible and reducible representations which are complex and anomaly-free. Complex irreducible representations can indeed be anomaly-free, although the number of such examples is very limited.

All AFICR with $D \leqslant 4 \times 10^9$ are listed in Table I up to SU(16). None of these representations satisfy the asymptotic freedom.

All complex fermion representations in SU(N) which satisfy the constraints of asymptotic freedom and anomaly cancellation are listed in Tables IV–VIII. The most general solution subject to the anomaly-free condition can be given by the sum of a complex representation C_a listed in Tables IV–VIII and a pseudoreal representation R_a whose general form is

$$R_a = \sum_{i=1}^{9} m_i(R_i \oplus R_i^*) \oplus \sum_j n_j r_j. \tag{29}$$

Here $\{R_i\}$ are the nine complex representations defined in Table III and j runs over all pseudoreal irreducible representations r_j. The multiplicity m_i and n_j are nonnegative integers; and the condition for the general solution, $C_a + R_a$, to be asymptotically free is simply[16]

$$T_2(C_a) + T_2(R_a) \leqslant \tfrac{11}{2}N. \tag{30}$$

Our results will be useful in model building within the context of grand unified theories (GUT) with elementary scalar fields, where all gauge interactions are unified into a simple gauge group and the constraints to the model include the two conditions we have imposed. Furthermore, we expect the role of pseudoreal representations to be minimal in view of Georgi's rules[2] for grand unification. Usually additional

TABLE VI. Complex solutions in SU(N) with $3 \leqslant N \leqslant 7$ which contain at least one irreducible representation of rank greater than 2. The representation $R_1, R_2, \ldots, R_9$ are defined in Table III. In a given row, the representation $\Sigma_{i=1}^{9} n_i R_i$ is denoted by the integer $n_1, \ldots, n_9$. Again, if $n_i < 0$, $n_i R_i$ is interpreted as $|n_i| R_i^*$. When a number of solutions of similar form exists, they are sometimes denoted collectively by introducing an integer variable P in the solution. In these cases, the values of P which give solutions are given in the last column. The maximum multiplicity of the solution l is given in the 10th column.

n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	l	P
SU(3)										
0	0	0	-1	0	0	1	0	7	1	
0	0	0	-1	0	0	2	0	0	1	
SU(4)										
0	0	0	0	0	-1	0	0	7	2	
0	0	0	0	0	-2	1	0	6	1	
0	0	0	0	0	1	-1	0	1	2	
0	0	0	0	0	-1	-1	0	15	1	
0	0	0	0	0	1	-2	0	9	1	
SU(5)										
0	0	0	0	-1	0	0	P	6-1P	1	$-6 \leq P \leq 0$
0	-1	0	0	0	0	0	P	15-1P	1	$-1 \leq P \leq 2$
0	-1	0	0	0	0	1	P	6-1P	1	$-1 \leq P \leq 3$
0	0	0	0	0	-1	0	P	16-1P	1	$-4 \leq P \leq 8$
0	0	0	0	0	-1	1	P	7-1P	1	$-4 \leq P \leq 8$
0	0	0	0	1	-1	1	0	1	1	
0	0	0	0	0	-1	2	P	-2-1P	1	$-5 \leqslant P \leqslant 4$
0	0	0	0	-1	0	1	P	-3-1P	1	$-6 \leq P \leq 5$
0	0	0	0	-1	0	-1	P	15-1P	1	$-2 \leq P \leq 4$
0	0	0	0	0	-1	-1	0	25	1	
0	1	0	0	0	0	-2	P	3-1P	1	$0 \leq P \leq 1$
0	0	0	0	1	0	-2	P	12-1P	1	$1 \leq P \leq 2$
0	0	0	0	0	1	-3	0	11	1	
SU(6)										
0	0	0	0	-1	0	0	P	4-2P	1	$-4 \leq P \leq 5$
0	0	0	0	0	-1	0	P	27-2P	1	$-1 \leq P \leq 3$
0	0	0	0	0	-1	1	P	17-2P	1	$-1 \leq P \leq 4$
0	0	0	0	0	-1	2	P	7-2P	1	$-1 \leq P \leq 4$
0	0	0	0	0	-1	3	P	-3-2P	1	$-2 \leq P \leq 1$
0	0	0	0	-1	0	1	P	-6-2P	1	$-4 \leq P \leq 2$
0	0	0	0	-1	0	-1	P	14-2P	1	$-1 \leq P \leq 3$
SU(7)										
0	0	0	0	-1	0	0	P	1-3P	1	$-2 \leq P \leq 2$
0	0	-1	0	0	0	0	P	2-3P	1	$-8 \leq P \leq -4, 4 \leq P \leq 8$
									2	p=-2, -3, 3
									3	p=-1, 2
									4	p=1
									6	p=0

TABLE VI (continued).

n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	ℓ		P
0	0	-1	0	1	0		0	P	1-3P	1	1≤P≤1
0	0	-1	0	-1	0		0	P	3-3P	1	-1≤P≤1
0	0	-2	0	0	0		0	P	4-3P	1	P=-5, -3, 3, 5, 7
										2	P=-1, 1
0	0	-3	0	0	0		0	P	6-3P	1	P=-5,-4,-2,-1,2,4,
										2	P=1
0	0	-4	0	0	0		0	P	8-3P	1	P=-3,-2,-1,1,2,3,5
0	0	-5	0	0	0		0	P	10-3P	1	P=-1,1,3
0	0	-6	0	0	0		1	P	1-3P	1	0≤P≤1
0	0	-6	0	0	0		0	1	9	1	
0	0	-4	0	0	0		1	P	-3-3P	1	-3≤P≤3
0	0	-5	0	0	0		1	P	-1-3P	1	-2≤P≤2
0	0	-3	0	0	0		1	P	-5-3P	1	-5≤P≤4
0	0	-1	0	0	0		1	P	-9-3P	1	-8≤P≤-4, 2≤P≤6
										2	-3≤P≤1
0	0	-2	0	0	0		1	P	-7-3P	1	-6≤P≤-2, 1≤P≤5, P=3
										2	P=0, -1
0	0	1	0	0	0		1	P	-13-3P	1	-8≤P≤-4, 1≤P≤5
										2	-3≤P≤0
0	0	2	0	0		0	1	P	-15-3P	1	-7≤P≤4
0	0	3	0	0		0	1	P	-17-3P	1	-6≤P≤2
0	0	-1	0	0		0	2	P	-20-3P	1	-8≤P≤3
0	0	-2	0	0		0	2	P	-18-3P	1	P=-7,-5,-3,-1,1
0	0	1	0	0		0	2	P	-24-3P	1	-9≤P≤3
0	0	0	0	1		0	-1	P	10-3P	1	0≤P≤1
0	0	0	0	-1		0	-1	0	12	1	
0	0	-4	0	0		0	-1	P	19-3P	1	-1≤P≤4
0	0	3	0	0		0	-2	P	16-3P	1	-1≤P≤5
0	0	4	0	0		0	-2	1	11	1	
0	0	-2	0	0		0	-2	P	26-3P	1	P=-1,1,3,5
0	0	-3	0	0		0	-2	0	28	1	
0	0	1	0	0		0	-3	P	31-3P	1	-1≤P≤4
0	0	2	0	0		0	-3	0	29	1	
0	0	-1	0	0		0	-3	P	35-3P	1	0≤P≤2

TABLE VII. Complex solutions in SU(N) with $8 \leqslant N \leqslant 10$ which contains at least one irreducible representation of rank greater than 2. The notation is the same as that of Table VI.

n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	·	P
SU(8)										
0	0	-1	0	0	0	0	P	5-4P	1	$-6 \leq P \leq -3$, $4 \leq P \leq 7$
									2	P=-2, -1,2,3
									4	P=0,1
0	0	-2	0	0	0	0	P	10-4P	1	P=-3,-1,3,5
									2	P=1
0	0	-3	0	0	0	1	P	3-4P	1	$-3 \leq P \leq 3$
0	0	-4	0	0	0	1	P	8-4P	1	$-1 \leq P \leq 2$
0	0	-5	0	0	0	0	P	15-4P	1	$-2 \leq P \leq 5$
0	0	-6	0	0	0	0	P	20-4P	1	$1 \leq P \leq 3$
0	0	0	0	-1	0	0	-1	1	1	
0	0	-2	0	0	0	1	P	-2-4P	1	$-5 \leq P \leq -1$, $1 \leq P \leq 4$
									2	P=0
0	0	-6	0	0	0	2	-1	0	1	
0	0	-1		0	0	1	P	-7-4P	1	$-7 \leq P \leq -3$, $2 \leq P \leq 5$
									2	$-2 \leq P \leq 1$
0	0	-3	0	0	0	2	P	-9-4P	1	$-3 \leq P \leq 1$
0	0	1	0	0	0	3	P	-17-4P	1	$-8 \leq P \leq -2$, $1 \leq P \leq 4$, p=4
									2	p=-1,0
0	0	-4	0	0	0	2	P	-19-4P	1	$-5 \leq P \leq 3$
0	0	-2	0	0	0	2	P	-14-4P	2	P=-5,-3,-1,1
0	0	2	0	0	0	1	P	-22-4P	1	$-7 \leq P \leq 2$
0	0	1	0	0	0	2	P	-29-4P	1	$-8 \leq P \leq 2$
0	0	-3	0	0	0	-1	P	27-4P	1	$0 \leq P \leq 3$
0	0	-2	0	0	0	-2	1	30	1	
0	0	1	0	0	0	-3	P	31-4P	1	$-3 \leq P \leq 6$
0	0	0	0	0	0	-3	P	26-4P	1	$0 \leq P \leq 1$
0	0	-1	0	0	0	-3	P	41-4P	1	$0 \leq P \leq 1$
SU(9)										
-1	0	0	0	0	0	0	P	5-5P	1	$-4 \leq P \leq -1$, $2 \leq P \leq 5$
									2	P=0,1
-2	0	0	0	0	0	0	P	10-5P	1	P=-1,1,3
-2	0	1	0	0	0	0	0	1	1	
0	0	-1	0	0	0	0	P	9-5P	1	$-5 \leq P \leq -2$, $4 \leq P \leq 7$
									2	P=-1,2,3
									3	P=0,1
1	0	-1	0	0	0	0	P	4-5P	1	$-3 \leq P \leq 3$
-1	0	-1	0	0	0	0	P	14-5P	1	$-2 \leq P \leq 4$
-1	0	-1	0	0	0	1	P	1-5P	1	$-2 \leq P \leq 2$
0	0	-2	0	0	0	1	P	5-5P	1	$-3 \leq P \leq 4$
0	0	-2	0	0	0	0	P	18-5P	1	P=-3,-1,1,3,5
1	0	-1	0	0	0	0	P	13-5P	1	$0 \leq P \leq 2$
1	0	-2	0	0	0	1	0	0	1	
-1	0	-2	0	0	0	1	0	10	1	
0	0	-3	0	0	0	1	P	14-5P	1	$0 \leq P \leq 3$
0	0	-3	0	0	0	2	P	1-5P	1	$-1 \leq P \leq 1$
0	0	-3	0	0	0	0	P	27-5P	1	P=1,2,4
-2	0	0	0	0	0	1	P	-3-5P	1	$-1 \leq P \leq 1$
0	0	-1	0	0	0	1	P	-4-5P	1	$-5 \leq P \leq -2$, $2 \leq P \leq 5$
									2	P=-1,0,1

n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	·	P
(SU(9))										
-1	0	0	0	0	0	1	P	-8-5P	1	$-5 \leq P \leq 3$
1	0	-1	0	0	0	1	P	-9-5P	1	$-3 \leq P \leq 1$
0	0	-2	0	0	0	2	P	-8-6P	1	P=-3,-1,1
1	0	0	0	0	0	1	P	-18-5P	1	$-5 \leq P \leq 2$
-1	0	1	0	0	0	1	P	-17-5P	1	$-4 \leq P \leq 1$
0	0	-1	0	0	0	2	P	-17-5P	1	$-6 \leq P \leq 3$
0	0	1	0	0	0	1	P	-27-5P	1	$-7 \leq P \leq 3$
-1	0	0	0	0	0	2	P	-21-5P	1	$-5 \leq P \leq 1$
0	0	-1	0	0	0	3	P	-30-5P	1	$-6 \leq P \leq 1$
0	0	1	0	0	0	2	P	-35-5P	1	$-7 \leq P \leq 1$
-1	0	-1	0	0	0	-1	P	27-5P	1	$0 \leq P \leq 2$
0	0	-2	0	0	0	-1	P	31-5P	1	$-1 \leq P \leq 6$
1	0	1	0	0	0	-2	P	12-5P	1	$0 \leq P \leq 2$
-1	0	0	0	0	0	-2	P	31-5P	1	$0 \leq P \leq 5$
0	0	2	0	0	0	-3	P	21-5P	1	$0 \leq P \leq 1$
SU(10)										
-1	0	0	0	0	0	0	P	14-6P	1	$-2 \leq P \leq 4$
-1	0	0	0	0	0	1	P	0-6P	1	$-3 \leq P \leq 3$
-1	0	1	0	0	0	0	P	0-6P	1	$-1 \leq P \leq 1$
0	0	-1	0	0	0	0	P	14-6P	1	$-4 \leq P \leq -1$, $3 \leq P \leq 6$
									2	P=0,1,2
0	0	-1	0	0	0	1	P	0-6P	1	$-5 \leq P \leq -2$, $2 \leq P \leq 5$
									2	p=-1,0,1
-1	0	-1	0	0	0	1	0	14	1	
-1	0	-1	0	0	0	2	0	0	1	
0	0	-2	0	0	0	1	P	14-6P	1	$-2 \leq P \leq 4$
0	0	-2	0	0	0	0	P	28-6P	1	P=-1,1,3,5
0	0	-2	0	0	0	2	P	0-6P	1	P=-1,1
-1	0	0	0	0	0	2	P	-14-6P	1	$-3 \leq P \leq 1$
0	0	-1	0	0	0	2	P	-14-6P	1	$-5 \leq P \leq 3$
0	0	1	0	0	0	1	P	-28-6P	1	$-7 \leq P \leq 3$
1	0	0	0	0	0	1	P	-28-6P	1	$-5 \leq P \leq 1$
0	0	-1	0	0	0	3	P	-28-6P	1	$-5 \leq P \leq 1$
0	0	1	0	0	0	2	P	-42-6P	1	$-7 \leq P \leq 1$
-1	0	1	0	0	0	-1	0	14	1	
1	0	-1	0	0	0	-1	0	14	1	
0	0	-2	0	0	0	-1	0	42	1	
0	0	2	0	0	0	-3	P	14-6P	1	$0 \leq P \leq 2$

TABLE VIII. Complex solutions in SU(N) with $11 \leqslant N \leqslant 17$ which contain at least one irreducible representation of rank greater than 2. No solutions of this type exist for $N \geqslant 18$. The notation is the same as that of Table VI.

	n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	n_9	ℓ	P
SU(11)											
	-1	0	0	0	0	0	0	P	28-7P	1	$0 \leq P \leq 4$
	-1	0	0	0	0	0	1	P	13-7P	1	$0 \leq P \leq 2$
	0	0	-1	0	0	0	0	P	20-7P	1	$-4 \leq P \leq -1$, $3 \leq P \leq 6$
										2	$0 \leq P \leq 2$
	0	0	-1	0	0	0	1	P	5-7P	1	$-4 \leq P \leq -1$, $2 \leq P \leq 4$
										2	P=0,1
	0	0	-2	0	0	0	1	P	25-7P	1	$0 \leq P \leq 3$
	0	0	-2	0	0	0	0	P	40-7P	1	P=1,3
	0	0	-2	0	0	0	2	1	3	1	
	0	0	-1	0	0	0	2	P	-10-7P	1	$-4 \leq P \leq 3$
	0	0	-1	0	0	0	3	P	-25-7P	1	$-4 \leq P \leq 1$
	0	0	1	0	0	0	1	P	-35-7P	1	$-6 \leq P \leq 2$
	1	0	0	0	0	0	-2	0	2	1	
	0	0	-1	0	0	0	-2	P	50-7P	1	$0 \leq P \leq 4$
	0	0	2	0	0	0	-3	0	5	1	
SU(12)											
	0	0	-1	0	0	0	0	P	27-8P	1	$-3 \leq P \leq 6$
	0	0	-1	0	0	0	1	P	11-8P	1	$-3 \leq P \leq 4$
	0	0	-1	0	0	0	2	P	-5-8P	1	$-3 \leq P \leq 5$
	0	0	-1	0	0	0	3	P	-21-8P	1	$-3 \leq P \leq 1$
	0	0	1	0	0	0	1	P	-43-8P	1	$-6 \leq P \leq 1$
	0	0	-1	0	0	0	-2	0	59	1	
SU(13)											
	0	0	-1	0	0	0	0	P	35-9P	1	$-2 \leq P \leq 6$
	0	0	-1	0	0	0	1	P	18-9P	1	$-2 \leq P \leq 4$
	0	0	-1	0	0	0	2	P	1-9P	1	$-2 \leq P \leq 2$
	0	0	-1	0	0	0	3	P	-16-9P	1	$-2 \leq P \leq 1$
	0	0	1	0	0	0	1	P	-52-9P	1	$-6 \leq P \leq 1$
SU(14)											
	0	0	1	0	0	0	0	P	44-10P	1	$-2 \leq P \leq 6$
	0	0	-1	0	0	0	1	P	26-10P	1	$-2 \leq P \leq 4$
	0	0	-1	0	0	0	2	P	8-10P	1	$-2 \leq P \leq 2$
	0	0	-1	0	0	0	3	P	-10-10P	1	$-2 \leq P \leq 1$
	0	0	-1	0	0	0	1	P	62-10P	1	$0 \leq P \leq 5$
SU(15)											
	0	0	-1	0	0	0	0	P	54-11P	1	$1 \leq P \leq 5$
	0	0	-1	0	0	0	1	P	35-11P	1	$1 \leq P \leq 4$
	0	0	-1	0	0	0	2	P	16-11P	1	$1 \leq P \leq 2$
	0	0	-1	0	0	0	3	P	-3-11P	1	$-1 \leq P \leq 1$
SU(16)											
	0	0	-1	0	0	0	0	P	65-12P	1	$0 \leq P \leq 5$
	0	0	-1	0	0	0	1	P	45-12P	1	$0 \leq P \leq 4$
	0	0	-1	0	0	0	2	P	25-12P	1	$0 \leq P \leq 2$
	0	0	-1	0	0	0	3	P	5-12P	1	$-1 \leq P \leq 1$
SU(17)											
	0	0	-1	0	0	0	0	P	77-13P	1	$0 \leq P \leq 2$
	0	0	-1	0	0	0	1	P	56-13P	1	$0 \leq P \leq 3$
	0	0	-1	0	0	0	2	P	35-13P	1	$0 \leq P \leq 2$
	0	0	-1	0	0	0	3	P	14-13P	1	$0 \leq P \leq 1$

constraints are needed for GUT to insure that fermions transform as 1, 3, and 3* only under the SU(3) color group.[3]

In dynamical models, a new gauge interaction is introduced which becomes strong at an energy scale much above presently available energies. These kinds of interactions usually have a simple compact group structure of the kinds studied here. Again the fermions must satisfy the conditions of asymptotic freedom and anomaly cancellation with respect to this new gauge interaction to be physically meaningful. Furthermore, the real representation content is relatively unimportant. In these models it is perfectly sensible to regard the ordinary quarks and leptons as bound states of more fundamental objects (preons), and the additional constraint that the representation is totally antisymmetric in SU(N) GUT need not apply.

Thus both schemes of unification requiries the same minimal conditions on the fermionic content[13]:

(a) existence of complex representations,

(b) asymptotic freedom,

(c) anomaly cancellation.

We have enumerated all solutions to these conditions in this paper.

ACKNOWLEDGMENTS

We would like to thank W. Bardeen, F. Feinberg, M. Fischler, H. Georgi, D. V. Nanopoulos, J. Patera, J. Preskill, R. T. Sharp, A. N. Schellekens, M. Wise, S. K. Yun, and A. Zee for helpful discussions. One of us (I.-G. K.) wishes to thank members of the Fermilab Theory Group for warm hospitality. The same author is supported in part by the Korea Traders Foundation and the Korea Science and Engineering Foundation.

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[13]See, for example, Ref. 9, in the case of preon dynamics, and P. H. Frampton, Phys. Lett. B **88**, 299 (1979), in the case of grand unification models.
[14]In the special case of equality in Eq. (25) an additional group theoretical constraint (arising in higher orders)

$$-\tfrac{34}{3}N^2 + \tfrac{10}{3}N\sum_{R_i} T_2(R_i) + 2\sum_{R_i} C_2(R_i)T_2(R_i) < 0$$

must be satisfied for the theory to be asymptotically free. We will, however, present all solutions of Eq. (25). The two loop beta function (from which the above constraint follows) was first calculated by W. E. Caswell, Phys. Rev. Lett. **33**, 244 (1974).
[15]Recently A. N. Schellekens has also independently compiled reducible anomaly-free and complex representations with a limit on dimension, instead of the asymptotic freedom requirement imposed here.
[16]The same comment as in Ref. 14 applies in the special case of equality in Eq. (28).

Complete set of states for microscopic nuclear collective models

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(Received 2 April 1982; accepted for publication 4 June 1982)

For several years the authors have been interested in determining complete sets of states for macroscopic nuclear collective models, such as the Bohr–Mottelson one (BM) and the interacting boson approximation (IBA), as well as in their use in nuclear structure calculations. In the present paper we obtain a complete set of states for microscopic nuclear collective models such as those of Vanagas and of Filippov and Smirnov. For calculations in these models, one requires a set of states for the A nucleon system, in appropriate coordinates which include the ones related with collective degrees of freedom. As is customary in nuclear physics, the complete set of states is derived more conveniently if one assumes an oscillator interaction between the nucleons. We obtain explicitly this set of states when $A \gg 1$, showing that it can be expressed in terms of wavefunctions whose dependence on the collective coordinates is similar to those appearing in the BM model and in the IBA. We briefly indicate how this set of states can be used in microscopic collective model calculations.

PACS numbers: 21.60.Ev

I. INTRODUCTION

For several years the authors[1-3] have been interested in determining complete sets of states for macroscopic nuclear collective models as well as in their use in nuclear structure calculations.

Some of the authors[1,2] first obtained the eigenfunctions of the Bohr–Mottelson (BM) Hamiltonian[4] associated with quadrupole vibrations, which implied the explicit derivation of the γ part of the BM eigenstates as the rest of the eigenfunction was known.[4] It was also realized in these papers,[1,2] that, using this γ part, one could obtain the reduced $3j$-symbols for the $O(5) \supset O(3)$ chain of groups, and with the help of the latter determine all relevant matrix elements that appear in the general BM Hamiltonian, i.e., one that contains higher-order terms than the quadratic ones in both potential and kinetic energy. These states and reduced $3j$-symbols were applied by one of the authors[5] and his collaborators to the study of the structure of several medium and heavy even–even nuclei, in the Greiner[6] version of the general BM Hamiltonian.

A few years later we became aware of the extensive work on the interacting boson approximation (IBA) that had been carried out by Arima and Iachello.[7] We managed to reformulate the problem in configuration space[3] and showed that a complete basis of states required in the IBA computations would be those of the BM vibrational Hamiltonian, multiplied by the eigenstate of a one-dimensional oscillator Hamiltonian associated with an s boson. The calculations of the matrix elements of the two-body interactions in the IBA required then the same reduced $3j$-symbols of the $O(5) \supset O(3)$ chain of groups, which were mentioned in the previous paragraph. Thus the stage was set for calculations in the IBA using the same techniques as for the generalized BM Hamiltonian. Some of the authors[8] and their collaborators carried out this IBA program for several medium and heavy even–even nuclei.

About the same time that we started to develop an interest in the IBA, we became aware of the extensive work done on microscopic nuclear collective models by the groups of Vanagas[9] and of Filippov *et al.*[10] For calculations in these models one requires, as in the macroscopic case, a complete set of states, but now for the A nucleon system, in appropriate coordinates[11,12] that include explicitly the ones related with collective degrees of freedom. As is customary in nuclear physics, the complete set of states is derived more conveniently if one assumes an oscillator interaction between the nucleons.[13] In the references mentioned[9,10] some of the states are derived with the help of the translationally invariant shell model,[10] as well as by using appropriate Wigner coefficients by the $U(A-1)$ group associated with the $A-1$ Jacobi vectors for the A nucleon system.[9]

It is the purpose of the present paper to derive the complete set of states explictly when $A \gg 1$, using for the collective parts the type of wavefunctions already introduced in the analysis of the general BM Hamiltonian and the IBA.[1-3] The matrix elements of the relevant operators with respect to this complete set of states can then be determined through procedures similar to those followed in the macroscopic nuclear collective models. The program has already been outlined in a short publication[14] in which the states were limited to the scalar representation of the $O(A-1)$ group, but in this paper an arbitrary one, characterized by the partition $(\omega_1\omega_2\omega_3)$ involving only three numbers, will be considered. This would allow us to discuss collective effects for open shell nuclei, where they are particularly important, and not only for the case of closed shells which is the one explicitly treated in Ref. 14.

[a] Supported by the Deutsche Forschungsgemeinschaft (DFG).
[b] Member of the Instituto Nacional de Investigaciones Nucleares and El Colegio Nacional.

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The paper will be mathematical in nature, but the experience of the previous publications[1–3] clearly indicates that, once a complete set of states becomes available, the applications to specific nuclei become feasible.[5,8]

II. THE COLLECTIVE DEGREES OF FREEDOM

In this section we shall introduce the collective degrees of freedom through the concept of an intrinsic quadrupole moment for an A-body system in three dimensional space, and then express the coordinates X'_{is}, $i = 1,2,3$, $s = 1,2,...,A$, of this system in terms of the collective ones plus others.

From the beginning we want to eliminate the center of mass motion, and thus our description will be given in terms of the Jacobi coordinates associated with the relative positions of the nucleons, i.e.,

$$X_{is} = [s(s+1)]^{-1/2}\left[\sum_{t=1}^{s} X'_{it} - sX'_{is+1}\right], \quad s = 1,2,...,A-1. \tag{2.1}$$

We now consider the quadrupole matrix for the A-body system which, in the frame of reference fixed in space whose origin is at the center of mass, is given by

$$\mathbf{q} = \|q_{ij}\| = \left\|\sum_{s=1}^{A-1} X_{is}X_{js}\right\|, \quad i,j = 1,2,3. \tag{2.2}$$

The intrinsic quadrupole matrix in the frame of reference fixed in the body is then a diagonal matrix whose elements are given by the roots[15] of the characteristic equation

$$\det\|\lambda\delta_{ij} - q_{ij}\| = 0. \tag{2.3}$$

Denoting these three real and positive roots by $\lambda = \rho_k^2$, $k = 1,2,3$, and expressing them in terms of three new parameters ρ,b,c through the relations[16]

$$\rho_k^2 = (\rho^2/3)[1 + 2b\cos(c - 2\pi k/3)], \tag{2.4}$$

we immediately find out, through the standard methods of solving a cubic equation with the help of trigonometric functions,[17] that

$$\rho^2 = \operatorname{tr} q, \quad b^2 = \tfrac{3}{2}\operatorname{tr} Q^2/(\operatorname{tr} q)^2,$$
$$\cos 3c = (54)^{1/2}\det Q/(\operatorname{tr} Q^2)^{3/2}, \tag{2.5}$$

with Q being the traceless quadrupole matrix defined by

$$\mathbf{Q} = \|q_{ij} - \tfrac{1}{3}\operatorname{tr} q\delta_{ij}\|.$$

The ρ_k^2's, $k = 1,2,3$, are the terms in the diagonal quadrupole matrix in the frame of reference fixed in the body. We expect then that they or, equivalently, ρ,b,c of (2.5), together with the Euler angles ϑ_k, $k = 1,2,3$, will be related with the collective degrees of freedom of an A-body system. But this system, once we have eliminated the center of mass coordinate, has $3A - 3$ degrees of freedom while the ρ_k,ϑ_k, $k = 1,2,3$, gives us only six. Is it possible to find $3A - 9$ new coordinates such that we can expand the X_{is}, $i = 1,2,3$, $s = 1,2,...,A-1$, in terms of them and the six ρ_k,ϑ_k, $k = 1,2,3$? The answer to this was given more than a decade ago by Zickendraht[11] and by Dzublik *et al.*,[12] and, in the notation of Vanagas,[9] the coordinate transformation takes the form

$$X_{is} = \sum_{k=1}^{3}\{\rho_k D^1_{ki}(\vartheta_j) D^1_{A-4+k,s}(\phi)\}. \tag{2.6}$$

In (2.6) the matrix $\mathbf{D}^1(\vartheta_j) = \|D^1_{ki}(\vartheta_j)\|$ is the defining representation (which is the reason for the $l = 1$ appearing as an upper index) of the O(3) group, in terms of the Euler angles and in its standard orthogonal form.[18] The matrix $\|D^1_{ts}(\phi)\|$, $t,s = 1,2,...,A-1$, has the same meaning for the $O(A-1)$ group and it depends on $(A-1)(A-2)/2$ angular coordinates denoted by ϕ. As in (2.6) we need only the last three rows of this matrix; the number of angular coordinates required will be those of the $O(A-1)$ group minus those of the $O(A-4)$ subgroup associated with rows 1 to $A-4$, i.e.,

$$\tfrac{1}{2}(A-1)(A-2) - \tfrac{1}{2}(A-4)(A-5) = 3A - 9, \tag{2.7}$$

which is the required number as indicated in the previous paragraph.

Furthermore, we note that from the orthogonal property of the matrices $\|D^1_{ts}(\phi)\|$ we have

$$\mathbf{q} = \tilde{\mathbf{D}}^1(\vartheta_k)\|\rho_i^2\delta_{ij}\|\mathbf{D}^1(\vartheta_k), \tag{2.8}$$

where $\sim$ indicates the transposed matrix. Thus the ρ_k's appearing in (2.6) are related to the diagonal quadrupole matrix $\|\rho_i^2\delta_{ij}\|$ while $\mathbf{D}^1(\vartheta_k)$ is the orthogonal matrix, function of the Euler angles, that takes us from the frame of reference fixed in space to the one fixed in the body. Note that from (2.2), (2.4), (2.5), and (2.8) we see that the ρ_k,ϑ_k, $k = 1,2,3$, are invariant under permutations of the single-particle coordinates, which is one of the reasons for identifying them with collective degrees of freedom.

The coordinate transformation (2.6) must be bijective (one-to-one onto) which implies the inequality[16] $0 \leqslant \rho_2 \leqslant \rho_1 \leqslant \rho_3 \leqslant \infty$ that translates into restrictions for b and c that limit them[16] to the lined triangle in Fig. 1, where $x = b\cos c$, $y = b\sin c$. The restrictions on c, i.e., $0 \leqslant c \leqslant \pi/3$ are the same[4] as those of γ in the BM model but, as we see from Fig. 1, b cannot exceed 1 so its range *is not* that of β, which is in the interval[4] $0 \leqslant \beta \leqslant \infty$.

From (2.6) the X_{is} are associated with the defining irreducible representation (irreps) of both the O(3) and $O(A-1)$ orthogonal groups. It is clear therefore that polynomial functions of the X_{is} can be expanded in terms of irreducible representations of these two groups, and, for our later developments, it will be important to understand the nature of these representations and introduce a convenient notation for them. For the O(3) group they are the well-known ones[19] that can be denoted by

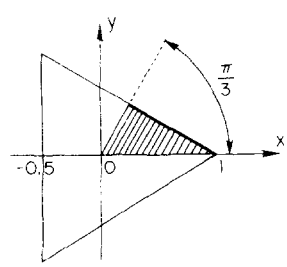


FIG. 1. The variables b and c appearing in Eqs. (2.4) and (2.5) are restricted to the lined triangle, where the coordinates are given by $x = b\cos c$ and $y = b\sin c$.

$$D^{L}_{KM}(\vartheta_j), \tag{2.9}$$

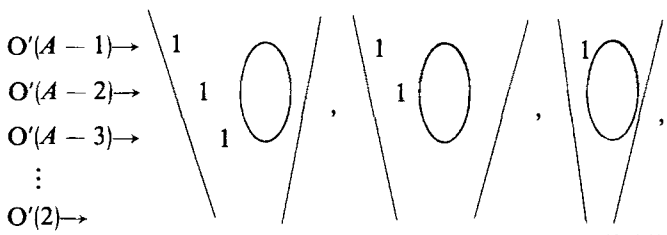
in which L gives the irrep of O(3) while K and M are, respectively, the irreps of O'(2) and O(2), the subgroups associated with rotations around the z axis in frames of reference fixed in the body and in space. The notation (2.9) is in agreement with the $D^{1}_{ki}(\vartheta_j)$ appearing in (2.6), but corresponds to the inverse rotation in the notation used in Rose's book.[19] Denoting by $\mathscr{D}^{L}_{KM}(\vartheta_j)$ the functions used in this reference,[19] we have the relation $D^{L}_{KM}(\vartheta_j) = \mathscr{D}^{L}_{MK}{}^{*}(\vartheta_j)$, where * indicates conjugation.

Passing now to the O($A-1$) group, the rows and columns of its irreps can again be characterized by subgroups of O($A-1$) in frames of reference fixed respectively in the "body" and in "space." We note that the O($A-1$) group is essentially related with particle indices and thus the "body" and "space" labels for the rows and columns in its representations is just a way of describing them which emphasizes the analogy, *but not the identity*, with a similar labeling in the O(3) group. We shall denote respectively with and without prime the chain of orthogonal groups in the "body" and "space" fixed frames. We shall also refer to "body" and "space" fixed frame generators (again to be denoted with and without prime) of these chains of groups as those which Vanagas[9] calls left and right shift operators.

In the case of the rows of the irreps of O($A-1$) we can take the Gel'fand–Zetlin[20] chain of orthogonal groups, i.e.,

$$O'(A-1)\supset O'(A-2)\supset O'(A-3)\supset\cdots\supset O'(2). \tag{2.10}$$

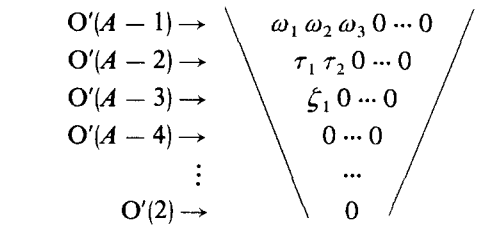
Looking now at the X_{is} of (2.6), we see that they are expressed in terms of $D^{1}_{A-4+k,s}(\phi)$, $k=1,2,3$, $s=1,2,\ldots,A-1$, so in the frame of reference fixed in the body (to which the row index $A-4+k$ corresponds) only the last three components $A-3$, $A-2$, $A-1$, appear. These components expressed as Gel'fand patterns[20] associated with the irreps of the chain of groups (2.10) are given respectively by



(2.11)

where the big zero indicates that all components in the pattern are zero except those explicitly indicated as 1.

Clearly, then if we now have instead of the X_{is} an arbitrary polynomial function of them, all irreps associated with the chain of subgroups $O'(A-4)\supset O'(A-5)\supset\cdots\supset O'(2)$ continue to be scalars, i.e., the corresponding rows in the Gel'fand pattern contain only zeros. Thus, by the inequalities[20] satisfied by the partitions characterizing the irreps of the chain of groups (2.10), a polynomial in the X_{is} can be expanded in irreps of O($A-1$) whose rows are associated with Gel'fand patterns of the type



(2.12)

From (2.12) we conclude that the only irreps of O($A-1$) of interest to us would be those characterized by a partition in three integers, i.e., $(\omega_1\omega_2\omega_3)$. Furthermore, the row or the representation will be characterized by the irreps $(\tau_1\tau_2)$ of O'($A-2$) and ζ_1 of O'($A-3$), which, from the Gel'fand–Zetlin rules[20] (at least when $A\geqslant 6$) satisfy the inequalities

$$\omega_1\geqslant\tau_1\geqslant\omega_2\geqslant\tau_2\geqslant\omega_3\geqslant 0, \tag{2.13a}$$

$$\tau_1\geqslant\zeta_1\geqslant\tau_2\geqslant 0, \tag{2.13b}$$

which are also those of a $U(3)\supset U(2)\supset U(1)$ chain of groups.

We now turn our attention to the column index in the irrep of O($A-1$) that will be relevant for our later development. As the X_{is} are expressed in terms of the $D^{1}_{A-4+k,s}(\phi)$, where the column index s takes now *all* values $s=1,2,\ldots,A-1$, it is clear that in the chain of groups (2.10), but now in the frame of reference fixed in "space" and not in the "body," we no longer have only scalar representations of the subgroups $O(A-4)\supset O(A-5)\supset\cdots\supset O(2)$. We can then still develop polynomial functions of the X_{is} in terms of irreps of O($A-1$) whose columns are characterized by Gel'fand patterns such as (2.12), but they would have, in general, three terms in every row. However, this characterization of the columns in the irrep of O($A-1$) is not very physical. It is more convenient to pass from O($A-1$) to the subgroup given by the representation $D^{(A-1,1)}(S_A)$ of the A-dimensional symmetric group S_A.[21] In this way the polynomial functions in the X_{is} will be characterized by irreps of the symmetric[21] group S_A associated with the partition $\{f\}=(f_1f_2\cdots f_A)$ of A, and could be combined with the spin–isospin part of the wavefunction to satisfy the Pauli principle. Considering also the chain of subgroups $S_A\supset S_{A-1}\supset\cdots\supset S_2$ of the symmetric group, the irrep of O($A-1$) is further characterized by Yamanouchi[21] symbol $(r)=(r_1r_2\cdots r_A)$ and, because a given irrep $\{f\}$ of S_A can appear several times in an irrep $(\omega_1\omega_2\omega_3)$ of O($A-1$), we need an extra set of indexes δ that distinguishes[22] these repeated representations. Thus we finally arrive at the conclusion that polynomial functions of the X_{is} can be expanded in terms of the irreps of O($A-1$), which we could denote by

$$D^{(\omega_1\omega_2\omega_3)}_{\tau_1\tau_2,\zeta_1;\delta\{f\}(r)}(\phi). \tag{2.14}$$

The explicit determination of these irreps is by no means trivial,[9,10] but, as we shall see later, in most applications we shall not require them. What will be important though is to find a complete set of states that we can write as sums of products of irreps of O(3), O($A-1$) in (2.9) and (2.14) and functions of ρ,b,c, which we shall proceed to determine.

III. THE OSCILLATOR HAMILTONIAN

As in many other problems in nuclear physics,[13] when we want to find complete sets of states we start by consider-

ing eigenstates of an A-body system in which the interactions are of the harmonic oscillator type. Choosing units in which $\hbar$, the mass of the nucleon, and an appropriate frequency[23] are 1, we have in terms of the Jacobi coordinates X_{is} and their corresponding momenta $P_{is} = -i\partial/\partial X_{is}$ that our Hamiltonian takes the form

$$H = \tfrac{1}{2}\sum_{s=1}^{A-1}\sum_{i=1}^{3}(P_{is}^2 + X_{is}^2). \tag{3.1}$$

It is clear that this Hamiltonian is invariant under both the O(3) and O($A-1$) orthogonal groups and thus the irreps L and $(\omega_1\omega_2\omega_3)$ can characterize the eigenstates of (3.1). To find these eigenstates explicitly, it is convenient to pass from the coordinates X_{is} to the six collective coordinates ρ_k, ϑ_k, $k = 1,2,3$ and the $3A-9$ angular coordinates ϕ, as indicated in (2.6). Under this transformation of coordinates the Hamiltonian (3.1) takes the form[9,10]

$$\begin{aligned} H = &\left\{\tfrac{1}{2}\sum_{k=1}^{3}\left[-\frac{\partial^2}{\partial\rho_k^2} - \frac{(A-4)}{\rho_k}\frac{\partial}{\partial\rho_k} + \rho_k^2\right]\right. \\ &\left. - \sum_{k>k'=1}^{3}(\rho_k^2 - \rho_{k'}^2)^{-1}\left(\rho_k\frac{\partial}{\partial\rho_k} - \rho_{k'}\frac{\partial}{\partial\rho_{k'}}\right)\right\} \\ &+ \left\{\tfrac{1}{2}\sum_{k>k'=1}^{3}(\rho_k^2 + \rho_{k'}^2)(\rho_k^2 - \rho_{k'}^2)^{-2}\right. \\ &\times[\mathscr{L}'^2_{A-4+k,A-4+k'} + L'^2_{kk'}] \\ &\left. + 2\sum_{k>k'=1}^{3}\rho_k\rho_{k'}(\rho_k^2 - \rho_{k'}^2)^{-2}\right. \\ &\left.\times\mathscr{L}'_{A-4+k,A-4+k'}L'_{kk'}\right\} \\ &+ \frac{1}{2}\sum_{k=1}^{3}\rho_k^{-2}\sum_{s=1}^{A-4}\mathscr{L}'^2_{A-4+k,s}, \end{aligned} \tag{3.2}$$

where

$L'_{k'k''} = \Sigma_{k=1}^{3}\epsilon_{k'k''k}L'_k$ with $\epsilon_{k'k''k}$ being the antisymmetric tensor and L'_k the component of the ordinary angular momentum vector in the frame of reference fixed in the body.[18] The $\mathscr{L}'_{st}$ are the generators of an O($A-1$) group also in a kind of "body" fixed reference frame, i.e., they are defined by

$$\mathscr{L}'_{st} = \sum_{u,v=1}^{A-1} D^1_{su}(\phi)D^1_{tv}(\phi)\mathscr{L}_{uv}, \tag{3.3}$$

where $\mathscr{L}_{uv}$ are the standard generators of the O($A-1$) group

$$\mathscr{L}_{uv} = -i\sum_{j=1}^{3}\left(X_{ju}\frac{\partial}{\partial X_{jv}} - X_{jv}\frac{\partial}{\partial X_{ju}}\right), \tag{3.4}$$

which in turn can be expressed as functions of only the angles ϕ's and derivatives with respect to them.

While the derivation of the expression (3.2) is carried out in the references mentioned,[9,10] the present authors have also looked at the problem from a point of view that leads to the explicit expressions of all the generators of a dynamical group Sp(6) [where one of these generators is the Hamiltonian (3.1)] in terms of the coordinates introduced in (2.6). This analysis is presented in Appendix A.

We want to transform the Hamiltonian (3.2) so as to be able to obtain from it the equation that will provide us with a complete set of states characterized by the irrep L of O(3) and $(\omega_1\omega_2\omega_3)$ of O($A-1$). For this purpose we note that the Casimir operator $G'(r)$, $r = 2,3,\ldots,A-1$, of an orthogonal group $O'(r)$ in a frame of reference fixed in the body is given by

$$G'(r) = \tfrac{1}{2}\sum_{s,t=1}^{r}\mathscr{L}'^2_{st}. \tag{3.5}$$

Looking then at $\Sigma_{s=1}^{A-4}\mathscr{L}'^2_{A-4+k,s}$, $k = 1,2,3$, which is the last term appearing in (3.2), we conclude from the fact that $\mathscr{L}'_{st} = -\mathscr{L}'_{ts}$, that we can write for $k = 1,2,3$,

$$\begin{aligned} &\sum_{s=1}^{A-4}\mathscr{L}'^2_{A-3,s} = G'(A-3) - G'(A-4), \\ &\sum_{s=1}^{A-4}\mathscr{L}'^2_{A-2,s} = G'(A-2) - G'(A-3) - \mathscr{L}'^2_3, \\ &\sum_{s=1}^{A-4}\mathscr{L}'^2_{A-1,s} = G'(A-1) - G'(A-2) - \mathscr{L}'^2_1 - \mathscr{L}'^2_2, \end{aligned} \tag{3.6}$$

in which

$$\mathscr{L}'_k \equiv \tfrac{1}{2}\sum_{k',k''}\epsilon_{kk'k''}\mathscr{L}'_{A-4+k',A-4+k''}. \tag{3.7}$$

We can write now the eigenfunction Ψ of H of (3.2) as

$$\Psi = (\rho_1\rho_2\rho_3)^{-(A-4)/2}(\rho_1^2 + \rho_2^2 + \rho_3^2)^{-2}\psi \tag{3.8}$$

and the corresponding Hamiltonian when acting on ψ as H'. Expressing then H' in terms of ρ,b,c, related to ρ_1,ρ_2,ρ_3 through (2.4) we see, in a straightforward though laborious way, that it becomes

$$H' = \frac{1}{2}\left(-\frac{\partial^2}{\partial\rho^2} + \frac{R^2}{\rho^2} + \rho^2\right), \tag{3.9}$$

where, using (3.6), we obtain that the operator $\frac{1}{2}R^2$ takes the form

$$\tfrac{1}{2}R^2 = \tfrac{1}{2}(R_1^2 + R_2^2 + R_3^2), \tag{3.10}$$

in which

$$\begin{aligned} \tfrac{1}{2}R_1^2 = &-(1 + b\cos 3c - 2b^2)\frac{\partial^2}{\partial b^2} + (2b\sin 3c)\frac{1}{b}\frac{\partial^2}{\partial b\partial c} \\ &- \frac{4}{b}\left[1 - \frac{b}{4}\cos 3c - \frac{9}{4}b^2\right] \\ &\times\frac{\partial}{\partial b} - \frac{1 - b\cos 3c}{b^2}\frac{\partial^2}{\partial c^2} \\ &- \frac{3}{b^2}\cot 3c\left[1 + \tfrac{2}{3}b\sin 3c\tan 3c - b\sec 3c\right]\frac{\partial}{\partial c} \\ &+ \frac{9}{2}\left[\left(\frac{A-5}{2}\right)^2 - \frac{1}{4}\right] \\ &\times\frac{1 - b^2}{1 - 3b^2 + 2b^3\cos 3c} + 6, \end{aligned} \tag{3.11a}$$

$$\begin{aligned} \tfrac{1}{2}R_2^2 = &\sum_{k=1}^{3}\frac{1 - bc_k}{4b^2s_k^2}(L'^2_k + \mathscr{L}'^2_k) \\ &+ \sum_{k=1}^{3}\frac{[1 - 2bc_k + 4b^2(c_k^2 - \frac{3}{4})]^{1/2}}{2b^2s_k^2}L'_k\mathscr{L}'_k, \end{aligned} \tag{3.11b}$$

$$\begin{aligned} \tfrac{1}{2}R_3^2 = &\tfrac{3}{2}(1 + 2bc_1)^{-1}[G'(A-3) - G'(A-4)] \\ &+ \tfrac{3}{2}(1 + 2bc_2)^{-1} \\ &\times[G'(A-2) - G'(A-3) - \mathscr{L}'^2_3] + \tfrac{3}{2}(1 + 2bc_3)^{-1} \\ &\times[G'(A-1) - G'(A-2) - \mathscr{L}'^2_1 - \mathscr{L}'^2_2], \end{aligned}$$

where we have used the shorthand notation

$$c_k \equiv \cos[c - (2\pi k/3)], \quad s_k \equiv \sin[c - (2\pi k/3)], \quad k = 1,2,3. \tag{3.12}$$

The reason for writing the $\frac{1}{2} R^2$ of (3.10) as a sum of three terms is to emphasize that R_1^2 and R_2^2 came respectively from the first and second curly brackets in (3.2) while R_3^2, when divided by $2\rho^2$, is the last term in (3.2).

As the Hamiltonian (3.1), and thus also the H' of (3.9), is invariant under the group $O(A-1)$, the eigenstates of H' can be characterized by the irrep $(\omega_1\omega_2\omega_3)$ of this group. Therefore, we can write the ψ in (3.8) in the form

$$\psi = \sum_{\tau_1,\tau_2,\zeta_1} f^{(\omega_1\omega_2\omega_3)}_{\tau_1\tau_2,\zeta_1}(\rho,b,c;\vartheta_k) D^{(\omega_1\omega_2\omega_3)}_{\tau_1\tau_2,\zeta_1;\delta\{f\}(r)}(\phi)$$

$$= [\,\mathbf{f}^{(\omega_1\omega_2\omega_3)}(\rho,b,c;\vartheta_k)\cdot\mathbf{D}^{(\omega_1\omega_2\omega_3)}(\phi)\,]_{\delta\{f\}(r)}, \tag{3.13}$$

where the D is given in (2.14) and $f^{(\omega_1\omega_2\omega_3)}$ is still to be determined. We have also expressed ψ as the component $\delta\{f\}(r)$ of the product of a row vector $\mathbf{f}^{(\omega_1\omega_2\omega_3)}$ and a matrix $\mathbf{D}^{(\omega_1\omega_2\omega_3)}$ associated with the irrep $(\omega_1\omega_2\omega_3)$ of $O(A-1)$. From the inequalities (2.13) it is clear that the row vector has as many components as the dimension of the irrep $[\omega_1\omega_2\omega_3]$ of a U(3) group.[24]

The only operators appearing in (3.9)–(3.11) that are related to the $O(A-1)$ group are the generators $\mathscr{L}'_k$, $k = 1,2,3$, of (3.7) and the Casimir operator $G'(r)$, $r = A-1$, $A-2$, $A-3$, $A-4$, both of them in the frame of reference fixed in the "body." Thus $\mathbf{f}^{(\omega_1\omega_2\omega_3)}(\rho,b,c;\vartheta_k)$ satisfies the equation

$$\mathbf{H}'\mathbf{f}^{(\omega_1\omega_2\omega_3)} = E\mathbf{f}^{(\omega_1\omega_2\omega_3)}, \tag{3.14}$$

where H' is the matrix operator given by (3.9)–(3.11) in which $\mathscr{L}'_k$ and $G'(r)$ are replaced by their matrices $\underline{\mathscr{L}}'_k$ and $\mathbf{G}'(r)$ with respect to the Gel'fand states (2.12). These matrices are well known; for the $G'(r)$ they are diagonal and if the irrep of $O'(r)$ is characterized by the partition $(K_1K_2\cdots K_{[r/2]})$ the factor along the diagonal is given by[24]

$$\sum_{s=1}^{[r/2]} K_s(K_s + r - 2s), \tag{3.15}$$

where $[r/2] = r/2$ or $(r-1)/2$ depending on whether r is even or odd. Thus we see that with respect to the states (2.12) we have the following diagonal matrices associated with the Casimir operators:

$$\mathbf{G}'(A-1) = [\omega_1(\omega_1 + A - 3) + \omega_2(\omega_2 + A - 5) + \omega_3(\omega_3 + A - 7)] \times \|\delta_{\tau'_1\tau_1}\delta_{\tau'_2\tau_2}\delta_{\zeta'_1\zeta_1}\|, \tag{3.16a}$$

$$\mathbf{G}'(A-2) = \|[\tau_1(\tau_1 + A - 4) + \tau_2(\tau_2 + A - 6)]\delta_{\tau'_1\tau_1}\delta_{\tau'_2\tau_2}\delta_{\zeta'_1\zeta_1}\|, \tag{3.16b}$$

$$\mathbf{G}'(A-3) = \|\zeta_1(\zeta_1 + A - 5)\delta_{\tau'_1\tau_1}\delta_{\tau'_2\tau_2}\delta_{\zeta'_1\zeta_1}\|, \tag{3.16c}$$

while $\mathbf{G}(A-4)$ vanishes. The matrix elements of $\mathscr{L}'_k$, $k = 1,2,3$, with respect to the states (2.12) have been obtained by Gel'fand and Zetlin,[20] and they will be discussed in the next section.

Thus we see that we have the perfectly definite problem (3.14) to solve if we want to find the components of the vector $\mathbf{f}^{(\omega_1\omega_2\omega_3)}(\rho,b,c,\vartheta_k)$, which we require if we want to get a complete set of states for microscopic collective models. Unfortunately, this problem seems quite difficult. The part of $\mathbf{f}^{(\omega_1\omega_2\omega_3)}(\rho,b,c,\vartheta_k)$ that depends on ρ can, from (3.9), be separated from the rest and expressed in terms of Laguerre polynomials.[1,2] The dependence of $\mathbf{f}^{(\omega_1\omega_2\omega_3)}$ on the Euler angles ϑ_k can be given[1,2] in terms of the Wigner function $D^L_{KM}(\vartheta_k)$ of (2.9). It is the dependence of $\mathbf{f}^{(\omega_1\omega_2\omega_3)}$ on b and c that is difficult to determine as, from (3.11) and (3.14), it would imply solving a complicated set of coupled partial differential equations in these variables. The experience that two of the authors had with the solution[1,2] of the Bohr–Mottelson vibrational Hamiltonian showed how hard (though still feasible with the help of group theoretical methods[1,2]) was the solution of the set of coupled *ordinary* differential equations associated with the single variable γ. The present problem is at least an order of magnitude harder, and thus, rather than attempt to solve it exactly, we shall consider in Sec. V the case when $A \gg 1$ and then show how to express $\mathbf{f}^{(\omega_1\omega_2\omega_3)}$ in terms of the eigenfunctions that appeared in the *BM* vibrational Hamiltonian[1,2].

To implement our program in the limit of large A's, it will be convenient to add and subtract to the matrix Hamiltonian appearing in (3.14) the term

$$\frac{3}{2}\sum_{k=1}^{3}\frac{\omega(\omega + A - 5)}{\{1 + 2b\cos[c - (2\pi k/3)]\}} = \frac{9}{2}\omega(\omega + A - 5)\frac{(1-b^2)}{1 - 3b^2 + 2b^3\cos 3c}, \tag{3.17}$$

where ω is related to the partition $(\omega_1\omega_2\omega_3)$ characterizing the irrep of $O(A-1)$ through the definition

$$\omega \equiv \tfrac{1}{3}(\omega_1 + \omega_2 + \omega_3). \tag{3.18}$$

The H' is then given by

$$\mathbf{H}' = \frac{1}{2}\left[-\frac{\partial^2}{\partial\rho^2} + \frac{\mathbf{R}^2}{\rho^2} + \rho^2\right], \tag{3.19}$$

where the matrix operator $\mathbf{R}^2$ can be written as

$$\tfrac{1}{2}\mathbf{R}^2 = \tfrac{1}{2}(\mathbf{R}'^2_1 + \mathbf{R}'^2_2 + \mathbf{R}'^2_3), \tag{3.20}$$

in which $\mathbf{R}'^2_k$, $k = 1,2,3$, are defined as follows: The operator $\frac{1}{2}\mathbf{R}'^2_1$ is given by (3.11a) in which, from the right-hand side of (3.17), the term $[(A-5)/2]^2$ appearing in it is replaced by $[\omega + (A-5)/2]^2$; $\frac{1}{2}\mathbf{R}'^2_2$ is given by (3.11b) in which $\mathscr{L}'_k$, $k = 1,2,3$ of (3.7) are replaced by the matrices $\underline{\mathscr{L}}'_k$ of these operators with respect to the states (2.12); finally $\frac{1}{2}\mathbf{R}'^2_3$ is given by (3.11c), where in each of the square brackets we have to add, from the left-hand side of (3.17), the term $-\omega(\omega + A - 5)$ and besides replace $\mathscr{L}'_k$ by $\underline{\mathscr{L}}'_k$ and the Casimir operators $G'(r)$, $r = A-1, A-2, A-3, A-4$, by the diagonal matrices $\mathbf{G}'(r)$ of (3.16).

It will be very convenient to have a compact symbol to

designate the new term appearing in $\frac{1}{2}\mathbf{R}_1'^2$, and thus we define

$$\sigma^2 = \omega_1 + \omega_2 + \omega_3 + \tfrac{3}{2}(A-5) = 3[\omega + (A-5)/2], \tag{3.21}$$

which will play an important role in all the following discussions.

We proceed now to derive the matrices of $\mathscr{L}_k'$ with respect to the Gel'fand–Zetlin[20] states (2.12) and see the interesting form that $\mathscr{L}_k'$ takes when $A \gg 1$, which will allow us to find in Sec. V a complete set of states for microscopic collective models of the nucleus.

IV. MATRIX ELEMENTS OF THE GENERATORS OF AN O($A-1$) GROUP IN A GEL'FAND–ZETLIN BASIS

In this section we wish to determine the matrix elements in the Gel'fand–Zetlin basis (2.12) of the operators $\mathscr{L}_k'$, $k = 1,2,3$, which, from (3.7), are given by the following generators of the O($A-1$) group in the frame of reference fixed in the "body"

$$\mathscr{L}_1' = \mathscr{L}_{A-2,A-1}', \qquad \mathscr{L}_2' = \mathscr{L}_{A-1,A-3}', \quad \mathscr{L}_3' = \mathscr{L}_{A-3,A-2}'. \tag{4.1}$$

The work of Gel'fand and Zetlin,[20] and later that of Pang and Hecht,[25] provided the general expression for the matrix element of a generator $\mathscr{L}_{st}$, $s,t = 1,2,\ldots,r$ of an O(r) group, with respect to the Gel'fand state characterized by the irreps of the chain of groups $O(r) \supset O(r-1) \supset \cdots \supset O(2)$. The $\mathscr{L}_{st}$ defined in the frame of reference fixed in "space" satisfy the commutation relations

$$[\mathscr{L}_{st}, \mathscr{L}_{s't'}] = (-i)(\mathscr{L}_{st'}\delta_{s't} + \mathscr{L}_{ts'}\delta_{t's} + \mathscr{L}_{t't}\delta_{ss'} + \mathscr{L}_{s's}\delta_{tt'}), \tag{4.2}$$

while the $\mathscr{L}_{st}'$ in the frame of reference fixed in the "body" satisfy the same commutation relation (4.2) but with the sign changed on the right-hand side. It is clear therefore that $-(-1)^{s-t}\mathscr{L}_{st}$ and $\mathscr{L}_{st}'$ satisfy the same commutation relations, and thus, if we multiply the matrix representations of Gel'fand and Zetlin[20,25] for $\mathscr{L}_{st}$ by the phase factor $-(-1)^{s-t}$, we get a representation of the generators in the frame of reference fixed in the "body," i.e., for the particular generators in (4.1), the matrix $\underline{\mathscr{L}}_k'$ associated with $\mathscr{L}_k'$. The choice of phase was also made so that it agrees with standard results[18] when we restrict ourselves to the group O(3).

The Gel'fand–Zetlin states (2.12) are not the more general ones possible for the group O($A-1$) but are restricted to those in which, in the frame of reference fixed in the "body," from O($A-4$) downwards we have only the scalar representations. We suppress all the zeros in the Gel'fand pattern (2.12), and thus what we want to determine are the matrix elements

$$\left\langle \begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1'\tau_2' \\ \zeta_1' \end{matrix} \middle| \mathscr{L}_k' \middle| \begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1 \end{matrix} \right\rangle, \quad k = 1,2,3. \tag{4.3}$$

We start by considering $\mathscr{L}_3' = \mathscr{L}_{A-3,A-2}'$, which obviously is not affected by the irrep $(\omega_1\omega_2\omega_3)$ of O($A-1$) as it corresponds to a generator of the subgroup O'($A-2$). Thus the matrix element of $\mathscr{L}_3'$ depends only on τ_1,τ_2,ζ_1 in ket and bra, is diagonal in the τ indices, and, from the analysis of Pang and Hecht[25] and the phase considerations discussed above, is given by

$$\begin{aligned} &\left\langle \begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1' \end{matrix} \middle| \mathscr{L}_3' \middle| \begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1 \end{matrix} \right\rangle \\ &\quad = i[(\tau_1-\zeta_1)(\zeta_1+1-\tau_2)]^{1/2} g_{\zeta_1}^{\tau_1\tau_2}\delta_{\zeta_1',\zeta_1+1} \\ &\quad - i[(\tau_1-\zeta_1+1)(\zeta_1-\tau_2)]^{1/2} g_{\zeta_1-1}^{\tau_1\tau_2}\delta_{\zeta_1',\zeta_1-1}, \end{aligned} \tag{4.4}$$

where $g_{\zeta_1}^{\tau_1\tau_2}$ is given by

$$g_{\zeta_1}^{\tau_1\tau_2} = \left[\frac{(\tau_1+\zeta_1+A-4)(\tau_2+\zeta_1+A-5)}{(2\zeta_1+A-5)(2\zeta_1+A-3)}\right]^{1/2}. \tag{4.5}$$

Turning now our attention to $\mathscr{L}_1' = \mathscr{L}_{A-2,A-1}'$, we see from (4.2) that it commutes with all the generators of O'($A-3$) and thus its matrix element will be diagonal in the ζ_1 index. Again from the analysis of Pang and Hecht[25] and the phase considerations discussed previously we obtain

$$\begin{aligned} &\left\langle \begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1'\tau_2' \\ \zeta_1 \end{matrix} \middle| \mathscr{L}_1' \middle| \begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1 \end{matrix} \right\rangle \\ &= i\left[\frac{(\tau_1-\zeta_1+1)(\omega_1-\tau_1)(\tau_1-\omega_2+1)(\tau_1-\omega_3+2)}{(\tau_1-\tau_2+1)(\tau_1-\tau_2+2)}\right]^{1/2} \\ &\quad \times g_{\tau_1-1}^{(\omega_1\omega_2\omega_3)(\tau_1+\tau_2)\zeta_1}\delta_{\tau_1',\tau_1-1}\delta_{\tau_2',\tau_2} \\ &\quad + i\left[\frac{(\zeta_1-\tau_2)(\omega_1-\tau_2+1)(\omega_2-\tau_2)(\tau_2-\omega_3+1)}{(\tau_1-\tau_2+1)(\tau_1-\tau_2+2)}\right]^{1/2} \\ &\quad \times g_{\tau_2}^{(\omega_1\omega_2\omega_3)(\tau_1+\tau_2)\zeta_1}\delta_{\tau_1',\tau_1}\delta_{\tau_2',\tau_2+1} \\ &\quad - i\left[\frac{(\tau_1-\zeta_1)(\omega_1-\tau_1+1)(\tau_1-\omega_2)(\tau_1-\omega_3+1)}{(\tau_1-\tau_2)(\tau_1-\tau_2+1)}\right]^{1/2} \\ &\quad \times g_{\tau_1-1}^{(\omega_1\omega_2\omega_3)(\tau_1+\tau_2)\zeta_1}\delta_{\tau_1',\tau_1-1}\delta_{\tau_2',\tau_2} \\ &\quad - i\left[\frac{(\zeta_1-\tau_2+1)(\omega_1-\tau_2+2)(\omega_2-\tau_2+1)(\tau_2-\omega_3)}{(\tau_1-\tau_2+1)(\tau_1-\tau_2+2)}\right]^{1/2} \\ &\quad \times g_{\tau_2-1}^{(\omega_1\omega_2\omega_3)(\tau_1+\tau_2)\zeta_1}\delta_{\tau_1',\tau_1}\delta_{\tau_2',\tau_2-1}, \end{aligned} \tag{4.6}$$

where

$$\begin{aligned} &g_{\tau_j}^{(\omega_1\omega_2\omega_3)(\tau_1+\tau_2)\zeta_1} \\ &\quad = \left[\frac{(\zeta_1+\tau_j-j+A-3)(\omega_1+\tau_j-j+A-2)}{(2\tau_j-2j+A)(2\tau_j-2j+A-2)}\right. \\ &\quad \left.\times\frac{(\omega_2+\tau_j-j+A-3)(\omega_3+\tau_j-j+A-4)}{(\tau_1+\tau_2+A-4)(\tau_1+\tau_2+A-5)}\right]^{1/2} \end{aligned} \tag{4.7}$$

and $j = 1,2$.

As for the matrix element (4.3) when $k = 2$, we do not need to calculate it explicitly as we can obtain it using the commutation relation

$$[\mathscr{L}'_3,\mathscr{L}'_1] = -i\mathscr{L}'_2. \tag{4.8}$$

Once we have the matrix elements (4.4), (4.6), and (4.8) of the $\mathscr{L}'_k$, $k = 1,2,3$, it becomes interesting to determine their asymptotic form when A becomes very large. It is convenient for this purpose to replace the numbers characterizing the irreps in the chain $O'(A-1)\supset O'(A-2)\supset O'(A-3)$ by the following parameters, which, as we show later, will be related to the irrep in the chain $U(3)\supset U(2)\supset U(1)$ and allow us to see more clearly the limits of the coefficients g in (4.5) and (4.7) when we have a large number of nucleons. We first define

$$\lambda = \omega_1 - \omega_2, \tag{4.9a}$$

$$\mu = \omega_2 - \omega_3, \tag{4.9b}$$

and, combining with the ω of (3.18), we obtain

$$\omega_1 = \omega + (2\lambda + \mu)/3, \tag{4.10a}$$

$$\omega_2 = \omega + (\mu - \lambda)/3, \tag{4.10b}$$

$$\omega_3 = \omega - (\lambda + 2\mu)/3. \tag{4.10c}$$

Furthermore, we define

$$2\tau = \tau_1 + \tau_2, \tag{4.11a}$$

$$2l = \tau_1 - \tau_2, \tag{4.11b}$$

which imply

$$\tau_1 = \tau + l, \tag{4.12a}$$

$$\tau_2 = \tau - l, \tag{4.12b}$$

and finally we introduce a parameter m by the relation

$$\zeta_1 = \tau + m. \tag{4.13}$$

From the inequalities (2.13a) we see that

$$\omega_1 + \omega_2 \geqslant \tau_1 + \tau_2 \geqslant \omega_2 + \omega_3, \tag{4.14}$$

and thus, if we define

$$\tau' = \tau - \omega, \tag{4.15}$$

we see that it takes values only in the range

$$-(2\lambda + \mu)/6 \leqslant \tau' \leqslant (\lambda + 2\mu)/6. \tag{4.16}$$

We note furthermore from (2.13b) that $\tau_1 \geqslant \tau_2$ and thus from (4.11b) l must be nonnegative. As we have also $\omega_1 \geqslant \tau_1$ we obtain from (4.10a), (4.12a), and (4.16) that

$$\lambda + \mu/2 \geqslant l \geqslant 0. \tag{4.17}$$

Finally from (2.13b) and (4.12),(4.13) we have

$$l \geqslant m \geqslant -l. \tag{4.18}$$

We proceed now to rewrite the g's of (4.5) and (4.7) in terms of λ,μ,l,m,τ', and instead of ω we substitute σ^2 through the relation (3.21). We then obtain for the g of (4.5)

$$g^{\tau_1\tau_2}_{\zeta_1} = \left[\frac{(\frac{2}{3}\sigma^2 + 2\tau' + l + m + 1)(\frac{2}{3}\sigma^2 + 2\tau' - l + m)}{(\frac{2}{3}\sigma^2 + 2\tau' + 2m)(\frac{2}{3}\sigma^2 + 2\tau' + 2m + 2)}\right]^{1/2}, \tag{4.19}$$

while for the g of (4.7) we get

$$g^{(\omega_1\omega_2\omega_3)[(\tau_1+\tau_2)\zeta_1}_{\tau_j} = \left\{\frac{[\frac{2}{3}\sigma^2 + 2\tau' + m + 1 + l_j][\frac{2}{3}\sigma^2 + \tau' + (2\lambda+\mu)/3 + 2 + l_j]}{(\frac{2}{3}\sigma^2 + 2\tau' + 3 + 2l_j)(\frac{2}{3}\sigma^2 + 2\tau' + 1 + 2l_j)} \times \frac{[\frac{2}{3}\sigma^2 + \tau' + (\mu-\lambda)/3 + 1 + l_j][\frac{2}{3}\sigma^2 + \tau' - (\lambda+2\mu)/3 + l_j]}{(\frac{2}{3}\sigma^2 + 2\tau' + 1)(\frac{2}{3}\sigma^2 + 2\tau')}\right\}^{1/2} \tag{4.20}$$

with j in l_j and τ_j taking the values $j = 1,2$ and $l_1 = l$, $l_2 = -l - 1$.

When, in Sec. VI, we discuss microscopic collective models in the versions of Vanagas[9] and Filippov,[10] we will show that for A of the order of a 100, the σ^2 is of the order of a1000, while λ,μ,τ',l,m are of the order of 10. This difference becomes even more pronounced when A continues to increase. Thus when $A\to\infty$ the g of (4.19) and (4.20) becomes 1 while for large A we can expand the g's in inverse powers of σ^2 so that, suppressing all upper and lower indices, we can write

$$g = 1 + (\bar{g}/\sigma^2), \tag{4.21a}$$

$$\bar{g} = \sum_{n=0}^{\infty} (\bar{g}_n/\sigma^{2n}). \tag{4.21b}$$

It is interesting now to compare, in the limit when $A\to\infty$, the matrix elements (4.4), (4.6), and (4.8) of $\mathscr{L}'_k$, with those of the generators C_{ij}, $i,j = 1,2,3$, of a U(3) group, again in a Gel'fand and Zetlin basis[26] but now for the unitary group chain $U(3)\supset U(2)\supset U(1)$. We shall designate this basis by a round bracket rather than the angular one for the orthogonal groups used in (4.3). The matrix elements

$$\begin{pmatrix} \omega_1\omega_2\omega_3 \\ \tau'_1\tau'_2 \\ \zeta'_1 \end{pmatrix} \left| C_{ij} \right| \begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1 \end{matrix} \tag{4.22}$$

have been obtained explicitly in Ref. 24 (p. 26). Comparing them with (4.4) and (4.6), we immediately obtain in the limit $A\to\infty$, for which $g = 1$, the correspondence

$$\mathscr{L}'_3 \to i(C_{12} - C_{21}) \equiv \mathsf{L}'_3, \tag{4.23a}$$

$$\mathscr{L}'_1 \to i(C_{23} - C_{32}) \equiv \mathsf{L}'_1, \tag{4.23b}$$

$$\mathscr{L}'_2 \to i(C_{31} - C_{13}) \equiv \mathsf{L}'_2, \tag{4.23c}$$

where the last relation is obtained by comparing the commutator (4.8) with[25]

$$[\mathsf{L}'_3,\mathsf{L}'_1] = -i\mathsf{L}'_2. \tag{4.24}$$

We denote now by boldface letters $\underline{\mathscr{L}}'_k$ and $\mathbf{L}'_k$, the matrices associated with the operator $\mathscr{L}'_k$ and L'_k, $k = 1,2,3$, in their respective basis (4.3),(4.22). In view of the expansion (4.21a) of g, and if we denote by $\overline{\mathscr{L}}'_k$ the matrices associated with (4.4) and (4.6) when we replace g by $\bar{g}$ of (4.21), we see that we can write now for arbitrary A that

$$\underline{\mathscr{L}}'_k = \mathbf{L}'_k + (\overline{\mathscr{L}}'_k/\sigma^2). \tag{4.25}$$

This will be the basic expansion needed in the next section to obtain a complete set of states for microscopic collective models.

V. COMPLETE SET OF STATES

We proceed now to discuss the matrix Hamiltonian $\mathbf{H}'$ of (3.19) to show that under an appropriate change of variables it can be expanded as σ^2 plus a series of inverse powers in σ, where this parameter is defined in (3.21), i.e.,

$$\mathbf{H}' = \sigma^2 + \sum_{n=0}^{\infty} \frac{\mathbf{H}'_n}{\sigma^n}. \tag{5.1}$$

We show in discussions in this and the following section that σ^2 is related with the ground state energy of the oscillator Hamiltonian (3.1). Thus we want to deal with $(\mathbf{H}' - \sigma^2)$ rather than with $\mathbf{H}'$ as the eigenvalues of the former will provide the excitation energies. When $A \to \infty$, we see from (3.21) that $\sigma \to \infty$ and thus $(\mathbf{H}' - \sigma^2)$ will go into the matrix operator $\mathbf{H}'_0$ which will be determined explicitly in this section as well as the complete set of its eigenstates. We can then use this set to find the matrices of $\mathbf{H}'_n$ and thus of $\mathbf{H}'$ or, more generally, to find the matrix representation of a Hamiltonian $\mathscr{H}'$ associated with an arbitrary two-body interaction potential.

The $\mathbf{H}'$ of (3.19) is given in terms of the $\mathbf{R}^2$ of (3.20), which, from the discussion following this last equation as well as from (3.11), is a matrix whose elements are operator functions of b, c, $\partial/\partial b$, $\partial/\partial c$, and L'_k. We shall first analyze $\mathbf{R}^2$ and then turn our attention to $\mathbf{H}'$.

We recall that b and c are restricted to the lined triangle in Fig. 1, where the abscissa and ordinate are given by $x = b\cos c$ and $y = b \sin c$. Thus the c is in the interval $0 \leqslant c \leqslant \pi/3$ while b can go from 0 to a value along the heavy line in the figure whose equation is

$$1 + 2b\cos[c - (4\pi/3)] = 0. \tag{5.2}$$

We now propose to substitute the variables b and c in $\mathbf{R}^2$ by new ones β and γ defined by

$$\gamma = c, \tag{5.3}$$

$$1 + 2(\beta^2/\sigma^2) = (1 - b^2)(1 - 3b^2 + 2b^3\cos 3c)^{-1} = \tfrac{1}{3}\sum_{k=1}^{3}\{1 + 2b\cos[c - (2\pi k/3)]\}^{-1}, \tag{5.4}$$

where σ^2 is defined by (3.21). The explicit expression $b = b(\beta,\gamma)$ can be obtained either by solving a cubic equation that we get for b if we replace c by γ in (5.4) or, more conveniently for our purposes, if we write

$$b(\beta,\gamma) = \sum_{n=1}^{\infty} \frac{b_n(\beta,\gamma)}{\sigma^n} \tag{5.5}$$

and use (5.4) to get a recurrence relation to obtain $b_n(\beta,\gamma)$. Note that when $b \ll 1$, $b \simeq (\beta/\sigma)$ and thus in (5.5) the summation starts with $n = 1$ and $b_1(\beta,\gamma) = \beta$.

By using (5.3) and (5.5) we can then express the R^2 given by (3.10) and (3.11), with the modifications added in the discussion following (3.20), as a matrix whose elements are operators which are functions of β, γ, $\partial/\partial\beta$, $\partial/\partial\gamma$, and L'_k.

When A, and thus also σ^2 of (3.21), becomes very large, we can see from the discussion of the previous paragraph that the new form of $\mathbf{R}^2/2$ can be obtained if we write $c = \gamma$ and $b \simeq (\beta/\sigma)$ and disregard all terms in the final result in which we have inverse powers of σ.

Looking at $\mathbf{R}'^2_1/2$ of (3.11a), we see that we have terms such as

$$\frac{\partial^2}{\partial b^2},\quad \frac{1}{b}\frac{\partial}{\partial b},\quad \frac{1}{b}\frac{\partial^2}{\partial b\partial c},\quad \frac{1}{b^2}\frac{\partial^2}{\partial c^2},\quad \frac{\cot 3c}{b}\frac{\partial}{\partial b}, \tag{5.6}$$

which will have the same form in β and γ but only with the extra factor σ^2. We have also in $\mathbf{R}'^2_1/2$ as indicated in the discussion following (3.20), a term

$$(\sigma^4/2)(1 - b^2)(1 - 3b^2 + 3b^3\cos 3c)^{-1} = \sigma^4/2 + \sigma^2\beta^2, \tag{5.7}$$

where the right-hand side follows from (5.4). All terms in $\mathbf{R}'^2_1/2$ that contain expressions of the type (5.6) multiplied by powers of b can be disregarded as $b \simeq \beta/\sigma$ and thus they will be small compared with the terms (5.6) themselves. We also notice that from the procedure by which we go from H' of (3.9) to the matrix $\mathbf{H}'$ of (3.14) the $\mathbf{R}'^2_1$ must contain as a factor the unit matrix

$$\mathbf{I} = \|\delta_{\tau'_1\tau_1}\delta_{\tau'_2\tau_2}\delta_{\tau'_3\tau_3}\|. \tag{5.8}$$

Turning now our attention to $\mathbf{R}'^2_2/2$, we note that it contains the factor $(1/b^2) \simeq (\sigma^2/\beta^2)$ but that all b present in the numerator can be disregarded as $b \simeq (\beta/\sigma)$. Furthermore, we saw from (4.25) that $\mathscr{L}'_k$ can be expressed as a sum of two terms, the second of which has a σ^2 in the denominator. Thus we can substitute $\mathscr{L}'_k$ by $\mathbf{L}'_k$ and write $\mathbf{R}'^2_2/2$ approximately as

$$\mathbf{R}'^2_2/2 \simeq \sigma^2 \sum_{k=1}^{3}\{4\beta^2\sin^2[\gamma - (2\pi k/3)]\}^{-1}\mathbf{J}'^2_k, \tag{5.9}$$

where

$$\mathbf{J}'_k = L'_k\mathbf{I} + \mathbf{L}'_k. \tag{5.10}$$

Finally we turn our attention to $\mathbf{R}'^2_3/2$, given by (3.11c) with the modifications discussed in the paragraph following Eq. (3.20). We have in it factors of the form $\{1 + 2b\cos[c - (2\pi k/3)]\}^{-1}$, which we can replace by 1 as $b \simeq \beta/\sigma$ is small.

We then see, using again (4.25), that $\mathbf{R}'^2_3/2$ can be written as

$$\mathbf{R}'^2_3/2 \simeq \tfrac{3}{2}\left\{[\mathbf{G}'(A-1) - 3\omega(\omega + A - 5)\mathbf{I}] - \sum_{k=1}^{3}\mathbf{L}'^2_k\right\} = [\lambda^2 + \mu^2 + \lambda\mu + 3(\lambda + \mu)]\mathbf{I} - \tfrac{3}{2}\sum_{k=1}^{3}\mathbf{L}'^2_k, \tag{5.11}$$

where $\mathbf{I}$ is the unit matrix of (5.8), and the right-hand side was obtained with the help of Eq. (3.16a), (3.18), and (4.10).

We note that $\mathbf{R}'^2_1, \mathbf{R}'^2_2$ contain factors σ^2 plus, from (5.7), a constant term $\frac{1}{2}\sigma^4\mathbf{I}$, while $\mathbf{R}'^2_3$ contains factors of the order of λ, μ or squares of them, which, as indicated in the previous section, are orders of magnitude smaller. Thus to the order that we have been carrying the analysis we can disregard $\mathbf{R}'^2_3$ as compared with $\mathbf{R}'^2_1$ and $\mathbf{R}'^2_2$ and write finally

$$\mathbf{R}^2/2 = (\sigma^4/2)\mathbf{I} + \sigma^2[2\mathbf{H}'_{BM} + O(1/\sigma)], \tag{5.12}$$

where $\mathbf{H}^J_{\rm BM}$ is the Bohr–Mottelson collective Hamiltonian associated with the angular momentum J of (5.10) in the frame of reference fixed in the body, i.e.,

$$\mathbf{H}^J_{\rm BM} = \frac{1}{2}\left(-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} - \frac{1}{\beta^2\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\frac{\partial}{\partial\gamma} + \beta^2\right)\mathbf{I} + \sum_{k=1}^{3}\frac{1}{4\beta^2\sin^2[\gamma-(2\pi k/3)]}\mathbf{J}'^2_k. \tag{5.13}$$

In (5.12) we write an equality rather than an approximate expression and this is the reason for including the term of order $O(1/\sigma)$, which, of course, can be disregarded as compared to $\mathbf{H}^J_{\rm BM}$ if $\sigma\to\infty$.

We now introduce this $\mathbf{R}^2$ in $\mathbf{H}'$ of (3.19) and proceed to show how we finally get the $\mathbf{H}'_0$ in the expansion (5.1) and then derive the explicit and complete set of eigenstates of the latter.

We again note that, for large A, σ^2 is large and thus the first term in (5.12) is much larger than the second so that the main part of the potential in $\mathbf{H}'$ of (3.19) is given by $\frac{1}{2}[\sigma^4/\rho^2+\rho^2]$ which has a minimum at $\rho=\sigma$. As a last step, we would like to change the variable ρ in the range $0\leqslant\rho\leqslant\infty$ to another one $\overline{\alpha}$ in the range $-\infty\leqslant\overline{\alpha}\leqslant\infty$ for which the potential would have its minimum value σ^2 at $\overline{\alpha}=0$. One possible way to introduce a coordinate with these characteristics is to write

$$\rho=\sigma\exp(\overline{\alpha}/\sqrt{2}\sigma)\simeq\sigma+\overline{\alpha}/\sqrt{2}+\cdots, \tag{5.14}$$

which gives for the main part of the potential in $\mathbf{H}'$ the expression

$$\tfrac{1}{2}[\sigma^4/\rho^2+\rho^2] = \sigma^2\cosh(\sqrt{2}\overline{\alpha}/\sigma) = \sigma^2+\overline{\alpha}^2+O(\sigma^{-2}). \tag{5.15}$$

Furthermore, we see from the right-hand side of (5.14) that we can write

$$-\frac{1}{2}\frac{\partial^2}{\partial\rho^2} = -\frac{\partial^2}{\partial\overline{\alpha}^2}+O(\sigma^{-1}). \tag{5.16}$$

Finally, as the term $2\sigma^2 H'^J_{\rm BM}$ in (5.12) that appears in the $\mathbf{H}'$ of (3.19) is divided by $\rho^2\simeq\sigma^2$, we obtain

$$\mathbf{H}' = \sigma^2\mathbf{I}+\mathbf{H}'_0+O(\sigma^{-1}), \tag{5.17}$$

where

$$H'_0 = \left(-\frac{\partial^2}{\partial\overline{\alpha}^2}+\overline{\alpha}^2\right)\mathbf{I}+2\mathbf{H}^J_{\rm BM}. \tag{5.18}$$

Comparing (5.17) with (5.1), we see that $\mathbf{H}'_0$ is the first term (i.e., corresponding to $n=0$) in the series of inverse powers of σ appearing in (5.1) while $O(\sigma^{-1})$ represents the rest of the series. It is interesting to note that the BM Hamiltonian will not change its spectrum if we replace L'_k by $\mathbf{J}'_k$ of (5.10) and thus it will remain[1] $\nu+5/2$, where ν is an integer. The spectrum of $\frac{1}{2}(-\partial^2/\partial\overline{\alpha}^2+\overline{\alpha}^2)$ will, of course, be $n+\frac{1}{2}$, where n is an integer. Thus the spectrum of $\sigma^2+\mathbf{H}'_0$ takes the value

$$\sigma^2+2N+6=\omega_1+\omega_2+\omega_3+\tfrac{3}{2}(A-1)+2N, \tag{5.19}$$

where $N=n+\nu$.

Turning now our attention to the oscillator Hamiltonian of (3.1), we show in the next section that its ground state for a given irrep $(\omega_1\omega_2\omega_3)$ of $O(A-1)$ has the energy (5.19) when $N=0$. Furthermore, as collective excited states can be obtained by applying to the ground state functions of the creation operators that are scalars of $O(A-1)$, i.e.,

$$\sum_{s=1}^{A-1}\eta_{is}\eta_{js},\quad i,j=1,2,3, \tag{5.20}$$

$$\eta_{is}=(1/\sqrt{2})(X_{is}-iP_{is}), \tag{5.21}$$

we see that collective excited states will increase their energy by jumps of two quanta as is also the case of (5.19). Thus, when considering all irreps $(\omega_1\omega_2\omega_3)$ of $O(A-1)$, $\sigma^2\mathbf{I}+\mathbf{H}'_0$ has already the same spectrum as H of (3.1) or, equivalently, as H' of (3.9) or (5.17). Therefore, the terms $O(\sigma^{-1})$ in (5.18) considered as perturbations can change the eigenstates of $\sigma^2\mathbf{I}+\mathbf{H}'_0$ but not its eigenvalues.

We now turn our attention to the derivation of a complete set of eigenstates of the Hamiltonian $\mathbf{H}'_0$ of (5.18). For this purpose we first note that the matrices $\mathbf{L}'_k$ are given with respect to Gel'fand states characterized by $U(3)\supset U(2)\supset U(1)$ chain of groups whose irreps are, respectively, $(\omega_1\omega_2\omega_3)$, $(\tau_1\tau_2)$, (ζ_1), i.e,

$$\mathbf{L}'_k = \left\| \begin{pmatrix} \omega_1\omega_2\omega_3 \\ \tau'_1\tau'_2 \\ \zeta'_1 \end{pmatrix} \middle| L'_k \middle| \begin{pmatrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1 \end{pmatrix} \right\|. \tag{5.22}$$

We can now consider the states characterized by the chain of groups $U(3)\supset O(3)\supset O(2)$, where the irreps will be respectively $(\omega_1\omega_2\omega_3)$, L,K and we need an extra quantum number Ω to distinguish[27] repeated representations L of O(3) in a given one $(\omega_1\omega_2\omega_3)$ of U(3). The kets can then be denoted by

$$\begin{pmatrix} \omega_1\omega_2\omega_3 \\ \Omega\mathsf{LK} \end{pmatrix} \tag{5.23}$$

and the matrices in this new basis, which we designate by a dot above, i.e., $\dot{\mathbf{L}}'_k$, will clearly be diagonal in Ω,L and independent of the former as well as of the $(\omega_1\omega_2\omega_3)$, as the $\dot{\mathbf{L}}'_k$ are the generators of $O(3)\supset O(2)$. In fact the $\dot{\mathbf{L}}'_k$ have the standard form, i.e., for $k=1,2$, we obtain

$$\dot{\mathbf{L}}'_k = \| \tfrac{1}{2} i^{k-1}\{[(\mathsf{L}-\mathsf{K})(\mathsf{L}+\mathsf{K}+1)]^{1/2}\delta_{\mathsf{K}',\mathsf{K}+1} + (-1)^{k-1}[(\mathsf{L}+\mathsf{K})(\mathsf{L}-\mathsf{K}+1)]^{1/2}\delta_{\mathsf{K}',\mathsf{K}-1}\}\delta_{\Omega'\Omega}\delta_{\mathsf{L}',\mathsf{L}}\| \tag{5.24a}$$

while for $k=3$ we have

$$\dot{\mathsf{L}}'_3 = \|\mathsf{K}\delta_{\mathsf{K}'\mathsf{K}}\delta_{\mathsf{L}'\mathsf{L}}\delta_{\Omega'\Omega}\|. \tag{5.24b}$$

We shall also designate by $\dot{\mathbf{I}}$ the matrix $\dot{\mathbf{I}}=\|\delta_{\Omega'\Omega}\delta_{\mathsf{L}'\mathsf{L}}\delta_{\mathsf{K}'\mathsf{K}}\|$ corresponding to $\mathbf{I}$ of (5.8).

The passage from the basis in $U(3)\supset U(2)\supset U(1)$ to the one in $U(3)\supset O(3)\supset O(2)$ is achieved with the help of the unitary transformation bracket

$$\begin{pmatrix} \omega_1\omega_2\omega_3 & \omega_1\omega_2\omega_3 \\ \Omega\mathsf{LK} & \tau_1\tau_2 \\ & \zeta_1 \end{pmatrix}, \tag{5.25}$$

which has been determined in previous publications,[28,29] with the explicit form summarized in Appendix B.

We can then use (5.25) to transform $\mathbf{H}^J_{\rm BM}$ of (5.13) into an $\dot{\mathbf{H}}^J_{\rm BM}$ in which the $\mathbf{J}'_k$ of (5.10) is replaced by

$$\dot{\mathbf{J}}'_k = L'_k\dot{\mathbf{I}}+\dot{\mathbf{L}}'_k. \tag{5.26}$$

Furthermore, from the discussion in Sec. II, we saw that the dependence of the eigenstates H' of (3.9) on the Euler angles is given in terms of the irreps of O(3), i.e., the Wigner functions $D^L_{KM}(\vartheta_j)$. Thus in (5.26) we can replace L'_k by its matrix $\mathbf{L}'_k$ defined by

$$\mathbf{L}'_k = \left|\left| \int D^{L*}_{K'M}(\vartheta_j) L'_k D^L_{KM}(\vartheta_j) d\Omega \right|\right| \tag{5.27}$$

and get a corresponding $\dot{H}^J_{\mathrm{BM}}$ given by (5.13) in which the $\mathbf{J}$ of (5.10) is replaced by

$$\dot{\mathbf{J}}_k = \mathbf{L}'_k \dot{\mathbf{I}} + \mathbf{I}\dot{\mathbf{L}}'_k . \tag{5.28}$$

The matrix $\mathbf{L}'_k$ is independent of M as the operator L'_k is the angular momentum in the frame of reference fixed in the body. The explicit form of this matrix is then given by (5.24) if we suppress the $\delta_{\Omega'\Omega}$ appearing there and replace L and K by L and K. Furthermore, the matrix $\mathbf{I}$ is the $(2L+1)\times(2L+1)$ unit matrix $\mathbf{I} = \|\delta_{K',K}\|$.

Note that the right-hand side of (5.28) is the sum of two terms. The first one is the matrix $\mathbf{L}'_k$ of the operator L'_k in the basis in which $\mathbf{L}'^2$ and $\mathbf{L}'_3$ are diagonal, multiplied by the unit matrix in the basis characterized by the $\mathrm{U}(3)\supset\mathrm{O}(3)\supset\mathrm{O}(2)$ chain of groups in which $\dot{\mathbf{L}}'^2$ and $\dot{\mathbf{L}}'_3$ are diagonal. The second is the unit matrix in the basis in which $\mathbf{L}'^2$ and $\mathbf{L}'_3$ are diagonal, multiplied by the matrix $\dot{\mathbf{L}}'_k$ of the operator $\mathbf{L}'_k$ in the basis characterized by the $\mathrm{U}(3)\supset\mathrm{O}(3)\supset\mathrm{O}(2)$ chain of groups in which $\dot{\mathbf{L}}'^2$ and $\dot{\mathbf{L}}'_3$ are diagonal. Clearly then from the very procedure used to derive the Clebsch–Gordan coefficients in Chapter III of Ref. 19, we see that if we apply to $\dot{J}'_k$ the unitary transformation $\dot{\mathbf{J}}'_k \equiv (\mathbf{U}^{L\mathsf{L}})^\dagger \dot{\mathbf{J}}'_k \mathbf{U}^{L\mathsf{L}}$, where $\mathbf{U}^{L\mathsf{L}}$, is given by

$$\mathbf{U}^{L\mathsf{L}} = \|U^{L\mathsf{L}}_{K\mathsf{K},J\mathscr{K}}\| = \|\langle LK\ \mathsf{L}\mathsf{K}|J\mathscr{K}\rangle\| , \tag{5.29}$$

we obtain that the matrix $\dot{\mathbf{J}}'_k$ takes the form (5.24) in which L and K is replaced by J and $\mathscr{K}$ with $|L-\mathsf{L}|\leqslant J\leqslant L+\mathsf{L}$. Thus the matrix $(\mathbf{U}^{L\mathsf{L}})^\dagger \dot{\mathbf{H}}^J_{\mathrm{BM}} \mathbf{U}^{L\mathsf{L}}$ whose elements are operator functions of β, γ, $\partial/\partial\beta$, $\partial/\partial\gamma$ are then exactly the same as those appearing in the Bohr–Mottelson (BM) vibrational Hamiltonian[1,2] with the only difference that now we have J and $\mathscr{K}$ while in the BM case we had L and K. It is clear, therefore, that, with the changes indicated, we can use for the eigenstates of $\mathbf{H}'_0$ of (5.18) the same functions of β and γ as in the BM case.

If we now put together all the steps discussed in the last paragraphs, we get a vectorial eigenfunction of the matrix operator of (5.18) whose components we can denote by $f^{(\omega_1\omega_2\omega_3)}_{\tau_1\tau_2\zeta_1}(\bar{\alpha},\beta,\gamma;\vartheta_k)$. Combining them with the irrep $D^{(\omega_1\omega_2\omega_3)}_{\tau_1\tau_2\zeta_1;\delta\{f\}(r)}(\phi)$ of $\mathrm{O}(A-1)$ as indicated in (3.13), we get a complete orthonormal set of states for an A-body problem, in the collective coordinates $\bar{\alpha},\beta,\gamma,\vartheta_k$ plus the angles ϕ associated with the group $\mathrm{O}(A-1)$, that is denoted by the ket

$$\begin{aligned}
&|N\nu,\Lambda t J,LM,\Omega\mathsf{L},(\omega_1\omega_2\omega_3)\delta\{f\}(r)\rangle \\
&\quad = \psi_{N-\nu}(\bar{\alpha})\, F^{\Lambda}_{(\nu\ \ \Lambda)/2}(\beta) \sum_{\mathscr{K}} \Phi^{\Lambda t J}_{\ \ \mathscr{K}}(\gamma) \\
&\qquad \times \sum_{K,\mathsf{K}} \{\langle LK,\mathsf{L}\mathsf{K}|J\mathscr{K}\rangle \\
&\qquad \times D^L_{KM}(\vartheta_j) \sum_{\tau_1\tau_2\zeta_1} \left[\begin{pmatrix} \omega_1\omega_2\omega_3 & \omega_1\omega_2\omega_3 \\ \Omega\mathsf{L}\mathsf{K} & \tau_1\tau_2 \\ & \zeta_1 \end{pmatrix} \right. \\
&\qquad \left. \times D^{(\omega_1\omega_2\omega_3)}_{\tau_1\tau_2\zeta_1;\delta\{f\}(r)}(\phi)\right]\} .
\end{aligned} \tag{5.30}$$

In (5.30) $\psi_{N-\nu}(\bar{\alpha})$ is a one-dimensional oscillator state of $N-\nu$ quanta associated with the operator $(-\partial^2/\partial\bar{\alpha}^2 + \bar{\alpha}^2)$ appearing in $\mathbf{H}'_0$ of (5.18). The rest of the state comes from the $\mathbf{H}^J_{\mathrm{BM}}$ of (5.13). The $F^{\Lambda}_{(\nu-\Lambda)/2}(\beta)$ and $\Phi^{\Lambda tJ}_{\ \ \mathscr{K}}(\gamma)$ are respectively the β- and γ-dependent part of the eigenstates of the Bohr–Mottelson vibrational Hamiltonian that were given explicitly in Ref. 2. The other terms appearing in (5.30) have already been defined and discussed in this article. We recall that in the BM problem[1,2] the ν and Λ are related, respectively, to the irreps of the U(5) symmetry group of the BM Hamiltonian and its O(5) subgroup. The J appearing in $\Phi^{\Lambda tJ}_{\ \ \mathscr{K}}(\gamma)$ is the irrep of an ordinary rotation group in the chain $\mathrm{O}(5)\supset D^2(\mathrm{O}(3))$. As a given J can appear more than once in a definite irrep Λ of O(5) the index t distinguishes between these repeated representations of O(3).[1,2]

The orthonormality properties of the ket (5.30) with respect to all the indices in it follow from the properties of the functions and transformation brackets appearing on the right-hand side. Furthermore, from the way the states (5.30) were derived, it follows that they will be eigenstates of H' of (3.9), when A and thus also σ^2 of (3.21), tends to infinity.

Having obtained an explicit and complete set of states for the A-body problem in terms of the collective coordinates $\bar{\alpha},\beta,\gamma,\vartheta_1,\vartheta_2,\vartheta_3$, as well as the angles ϕ characterizing the relevant part of an $(A-1)\times(A-1)$ orthogonal matrix, we proceed, in the next section, to discuss its application to microscopic nuclear collective models.

VI. MICROSCOPIC NUCLEAR COLLECTIVE MODELS

In the previous section we gave explicitly a complete set of orthonormal states for the translationally invariant part of an A-body problem, which would be the eigenstates, in collective coordinates plus others, of the oscillator Hamiltonian (3.1) when $A\to\infty$. In this section we would like to consider an A-body Hamiltonian with an arbitrary two-body interaction between the nucleons rather than the oscillator one, and with $A\gg 1$ but not infinite. We shall in particular restrict ourselves to the collective part of this Hamiltonian along the lines that have been proposed, from one viewpoint, by Filippov[10] and his collaborators, and, from another, by the group of Vanagas.[9]

In both of these approaches one restricts oneself, in the first step, to a definite irrep $(\omega_1\omega_2\omega_3)$ of $\mathrm{O}(A-1)$. Before proceeding with the analysis, we first want to indicate how this irrep is suggested by the Pauli principle and the SU(3) symmetry of the oscillator.

A. Determination of the irrep $(\omega_1\omega_2\omega_3)$ of O$(A-1)$

If we start with the oscillator Hamiltonian (3.1), we know that we can get its lowest energy states[30] that satisfy the Pauli principle as Slater determinants in which we fill the levels compactly with Z protons and $A-Z$ neutrons. In the case of closed proton and neutron shells we have a single state, while in the open case we have many, but in both the dependence on the center of mass coordinate

$$X_{iA} = (A)^{-1/2} \sum_{s=1}^{A} X'_{is} \tag{6.1}$$

is given[30] by the multiplicative factor $\exp[-\frac{1}{2}\sum_{i=1}^{3} X_{iA}^2]$, which corresponds to zero quanta. Thus the number of quanta $\mathcal{N}_p$ and $\mathcal{N}_n$ that we have respectively for protons and neutrons can be calculated in the following way: Let us consider first the Z protons and call N the number of quanta in the last shell of the oscillator that is completely filled. As each shell $n = 0,1,...,N$ of the oscillator has a capacity for $(n+1)(n+2)$ protons (taking into account the spin $\frac{1}{2}$ of these particles) it is clear that

$$\mathcal{N}_p = \left[Z - \sum_{n=0}^{N}(n+1)(n+2)\right](N+1) + \sum_{n=0}^{N} n(n+1)(n+2). \tag{6.2}$$

Using well-known formulas[31] for $\Sigma_{n=0}^{N} n^r$, where $r = 0,1,2,3$, we obtain

$$\mathcal{N}_p = (N+1)Z - \tfrac{1}{12}N(N+1)(N^2+9N+2) - 2(N+1)^2. \tag{6.3}$$

In a similar way for the neutron case, if N' is the number of quanta in the last filled shell of the oscillator, we can write

$$\mathcal{N}_n = (N'+1)(A-Z) - \tfrac{1}{12} \times N'(N'+1)(N'^2+9N'+2) - 2(N'+1)^2. \tag{6.4}$$

If the last shell, i.e., the one corresponding to $N+1$ or $N'+1$ quanta for protons or neutrons respectively, is not empty then, as was indicated above, there are a variety of ways of constructing the Slater determinants giving states of lowest energy. One could combine these states linearly so as to characterize them by definite irreps $(\lambda\mu)$ of the SU(3) symmetry group of the oscillator; for medium and heavy nuclei, there would not only be many of these $(\lambda\mu)$, but, in general, each one would appear many times. Sabaliauskas[32] has shown, that the irrep $(\lambda\mu)_{max}$ corresponding to the maximal eigenvalue of the quadratic Casimir operator of the SU(3) group usually appears only once and suggests that the states characterized by this irrep would give rise to the ground state band. This happens for many nuclei in the *s-d* shell as shown in the SU(3) model of Elliott.[33] The strong spin–orbit coupling effects in medium heavy and heavy nuclei seem to break this symmetry, but the low multiplicity that Sabaliauskas[32] finds for $(\lambda\mu)_{max}$ may indicate that SU(3), as happened before for isospin in the case of isobaric analog states,[34] remains a good symmetry even in a region in which one would not expect it to be valid.

We shall follow Sabaliauskas' suggestion, so that the linear combination of Slater determinants corresponding to the ground state band will be characterized by the number of quanta $\mathcal{N} = \mathcal{N}_p + \mathcal{N}_n$ and the irrep $(\lambda\mu)_{max}$ of SU(3). From its construction it is clear that the configuration part of these states will be characterized, if Z and A are even, by the irrep $\{f\} = \{4^{Z/2}\,2^{(A/2-Z)}\}$ of the symmetric group S_A. Furthermore, this configuration part is also characterized by the chain of groups[22]

$$\begin{array}{lcll} U(3A-3) \supset & U(3) & \times & U(A-1) \quad [h_1h_2h_3] \\ & \cup & & \cup \\ & O(3) & L & O(A-1) \quad (\omega_1\omega_2\omega_3) \\ & \cup & & \cup \\ & O(2) & M & S_A \qquad \{f\}, \end{array} \tag{6.5}$$

where to the right of each group we have indicated its irrep, noting that the irreps $[h_1h_2h_3]$ of U(3) and U$(A-1)$ are the same.[22]

The ground state band constructed by the procedure indicated in the previous paragraph is also characterized by a definite irrep $(\omega_1\omega_2\omega_3)$ of O$(A-1)$ which coincides with the irrep $[h_1h_2h_3]$ of U$(A-1)$. This can be seen from the fact that the ground state was formed by a combination of Slater determinants in which the levels were filled compactly. Thus when we apply the O$(A-1)$ scalar quadratic functions of the annihilation operators $\xi_{is} = (1/\sqrt{2})(X_{is} + iP_{is})$ of the form

$$B_{ij} = \sum_{s=1}^{A-1} \xi_{is}\,\xi_{js}, \tag{6.6}$$

which are also invariants of the symmetric group S_A, to the ground state, we get zero, as we cannot obtain states with lower number of quanta that satisfy the Pauli principle.

We conclude then from the relations of the irreps of U(3) and SU(3), U(3) and U$(A-1)$, and the fact that $(\omega_1\omega_2\omega_3) = [h_1\,h_2\,h_3]$ that

$$\omega_1 + \omega_2 + \omega_3 \equiv 3\omega = \mathcal{N}, \tag{6.7a}$$

$$\omega_1 - \omega_2 = \lambda, \tag{6.7b}$$

$$\omega_2 - \omega_3 = \mu, \tag{6.7c}$$

where we used (3.18); λ and μ belong to $(\lambda\mu)_{max}$ for the nucleus in question as given in the tables of Sabaliauskas,[32] and $\mathcal{N} = \mathcal{N}_p + \mathcal{N}_n$ is given in (6.3) and (6.4) as function of (A,Z). We give in Table I for some nuclei the irrep $(\omega_1\omega_2\omega_3)$ of O$(A-1)$ together with the $\sigma^2 = \omega_1 + \omega_2 + \omega_3 + \frac{3}{2}(A-5)$. Using the tables of $(\lambda\mu)_{max}$ of Sabaliauskas,[32] it would be an

TABLE I. The irreps $(\omega_1\omega_2\omega_3)$ of O$(A-1)$ for several nuclei. The table also includes the irrep $(\lambda\mu)_{max}$ corresponding to the maximum eigenvalue of the quadratic Casimir operator of the SU(3) group, that is consistent with the Pauli principle for the most symmetric partition $\{f\}$ characterizing the irrep of S_A. The table includes the total of number of quanta $\mathcal{N}$ when filling compactly the levels of the oscillator with nucleons and the parameter σ^2 defined by (3.21).

Nucleus	$^{16}_{8}O_8$	$^{40}_{20}Ca_{20}$	$^{152}_{62}Sm_{90}$	$^{168}_{68}Er_{100}$	$^{238}_{92}U_{146}$
$(\lambda\mu)_{max}$	(0,0)	(0,0)	(12,52)	(0,44)	(8,96)
$\mathcal{N}$	12	60	488	562	944
$\{f\}$	$\{4^4\}$	$\{4^{10}\}$	$\{4^{31},2^{14}\}$	$\{4^{34},2^{16}\}$	$\{4^{46},2^{27}\}$
$(\omega_1\omega_2\omega_3)$	(4,4,4)	(20,20,20)	(188,176,124)	(202,202,158)	(352,344,248)
σ^2	28.5	112.5	708.5	806.5	1293.5

easy matter to get these values for all nuclei between $Z = 32$, $A = 68$ and $Z = 102$, $A = 254$.

We see from Table I that, for $A > 100$, σ^2 is at least an order of magnitude higher than λ or μ of $(\lambda\mu)_{\max}$, and thus the type of development in inverse powers of σ discussed in the previous sections seems justified.

In the microscopic collective models of the nucleus discussed by both Vanagas[9] and Filippov,[10] the actual Hamiltonian for an A nucleon system is projected on a definite irrep $(\omega_1\omega_2\omega_3)$ of the $O(A-1)$ group. This irrep is suggested by the Pauli principle for the ground state, along the lines discussed in the present subsection. For a Hamiltonian with an oscillator two-body interaction this projection was carried out in Sec. III and, as the potential energy is only $(\rho^2/2)$, it means that it can also be carried out for the kinetic energy in an arbitrary Hamiltonian. It remains then to carry out the projection for a two-body potential interaction, and, in the next subsection, we briefly summarize the procedures followed by Filippov *et al.*[10] and by Vanagas,[9] where for simplicity we assume the potential V to be a central one.

B. The collective part of the potential

As the interaction is symmetric under permutations of the particles and depends only on the relative coordinates between them, we can make the replacement

$$\sum_{s<t=2}^{A} V\left(\left[\sum_{i=1}^{3}(X'_{is}-X'_{it})^2\right]^{1/2}\right)\to\frac{A(A-1)}{2}\times V\left(\sqrt{2}\left[\sum_{i=1}^{3}(X_{i1}^2)\right]^{1/2}\right), \tag{6.7}$$

where X_{i1}, $i = 1,2,3$, is the first Jacobi vector, and thus, using (2.6) and the orthogonal character of $D^1_{ki}(\vartheta_j)$, we obtain

$$\sum_{i=1}^{3} X_{i1}^2 = \sum_{k=1}^{3}\rho_k^2\,[D^1_{A-4+k,1}(\phi)]^2. \tag{6.8}$$

The collective potential used by Filippov is then obtained by projecting (6.7) on a definite irrep $(\omega_1\omega_2\omega_3)$ of $O(A-1)$, i.e.,

$$\mathscr{V}^{(\omega_1\omega_2\omega_3)\,|\,f\,|}_{\tau_1'\tau_2'\xi_1'\xi_2';\delta';\tau_1\tau_2\xi_1\xi_2;\delta}(\rho_1\rho_2\rho_3) = \int D^{(\omega_1\omega_2\omega_3)*}_{\tau_1'\tau_2'\xi_1'\xi_2';\delta'\,|\,f\,|(r)}(\phi)\times\left\{\frac{A(A-1)}{2}V\left(\sqrt{2}\left[\sum_{i=1}^{3}(X_{i1}^2)\right]^{1/2}\right)\right\}\times D^{(\omega_1\omega_2\omega_3)}_{\tau_1\tau_2\xi_1\xi_2;\delta\,|\,f\,|(r)}(\phi)\,d\tau(\phi), \tag{6.9}$$

where $d\tau(\phi)$ is the volume element in the angles ϕ corresponding to the $O(A-1)$ group. From (6.7) the potential is independent of the Euler angles ϑ_j, as could have also been predicted from the invariance of V under rotations. Filippov[10] has given an algorithm for the calculation of the potential (6.9) for closed shells and other special cases.

Another possibility for the collective potential was given by Vanagas,[9] who suggested that one decompose the two-body interaction into its irreducible parts associated with the group $O(A-1)$ and consider in the first step just the scalar part with respect to this group. The collective potential is then given by[9]

$$\mathscr{V}(\rho_1\rho_2\rho_3) = \frac{A(A-1)}{2}\int V\times\left(\sqrt{2}\left[\sum_{i=1}^{3}(X_{i1}^2)\right]^{1/2}\right)d\tau(\phi). \tag{6.10}$$

For a Gaussian interaction $V(r) = -V_0\exp(-a^{-2}r^2)$ we show in Appendix C that the Vanagas collective potential takes the form

$$\mathscr{V}(\rho_1\rho_2\rho_3) = -\frac{V_0A(A-1)}{2}\times\sum_{k,l,m}\frac{(\tfrac{1}{2})_k(\tfrac{1}{2})_l(\tfrac{1}{2})_m(-2a^{-2}\rho_1^2)^k(-2a^{-2}\rho_2^2)^l(-2a^{-2}\rho_3^2)^m}{k!\,l!\,m!\,((A-1)/2)_{k+l+m}}, \tag{6.11}$$

where $\alpha_m = \alpha(\alpha+1)\cdots(\alpha+m-1)$ is a Pochhammer symbol. In the case when $A \gg 1$, as also shown in Appendix C, the collective potential (6.11) takes the simpler form

$$\mathscr{V}(\rho_1\rho_2\rho_3) \simeq -\frac{V_0A(A-1)(A-5)^{3/2}}{2[(A+4\rho_1^2/a^2)(A+4\rho_2^2/a^2)(A+4\rho_3^2/a^2)]^{1/2}}. \tag{6.12}$$

Having a procedure for the calculation of the collective potential energy in both the Filippov[10] and Vanagas[9] cases, and in the latter even the explicit expression of the potential for a Gaussian interaction, we then obtain the collective Hamiltonian used by these authors if we add to the potential energy expressions (6.9) or (6.10) the kinetic energy given by (3.2) when we subtract from it $(\rho^2/2)$. We briefly outline in the next subsection how to carry out calculations for eigenvalues and eigenstates for these collective Hamiltonians with the help of the complete set of states (5.30).

C. Outline for the calculation of matrix elements

In the Hamiltonian discussed in the previous section we first replace, with the help of (2.4), ρ_k, $k = 1,2,3$, by ρ,b,c. If we then substitute the eigenstate Ψ of this Hamiltonian by a ψ related to it through (3.8), we see that $\mathscr{H}\psi = E\psi$ in which

$$\mathscr{H} = \frac{1}{2}\left(-\frac{\partial^2}{\partial\rho^2}+\frac{R^2}{\rho^2}\right)+\mathscr{V}(\rho,b,c), \tag{6.13}$$

where R^2 is given by (3.10), (3.11), and $\mathscr{V}(\rho,b,c)$ by (6.9) or (6.10) in which ρ_k is replaced by ρ,b,c. Finally, we write $\mathscr{H}$ in terms of $\overline{\alpha},\beta,\gamma$ and their derivatives by replacing ρ,b,c by the former through the relations (5.3), (5.4), and (5.14). We then have that $\mathscr{H}$ depends on

$$\mathscr{H}\left(\overline{\alpha},\beta,\gamma;\frac{\partial}{\partial\overline{\alpha}},\frac{\partial}{\partial\beta},\frac{\partial}{\partial\gamma};L'_k,\mathscr{L}'_k,G'(A-k)\right), \tag{6.14}$$

where L'_k, $k = 1,2,3$, are the components of the angular momentum in the frame of reference fixed in the body, while $G'(A-k)$ and $\mathscr{L}'_k$, $k = 1,2,3$, are respectively the Casimir operators and generators of $O'(A-1)$ given by (3.5) and (3.7).

We are now in a position to calculate the matrix elements of $\mathscr{H}$ of (6.14) with respect to the states (5.30). This implies that $G'(A-k)$, $\mathscr{L}'_k$, and L'_k have to be replaced respectively by the matrices $\mathbf{G}'(A-k)$, $\mathscr{L}'_k$, and $\mathbf{L}'_k$ given in (3.16), (4.25), and (5.27). Furthermore, we need to calculate the matrix of operators functions of $\overline{\alpha},\beta,\gamma,\partial/\partial\overline{\alpha},\partial/\partial\beta,\partial/\partial\gamma$

with respect to the functions $\psi_{N-\nu}(\overline{\alpha})$, $F^{\Lambda}_{(\nu-\Lambda)/2}(\beta)$, $\Phi^{\Lambda l l}_{\lambda'}(\gamma)$ appearing in (5.30). For the potential energy part this requires the same type of calculations that were carried out in the generalized BM model.[2,5] For the kinetic energy a somewhat different approach is required that will be discussed in a future publication. In principle, though, the evaluation of the matrix elements of $\mathscr{H}$ with respect to the states (5.30) of up to N quanta is straightforward, and the corresponding matrix can be diagonalized to give the eigenvalues and eigenstates. We also plan to discuss in future publications the best way to select the frequency of the oscillator functions (5.30) so as to get the most effective variational procedure.

VII. CONCLUSIONS

The main objective of this paper is achieved through Eq. (5.30), i.e., the determination of a complete set of states for the A nucleon system in terms of the collective coordinates of (5.14), (5.3), (5.4), the Euler angles ϑ_k, $k = 1, 2, 3$, and the angles ϕ, related respectively to the O(3) and O($A-1$) groups. Furthermore, in Sec. VI, we indicate how to use these states for the determination of the matrix elements of microscopic collective Hamiltonians, although some of the steps required in this determination need further elucidation, which we expect to implement in future publications.

It may be fitting to conclude this paper by indicating some "hidden" symmetries in the Hamiltonian (3.1) for a system of particles interacting through harmonic oscillator forces. If we first consider the case of the scalar representation $(\omega_1\omega_2\omega_3) = (000)$ of O($A-1$) we note that, when $A\to\infty$, we get the Hamiltonian $\mathbf{H}' = \mathbf{H}'_0$ of (5.18) of the form

$$H'_0 = (-\partial^2/\partial\overline{\alpha}^2 + \overline{\alpha}^2) + 2H^L_{\rm BM}\,, \tag{7.1}$$

as in the irrep (000) the $\mathscr{L}'_k$ and thus also the $\mathbf{L}'_k$ in (5.10) vanish. If we then introduce, as was shown in the original work of Bohr and Mottelson,[4] the coordinates

$$\alpha_m = (1/\sqrt{2})\beta\sin\gamma\,[D^2_{2m}(\vartheta_k) + D^2_{-2m}(\vartheta_k)] + \beta\cos\gamma D^2_{20}(\vartheta_k)\,, \tag{7.2}$$

we get

$$2H^L_{\rm BM} = \sum_{m=-2}^{2}(\alpha_m\alpha^m + \pi_m\pi^m), \tag{7.3}$$

where $\alpha^m = (-1)^m\alpha_{-m}$ and $\pi_m = -i\partial/\partial\alpha^m$. Thus $H'_0/2$ is the Hamiltonian of a six-dimensional harmonic oscillator and its symmetry group would be U(6), as was indicated in a recent publication,[14] where the Hamiltonian (3.1) was considered in the scalar representation (000) of O($A-1$). This symmetry is not restricted to (3.1) when $A\to\infty$, but actually appears for any A as was shown by one of the authors (M.M.)[35] and derived, from another viewpoint and in a very explicit fashion, by Deenen and Quesne.[36]

What happens in the case of an arbitrary representation $(\omega_1\omega_2\omega_3)$ of O($A-1$)? It is clear then that the $\mathbf{L}'_k$ appearing in (5.10) and (5.13) does not vanish, and thus at first sight one could think that this breaks the U(6) symmetry. A recent discussion by Moshinsky and Quesne[37] of a three-dimensional harmonic oscillator Hamiltonian with a particular spin–orbit interaction and an extra centrifugal term indicates that the U(3) symmetry is *not* broken, at least in the classical limit. The analogy of this problem with the one appearing in (5.18) for arbitrary $(\omega_1\omega_2\omega_3)$ indicates the possibility that in this case U(6) will not be broken either. Some of the authors plan to discuss this problem in a future publication.

APPENDIX A: THE GENERATORS OF Sp(6)

It is well known that the translationally invariant states for a system of A particles in a three-dimensional space, interacting under harmonic oscillator forces, have the Sp($6A-6$) group as a dynamical group[38] whose generators are the $(6A-6)(6A-5)/2$ bilinear operators

$$\eta_{is}\eta_{jt},\quad \xi_{is}\xi_{jt},\quad \tfrac{1}{2}(\eta_{is}\,\xi_{jt} + \xi_{jt}\,\eta_{is})\,, \tag{A1}$$
$$i,j = 1,2,3,\quad s,t = 1,2,\ldots,A-1,$$

where the η's and ξ's are the creation and annihilation operators associated with the Jacobi coordinates [see Eq. (2.1)] through the relations

$$\eta_{is} = (1/\sqrt{2})(X_{is} - iP_{is}),\quad \xi_{is} = (1/\sqrt{2})(X_{is} + iP_{is})\,. \tag{A2}$$

Contracting the generators given in (A1) with respect to the particle index s, we get the generators of the Sp(6) subgroup of Sp($6A-6$):

$$B^\dagger_{ij} = \sum_{s=1}^{A-1}\eta_{is}\,\eta_{js},\quad i,j = 1,2,3, \tag{A3a}$$

$$B_{ij} = \sum_{s=1}^{A-1}\xi_{is}\,\xi_{js},\quad i,j = 1,2,3, \tag{A3b}$$

$$C_{ij} = \tfrac{1}{2}\sum_{s=1}^{A-1}(\eta_{is}\,\xi_{js} + \xi_{js}\,\eta_{is}) \equiv \mathscr{C}_{ij} + \tfrac{1}{2}(A-1)\,\delta_{ij},\quad i,j = 1,2,3, \tag{A3c}$$

which satisfy the following commutation relations:

$$\begin{aligned}
&[C_{ij},C_{i'j'}] = C_{ij'}\delta_{ji'} - C_{ji'}\delta_{ij'}\,,\\
&[C_{ij},B^\dagger_{i'j'}] = B^\dagger_{ij'}\,\delta_{ji'} + B^\dagger_{ii'}\,\delta_{jj'}\,,\\
&[C_{ij},B_{i'j'}] = -B_{jj'}\,\delta_{ii'} - B_{ji'}\,\delta_{ij'}\,,\\
&[B^\dagger_{ij},B^\dagger_{i'j'}] = [B_{ij},B_{i'j'}] = 0\,,\\
&[B_{ij},B^\dagger_{i'j'}] = C_{j'j}\,\delta_{ii'} + C_{i'j}\,\delta_{ij'} + C_{j'i}\,\delta_{ji'} + C_{i'i}\,\delta_{jj'}\,.
\end{aligned} \tag{A4}$$

In Eq. (A3c), we have introduced the operators

$$\mathscr{C}_{ij} \equiv \sum_{s=1}^{A-1}\eta_{is}\,\xi_{js},\quad i,j = 1,2,3, \tag{A5}$$

which are the generators of the U(3) subgroup of Sp(6), and satisfy the same commutation relations as the C_{ij} operators.

Using Eq. (A2), the generators (A3) can be written in terms of the Jacobi coordinates:

$$C_{ij} = \tfrac{1}{2}(q_{ij} + T_{ij} + iL_{ij}),\quad i,j = 1,2,3, \tag{A6a}$$

$$B^\dagger_{ij} = \tfrac{1}{2}\Big[q_{ij} - T_{ij} - (A-1)\delta_{ij} - i\times\sum_{s=1}^{A-1}(X_{is}\,P_{js} + X_{js}\,P_{is})\Big], \tag{A6b}$$

$$B_{ij} = \tfrac{1}{2}\Big[q_{ij} - T_{ij} + (A-1)\,\delta_{ij} + i\times\sum_{s=1}^{A-1}(X_{is}\,P_{js} + X_{js}\,P_{is})\Big], \tag{A6c}$$

where q_{ij} is given in Eq. (2.8) and the operators T_{ij} and L'_{ij} are given by

$$T_{ij} = \sum_{s=1}^{A-1} P_{is} P_{js}, \quad i,j = 1,2,3, \tag{A7a}$$

$$L_{ij} = \sum_{s=1}^{A-1} (X_{is} P_{js} - X_{js} P_{is}), \quad i,j = 1,2,3, \tag{A7b}$$

where the latter are the components of the total angular momentum in the frame of reference fixed in space.

To write the operators $\Sigma_{s=1}^{A-1} X_{is} P_{js}$ and T_{ij} in terms of the coordinates introduced in (2.6), we need to consider the classical expression of the kinetic energy, i.e.,

$$2T = \sum_{i=1}^{3} T_{ii} = \sum_{i,s} (\dot{X}_{is})^2, \tag{A8}$$

with $\dot{X}_{is} = dX_{is}/dt$ and where we use units in which the mass of the particles is 1.

Carrying out the time derivative of Eq. (2.6), one finds

$$\dot{X}_{is} = \sum_{k=1}^{3} (\dot{\rho}_k D_{ki} \Delta_{Ks} + \rho_k \dot{D}_{ki} \Delta_{Ks} + \rho_k D_{ki} \dot{\Delta}_{Ks}), \tag{A9}$$

where $D^{1}_{ki}(\vartheta_j) \equiv D_{ki}$, $D^{1}_{A-4+k,s}(\phi) \equiv \Delta_{Ks}$, and $K = A - 4 + k$.

Thus, the kinetic energy takes the form

$$\begin{aligned} 2T = &\sum_{k=1}^{3} \dot{\rho}_k^2 + \sum_{k=1}^{3} \rho_k^2 \sum_{i=1}^{3} \dot{D}_{ki} \dot{D}_{ki} \\ &+ \sum_{k=1}^{3} \rho_k^2 \sum_{s=1}^{A-1} \dot{\Delta}_{Ks} \dot{\Delta}_{Ks} \\ &+ 2 \sum_{k,k'=1}^{3} \rho_k \rho_{k'} \sum_{i=1}^{3} D_{ki} \dot{D}_{k'i} \sum_{s=1}^{A-1} \Delta_{K's} \dot{\Delta}_{Ks}, \end{aligned} \tag{A10}$$

where we have used the orthogonality properties of the $\|D_{ki}\|$ and $\|\Delta_{Ks}\|$ matrices.

To calculate the time derivative of these matrices, we use the general result[39]

$$\dot{\mathbf{D}} = \boldsymbol{\Omega} \mathbf{D}, \tag{A11}$$

where $\Omega_{\alpha\beta} = -\Omega_{\beta\alpha}$ and $\mathbf{D}$ is a rotation matrix in n dimensions. The matrix elements $\Omega_{\alpha\beta}$, when $\mathbf{D}$ rotates a vector, give the angular velocity in the plane defined by the axes (α,β) of the "body" frame. The $\dot{\mathbf{D}}$ and $\dot{\boldsymbol{\Delta}}$ matrices can thus be written as

$$\dot{D}_{kk'} = \sum_{i=1}^{3} \omega_{ki} D_{ik'}, \quad k,k' = 1,2,3, \tag{A12a}$$

and

$$\begin{aligned} &\dot{\Delta}_{Kt} = \sum_{s=1}^{A-1} \Omega_{Ks} \Delta_{st}, \\ &K = A - 4 + k, \ k = 1,2,3, \ t = 1,2,\ldots,A-1. \end{aligned} \tag{A12b}$$

Substituting Eq. (A12) in (A10), we find the final result:

$$\begin{aligned} 2T = &\sum_{k=1}^{3} \dot{\rho}_k^2 + \sum_{k<k'=2}^{3} (\rho_k^2 + \rho_{k'}^2)(\omega_{kk'}^2 + \Omega_{KK'}^2) \\ &- 4 \sum_{k<k'=2}^{3} \rho_k \rho_{k'} \omega_{kk'} \Omega_{KK'} \\ &+ \sum_{k=1}^{3} \sum_{r=1}^{A-4} \rho_k^2 \Omega_{Kr}^2. \end{aligned} \tag{A13}$$

The momenta associated with the ρ's, ϑ's, and ϕ's are then given by[39]

$$P_k = \frac{\partial T}{\partial \dot{\rho}_k} = \dot{\rho}_k, \quad k = 1,2,3, \tag{A14a}$$

$$\begin{aligned} L'_{ij} = \frac{\partial T}{\partial \omega_{ij}} &= (\rho_i^2 + \rho_j^2)\omega_{ij} \\ &- 2\rho_i \rho_j \Omega_{A-4+i,A-4+j}, \quad i,j = 1,2,3, \end{aligned} \tag{A14b}$$

$$\mathscr{L}'_{tt'} = \frac{\partial T}{\partial \Omega_{tt'}}$$

$$= \begin{cases} 0 \quad \forall \ t \leqslant A-4, \\ (\rho_t^2 + \rho_{t'}^2)\Omega_{tt'} - 2\rho_t \rho_{t'} \omega_{tt'}, \quad t,t' = A-4+i, \\ i = 1,2,3, \\ \rho_t^2 \Omega_{tt'}, \quad t = A-4+i, \\ i = 1,2,3, \quad t' = 1,2,\ldots,A-1. \end{cases} \tag{A14c}$$

From Eq. (A14) we can obtain $\omega_{kk'}$ and Ω_{Ks} in terms of their canonically conjugated momenta, so the P_{is} take the form

$$\begin{aligned} P_{is} = &\sum_{k=1}^{3} D_{ki} \Delta_{Ks} P_k \\ &+ \sum_{k \neq k'=1}^{3} \frac{D_{k'i} \Delta_{Ks}}{\rho_k^2 - \rho_{k'}^2} (\rho_k L'_{kk'} + \rho_{k'} \mathscr{L}'_{KK'}) \\ &+ \sum_{k=1}^{3} \sum_{t=1}^{A-4} \frac{1}{\rho_k} D_{ki} \Delta_{ts} \mathscr{L}'_{Kt}. \end{aligned} \tag{A15}$$

The corresponding quantum expression is obtained by doing the standard replacements

$$P_{is} \to \frac{1}{i} \frac{\partial}{\partial X_{is}}, \quad P_k \to \frac{1}{i} \frac{\partial}{\partial \rho_k},$$

$$L'_{kk'} \to \hat{L}'_{kk'} = \frac{1}{i} \frac{\partial}{\partial \vartheta_{kk'}}, \quad \mathscr{L}'_{Kt} \to \hat{\mathscr{L}}'_{Kt} = \frac{1}{i} \frac{\partial}{\partial \phi_{Kt}},$$

where $\vartheta_{kk'}$ and ϕ_{Kt} are the angles associated with the rotation matrices, and we have taken $\hbar = 1$. Thus we have

$$\begin{aligned} \frac{\partial}{\partial X_{is}} = &\sum_{k=1}^{3} D_{ki} \Delta_{Ks} \frac{\partial}{\partial \rho_k} \\ &+ i \sum_{k \neq k'=1}^{3} \frac{\Delta_{Ks} D_{k'i}}{\rho_k^2 - \rho_{k'}^2} (\rho_k \hat{L}'_{kk'} + \rho_{k'} \hat{\mathscr{L}}'_{KK'}) \\ &+ i \sum_{k=1}^{3} \sum_{t=1}^{A-4} \frac{1}{\rho_k} D_{ki} \Delta_{ts} \hat{\mathscr{L}}'_{Kt}, \\ s = 1,2,\ldots,A-1, \ i = 1,2,3. \end{aligned} \tag{A16}$$

Now we can construct the operator $\Sigma_s X_{is} P_{is}$ straightforwardly:

$$\begin{aligned} \sum_s X_{is} \frac{\partial}{\partial X_{js}} = &\sum_{k=1}^{3} D_{ki} D_{kj} \rho_k \frac{\partial}{\partial \rho_k} \\ &+ i \sum_{k<k'=2}^{3} \frac{1}{\rho_k^2 - \rho_{k'}^2} (\rho_k^2 D_{ki} D_{k'j} \\ &+ \rho_{k'}^2 D_{k'i} D_{kj}) \hat{L}'_{kk'} \\ &+ i \sum_{k<k'=2}^{3} \frac{\rho_k \rho_{k'}}{\rho_k^2 - \rho_{k'}^2} [D_{ki} D_{k'j} \\ &+ D_{k'i} D_{kj}] \hat{\mathscr{L}}'_{KK'}, \end{aligned} \tag{A17}$$

which coincides with the result of Vanagas.[9]

To write T_{ij} in terms of the Zickendraht–Dzublik coordinates, we need to know the action of the operators $\hat{L}'_{kk'}$ (or $\hat{\mathscr{L}}'_{Kt}$) on their corresponding rotation matrix $\mathbf{D}$ (or $\mathbf{\Delta}$). Consider a rotation matrix $\mathbf{D}$ in an n-dimensional space and $\mathscr{L}_{kk'}$ the corresponding canonically conjugated momenta associated with the angles $\chi_{kk'}$ of the matrix $\mathbf{D}$. Then, using Eq. (A11), we have

$$\dot{D}_{ik} = \sum_{l=1}^{n} \omega_{il} D_{lk} = \sum_{l,m=1}^{n} \delta_{l,m}\, \omega_{im}\, D_{mk} = \sum_{l<m=2}^{n} \omega_{ml}(\delta_{im} D_{lk} - \delta_{il} D_{mk})\,. \tag{A18}$$

The left-hand side of this equation can now be written in the following way:

$$\dot{D}_{ik} = \frac{\partial}{\partial t} D_{ik} = \sum_{l<m=2}^{n} \frac{\partial \chi_{ml}}{\partial t} \frac{\partial}{\partial \chi_{ml}} D_{ik} = \sum_{l<m=2}^{n} i\omega_{ml}\, \hat{\mathscr{L}}_{ml}\, D_{ik}\,, \tag{A19}$$

where we define $\hat{\mathscr{L}}_{ml} \equiv (1/i)\partial/\partial\chi_{ml}$ and $\omega_{ml} \equiv \partial\chi_{ml}/\partial t$.

Comparing (A18) with (A19), we arrive to the result:

$$\hat{\mathscr{L}}_{ml}\, D_{ik} = i(\delta_{il} D_{mk} - \delta_{im} D_{lk})\,. \tag{A20}$$

Thus, the operator T_{ij} given in terms of the Zickendraht–Dzublik coordinates takes the form

$$\begin{aligned} T_{ij} = & -\sum_{s=1}^{A-1} \frac{\partial}{\partial X_{is}\, \partial X_{js}} \\ = & \left\{ \sum_{k=1}^{3} D_{ki} D_{kj} \left[-\frac{\partial^2}{\partial \rho_k^2} - \frac{(A-4)}{\rho_k} \frac{\partial}{\partial \rho_k} \right] \right. \\ & - \sum_{k\neq k'} \frac{D_{ki} D_{kj}}{\rho_k^2 - \rho_{k'}^2} \left(\rho_k \frac{\partial}{\partial \rho_k} - \rho_{k'} \frac{\partial}{\partial \rho_{k'}} \right) \\ & - i \sum_{k\neq k'=1}^{3} \frac{D_{ki} D_{k'j}}{\rho_k^2 - \rho_{k'}^2} \left[\left(\rho_k \frac{\partial}{\partial \rho_k} + \rho_{k'} \frac{\partial}{\partial \rho_{k'}} \right) \right. \\ & \times \hat{L}'_{kk'} + \left. \left(\rho_{k'} \frac{\partial}{\partial \rho_k} + \rho_k \frac{\partial}{\partial \rho_{k'}} \right) \hat{\mathscr{L}}'_{KK'} \right] \\ & + \sum_{\substack{k\neq k'=1 \\ k\neq \bar{k}}}^{3} \frac{D_{k'i} D_{\bar{k}'j}}{(\rho_k^2 - \rho_{k'}^2)(\rho_k^2 - \rho_{\bar{k}}^2)} \\ & \times (\rho_k \hat{L}'_{kk'} + \rho_{k'} \hat{\mathscr{L}}'_{KK'}) \\ & \times (\rho_k \hat{L}'_{k\bar{k}} + \rho_{\bar{k}} \hat{\mathscr{L}}'_{K\bar{K}}) \\ & + i \sum_{k\neq k'\neq \bar{k}} \frac{D_{k'i} D_{\bar{k}'j}}{(\rho_k^2 - \rho_{k'}^2)(\rho_{k'}^2 - \rho_{\bar{k}}^2)} \\ & \times (\rho_k^2 \hat{L}_{k'\bar{k}} + \rho_k \rho_{\bar{k}} \hat{\mathscr{L}}'_{K'\bar{K}}) \\ & - i(A-4) \sum_{k\neq k'} \frac{D_{ki} D_{k'j}}{\rho_k^2 - \rho_{k'}^2} \left(\hat{L}'_{kk'} + \frac{\rho_{k'}}{\rho_k} \hat{\mathscr{L}}'_{KK'} \right) \\ & \left. + \sum_{t=1}^{A-4} \sum_{k,k'=1}^{3} \frac{D_{ki} D_{k'j}}{\rho_k \rho_{k'}} \hat{\mathscr{L}}'_{Kt} \hat{\mathscr{L}}'_{Kt} \right\}. \end{aligned} \tag{A21}$$

Finally, substituting the operators q_{ij}, $\Sigma_s X_{is} P_{js}$, and T_{ij} in Eq. (A6), we get the generators of the Sp(6) group in terms of the Zickendraht–Dzublik coordinates.

The quantum kinetic energy of the system is obtained by taking $j = i$ and summing over i in the last expression. The result is given by Eq. (3.2) when we subtract from it $\rho^2/2$.

APPENDIX B: THE TRANSFORMATION BRACKET (5.25)

In this appendix we shall denote the bracket (5.25) by the shorthand notation

$$(\tau_1\tau_2\zeta_1|\Omega LK) \equiv \left(\begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1 \end{matrix} \middle| \begin{matrix} \omega_1\omega_2\omega_3 \\ \Omega LK \end{matrix} \right), \tag{B1}$$

where we interchanged bra and ket as the transformation bracket is real. When $K = L$, a bracket closely related to (B1) was determined in Refs. 28 and 29. The result obtained there differs from $(\tau_1\tau_2\zeta_1|\Omega LL)$ because of two facts. One is that in Ref. 28 the U(3)⊃O(3) basis was a complete but nonorthogonal set of states where states degenerate in L were distinguished by means of an integer label q. If we want to classify the basis by the quantum number Ω indicated in (B1), we must diagonalize, with respect to the states of Ref. 28, a Hermitian operator $\hat{\Omega}$; a suitable operator of this type is discussed in Ref. 27.

The second fact to be noticed is that in Ref. 28 the Gel'fand states of U(3), i.e., the U(3)⊃U(2)⊃U(1) states, were written in a realization involving the spherical components η_m, $m = \pm 1, 0$, of the boson creation operators η_μ, $\mu = 1,2,3$. Since $\eta_0 = \eta_3$ and

$$\begin{pmatrix} \eta_{+1} \\ \eta_{-1} \end{pmatrix} = i^{1/2}\, \mathbf{M} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}, \quad \mathbf{M} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i^{-1/2} - i^{1/2} \\ i^{-1/2} - i^{1/2} \end{pmatrix}, \tag{B2}$$

where $\mathbf{M}$ is an SU(2) matrix corresponding to the Euler angles

$$\vartheta_1 = \pi, \quad \vartheta_2 = \pi/2, \quad \vartheta_3 = 3\pi/2\,, \tag{B3}$$

it follows that the Gel'fand state $|\tau_1\tau_2\zeta_1)$, which appears as the bra in (B1), is related to the Gel'fand states $|\tau_1\tau_2\zeta'_1\rangle$ of Ref. 28 by

$$\begin{aligned} |\tau_1\tau_2\zeta_1) &= i^{\nu} \sum_{\zeta'_1} D^{j}_{\zeta_1 - \nu, \zeta'_1 - \nu}(\pi, \pi/2, 3\pi/2) |\tau_1\tau_2\, \zeta'_1\rangle \\ &= \sum_{\zeta'_1} i^{\zeta'_1} (-)^{\zeta_1 - \nu} d^{j}_{\zeta_1 - \nu, \zeta'_1 - \nu}\left(\frac{\pi}{2}\right) \\ &\quad \times |\tau_1\tau_2\, \zeta'_1\rangle\,, \end{aligned} \tag{B4}$$

where $\nu = \frac{1}{2}(\tau_1 + \tau_2)$, $j = \frac{1}{2}(\tau_1 - \tau_2)$, and $\mathbf{D}^j(\vartheta_1, \vartheta_2, \vartheta_3)$ are the standard irrep matrices[19] of SU(2).

Thus we have

$$\left(\begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1 \end{matrix} \middle| \begin{matrix} \omega_1\omega_2\omega_3 \\ qLL \end{matrix} \right) = \sum_{\zeta'_1} (-i)^{\zeta'_1} (-)^{\zeta_1 - \nu} \times d^{j}_{\zeta_1 - \nu, \zeta'_1 - \nu}\left(\frac{\pi}{2}\right) \left(\begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta'_1 \end{matrix} \middle| \begin{matrix} \omega_1\omega_2\omega_3 \\ qLL \end{matrix} \right), \tag{B5}$$

where, from Ref. 28,

$$\left\langle \begin{matrix} \omega_1\omega_2\omega_3 \\ \tau_1\tau_2 \\ \zeta_1' \end{matrix} \middle| \begin{matrix} \omega_1\omega_2\omega_3 \\ qLL \end{matrix} \right\rangle = q!(-2)^{\nu-L/2-\omega_3}$$
$$\times\left[\frac{(2j+1)(j+L/2)!(\tau_2-\omega_3)!(\tau_1-\omega_3+1)!(\omega_1-\tau_2+1)!(\tau_1-\omega_2)!(\omega_1-\tau_1)!}{(j-L/2)!(\omega_1-\omega_2+1)!(\omega_2-\tau_2)!}\right]^{1/2}$$
$$\times\sum_{\sigma,\beta}\frac{(-)^{\sigma}\left[\frac{1}{2}(\omega_1-\omega_3-L-\epsilon)-\sigma\right]!(2\sigma+\epsilon)!(\omega_2-\omega_3-\beta)!}{2^{\beta}\sigma!(q-\sigma)!\left[\frac{1}{2}(\omega_1+\omega_3-\epsilon)-\nu-\sigma+\beta\right]!(\tau_2-\omega_3-\beta)!(2\sigma+\epsilon-\beta)!\beta!(\tau_1-\omega_3+1-\beta)!}. \tag{B6}$$

Here $\epsilon=0$ when $\omega_1-\omega_3-L$ is even, and $\epsilon=1$ when $\omega_1-\omega_3-L$ is odd.

For values of $K<L$, the bracket (B1) can be obtained by using the fact that

$$\left|\begin{matrix}\omega_1\omega_2\omega_3\\ qLK\end{matrix}\right\rangle=\left[\frac{(L+K)!2^{L-K}}{(L-K)!(2L)!}\right]^{1/2}$$
$$\times(C^{1}_{0}+C^{0}_{-1})^{L-K}\left|\begin{matrix}\omega_1\omega_2\omega_3\\ qLL\end{matrix}\right\rangle, \tag{B7}$$

where $C^{m'}_{m}$ are generators of U(3). We take the scalar product of (B7) with

$$\left|\begin{matrix}\omega_1\omega_2\omega_3\\ \tau_1\tau_2\\ \zeta_1\end{matrix}\right\rangle \tag{B8}$$

expressed in the form (B4) and apply the powers of the generators on the bra using the known formulas[26] for the matrix elements of generators of U(3) with respect to Gel'fand states. In this way we obtain the bracket with arbitrary K as a linear combination of the brackets with $K=L$ given in (B5) and (B6).

APPENDIX C: THE VANAGAS POTENTIAL ENERGY FOR A GAUSSIAN INTERACTION AND ITS LIMIT FOR LARGE A

The type of interaction we consider [in units in which $\hbar$, the mass m of the nucleon, and the frequency of the oscillator used in (3.1) are taken as 1] has the form

$$-V_0\sum_{s<s'=1}^{A}\exp\left[-|\bar{r}_s'-\bar{r}_{s'}'|^2/a^2\right], \tag{C1}$$

where $\bar{r}_s'=\{X'_{is}, i=1,2,3\}$, $s=1,2,\ldots,A$, and "a" gives the range.

As the matrix element of the exponential function with respect to an antisymmetric system of identical particles gives the same result for any combination of (s,s'),[9] it is enough to consider

$$-\tfrac{1}{2}V_0A(A-1)\exp\left[-|\bar{r}_1'-\bar{r}_2'|^2/a^2\right]. \tag{C2}$$

As shown in Ref. 9, the interaction can be written in terms of $\{\rho_k,\phi\}$ as

$$-\tfrac{1}{2}V_0(A-1)A\exp\left[-(2/a^2)(\rho_1^2c_3^2s_2^2s_1^2+\rho_2^2c_2^2s_1^2+\rho_3^2c_1^2)\right], \tag{C3}$$

with

$$c_k=\cos\phi_k,\quad s_k=\sin\phi_k,\quad k=1,2,3,$$

where $\{\phi_k, k=1,2,3\}$ are the last three angles in the $(A-1)$-dimensional Jacobi coordinate space of (2.1) and (2.6).

In order to calculate the collective potential, we have according to Vanagas[9] to integrate (C3) with respect to the volume element

$$d\tau_\phi=\{\Gamma[(A-1)/2]/\pi^{3/2}\Gamma[(A-4)/2]\}(\sin\phi_3)^{A-5}$$
$$\times(\sin\phi_2)^{A-4}(\sin\phi_1)^{A-3}\,d\phi_1d\phi_2d\phi_3, \tag{C4}$$

with the range of the ϕ_k's being $0\leqslant\phi_k\leqslant\pi$, $k=1,2,3$. The normalization coefficient is determined via the condition $\int d\tau_\phi=1$.

To do the integration, we have to use formulas No. 9.212 and 3.383 of Ref. 31, i.e.,

$$\int_0^1 x^{\nu-1}(1-x)^{\mu-1}e^{\beta x}\,dx=B(\mu,\nu)\Phi(\nu,\mu+\nu,-\beta)$$
$$=B(\mu,\nu)e^{\beta}\Phi(\mu,\mu+\nu,-\beta), \tag{C5a}$$

where

$$B(\mu,\nu)=\Gamma(\mu)\Gamma(\nu)/\Gamma(\mu+\nu), \tag{C5b}$$

and Φ is the confluent hypergeometric function.

Let us now consider the integral

$$I=\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}e^{-(2/a^2)(\rho_1^2c_3^2s_2^2s_1^2+\rho_2^2c_2^2s_1^2+\rho_3^2c_1^2)}$$
$$\times s_3^{A-5}s_2^{A-4}s_1^{A-3}\,d\phi_3d\phi_2d\phi_1. \tag{C6}$$

First we integrate over the ϕ_3-dependent part and writing $c_3^2=1-s_3^2=1-x$, we get

$$e^{-(2/a^2)\rho_1^2s_2^2s_1^2}\int_0^1 e^{-(2/a^2)\rho_1^2s_2^2s_1^2x}x^{(A-6)/2}(1-x)^{-1/2}\,dx, \tag{C7a}$$

which from (C5) becomes

$$B(\tfrac{1}{2},(A-4)/2)\,\Phi(\tfrac{1}{2},(A-3)/2,-(2/a^2)\rho_1^2s_2^2s_1^2). \tag{C7b}$$

The integral (C6) now takes the form

$$I=B(\tfrac{1}{2},(A-4)/2)\int_0^{\pi}\int_0^{\pi}$$
$$\times\Phi(\tfrac{1}{2},(A-3)/2,-(2/a^2)\rho_1^2s_2^2s_1^2)$$
$$\times\exp\left[-(2/a^2)(\rho_2^2c_2^2s_1^2+\rho_3^2c_1^2)\right]$$
$$\times s_2^{A-4}s_1^{A-3}\,d\phi_1d\phi_2, \tag{C8a}$$

which, when expanding Φ as a series, gives

$$I = B(\tfrac{1}{2},(A-4)/2)\sum_K \left\{ \frac{(\tfrac{1}{2})_K}{((A-3)/2)_K} \frac{(-(2/a^2)\rho_1^2)^K}{K!} \right.$$
$$\times \int_0^\pi \int_0^\pi \exp[-(2/a^2)(\rho_2^2 c_2^2 s_1^2 + \rho_3^2 c_1^2]$$
$$\left. \times s_2^{A-4+2K} s_1^{A-3+2K} d\phi_1 d\phi_2 \right\}, \quad \text{(C8b)}$$

where $(x)_n$ is the Pochhammer symbol $(x)_n = x(x+1)\cdots(x+n-1)$. We use the same steps to determine the remaining integrals, getting finally $\mathscr{V}(\rho_1\rho_2\rho_3)$ of Eq. (6.11). It is obvious that the $\mathscr{V}(\rho_1\rho_2\rho_3)$ of (6.11) is invariant under permutation of the particle indices, or equivalently of the $\{\rho_k\}$, $k = 1,2,3$.

In order to investigate the dependence of $\mathscr{V}(\rho_1\rho_2\rho_3)$ on ρ, b, c, it is better to consider the limit $A \gg 1$ for which the factors s_1^{A-5}, s_2^{A-4}, and s_1^{A-3} in the volume element contribute only in the vicinity of $\phi_K = \pi/2$, $K = 1,2,3$. Making then the transformation

$$\phi_K = \pi/2 + \epsilon_K, \quad K = 1,2,3, \quad d\phi_i = d\epsilon_i, \quad \text{(C9a)}$$
$$\sin\phi_i = \cos\epsilon_i \quad \text{and} \quad \cos\phi_i = -\sin\epsilon_i, \quad \text{(C9b)}$$

and, if we disregard terms of order higher than ϵ_K^2, we can use the relation

$$\cos\epsilon_K \simeq 1 - \epsilon_K^2/2 \simeq \exp(-\epsilon_K^2/2), \quad \text{(C10)}$$
$$\sin\epsilon_K \simeq \epsilon_K, \quad K = 1,2,3,$$

so we finally get

$$I = \prod_{K=1}^{3} \int_{-\infty}^{\infty} \exp\left[-\left(\frac{A-6+K}{2} + 2a\rho_k^2 \right) \epsilon_{4-K}^2 \right] d\epsilon_{4-K}$$
$$= \pi^{3/2} \left\{ \prod_{K=1}^{3} [\tfrac{1}{2}(A-6+K) + 2\rho_K^2/a^2] \right\}^{-1/2}, \quad \text{(C11)}$$

where we enlarged the limits of the integrals from $(0,\pi)$ to $(-\infty, +\infty)$ because the whole expression only contributes in the vicinity of $\pi/2$. We obtain then

$$\mathscr{V}(\rho_1\rho_2\rho_3) = -\frac{v_0 A(A-1)}{2} \frac{I(a)}{I(0)}, \quad \text{(C12)}$$

which gives rise to Eq. (6.12). Substituting the ρ_K^2 by their values (2.4) in terms of ρ,b,c, we can write, when $A \gg 1$,

$$\mathscr{V}(\rho,b,c) \simeq -\frac{v_0 A^{7/2}}{2} \times \left[\frac{64}{27} \frac{\rho^6}{a^6} (1 - 3b^2 + 2b^3 \cos 3c) + \frac{16\rho^4}{3a^4} \times (1-b^2)A + \frac{4\rho^2}{a^2} A^2 + A^3 \right]^{-1/2}. \quad \text{(C13)}$$

Note that when $A \gg 1$, we have $\gamma = c$, $b \simeq \beta/\sigma$ and $\rho \simeq \sigma + \overline{\alpha}/\sqrt{2}$, where σ is given by (3.21). Thus we could also write the Vanagas potential in terms of $\overline{\alpha},\beta,\gamma$.

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Viscous fluid interpretation of electromagnetic fields. II

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(Received 10 June 1981; accepted for publication 7 August 1981)

The paper examines the possibility of interpreting the energy-stress tensor of an electromagnetic field with or without a perfect fluid as due to a viscous fluid without any electromagnetic field. Some results obtained previously by Tupper are recovered and the time irreversibility brought about by viscosity is emphasized.

PACS numbers: 41.10.Hv, 03.50.De

I. INTRODUCTION

Following the observations of Tupper[1] that some non-null electrovac metrics could be interpreted alternatively as due to a viscous-fluid distribution, the present authors[2] found that a necessary condition for such a dual interpretation is a symmetry property of the metric and the electric (or magnetic) field. We could thus exhibit some cases where this viscous fluid interpretation did not work.

More recently Tupper[3] has made a very thorough investigation of the problem of dual interpretation involving electromagnetic fields and viscous fluids and has given examples from known solutions of how different types of situation can arise. In the present paper we attempt a similar investigation, but our mathematical procedure is somewhat different from that of Tupper and appears to us simpler. Also some points which have not been properly emphasized in Tupper's paper are here brought into relief.

Let us first state the problem clearly: we have a metric $g_{\mu\nu}$ such that the corresponding Einstein tensor $G_{\mu\nu}\,(\equiv R_{\mu\nu}-\frac{1}{2}Rg_{\mu\nu})$ satisfies the following equation

$$G_{\mu\nu}=[(p+\rho)\vartheta_\mu\vartheta_\nu-pg_{\mu\nu}+E_{\mu\nu}], \tag{1}$$

where p and ρ are the pressure and density of the fluid respectively, ϑ_μ is the fluid velocity vector, and $E_{\mu\nu}$ is the energy stress tensor for an electromagnetic field. The coupling constant here and in the following discussion have been omitted.

Now following Lichnerowicz,[4] we can write

$$E_{\mu\nu}=-(\tfrac{1}{2}g_{\mu\nu}-\vartheta_\mu\vartheta_\nu)(E^2+B^2)-(E_\mu E_\nu+B_\mu B_\nu)-(\vartheta_\mu S_\nu+\vartheta_\nu S_\mu), \tag{2}$$

where E_μ and B_μ are the electric and magnetic fields as seen by an observer moving with the fluid and are given by

$$E_\nu=F_{\mu\nu}\vartheta^\mu,\quad B_\nu=\tfrac{1}{2}\eta_{\mu\nu\alpha\beta}\vartheta^\mu F^{\alpha\beta},$$

where $F_{\mu\nu}$ is the electromagnetic field tensor and the Poynting vector S_μ is defined by

$$S_\mu=\eta_{\mu\alpha\beta\gamma}E^\alpha B^\beta\vartheta^\gamma. \tag{3}$$

We are now ready to investigate whether the same metric field can be interpreted as being due to a viscous fluid, i.e., whether we can satisfy the equation

$$G_{\mu\nu}=[(\bar p+\bar\rho)u_\mu u_\nu-\bar pg_{\mu\nu}+2\eta\sigma_{\mu\nu}], \tag{4}$$

where we must have the algebraic relations

$$u^\mu u_\mu=1, \tag{5}$$

$$\sigma_{\mu\nu}u^\mu=0, \tag{6}$$

$$\sigma^\mu_\mu=0, \tag{7}$$

along with the differential relation connecting the shear tensor with the derivatives of the velocity vector

$$\sigma_{\mu\nu}=u_{(\mu;\nu)}-\tfrac{1}{3}\theta(g_{\mu\nu}-u_\mu u_\nu)-u_{(\mu}\dot u_{\nu)}. \tag{8}$$

As $G_{\mu\nu}$ is assumed given, Eqs. (4)–(7) provide us with 16 algebraic equations to determine the sixteen unknowns (four components of u^μ + ten components of $\eta\sigma_{\mu\nu}$ + the two scalars $\bar p$ and $\bar\rho$). Hence in general they will be uniquely determined. In order that the interpretation may be valid once the $\sigma_{\mu\nu}$ and u^μ are thus determined, the differential relation (8) must be identically satisfied and besides, the values of $\bar p,\bar\rho$, and η must be physically acceptable. Obviously this would not be the case in general.

II. SOLUTIONS OF THE ALGEBRAIC EQUATIONS

We note that in view of Eq. (4) and (6), u^μ is an eigenvector of $G_{\mu\nu}$ and hence in the case of nondegeneracy the other three eigenvectors of $G_{\mu\nu}$ will be spacelike (in the case of degeneracy one may choose the other three to be spacelike). It is easy to see that $G_{\mu\nu}$ and $\sigma_{\mu\nu}$ have the same eigenvectors—a result which will be used later.

We now investigate the eigenvectors of $G_{\mu\nu}$.

Using (1) and (2), we have

$$G_{\mu\nu}E^\mu=[\tfrac{1}{2}(E^2-B^2)-p]E_\nu-(E_\alpha B^\alpha)B_\nu, \tag{9}$$

$$G_{\mu\nu}B^\mu=[\tfrac{1}{2}(B^2-E^2)-p]B_\nu-(E_\alpha B^\alpha)E_\nu. \tag{10}$$

Hence there will be two eigenvectors (both spacelike) in the two space spanned by E^μ and B^μ. These are $E^\mu+\lambda_{\pm}B^\mu$, where

$$\lambda_{\pm}=\frac{1}{2(E_\alpha B^\alpha)}\times\{(E^2-B^2)\pm[(E^2-B^2)^2+4(E_\alpha B^\alpha)^2]^{1/2}\}. \tag{11}$$

λ is indeterminate in the case of null fields where $E^2-B^2=(E_\alpha B^\alpha)=0$. For non-null fields, the eigenvalues corresponding to the eigenvectors $E^\mu+\lambda_{\pm}B^\mu$ are from (9)–(11),

$$-p\pm\tfrac{1}{2}[(E^2-B^2)^2+4(E_\alpha B^\alpha)^2]^{1/2}. \tag{12}$$

For null fields the degenerate eigenvalue is $-p$. The two other eigenvectors will be in the orthogonal plane, i.e., in the plane spanned by S^μ and ϑ^μ. A simple calculation shows that the eigenvectors are $S^\mu+\alpha_{\pm}\vartheta^\mu$, where

$$\alpha_{\pm}=\tfrac{1}{2}\{-[(E^2+B^2)+p+\rho]\pm\xi\} \tag{13}$$

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with

$$\xi \equiv [(E^2 + B^2 + p + \rho)^2 - 4S^2]^{1/2} \tag{14}$$

and

$$S^2 \equiv -S_\mu S^\mu.$$

Of these two, $S^\mu + \alpha_- \vartheta^\mu$ is timelike and as u^μ is known to be the timelike eigenvector, we have

$$u^\mu = \beta [S^\mu + \alpha_- \vartheta^\mu], \tag{15}$$

where the normalizing factor β ensures that Eq. (5) is satisfied and is given by

$$\beta^2 = 1/[\alpha_-^2 - S^2]. \tag{16}$$

Thus, u^μ will be identical with ϑ^μ iff S^μ vanishes. The eigenvalues corresponding to these eigenvectors $S^\mu + \alpha_\pm \vartheta^\mu$ are, from (1), (2), (13), and (14),

$$\tfrac{1}{2}[(\rho - p) \mp \xi]. \tag{17}$$

From Eq. (4) the eigenvalue of $G_{\mu\nu}$ corresponding to the eigenvector u^μ is $\bar{\rho}$ while from (17) it is equal to $\frac{1}{2}[(\rho - p) + \xi]$.

Therefore

$$\bar{\rho} = \tfrac{1}{2}[(\rho - p) + \xi]. \tag{18}$$

Again contracting (1) and (4), we get

$$\rho - 3p = \bar{\rho} - 3\bar{p}. \tag{19}$$

Thus from (18) and (19)

$$\bar{p} = \tfrac{1}{6}[(5p - \rho) + \xi]. \tag{20}$$

From (1), (2), and (4), substituting the values of $\bar{p}$ and $\bar{\rho}$ from (18) and (20) we get

$$2\eta\sigma_{\mu\nu} = \{(p+\rho)[1 - \tfrac{1}{3}\beta^2(\alpha_-)^2] - \tfrac{2}{3}\beta^2(\alpha_-)^2\xi + (E^2 + B^2)\}\vartheta_\mu\vartheta_\nu - \tfrac{1}{6}[(p+\rho) - \xi + 3(E^2 + B^2)]g_{\mu\nu}$$
$$- (\vartheta_\mu S_\nu + \vartheta_\nu S_\mu)\{1 + \tfrac{1}{3}\beta^2\alpha_-[p + \rho + 2\xi]\} - \tfrac{1}{3}\beta^2[p + \rho + 2\xi]S_\mu S_\nu - (E_\mu E_\nu + B_\mu B_\nu). \tag{21}$$

Thus from (15), (16), (18), (20), and (21), the sixteen unknowns are determined in terms of the known quantities.

Again from (21), corresponding to the eigenvectors $S^\mu + \alpha_\mp \vartheta^\mu, E^\mu + \lambda_\pm B^\mu$, the eigenvalues of $\sigma_{\mu\nu}$ are

$$0, \quad \frac{1}{6\eta}[p + \rho - \xi],$$

$$\frac{1}{12\eta}[\xi - (p+\rho)] - \frac{1}{4\eta}[(E^2 - B^2) + 4(E_\alpha B^\alpha)^2]^{1/2},$$

$$\frac{1}{12\eta}[\xi - (p+\rho)] + \frac{1}{4\eta}[(E^2 - B^2)^2 + 4(E_\alpha B^\alpha)^2]^{1/2}.$$

The condition for the viscous fluid interpretation to work is that the shear calculated for the vector given by (15) must agree with (21). However in general this leads to a too complicated equation. Leaving aside the general discussion we now consider special cases.

III. SPECIAL CASES

A. Electrovac universe

Let us first take the case of an electrovac universe with $S_\mu = 0$. This is the case considered in our previous paper where the field was considered to be a simple electric or magnetic field (this can be done by a duality rotation); we have from (14), as $p = \rho = 0$,

$$\xi = E^2 \quad \text{(when only an electric field exists)},$$
$$= B^2 \quad \text{(for a simple magnetic field)},$$

and the eigenvalues of the shear tensor are

$$0, \frac{E^2}{3\eta}, -\frac{E^2}{6\eta}, -\frac{E^2}{6\eta},$$

(with similar expressions for the magnetic field case) belonging, respectively, to the eigenvectors, u^μ, E^μ (or B^μ) and two vectors orthogonal to E^μ and u^μ, there being a degeneracy for the last two. This was the main result arrived at in our previous paper.

B. Perfect fluid with null field

The null-field condition gives $E_\alpha B^\alpha = E^2 - B^2 = 0$.

If there is no fluid along with the null field, Eqs. (13) and (14) show that the eigenvalues corresponding to the eigenvectors $S_\mu + \alpha_\pm \vartheta^\mu$ both vanish and the eigenvectors are both null vectors (note the self-orthogonality of null vectors) and thus no timelike eigenvector u^μ exists. Thus, as was observed previously by Tupper, one cannot have a viscous-fluid interpretation in this case.

If a fluid is present along with the null field we have already noted from Eq. (11) that $\lambda_\pm$ is indeterminate. This corresponds to the fact that belonging to the degenerate eigenvalue $-p$ for the tensor $G_{\mu\nu}$ [cf. Eqs. (9) and (10)] any vector in the E^μ, B^μ space (i.e., any vector orthogonal to ϑ^μ and S^μ) is an eigenvector.

The eigenvalues of $\sigma_{\mu\nu}$ in this case are

$$0, \frac{1}{6\eta}(p + \rho - \xi), \frac{1}{12\eta}[\xi - (p+\rho)],$$
$$\frac{1}{12\eta}[\xi - (p+\rho)],$$

and show the same degeneracy as the $G_{\mu\nu}$ tensor.

It is clear that these degeneracies can be ensured automatically if the metric has a rotational symmetry in the space spanned by E^μ and B^μ (i.e., the two space orthogonal to ϑ^μ and S^μ). Once this is satisfied, the shear tensor given by (8) will have an eigenvalue pattern $(0, -2\alpha, \alpha, \alpha)$. If, as is likely due to symmetry reasons, the eigenvectors coincide, one can, by choice of the parameter η, make the shear tensor agree with the tensor (21). However, it may be noted that in view of Eq. (14), for this null-field case, $\xi > (p + \rho)$, and hence the degenerate eigenvalues are to be positive if η is to be positive.

As a distribution of fluid cum null field, we recall the metric given by Raychaudhuri and Dutta,[5]

$$ds^2 = \tfrac{1}{2}t^{2(\alpha+1)}[dt^2 - dr^2] - t^2(dx^2 + dy^2) \tag{22}$$

for matter plus radiation.

Using the above metric for a viscous fluid solution we

get

$$\bar{\rho} = \frac{1}{4\pi}(2\alpha + 3)t^{-2(\alpha+2)},$$

$$\bar{p} = \frac{1}{12\pi}(4\alpha + 3)t^{-2(\alpha+2)},$$

with the nonvanishing velocity component being

$$u^0 = \sqrt{2}\, t^{-(\alpha+1)}.$$

The shear tensor components, i.e., diagonal components are

$$\left[0, \frac{2\sqrt{2}\alpha}{3} t^{-(\alpha+2)}, -\frac{\sqrt{2}}{3}\alpha t^{-(\alpha+2)}, -\frac{\sqrt{2}}{3}\alpha t^{-(\alpha+2)}\right]$$

and

$$\eta = -\frac{t^{-(\alpha+2)}}{8\sqrt{2}\pi}$$

so here η may be positive if $t<0$ and α is odd. We shall return later to this point of η having positive values only for $t<0$.

C. Case of a perfect fluid distribution (with either an electric field or magnetic field)

When we have either an electric or magnetic field but not both, $S_\mu = 0$. Here from (16) we find $\beta\alpha_- = 1$ and hence from (15) $u^\mu = \vartheta^\mu$. From (14), $\xi = E^2 + p + \rho$ (if we have an electric field).

Using these conditions, Eq. (21) reduces to

$$2\eta\sigma_{\mu\nu} = \tfrac{1}{3}E^2(\vartheta_\mu\vartheta_\nu - g_{\mu\nu}) - E_\mu E_\nu. \tag{23}$$

From (18) and (19)

$$\left.\begin{aligned}\bar{\rho} - \rho &= \tfrac{1}{2}E^2\\ \bar{p} - p &= \tfrac{1}{6}E^2\end{aligned}\right\}. \tag{24}$$

Substituting (23) and (24) in Eq. (2) we get

$$E^\mu_\nu = [\,\bar{\rho} - \rho + \bar{p} - p\,]\vartheta^\mu\vartheta_\nu - (\bar{p} - p)\delta^\mu_\nu + 2\eta\sigma^\mu_\nu. \tag{25}$$

This is also evident from (1) and (4), since $u^\mu \equiv \vartheta^\mu$. Equation (25) is the same as that obtained in our previous paper in the case of electrovac universes—only we no longer have any freedom in choosing the velocity vector—here it must be the velocity vector of the original perfect fluid. Thus we now have the additional condition that this velocity vector of the original fluid must be shearing, the shear ellipsoid is a spheroid with the electric (or magnetic) vector orthogonal to the symmetry plane of the spheroid. In particular, for a static fluid cum electromagnetic field, due to the static nature the velocity vector is shear-free and hence no viscous fluid interpretation is possible.

Any nonstatic spherically-symmetric fluid distribution with a radial electric field can, in general admit a viscous fluid interpretation for, as known from the investigations of De,[6] Mashoon and Partovi,[7] in such a case shear is always present except for a very special equation of state, and radial symmetry ensures that the shear components

$$\sigma^\theta_\theta = \sigma^\phi_\phi.$$

The case of stationary, axially-symmetric rotating models[8] offers an interesting point. In this case there are two Killing vectors—one timelike and the other spacelike—with closed orbits. Consistent with the symmetry the velocity vector may be taken to be a linear combination of these two vectors—it then turns out that it is either nonshearing or the shear tensor has the eigenvalue pattern $(0, 0, -\alpha, +\alpha)$. As this does not agree with the necessary pattern for a viscous fluid interpretation, no such interpretation is possible in this case.

We next consider, as an example, a plane symmetric metric given by Thorne[9]

$$ds^2 = dt^2 - A^2(dx^2 + dy^2) - W^2dz^2, \tag{26}$$

with

$$t = a_0(A + 2\beta)(A - \beta)^{1/2},$$

$$W = A + 4\beta + \frac{q(A-\beta)^{1/2}}{A} - \frac{8\beta^2}{A}.$$

a_0 q, and β are constants, a_0 and β being limited to positive values. The metric was interpreted as due to a pressureless fluid of density $\rho = (6\pi a_0^2 WA^2)^{-1}$ and in the rest frame of the fluid, the electromagnetic field is a simple magnetic field in the Z direction, of magnitude

$$B = (2\beta^{1/2}/3a_0)A^{-2}.$$

Obviously in this case, the conditions for the viscous fluid interpretation to work are all satisfied. In particular, we have $\vartheta^\mu \equiv \delta^\mu_0$ and by direct calculation

$$\bar{\rho} = \rho + \frac{B^2}{8\pi} = \frac{1}{6\pi a_0^2 A^2}\left[\frac{1}{W} + \frac{\beta}{3A^2}\right], \tag{27}$$

$$\bar{p} = \frac{B^2}{24\pi} = \frac{\beta}{54\pi a_0^2 A^4}, \tag{28}$$

$$\sigma^z_z = -2\sigma^x_x = -2\sigma^y_y = \frac{2}{3}\frac{d}{dt}\ln[\,W/A\,], \sigma^0_0 = 0, \tag{29}$$

$$\eta = \beta/(18\pi a_0^2 A^4 \frac{d}{dt}[\ln(W/A)]). \tag{30}$$

η is thus a complicated function of time. Note the degeneracy of the shear-tensor components. The general behavior of the universe may be thus described: A has a minimum value β at $t = 0$ and increases monotonically as $t \to \infty$. However, at some intermediate value of t, say t_0, W vanishes—one then has a singularity of $\bar{\rho}$ as well as the shear tensor $\sigma_{\mu\nu}$, but the pressure $\bar{p}$ remains finite and is always less than $\bar{\rho}/3$. After $t = t_0$, W may have quite complicated behavior but if for simplicity we take $q = 0$, W also is monotonically increasing and ultimately as $t \to \infty$, W/A approaches unity and the shear tensor as well as the density and pressure vanish. η is always finite in the domain $t_0 \leqslant t < \infty$ and vanishes at both $t = t_0$ and $t \to \infty$, but is negative at large enough values of t.

IV. CONCLUDING REMARKS

To sum up we may classify the solutions using the electromagnetic field into the following cases and the relevant conclusions for the viscous-fluid interpretation to be possible.

(i) Electrovac with non-null field. For the viscous-fluid interpretation of such a solution there must be a symmetry of the $\sigma_{\mu\nu}$ tensor.

(ii) Electrovac with null field. A viscous-fluid solution is

not possible as such but may be possible with the introduction of the heat-flux term as well, as shown by Tupper.

(iii) Fluid cum electromagnetic null field. For the dual interpretation of such a solution, the velocity vector of the viscous fluid is given by $u_\mu = \beta(S_\mu + \alpha_- \vartheta_\mu)$ and a symmetry of the $\sigma_{\mu\nu}$ tensor is required.

(iv) Fluid cum non-null field with $S_\mu \neq 0$. For the equivalence of such a solution with viscous fluid, the velocity vector of viscous fluid is given by $u_\mu = \beta(S_\mu + \alpha_- \vartheta_\mu)$. The shear tensor calculated from this velocity vector must agree with that given by (21) and there is no symmetry restriction on $\sigma_{\mu\nu}$. This is the most general case and thus complicated.

(v) Fluid cum non-null field with $S_\mu = 0$. Here the velocity vector of the original fluid is equal to the velocity vector of the viscous fluid, i.e., $u^\mu \equiv \vartheta^\mu$. A symmetry of the shear tensor is required for the dual interpretation. In particular, if the original distribution is static so that the shear vanishes, no viscous-fluid interpretation is possible.

Lastly we note the following regarding the requirement that η must be positive.

Equating the divergence of the r.h.s. of Eq. (4) with zero and then contracting with u_ν, we get

$$\bar{\rho}_{,\mu} u^\mu + (\bar{p} + \bar{\rho})\theta - 4\pi\sigma^2 = 0. \tag{31}$$

The above relation shows that the constraint $\eta > 0$ would place some restrictions on $\bar{\rho}$, $\bar{p}$, and the expansion θ. In general one can say little further from Eq. (31); however most of the known solutions of a fluid cum—electromagnetic field are spatially homogeneous as given by Dunn and Tupper[10] (cited by Tupper)—admitting three linearly independent spacelike Killing vectors. In that case the Lie derivatives of $\bar{\rho}$, $\bar{p}$, with respect to all three Killing vectors vanish—i.e., they are functions of "t" alone where t lines are the orthogonals to the three trajectries of the group. We can have then a functional relationship between $\bar{p}$ and $\bar{\rho}$ and if, further, we take the simple special case $\bar{p} = \alpha\bar{\rho}$ where α is a constant for $\eta > 0$, the above equation requires $\rho(\sqrt{-g})^{(1+\alpha)/2}$ be a monotonically increasing function along the future directed t lines. Thus, while a particular metric may give rise to negative η, its time-reversed may satisfy the condition $\eta > 0$. This may be expected for viscosity, being a dissipative process, introduces an irreversibility and hence may fix a direction of time-flux. Indeed, it is due to this fact that we have found that the metric (22) can be interpreted as being due to a viscous fluid for $t < 0$. Similarly some cases where the viscous fluid interpretation has been considered untenable by Tupper because of negative η (as he has concentrated on $t > 0$) may yield $\eta > 0$ with $t < 0$.

ACKNOWLEDGMENTS

The authors' thanks are due to Professor B. O. J. Tupper for a preprint copy of his paper and some interesting correspondence. One of the authors (SKS) also thanks the U. G. C. (India) for the award of a Teacher Fellowship.

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Electron motion in longitudinal electromagnetic fields

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(Received 4 August 1981; accepted for publication 18 September 1981)

A complete study of a charged particles motion in such electromagnetic fields, where vectors of electric and magnetic fields are parallel to each other and to some constant vector, is made. It lists all classes of fields, permitting the solution of the problem by the method of separation of variables, and all concrete kinds of fields in which Dirac's and Klein–Gordon's equations can be expressed through the known specifications and are given for the first time.

PACS numbers: 41.70. + t

Consider a charged particles motion in such electromagnetic fields where in some Lorentz coordinate system vectors of electric and magnetic intensity are parallel to each other and to the constant vector $\mathbf{n}$.

$$\mathbf{E} = \mathbf{n}E, \quad \mathbf{H} = \mathbf{n}H. \tag{1}$$

Such fields will be called longitudinal. Without limitation of generality we consider $\mathbf{n}$ to be oriented along the Z axis, i.e., $\mathbf{n} = (0,0,1)$. In this case from Maxwell's equations we have (The system of units and designations of Refs. 1 and 14 is used here.)

$$E = E(x_0,x_3), \quad H = H(x_1,x_2). \tag{2}$$

Thus the magnetic field is stationary while the electric one can be nonstationary. For an electromagnetic current density we find

$$\rho = \partial_3 E, \quad \mathbf{j} = -[\mathbf{n}\nabla H] - \mathbf{n}\partial_0 E. \tag{3}$$

From (3) it follows that free ($\rho = \mathbf{j} = 0$) longitudinal fields can be only stationary and uniform. It is also obvious that the fields[1,2] in the general case may be given by the potentials

$$A_0 = A_0(x_0,x_3), \quad A_1 = A_1(x_1,x_2), \quad E = \partial_0 A_3 - \partial_3 A_0, \tag{4}$$

$$A_3 = A_3(x_0,x_3), \quad A_2 = A_2(x_1,x_2), \quad H = \partial_2 A_1 - \partial_1 A_2.$$

A_μ are arbitrary functions of their arguments. Lorentz classic relativistic equations in longitudinal fields fall into two independent systems (Differentiation with respect to τ interval is marked with a point.)

$$m\ddot{x}_0 + E\dot{x}_3 = 0, \quad m\ddot{x}_3 + E\dot{x}_0 = 0, \tag{5}$$

$$m\ddot{x}_1 + H\dot{x}_2 = 0, \quad m\ddot{x}_2 - H\dot{x}_1 = 0. \tag{6}$$

Each of the systems may have the first obvious integral k_1,

$$m^2(\dot{x}_0^2 - \dot{x}_3^2) = m^2 + k_1^2, \quad m^2(\dot{x}_1^2 + \dot{x}_2^2) = k_1^2. \tag{7}$$

Thus the classical motion in longitudinal fields falls into two independent ones—the motion in two-dimensional subspace x_0, x_3, determined by an electrical field only; and the motion in two-dimensional subspace x_1, x_2, determined only by a magnetic field.

Accordingly the classical action function can also be presented in the form of a two term sum,

$$S = S_0 + S_1, \quad S_0 = S_0(x_1,x_2), \quad S_1 = S_1(x_0,x_3), \tag{8}$$

satisfying two independent equations

$$(\partial_1 S_0 + A_1)^2 + (\partial_2 S_0 + A_2)^2 = k_1^2, \tag{9}$$

$$(\partial_0 S_1 + A_0)^2 - (\partial_3 S_1 + A_3)^2 = m^2 + k_1^2, \tag{10}$$

and describing independent motions in magnetic and electric fields.

In quantum theory k_1 is an integral of motion as well. The solutions of Klein–Gordon's equations that determine the states with the definite k_1, in the general case, can be represented as

$$\Psi = N_0 \psi(x_1,x_2)\varphi(x_0,x_3). \tag{11}$$

Here N_0 is a normalization factor, function ψ is a solution to equation

$$(\mathscr{P}_1^2 + \mathscr{P}_2^2 - k_1^2)\psi = 0, \tag{12}$$

that is, to Schrödinger's two-dimensional stationary equation. The function φ satisfies the equation

$$(\mathscr{P}_0^2 - \mathscr{P}_3^2 - m^2 - k_1^2)\varphi = 0. \tag{13}$$

In (12) and (13) we assumed $\mathscr{P}_\mu = i\partial_\mu + A_\mu$.

The Dirac wave function for longitudinal fields is more conveniently represented as "blocks" through Pauli's two-dimensional matrices $\boldsymbol{\sigma}$:

$$\Psi_D = NQ\begin{pmatrix} m + F - ik_1\sigma_2 \\ (m - F)\sigma_3 - k_1\sigma_1 \end{pmatrix}\tilde{\varphi}^\alpha, \quad F = \mathscr{P}_0 + \mathscr{P}_3. \tag{14}$$

Here α is a constant arbitrary double component spinor, the scalar function $\tilde{\varphi} = \tilde{\varphi}(x_0,x_3)$ is a solution of the equation,

$$(\mathscr{P}_0^2 - \mathscr{P}_3^2 - m^2 - k_1^2 + iE)\tilde{\varphi} = 0, \tag{15}$$

similar to (13). The two-dimensional matrix Q has the form

$$2Q = (1 + \sigma_3)f_1(x_1,x_2) + (1 - \sigma_3)f_{-1}(x_1,x_2), \tag{16}$$

and functions f_s ($s = \pm 1$) are the solution of the first-order equations system:

$$(\boldsymbol{\sigma}\mathbf{p})G = k_1 G, \quad \mathbf{p} = (\mathscr{P}_1,\mathscr{P}_2,0), \quad G = \begin{pmatrix} f_1 \\ f_{-1} \end{pmatrix}. \tag{17}$$

This system in general form is readily squared. Supposing

$$G = [(\boldsymbol{\sigma}\mathbf{p}) + k_1]\bar{G}, \quad \bar{G} = \begin{pmatrix} \psi_1 \\ \psi_{-1} \end{pmatrix}. \tag{18}$$

 0022-2488/82/122558-04$02.50

From (17) we find the second-order independent equations

$$(\mathscr{P}_1^2 + \mathscr{P}_2^2 - k_1^2 + sH)\psi_s = 0, \quad s = \pm 1 \tag{19}$$

that are analogs to Eq. (12). It is useful to note that the Q matrix, as follows from (16) and (17), satisfies the equation

$$(\boldsymbol{\sigma}\mathbf{p})Q = k_1 Q \sigma_1. \tag{20}$$

Thus the quantum-mechanical problem, like the classical one, resulted in the investigation of independent two-dimensional equations that describe independent motions in electric and magnetic fields.

The availability, as usual, of the arbitrary constant spinor α in Dirac's wave function (14) is evidence of integral motion existence with no classical analog (spin integral of motion). From Refs. 2–4 and 14 it follows that such a spin integral of motion for longitudinal fields can be found in the obvious form. For the fields of a structure[1,2] the operator

$$\hat{L} = (\boldsymbol{\Sigma}\mathbf{n})[m\cos\gamma + i(\boldsymbol{\Sigma}\mathbf{p})(\rho_3 \sin\gamma - \rho_2 \cos\gamma)], \tag{21}$$

where γ is an arbitrary constant, $\boldsymbol{\Sigma}, \rho_k$ are Dirac's matrices corresponding to the motion integral, and the function (14) can be subordinated to the additional equation

$$\hat{L}\Psi_D = \zeta L \Psi_D, \quad \zeta = \pm 1, \tag{22}$$

that taking of (20) results in an algebraic equation on the α spinor:

$$(\boldsymbol{\sigma}\mathbf{l})\alpha = \zeta\alpha, \quad L = (m^2\cos^2\gamma + k_1^2)^{1/2}, \tag{23}$$

$$\mathbf{l} = L^{-1}(-k_1\cos\gamma, -k_1\sin\gamma, m\cos\gamma), \quad \mathbf{l}^2 = 1.$$

The solution of such an equation is well known.

Thus, the classification of Dirac wave functions by spin is carried out in longitudinal fields.

One can manage to find the concrete solutions of Eqs. (12) and (19) and (13) and (15) only for such fields as allow separation of variables in these equations.

The problem of finding all the fields allowing a complete separation of variables in Klein–Gordon's equation was solved in Refs. 5 and 6 in full. Similar investigations of Dirac's equations were made in Ref. 7. According to Refs. 5–7 there are four classes of electrical and two classes of magnetic fields of such a kind. Numbers are given of these classes according to the classification of Ref. 5; in brackets are those of Ref. 7: 9(2), 11a(4), 16(11), 18a(12), 20(13), 23(14), 30b(25), 37a(26). In all the cases the classical equations (5) and (6) permit obviously one more, besides (7), first integrals of motion, and may be integrated in quadratures. The solutions of Eqs. (9) and (10) are just found by quadratures. In quantum theory the use of these integrals of motion permits reduction of the solutions of Eqs. (12), (13), (15), and (19) to a solution of usual differential equations.

Some rather particular cases of exact Dirac's and Klein–Gordon's equations for longitudinal fields were studied previously.[8–13]

Consider the kinds of electric fields permitting separation of variables in equations of motion and exact solutions of such equations.

(1) $A_0 = A(x_3), \quad A_3 = 0, \quad E = -A'.$

The first integrals of the classical equations (5) are

$$m\dot{x}_0 - k_0 - A = 0,$$

$$m^2\dot{x}_3^2 = R(x_3) = (k_0 + A)^2 - m^2 - k_1^2. \tag{24}$$

The conditions $k_0 + A \geqslant 0$, $R \geqslant 0$ determine classically accessible regions of motion. The solution of Eqs. (24) and (10) in quadratures with $A(x_3)$ being an arbitrary function has the form

$$x_0 = \int (k_0 + A)R^{-1/2}dx_3, \quad \tau = m\int R^{-1/2}dx_3,$$

$$S_1 = k_0 x_0 - \int R^{1/2}dx_3. \tag{25}$$

To solve Eqs. (13) and (15) we find

$$\varphi = \exp(-ik_0x_0)\chi(x_3), \quad \chi'' + R\chi = 0, \tag{26}$$

$$\tilde{\varphi} = \exp(-ik_0x_0)\tilde{\chi}(x_3), \quad \tilde{\chi}'' + (R - iA')\tilde{\chi} = 0,$$

$$F = i\partial_3 + k_0 + A.$$

One can manage to find exact solutions of Eq. (26) with the following choice of the $A(x_3)$ function:

$$A(x) = \alpha x, \quad A(x) = \alpha x^{-1}, \quad A(x) = \alpha\exp\beta x, \tag{27}$$

$$A(x) = \alpha\tan\beta x, \quad A(x) = \alpha\tanh\beta x,$$

$$A(x) = \alpha\coth\beta x.$$

Here α, β are constants. The solutions themselves of Eqs. (26) with the $A(x_3)$ choice in the form of one of the functions (27) can be expressed through the known special functions. This record, for example, was studied in Refs. 1 and 14 in detail and there is no need to repeat these calculations.

(2) $A_0 = 0, \quad A_3 = A(x_0), \quad E = A'.$

In classical theory, with $A(x_0)$ being an arbitrary function, we have

$$m^2\dot{x}_0^2 = R(x_0) = m^2 + k_1^2 + (k_3 + A)^2,$$

$$m\dot{x}_3 + k_3 + A = 0, x_3 = -\int (k_3 + A)R^{-1/2}dx_0,$$

$$\tau = m\int R^{-1/2}dx_0, \quad S_1 = k_3x_3 + \int R^{1/2}dx_0. \tag{28}$$

In quantum theory we find

$$\varphi = \exp(-ik_3x_3)\chi(x_0), \quad \chi'' + R\chi = 0,$$

$$\tilde{\varphi} = \exp(-ik_3x_3)\tilde{\chi}(x_0), \quad \tilde{\chi}'' + (R - iA')\tilde{\chi} = 0,$$

$$F = i\partial_0 + k_3 + A. \tag{29}$$

Here exact solutions of Eqs. (29) obviously can just be obtained with the $A(x_0)$ function choice in the form of (27).

(3) Introduce variables

$$u_0 = x_0 - x_3, \quad u_3 = x_0 + x_3, \tag{30}$$

and give them potentials

$$A_0 = 0, \quad 2A_3 = A(u_0), \quad E = A'(u_0).$$

In classics one may readily obtain

$$m\dot{u}_0 - k_0 - A = 0,$$
$$m(k_0 + A)\dot{u}_3 - m^2 - k_1^2 = 0, \quad k_0 + A \geqslant 0, \tag{31}$$
$$\tau = m\int (k_0 + A)^{-1} du_0, \quad u_3 = (m^2 + k_1^2)\int (k_0 + A)^{-2} du_0,$$
$$2S_1 = k_0 u_3 + (m^2 + k_1^2)\int (k_0 + A)^{-1} du_0.$$

In quantum theory the explicit solution is also possible for an arbitrary function $A(u_0)$,

$$\varphi = (k_0 + A)^{-1/2}\exp(-iS_1),$$
$$\tilde{\varphi} = (k_0 + A)^{-1}\exp(-iS_1), \quad F = k_0 + A. \tag{32}$$

(4) For the variables

$$u_0 = x_0^2 - x_3^2, \quad u_3 = \frac{1}{2}\ln\left|\frac{x_0 + x_3}{x_0 - x_3}\right|, \tag{33}$$

assign the potentials

$$A_0 = 0, \quad 2A_3 = A(u_0), \quad E = A'(u_0).$$

The classical motion is described by the following equations:

$$2mu_0\dot{u}_3 + k_3 + A = 0,$$
$$m^2\dot{u}_0^2 = R(u_0) = (k_3 + A)^2 + 4u_0(m^2 + k_1^2), \quad R \geqslant 0$$
$$\tau = m\int R^{-1/2} du_0,$$
$$2u_3 = -\int (k_3 + A)u_0^{-1} R^{-1/2} du_0,$$
$$2S_1 = k_3 u_3 + \int (2u_0)^{-1} R^{1/2} du_0. \tag{34}$$

In quantum theory we have

$$\varphi = \exp(-ik_3 u_3/2)\chi(u_0),$$
$$16u_0^2\chi'' + 16u_0\chi' + R\chi = 0,$$
$$\tilde{\varphi} = \exp(-ik_3 u_3/2)\tilde{\chi}(u_0), \tag{35}$$
$$16u_0^2\tilde{\chi}'' + 16u_0\tilde{\chi}' + (R - iA')\tilde{\chi} = 0,$$
$$F = [2(x_0 + x_3)]^{-1}(4iu_0\partial_0 + k_3 + A).$$

The exact solution here is possible with $A = \alpha u_0$; however, in this case the electric field is constant and uniform and more simple solutions exist in such a field (see the previous solutions of the paper). A solution is also possible if $A = \alpha\sqrt{|u_0|}$. By substituting $x^2 = |u_0|$ Eqs. (35) are reduced to the ones studied in Ref. 1.

In this case the electric field is nonstationary and nonuniform.

Other electric fields permitting exact solutions of Eqs. (13) and (15) have not been found yet.

There are two classes of magnetic fields permitting separation of variables in Eqs. (12) and (19).

(1) $A_1 = 0, \quad A_2 = A(x_1), \quad H = -A'.$

Classical equations (6), (7), and (9) permit in the explicit form the two first integrals, their solutions being expressed by quadratures.

$$m^2\dot{x}_1^2 = R(x_1) = k_1^2 - (k_2 + A)^2,$$
$$m\dot{x}_2 + k_2 + A = 0, \quad R \geqslant 0 \tag{36}$$
$$\tau = m\int R^{-1/2} dx_1, \quad x_2 = -\int (k_2 + A)R^{-1/2} dx_1,$$
$$S_0 = k_2 x_2 - \int R^{1/2} dx_1.$$

Quantum-mechanical equations (12) and (19) are reduced to the ordinary ones,

$$\psi = \exp(-ik_2 x_2)\chi(x_1), \quad \chi'' + R\chi = 0,$$
$$\psi_s = \exp(-ik_2 x_2)\chi_s(x_1), \quad \chi_s'' + (R + sA')\chi_s = 0. \tag{37}$$

These equations are absolutely analogous to Eqs. (26) and their solutions can be written in the explicit form through the known special functions, $A(x_1)$ being taken in the form of (27).

(2) Introduce polar coordinates

$$x_1 = u_1\cos u_2, \quad x_2 = u_1\sin u_2,$$

and assign potentials

$$A_1 = 0, \quad A_2 = A(u_1), \quad H = -u_1^{-1}A'(u_1).$$

Integration of classical equations leads to the expressions

$$m^2\dot{u}_1^2 = R(u_1) = k_1^2 - (k_2 + A)^2 u_1^{-2}, \quad mu_1^2\dot{u}_2 + k_2 + A = 0, \quad R \geqslant 0$$
$$\tau = m\int R^{-1/2} du_1, \quad u_2 = -\int (k_2 + A)u_1^{-2} R^{-1/2} du_1, \tag{38}$$
$$S_0 = k_2 u_2 - \int R^{1/2} du_1.$$

In quantum theory we find

$$\psi = \exp(-ik_2 u_2)\chi(u_1), \quad \chi'' + u_1^{-1}\chi' + R\chi = 0,$$
$$\psi_s = \exp(-ik_2 u_2)\tilde{\chi}_s(u_1),$$
$$\tilde{\chi}_s'' + u_1^{-1}\tilde{\chi}_s' + (R + su_1^{-1}A')\tilde{\chi}_s = 0. \tag{39}$$

Here k_2 is an integer for Klein–Gordon's equation and half-integer for that of Dirac's. The solutions are expressed in the explicit form through the known special functions only as $A = \alpha u_1^2$ (with stationary and longitudinal magnetic field). The field of this structure $A = \alpha u_1$ was investigated in Ref. 9.

Other magnetic fields allowing solution of Eqs. (12) and (19) in explicit form have not yet been found.

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Inverse scattering: determination of inhomogeneities in sound speed

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(Received 17 March 1982; accepted for publication 30 July 1982)

The one-dimensional wave equation is examined for the purpose of developing a method applicable to indirect probing of propagation speed inhomogeneities. The examination utilizes the theory of inverse scattering and results in the development of a new method. The method consists of an algorithm which derives the inhomogeneities through processing in a special way the backscattered waves generated by an incident δ-function.

PACS numbers: 43.20.Bi, 02.30.Jr

1. INTRODUCTION

Inverse scattering theory originated in a paper of Gel'fand and Levitan.[1] They employed spectral theory to develop a method for obtaining the Schrödinger potential from the spectral function. Further work illuminating mathematical and quantum mechanical aspects of the method was carried out by, among others, Levinson[2] and Faddeev.[3] Kay[4] added applications to electromagnetic propagation through plasmas where Schrödinger's equation is also useful. A survey of developments on inverse scattering and other inverse methods can be found in Ref. 5.

A re-examination of the method by the author showed that (a) the time domain formulation,[6] rather than the frequency domain formulation used earlier, is the most natural and that (b) there exists a simple intuitive derivation[7] of the key results which may lead to inverse scattering methods for other equations. Soliton theory, where again Schrödinger's equation crops up, found applications for the time domain formulation.[8,9]

Herein, the method is applied to a different equation, namely the wave equation. As is the case with Schrödinger's equation, the present application also leads to an algorithm involving the solution of an integral equation.

The application dealt with in this paper is relevant to the problem of indirect probing of sound speed inhomogeneities. This problem has recently received wide attention. Cohen and Bleistein have successfully considered the case of small inhomogeneities.[10,11] Refinements to their method were added by Gray.[12] Backus and Gilbert[13] examined uniqueness questions. Their technique was utilized by Chen and Tsien[14] in devising a numerical method for deducing weak inhomogeneities from spectral data at discrete frequencies.

Unfortunately, the methods referenced above treat only the case of small inhomogeneities. Methods that rely on inverse scattering are not constrained by the restriction to small inhomogeneities. An inverse scattering example that is directly applicable to the problem examined here is the method of Ware and Aki,[15] and its improved version provided by Coen.[16] These authors show that the reflected wave and the inhomogeneities are related through the Gel'fand–Levitan integral equation. The tie to the Gel'fand–Levitan equation is achieved by means of a change of variables that transforms the main equation to the Schrödinger equation.

The method presented herein examines the same problem analyzed by Ware, Aki, and Coen. However, herein the main equation is examined by a new inverse scattering method which was developed without use of either (a) a transformation to the Schrödinger equation, or (b) the Gel'fand–Levitan integral equation. Variations in the speed are obtained exactly by solving a new linear integral equation involving the reflected wave generated by an incident δ-function and a kernel related to the speed. Solution of the equation produces the kernel from which the speed is found.

The body of the paper is divided into four sections. The first section derives the method. We examine the main equation

$$\frac{\partial^2}{\partial\tau^2}U-\frac{\partial^2}{\partial t^2}U-\gamma(\tau)\frac{\partial U}{\partial\tau}=0,$$

where $\gamma(\tau)$ is continuous and

$$\gamma(\tau)=0 \quad \text{for } \tau\leqslant 0 \text{ and for } \tau\to\infty.$$

We relate $\gamma(\tau)$ to the reflected wave due to an incident δ-function,

$$U(\tau,t)=\delta(\tau-t)+R(\tau+t) \quad \text{for } \tau\leqslant 0,$$

by means of a new integral equation involving a kernel which determines $\gamma(\tau)$.

The section section contains the application to the inhomogeneous propagation speed. Here, we show that the wave equation

$$\frac{\partial^2}{\partial z^2}u-\frac{1}{c^2(z)}\frac{\partial^2 u}{\partial t^2}=0,$$

can be transformed to the previously examined equation, and we utilize the method of the previous section to obtain the variations of the propagation speed.

The third section provides an illustration of the theory by means of an example. Here the reflected wave and the kernel of the integral equation are evaluated by independent means for a particular speed profile. We show that (a) the kernel is the solution of the integral equation, and (b) the kernel reproduces the speed profile.

Finally, the fourth section considers the relation of the present method to that by Cohen and Bleistein as refined by Gray. We consider small variations and show that their results follow as a special case.

2. ANALYSIS

We consider the equation

$$\frac{\partial^2 U}{\partial\tau^2}-\frac{\partial^2 U}{\partial t^2}-\gamma(\tau)\frac{\partial U}{\partial\tau}=0, \tag{2.1}$$

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where

$\gamma(\tau)$ is continuous,

$\gamma(\tau) = 0$ for $\tau \leqslant 0$ and for $\tau \to \infty$, and

$$U(\tau,t) = \delta(\tau - t) + R(\tau + t) \quad \text{for } \tau \leqslant 0. \tag{2.2}$$

We shall derive a method for determining $\gamma(\tau)$ from the reflected wave $R(t)$.

Let us assume a representation of U of the form[17]

$$U(\tau,t) = \delta(\tau - t) + R(\tau + t) - \frac{\partial}{\partial t} K(\tau,t) + \int_{-\tau}^{\tau} K(\tau, y)\dot{R}(y + t)\, dy, \tag{2.3}$$

where $\dot{R}(\xi)$ means the total derivative of R with respect to its argument ξ. In Appendix A we show that the representation exists provided

$$\frac{\partial^2 K}{\partial \tau^2} - \frac{\partial^2 K}{\partial t^2} - \gamma(\tau)\frac{\partial K}{\partial \tau} = 0, \tag{2.4}$$

$$K(\tau,t) = 0 \quad \text{for } t < -\tau \text{ and } t > \tau, \tag{2.5}$$

$$K(\tau, -\tau) = 0,$$

and

$$2\frac{d}{d\tau} K(\tau,\tau) - \gamma(\tau) K(\tau,\tau) = \gamma(\tau). \tag{2.6}$$

The generated U cannot travel with a speed greater than one. Hence,

$$U(t,\tau) = 0 \quad \text{for } t > \tau. \tag{2.7}$$

It follows from (2.3) that

$$\int_0^{t+\tau} R(\xi)\, d\xi - K(\tau,t) + \int_{-t}^{\tau} K(\tau, y)R(y + t)\, dy = 0 \quad \text{for } |t| < \tau, \tag{2.8}$$

where we utilized the fact that

$$R(t) = 0 \quad \text{for } t < 0. \tag{2.9}$$

The inverse scattering method consists of solving the integral equation (2.8) to find $K(\tau,t)$. Then, one obtains $\gamma(\tau)$ from (2.6). Appendix B shows that the solution of (2.8) is unique, provided

$$0 \leqslant |\hat{R}(\omega)| < 1 \quad \text{for all real } \omega, \tag{2.10}$$

where $R(\omega)$ is the reflection coefficient

$$\hat{R}(\omega) = \int_{-\infty}^{\infty} R(t) e^{i\omega t}\, dt. \tag{2.11}$$

3. APPLICATION–WAVE EQUATION WITH INHOMOGENEOUS SPEED

Consider the wave equation

$$\frac{\partial^2 u}{\partial z^2} - \frac{1}{c^2(z)}\frac{\partial^2 u}{\partial t^2} = 0, \tag{3.1}$$

where $c(z)$ has a continuous derivative and

$$c(z) = \bar{c} \quad \text{for } z \leqslant 0 \text{ and } z \to \infty. \tag{3.2}$$

Let an incident δ-function generate a reflected wave,

$$u(z,t) = \delta[(z/\bar{c}) - t] + R[(z/\bar{c}) + t] \quad \text{for } z \leqslant 0. \tag{3.3}$$

introduce the transformation

$$\tau = \int_0^z \frac{d\xi}{c(\xi)}. \tag{3.4}$$

Then, the above problem reduces to the one discussed earlier, i.e.,

$$\frac{\partial^2 U}{\partial \tau^2} - \frac{\partial^2 U}{\partial t^2} - \gamma(\tau)\frac{\partial U}{\partial \tau} = 0, \tag{3.5}$$

where

$$U(\tau,t) = u(z,t), \tag{3.6}$$

$$\gamma(\tau) = \frac{1}{c[z(\tau)]}\frac{d}{d\tau} c[z(\tau)]. \tag{3.7}$$

We utilize the previously developed method in order to determine the propagation speed. We solve (2.8) in order to find[18] $K(\tau,t)$. Then, we find the speed value from[19] Eq. (3.8),

$$c[z(\tau)] = \bar{c}[1 + K(\tau,\tau)]^2, \tag{3.8}$$

and the position of this value from an alternative form of (3.4),

$$z(\tau) = \bar{c}\int_0^{\tau} [1 + K(\xi,\xi)]^2\, d\xi. \tag{3.9}$$

4. EXAMPLE

Consider the following speed profile

$$c(z) = \begin{cases} \bar{c}; & z < 0, \\ \bar{c}(1 + 6z)^{4/3}, & z > 0, \end{cases} \tag{4.1}$$

whose corresponding reflected signal is derived in Appendix C. The signal and the kernel are as follows,

$$R(t) = \begin{cases} 0, & t < 0, \\ \bar{c}e^{2\bar{c}t}[2\cos\sqrt{2}\bar{c}t - \sqrt{2}\sin\sqrt{2}\bar{c}t\,], & t > 0, \end{cases} \tag{4.2}$$

and

$$K(\tau,t) = \begin{cases} 0, & |t| > \tau, \\ \dfrac{1}{(1 - 2\bar{c}\tau)^3}[\bar{c}\tau(2 - 5\bar{c}\tau + 4\bar{c}^2\tau^2) \\ \quad + \bar{c}t(2 - 6\bar{c}\tau + t\bar{c}^2\tau^2) - \bar{c}^2t^2 - 2\bar{c}^3t^3], & |t| < \tau \end{cases} \tag{4.3}$$

We shall show that the kernel expression (4.3) is indeed the solution to the integral equation (2.8) and that the kernel produces the sound speed.

Let us for the moment assume that the kernel given in (4.3) is indeed the solution to the integral equation. Then, the speed profile should be obtainable from the kernel according to (3.8) where the corresponding value of z is given from (3.9). We verify this in the following manner. Equation (4.3) shows that

$$K(\tau,\tau) = \frac{1}{(1 - 2\bar{c}\tau)^2} - 1. \tag{4.4}$$

Thus, (3.8) gives

$$c[z(\tau)] = \bar{c}[1 + K(\tau,\tau)]^2,$$

or

$$c[z(\tau)] = \frac{\bar{c}}{[1 - 2\bar{c}\tau]^4}. \tag{4.5}$$

The corresponding value of z is

$$z(\tau) = \bar{c} \int_0^{\tau} [1 + K(\xi,\xi)]^2 \, d\xi,$$

or

$$z(\tau) = \frac{1}{6}\left(\frac{1}{(1 - 2\bar{c}\tau)^3} - 1\right). \tag{4.6}$$

Substitution of (4.6) into (4.5) verifies that the speed profile is indeed that given in (4.1).

Now, let us proceed to show that the kernel satisfies the integral equation (2.8). This equation can be rewritten as

$$I = K(\tau,t), \tag{4.7}$$

where

$$I = \int_0^{\tau + t} R(\xi)[1 + K(\tau,\xi - t)] \, d\xi. \tag{4.8}$$

Substitution of the expressions for R and K leads to

$$I = I_1 + I_2, \tag{4.9}$$

where

$$I_2 = I_1^*, \tag{4.10}$$

$$I_1 = \frac{A}{(1 - 2\tau')^3} \int_0^{\tau' + t'} e^{(2 + i\sqrt{2})\xi'} \times [C + D\xi' + E\xi'^2 + F\xi'^3] \, d\xi, \tag{4.11}$$

and

$$A = \frac{2 + i\sqrt{2}}{2}, \tag{4.12}$$

$$C' = 1 - 4\tau' + 7\tau'^2 - 4\tau'^3 - 2t' + 6t'\tau' - t'^2 - 6t'\tau'^2 + 2t'^3, \tag{4.13}$$

$$D = 2 + 2t' - 6\tau' + 6\tau'^2 - 6t'^2, \tag{4.14}$$

$$E = -1 + 6t', \tag{4.15}$$

$$F = -2, \tag{4.16}$$

$$t' = \bar{c}t, \tag{4.17}$$

$$\tau' = \bar{c}\tau, \tag{4.18}$$

and I_1^* denotes the complex conjugate of I_1.
Now, we note that

$$\int e^{\alpha\xi} \, d\xi = \frac{e^{\alpha\xi}}{\alpha},$$

$$\int \xi e^{\alpha\xi} \, d\xi = e^{\alpha\xi}\left(\frac{\xi}{\alpha} - \frac{1}{\alpha^2}\right),$$

$$\int \xi^2 e^{\alpha\xi} \, d\xi = e^{\alpha\xi}\left(\frac{\xi^2}{\alpha} - \frac{2\xi}{\alpha^2} + \frac{2}{\alpha^3}\right),$$

$$\int \xi^2 e^{\alpha\xi} \, d\xi = e^{\alpha\xi}\left(\frac{\xi^2}{\alpha} - \frac{3\xi^2}{\alpha^2} + \frac{6\xi}{\alpha^3} - \frac{6}{\alpha^4}\right).$$

Using the above in (4.11) and doing the algebra leads to

$$I = I_{1,0} + I_{1,0}^* + I_{1,1} + I_{1,1}^*, \tag{4.19}$$

where

$$I_{1,0} = \frac{A}{(1 - 2\tau')^3}\left(-\frac{C}{2 + i\sqrt{2}} + \frac{D}{(2 + i\sqrt{2})^2} - \frac{2E}{(2 + i\sqrt{2})^3} + \frac{6F}{(2 + i\sqrt{2})^4}\right), \tag{4.20}$$

$$I_{1,1} = \frac{AQ}{(1 - 2\tau')^3} e^{(2 + i\sqrt{2})(\tau' + t')}, \tag{4.21}$$

and

$$Q = \frac{C}{2 + i\sqrt{2}} + D\left(\frac{\tau' + t'}{2 + i\sqrt{2}} - \frac{1}{(2 + i\sqrt{2})^2}\right) + E\left(\frac{(\tau' + t')^2}{2 + i\sqrt{2}} - \frac{2(\tau' + t')}{(2 + i\sqrt{2})^2} + \frac{2}{(2 + i\sqrt{2})^3}\right) + F\left(\frac{(\tau' + t')^3}{2 + i\sqrt{2}} - \frac{3(\tau' + t')^2}{(2 + i\sqrt{2})^2} + \frac{6(\tau' + t')}{(2 + i\sqrt{2})^3} - \frac{6}{(2 + i\sqrt{2})^4}\right). \tag{4.22}$$

The expressions for A, C, D, E, and F which are given in equations (4.12)–(4.16), are substituted into the expressions for $I_{1,0}$ and $I_{1,1}$. After like order terms are collected, one finds out the following results

$$Q = 0,$$

$$I_{1,1} + I_{1,1}^* = 0,$$

$$I_{1,0} + I_{1,0}^* = K(\tau,t),$$

and

$$I = I_{1,0} + I_{1,0}^* + I_{1,1} + I_{1,1}^* = K(\tau,t).$$

So, the kernel given in (4.3) is indeed the solution to the integral equation.

Although the speed profile used as an example is very useful for analysis purposes because its reflected wave is expressible in terms of elementary functions, nevertheless, this profile violates two restrictions of the method. In particular, the example has a speed that goes to infinity at large z's whereas the method required that at large z's the speed returned to its value for $z < 0$. In addition, the speed has a discontinuous first derivative at $z = 0$ whereas the method required a continuous first derivative.

The restrictions placed by the method on the speed appear to be too strong. Quite clearly, abnormal behavior of the sound speed in some spatial region will not be accounted in the reflected wave until the first reflection from this region arrives at $z = 0$. Thus, as long as the inversion process is limited to finite z's, the speed behavior at infinity is irrelevant. Furthermore, the fact that the analysis goes through for this example indicates that the inversion process may go through even for speeds whose first derivative is discontinuous.

5. CASE OF SMALL INHOMOGENEITIES

Weak inhomogeneities give rise to small reflections. Thus, the solution of the integral equation may be expressed in terms of a series of terms whose order increases with the sequence number. In particular, the solution to (2.8) may be written as

$$K(\tau,t) = \sum_{n=0}^{\infty} K_n(\tau,t), \tag{5.1}$$

where

$$K_0(\tau,t) = \int_0^{t+\tau} R(\xi)\, d\xi, \tag{5.2}$$

$$K_n(\tau,t) = \int_{-t}^{\tau} K_{n-1}(\tau,y) R(y+t)\, dy. \tag{5.3}$$

The sound speed becomes

$$c[z(\tau)] = \bar{c}\left[1 + \sum_{n=0}^{\infty} K_n(\tau,\tau)\right]^2, \tag{5.4}$$

whereas the corresponding z is

$$z(\tau) = \bar{c}\int_0^{\tau}\left[1 + \sum_{n=0}^{\infty} K_n(\xi,\xi)\right]^2 d\xi. \tag{5.5}$$

A first order analysis of equations (5.4) and (5.5) shows that the sound speed is given by

$$c(z) = \bar{c} + c_0(z),$$

where the first order term c_0 is given by

$$c_0(z) = 2\bar{c}K_0(z/\bar{c}, z/\bar{c}),$$

or

$$\frac{d}{dz}c_0(z) = 4R(2z/\bar{c}),$$

or

$$\frac{d}{dz}c_0(z) = \frac{2}{\pi}\int_{-\infty}^{+\infty} \exp\left(-2i\frac{z}{\bar{c}}\omega\right)\hat{R}(\omega)\, d\omega, \tag{5.6}$$

where $\hat{R}(\omega)$ is the reflection coefficient,

$$R(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \hat{R}(\omega) e^{-i\omega t}\, d\omega.$$

The result shown in (5.6) is the same as that obtained in Ref. 12.

6. CONCLUSION

Earlier work, which had presented a simple derivation of the inverse scattering problem for Schrödinger's equation, was used in order to develop a new inverse scattering method for the determination of the variations of the propagation speed from the scattered wave. The method results in an integral equation involving two functions, (a) a kernel which is determined by the inhomogeneities, and (b) the wave reflected by the inhomogeneities when a δ-function wave is incident upon them. In general, the integral equation may be solved numerically. However, iteration may be used to solve the equation in the case where the inhomogeneities are small. In both cases, the propagation speed is obtained from the kernel.

ACKNOWLEDGMENT

The author would like to thank the reviewer for his many contributions to improvements in the clarity of the presentation of this work.

APPENDIX A

We will show here that $U(\tau,t)$,

$$U(\tau,t) = \delta(\tau - t) + R(\tau + t) - \frac{\partial}{\partial t}K(\tau,t) + \int_{-\tau}^{\tau} K(\tau,y)\dot{R}(y+t)\, dy, \tag{A1}$$

satisfies

$$\frac{\partial^2 U}{\partial \tau^2} - \frac{\partial^2 U}{\partial t^2} - \gamma(\tau)\frac{\partial U}{\partial \tau} = 0, \tag{A2}$$

provided

$$\frac{\partial^2 K}{\partial \tau^2} - \frac{\partial^2 K}{\partial t^2} - \gamma(\tau)\frac{\partial K}{\partial \tau} = 0 \quad \text{for } |t| < \tau, \tag{A3}$$

$$2\frac{d}{d\tau}K(\tau,\tau) - \gamma(\tau)K(\tau,\tau) = \gamma(\tau) \quad \text{and} \quad K(\tau,-\tau) = 0, \tag{A4}$$

and

$$K(\tau,t) = 0 \quad \text{for } t < -\tau, \text{ and } t > \tau. \tag{A5}$$

To show the contention, we insert (A1) into the left side of (A2). The terms are as follows

$$\frac{\partial U}{\partial \tau} = \dot{\delta}(\tau - t) + \dot{R}(\tau + t) - \frac{\partial^2}{\partial t\,\partial \tau}K(\tau,t) + K(\tau,\tau)\dot{R}(\tau + t) + K(\tau,-\tau)\dot{R}(t-\tau) + \int_{-\tau}^{\tau}\frac{\partial}{\partial \tau}K(\tau,y)\dot{R}(y+t)\, dy,$$

$$\frac{\partial^2 U}{\partial \tau^2} = \ddot{\delta}(\tau - t) + \ddot{R}(\tau + t) - \frac{\partial^3}{\partial t\,\partial \tau^2}K(\tau,t) + \frac{d}{d\tau}K(\tau,\tau)\dot{R}(\tau + t) + K(\tau,\tau)\ddot{R}(\tau + t) + \frac{d}{d\tau}K(\tau,-\tau)\dot{R}(t-\tau) - K(\tau,-\tau)\ddot{R}(t-\tau) + \frac{\partial}{\partial \tau}K(\tau,y)\Big|_{y=+\tau}\dot{R}(t+\tau) + \frac{\partial}{\partial \tau}K(\tau,y)\Big|_{y=-\tau}\dot{R}(t-\tau) + \int_{-\tau}^{\tau}\frac{\partial^2}{\partial \tau^2}K(\tau,t)\dot{R}(y+t)\, dy,$$

$$\frac{\partial^2 U}{\partial t^2} = \ddot{\delta}(\tau - t) + \ddot{R}(\tau + t) - \frac{\partial^3}{\partial t^3}K(\tau,t) + K(\tau,\tau)\ddot{R}(t+\tau) - K(\tau,-\tau)\ddot{R}(t-\tau) - \frac{\partial}{\partial y}K(\tau,y)\Big|_{y=\tau}\dot{R}(t+\tau) + \frac{\partial}{\partial y}K(\tau,y)\Big|_{y=-\tau}\dot{R}(t-\tau) + \int_{-\tau}^{\tau}\frac{\partial^2}{\partial y^2}K(\tau,y)\dot{R}(t+y)\, dy,$$

where we used integration by parts to obtain the last equation. When we sum the terms we find that

$$\frac{\partial^2}{\partial\tau^2}U-\frac{\partial^2}{\partial t^2}U-\gamma(\tau)\frac{\partial U}{\partial\tau}$$
$$=-\frac{\partial}{\partial t}\left(\frac{\partial^2}{\partial\tau^2}K(\tau,t)-\frac{\partial^2}{\partial t^2}K(\tau,t)\right.$$
$$\left.-\gamma(\tau)\frac{\partial}{\partial\tau}K(\tau,t)-\gamma(\tau)\delta(\tau-t)\right)$$
$$+\dot{R}(\tau+t)\left(2\frac{d}{d\tau}K(\tau,\tau)-\gamma(\tau)K(\tau,\tau)-\gamma(\tau)\right)$$
$$+\dot{R}(t-\tau)\left(2\frac{2}{d\tau}K(\tau,\tau)-\gamma(\tau)K(\tau,-\tau)\right)$$
$$+\int_{-\tau}^{\tau}\left(\frac{\partial^2}{\partial\tau^2}K(\tau,y)-\frac{\partial^2}{\partial y^2}K(\tau,y)\right.$$
$$\left.-\gamma(\tau)\frac{\partial K}{\partial\tau}(\tau-y)\right)\dot{R}(\tau+y)\,dy. \tag{A6}$$

Now, the contention is true because Eqs. (A3)–(A5) and

$$K(\tau,-\tau)=\frac{d}{d\tau}K(\tau,-\tau)=0,$$

drive to zero all the terms on the right hand side of equation (A6) except the first. To show the zeroing out of the first term we note that this term involves the values of K over the full t interval. However, we can express the values of K over the full t interval in terms of the values of K over the semi-infinite t interval as follows:

$$K(\tau,t)=H(\tau-t)f(\tau,t), \tag{A7}$$

where H is the Heaviside function

$$H(\xi)=\begin{cases}1, & \xi\geqslant 0,\\ 0, & \xi<0,\end{cases}$$

and

$$f(\tau,t)\equiv K(\tau,t)\quad\text{for } t\leqslant\tau. \tag{A8}$$

In this fashion we can rewrite the first term of (A6) as follows:

$$-\frac{\partial}{\partial t}\left(\frac{\partial^2}{\partial\tau^2}K(\tau,t)-\frac{\partial^2}{\partial t^2}K(\tau,t)-\gamma(\tau)\frac{\partial K}{\partial\tau}(\tau,t)-\gamma(\tau)\delta(\tau-t)\right)$$
$$=-\frac{\partial}{\partial t}\left\{\delta(\tau-t)\left[2\frac{\partial}{\partial\tau}f(\tau,t)+2\frac{\partial}{\partial t}f(\tau,t)-\gamma(\tau)f(\tau,t)-\gamma(\tau)\right]\right.$$
$$\left.+H(\tau-t)\left[\frac{\partial^2}{\partial\tau^2}f(\tau,t)-\frac{\partial^2}{\partial t^2}f(\tau,t)-\gamma(\tau)\frac{\partial f}{\partial\tau}(\tau,t)\right]\right\}$$
$$=-\frac{\partial}{\partial t}\left\{\delta(\tau-t)\left[2\frac{\partial}{\partial\tau}f(\tau,y)\Big|_{y=\tau}+2\frac{\partial}{\partial y}f(\tau,y)\Big|_{y=\tau}-\gamma(\tau)f(\tau,\tau)-\gamma(\tau)\right]\right.$$
$$\left.+H(\tau-t)\left[\frac{\partial^2}{\partial\tau^2}f(\tau,t)-\frac{\partial^2}{\partial t^2}f(\tau,t)-\gamma(\tau)\frac{\partial f}{\partial\tau}(\tau,t)\right]\right\}$$
$$=-\frac{\partial}{\partial t}\left\{\delta(\tau-t)\left[2\frac{d}{d\tau}K(\tau,\tau)-\gamma(\tau)K(\tau,\tau)-\gamma(\tau)\right]+H(\tau-t)\left[\frac{\partial^2}{\partial\tau^2}K(\tau,t)-\frac{\partial^2}{\partial t^2}K(\tau,t)-\gamma(\tau)\frac{\partial K}{\partial\tau}(\tau,t)\right]\right\}.$$

Clearly, this last form of the first term is zero because of (A3)–(A5).

APPENDIX B

The integral equation

$$\int_0^{t+\tau}R(\xi)\,d\xi-K(\tau,t)$$
$$+\int_{-\infty}^{\tau}K(\tau,y)R(y+t)\,dy=0,\quad t<\tau, \tag{B1}$$

has a unique solution provided

$$0\leqslant|\hat{R}(\omega)|<1\quad\text{for all real }\omega. \tag{B2}$$

To show the above, we note that $K(\tau,t)$ is unique provided the following equation has only the null solution,

$$\int_{-\infty}^{\tau}W(\tau,y)[\delta(y-t)-R(y+t)]\,dy=0,\quad t<\tau. \tag{B3}$$

However,

$$\delta(y-t)-R(y+t)$$
$$=\frac{1}{2\pi}\int_{-\infty}^{+\infty}(e^{-i\omega(y-t)}-\hat{R}(\omega)e^{-i\omega(y+t)})\,d\omega. \tag{B4}$$

Now, after we substitute the right hand side of (B4) in place of the term of (B3) appearing inside the brackets and we multiply the result by $W(\tau,t)$ and integrate over t, we find

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty}\{|\hat{W}(\tau,\omega)|^2-\hat{R}(\omega)[\hat{W}^*(\tau,\omega)]^2\}\,d\omega=0, \tag{B5}$$

or

$$\frac{1}{\pi}\int_0^{\infty}\{2|\hat{W}(\tau,\omega)|^2-\hat{R}(\omega)[\hat{W}^*(\tau,\omega)]^2$$
$$-\hat{R}^*(\omega)[\hat{W}(\tau,\omega)]^2\}\,d\omega=0, \tag{B6}$$

where $\hat{W}(\tau,\omega)$ is the Fourier Transform of $W(\tau,t)$,

$$\hat{W}(\tau,\omega)=\int_{-\infty}^{\tau}W(\tau,y)e^{i\omega y}\,dy, \tag{B7}$$

and

$$\hat{W}(\tau,-\omega)=\hat{W}^*(\tau,\omega). \tag{B8}$$

Equation (B6) can be put into an alternative form that is more useful for our purposes. Let a and b be the real and imaginary parts of $\hat{R}(\omega)$ and A and B the corresponding parts of $\hat{W}(\tau,\omega)$. Then, (B6) becomes

$$\frac{1}{\pi}\int_0^\infty \{2(1-a)A^2 + 2(1+a)B^2 - 4bAB\}\, d\omega = 0, \tag{B9}$$

or, alternatively,

$$\frac{1}{\pi}\int_0^\infty \{(1+r)[\sqrt{1-\cos\theta}\,A - \sqrt{1+\cos\theta}\,B]^2 + (1-r)[\sqrt{1+\cos\theta}\,A + \sqrt{1-\cos\theta}\,B]^2\}\, d\omega = 0, \tag{B10}$$

where

$$r = |\hat{R}| = \sqrt{a^2+b^2}, \tag{B11}$$

and

$$\cos\theta = \frac{a}{r}, \tag{B12}$$

$$\sin\theta = \frac{b}{r}. \tag{B13}$$

Now it follows from (B10) that

$$\sqrt{1-\cos\theta}\,A - \sqrt{1+\cos\theta}\,B = 0,$$

$$\sqrt{1+\cos\theta}\,A + \sqrt{1-\cos\theta}\,B = 0,$$

at all frequencies ω where $0 \leqslant r(\omega) < 1$. The above system of equations will have the solution $A = 0$ and $B = 0$ if the determinant Δ of the corresponding matrix is not equal to zero,

$$\Delta = \det\left(\begin{bmatrix} \sqrt{1-\cos\theta} & -\sqrt{1+\cos\theta} \\ \sqrt{1+\cos\theta} & \sqrt{1-\cos\theta} \end{bmatrix}\right).$$

However, Δ is equal to 2. Thus, both A and B, and therefore W, are equal to zero and the integral equation has a unique solution $K(\tau,t)$.

APPENDIX C

Consider the wave equation

$$\frac{\partial^2 u}{\partial z^2} - \frac{1}{c^2(z)}\frac{\partial^2 u}{\partial t^2} = 0, \tag{C1}$$

where

$$c(z) = \begin{cases} \bar{c}, & z < 0, \\ \bar{c}(1+6z)^{4/3}, & z > 0. \end{cases} \tag{C2}$$

We will develop the reflected wave that results from a δ-function wave incident from the region $z < 0$. We will carry out the development by going through the spectal domain. In going back to the time domain we will choose the integration contour in a fashion that will make the reflected signal at $z = 0$ to be causal. Furthermore, because the introduction of the variable τ, where

$$\tau = \int_0^z \frac{d\xi}{c(\xi)} = \frac{1}{2\bar{c}}[1 - (1+6z)^{-1/3}], \tag{C3}$$

is most convenient we shall eliminate z in favor of τ.

The incident wave generates a forward moving wave inside the inhomogeneous medium. It can be verified by direct substitution into the frequency domain form of (C1) that the forward wave is given by

$$\hat{u}[z(\tau),\omega] = A(\omega)e^{ik\bar{c}\tau}(1-2\bar{c}\tau)^{-2}[1 - (2i/k)(1-2\bar{c}\tau)^{-1}], \tag{C4}$$

where

$$k = \frac{\omega}{\bar{c}}.$$

The reflected wave is determined by the smoothness conditions at $z = 0$,

$$\hat{u}[0,\omega] = 1 + \hat{R}(\omega), \tag{C5}$$

$$\frac{\partial \hat{u}}{\partial z}(0,\omega) = ik[1 - \hat{R}(\omega)]. \tag{C6}$$

Substitution of (C4) into (C5) and (C6) yields the reflection wave spectrum,

$$\hat{R}(\omega) = \frac{1}{2}\left\{\frac{2i+\sqrt{2}}{k-(2i+\sqrt{2})} + \frac{2i-\sqrt{2}}{k-(2i-\sqrt{2})}\right\}. \tag{C7}$$

The reflected wave at $z = 0$ is found from $\hat{R}(\omega)$ by contour integration

$$R(t) = \frac{1}{2\pi}\int_\Gamma \hat{R}(\omega)e^{-i\omega t}\, d\omega, \tag{C8}$$

where the contour Γ is chosen so that it runs along the real ω-axis but departs from it near the imaginary ω-axis to pass above the upper half-plane singularity of $\hat{R}(\omega)$. Performing the indicated contour integration we find the reflected signal given in (4.2).

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$$|\hat{T}(\omega)| = (1 - |\hat{R}(\omega)|^2)^{1/2} ,$$

Thus, one expects that $0 \leqslant |\hat{R}(\omega)| < 1$ for all real frequencies ω. Hence, one expects the solution of (2.8) to be unique.

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Semiclassical statistical mechanics of a two-dimensional fluid

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(Received 15 December 1980; accepted for publication 4 September 1981)

Expansions are obtained for the radial distribution function and free energy for a two-dimensional hard-core fluid in the semiclassical limit, using the "modified" Wigner–Kirkwood expansion method. These results are used to obtain expressions for the density-independent part of the radial distribution function and the first-order density correction to it. Quantum corrections to the second and third virial coefficients are discussed in detail. Explicit results are given for the Sutherland, Yukawa-tail, Wood–Saxan, square-well, and Lennard-Jones (12-6) pair potential models.

PACS numbers: 47.10. + g, 05.20. − y

I. INTRODUCTION

This paper is concerned with the evaluation of thermodynamic properties and low-order correlation functions of two-dimensional fluids in the semiclassical limit, where quantum effects are small and can be treated as a correction to the classical system. Although an ideally flat system seldom occurs in nature, a strictly two-dimensional picture has been used in predicting the properties of an adsorbed film.[1] For classical fluids, considerable progress has been made in recent years.[2–4] However, our understanding of the two-dimensional quantum fluids is less satisfactory.[5] Although the influence of dimensionality on the quantum effect is of much interest,[6] it has not yet been investigated systematically.

The usual way of studying the contribution of the quantum corrections is to expand the physical property of interest in ascending powers of Planck's constant h. The first term of this series is the classical value, the other terms collectively give the contributions arising due to quantum effects. In the Wigner–Kirkwood (WK) method,[7] the expansion is made in powers of the kinetic energy operator $\hbar^2\nabla^2$, which leads to a series in powers of $\hbar^2$. Since ∇^2 operates on the potential energy term, the WK method fails in cases where the intermolecular potential is a nonanalytic function of distance. The other shortcoming of the WK method is the slow convergence of the expansion series. This limits the applicability of the method to systems at high temperatures and low densities.

The problems of nonanalytic potentials are dealt with by using the Hemmer–Jancovici[8] (HJ) method in which expansion is done in terms of the modified Ursell functions U_l^m, leading to a series in powers of $\hbar$. The value of U_l^m can, in principle, be found from the solution of the quantum mechanical l-body problem. Unfortunately, the actual calculation is too involved to be feasible. It is only for hard spheres[9–11] and hard disks[6]-systems that U_2^m and U_3^m have been evaluated. For potentials, which have an attractive tail, the solution of even the two-body problem becomes difficult. However, for such potentials, a different type of expansion commonly known as the perturbation method[12] or modified WK method[13] can be adopted. In the modified WK expansion, hard-sphere basis fucntions are used instead of free-particle basis functions. The use of the hard-sphere basis functions remove, at least partially, the shortcoming of the WK method.

The problems concerning the evaluation of the equilibrium properties (virial coefficients, pair correlation functions, and thermodynamic properties) for nonanalytic potentials have been discussed using the modified WK method.[14–17] But all these attempts are confined to three-dimensional fluids. To the best of our knowledge, no work is available for a two-dimensional fluid, the constituent particles of which interact via a potential which has a hard core plus an attractive tail.

In Sec. II we discuss a general theory for calculating the equilibrium properties of a two-dimensional fluid whose particles interact via a hard core plus weak attractive tail potential. Section III is devoted to obtaining the density-independent radial distribution function and the first-order density correction to it. In Sec. IV we calculate the second and third virial coefficients for a two-dimensional hard-core fluid in the semiclassical limit. We discuss the second and third virial coefficients for some specific potential models in Sec. V. The results are summarized in Sec. VI.

II. GENERAL THEORY

In quantum statistical mechanics the grand canonical partition function of a two-dimensional fluid is defined as

$$\Xi^q = \sum_{N\geq 0} \frac{z^N}{N!} \int\cdots\int W_N^q(1, 2, ..., N) \prod_{i=1}^{N} d\mathbf{r}_i, \tag{2.1a}$$

where z is the fugacity and W_N^q is known as the *Slater sum*. For a two-dimensional fluid the Slater sum is written as

$$W_N^q(1, 2, ..., N) = N!\lambda^{2N} \sum_x \psi_x^*(1, 2, ..., N)\exp(-\beta\hat{H}_N)\psi_x(1, 2, ..., N), \tag{2.1b}$$

where $\lambda = (2\pi\hbar^2\beta/m)^{1/2}$ is the thermal wavelength, $\beta = (kT)^{-1}$, and the ψ's are a complete set of an orthogonal N-particle wave function. The summation in Eq. (2.1b) extends over all states. $\hat{H}_N$ is the Hamiltonian of the system

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$$\hat{H}_N = \frac{-\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + U(1, 2, ..., N), \tag{2.2a}$$

with

$$U(1, 2, ..., N) = \sum_{i<j} u(i, j). \tag{2.2b}$$

The quantity $W_N(1, ..., N)\mathrm{II}_N^{i=1} d\mathbf{r}_i$ is the measure of the probability that the configuration of the system is found to be within the interval

$$\{(\mathbf{r}_1, ..., \mathbf{r}_N), (\mathbf{r}_1 + d\mathbf{r}_1 ..., \mathbf{r}_N + d\mathbf{r}_N)\}.$$

Assuming that the quantum effects are largely determined by the repulsion due to the hard core, we choose the basis function, which is the eigenfunction of the hard-disk Hamiltonian. Let ψ_x^0 be the eigenfunction of the hard-disk Hamiltonian $\hat{H}_N^0$ given by

$$\hat{H}_N^0 = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + U_{\mathrm{hd}}(1, 2, ..., N), \tag{2.3a}$$

with

$$U_{\mathrm{hd}}(1, 2, ..., N) = \sum_{i<j} u_{\mathrm{hd}}(i, j). \tag{2.3b}$$

Then

$$\hat{H}_N^0\,\psi_x^0 = E_x^0\,\psi_x^0. \tag{2.4}$$

Treating the attractive interaction as a perturbation, Eq. (2.2a) can be written as

$$\hat{H}_N = \hat{H}_N^0 + U_p(1, 2, ..., N), \tag{2.5a}$$

where

$$U_p(1, 2, ..., N) = \sum_{i<j} u_p(i, j); \tag{2.5b}$$

$u_p(i, j)$ is the intermolecular perturbation potential, which is zero for $r_{ij} < d$, where d is the hard-disk diameter.

In terms of the hard-disk wave function ψ_x^0, The Slater sum can be expressed as

$$W_N^q(1, 2, ..., N)$$

$$= N!\lambda^{2N}\sum_x \psi_x^{0*}(1, 2, ..., N) \times \exp[-\beta(\hat{H}_N^0 + U_p)]\psi_x^0(1, 2, ..., N). \tag{2.6}$$

We follow the method of Friedman[18] and write

$$\exp[-t\beta(\hat{H}_N^0 + U_p)] = \exp[-t\beta U_p]\,T(t)\exp[-t\beta\hat{H}_N^0], \tag{2.7}$$

where

$$T(t) = 1 + T_1(t) + T_2(t) + \cdots, \tag{2.8}$$

with

$$T_1(t) = \int_0^t dt_1 \exp(t_1\beta U_p)[\exp(-t_1\beta U_p), \beta\hat{H}_N^0], \tag{2.9a}$$

$$T_2(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \exp(t_1\beta U_p)[\exp(-t_1\beta U_p) \times \exp(t_2\beta U_p)[\exp(-t_2\beta U_p), \beta\hat{H}_N^0], \beta\hat{H}_N^0]. \tag{2.9b}$$

The term T_{n+1} is given by the recursion relation

$$T_{n+1}(t) = \int_0^t dt_1 \exp(t_1\beta U_p)[\exp(-t_1\beta U_p)[T_n(t_1), \beta\hat{H}_N^0]$$

$$= \left(-\frac{\hbar^2\beta}{2m}\right)\int_0^t dt_1 \sum_{i=1}^{N}([-\nabla_i^2 T_n(t_1) + t_1\beta\{\nabla_i^2 U_p T_n(t_1) + 2\nabla_i U_p \nabla_i T_n(t_1)\} - t_1^2\beta^2(\nabla_i U_p)^2 T_n(t_1)] + [-2\nabla_i T_n(t_1) + 2t_1(\nabla_i U_p)T_n(t_1)]\cdot\nabla_i). \tag{2.10}$$

From Eqs. (2.6)–(2.10), we get

$$W_N^q(1, 2, ..., N) = W_N^0(1, 2, ..., N) + W_N^1(1, 2, ..., N) + W_N^2(1, 2, ..., N) + \cdots, \tag{2.11}$$

where

$$W_N^0(1, 2, ..., N) = N!\lambda^{2N}\sum_x \psi_x^{0*} e^{-\beta U_p} e^{-\beta\hat{H}_N^0}\psi_x^0 = e^{-\beta U_p} W_N^{\mathrm{hd}}(1, 2, ..., N), \tag{2.12}$$

$$W_N^1(1, 2, ..., N) = N!\lambda^{2N}\sum_x \psi_x^{0*} e^{-\beta U_p}\left(-\frac{\lambda^2\beta}{4\pi}\right)\sum_{i=1}^{N}\left[\frac{1}{2}\nabla_i^2 U_p - \frac{1}{3}\beta(\nabla_i U_p)^2 + \frac{1}{2}\nabla_i U_p\cdot\nabla_i\right]e^{-\beta\hat{H}_N^0}\psi_x^0$$

$$= \left(-\frac{\lambda^2\beta}{4\pi}\right)e^{-\beta U_p}\sum_{i=1}^{N}\left[\frac{1}{2}\nabla_i^2 U_p - \frac{1}{3}\beta(\nabla_i U_p)^2 + \frac{1}{2}\nabla_i U_p\cdot\nabla_i\right]W_N^{\mathrm{hd}}(1, 2, ..., N), \tag{2.13}$$

$$W_N^2(1, 2, ..., N) = N!\lambda^{2N}\sum_x \psi_x^{0*} e^{-\beta U_p} T_2(1) e^{-\beta\hat{H}_N^0}\psi_x^0, \tag{2.14}$$

and

$$W_N^{\mathrm{hd}}(1, 2, ..., N) = N!\lambda^{2N}\sum_x \psi_x^{0*} e^{-\beta\hat{H}_N^0}\psi_x^0 \tag{2.15}$$

is the Slater sum of the hard-disk fluid.

To evaluate Eq. (2.14), we use the superposition approximation and write the Slater sum as

$$W_N^q(1, 2, ..., N) = \prod_{i<j} W_2^q(i, j), \tag{2.16a}$$

where $W_2^q(i, j)$ is the Slater sum of a pair of particles i and j. It can be expressed as

$$W_2^q(i, j) = W_2^0(i, j) + W_2^1(i, j) + W_2^2(i, j) + \cdots. \tag{2.16b}$$

Equation (2.16a) is exact in the classical limit. For a quantum mechanical system, it is accurate at $\rho \to 0$. In the semiclassical limit we may expect it to be a reasonable approximation, except perhaps, for configurations in which three or more particles are very close and there is considerable interference of the wave functions. Under this approximation

$$W_N^2(1,2,...,N) = W_N^{hd}(1,2,...,N) \times \sum_{i<j} [W_2^2(i,j)/W_2^{hd}(i,j)], \quad (2.17)$$

which leads to

$$W_N^2(1,2,...,N) = (\lambda^2\beta) e^{-\beta U_p} W_N^{hd}(1,2,...,N) \sum_{i<j} [W_2^{hd}(i,j)]^{-1} \times \left\{ \left[\frac{\partial^2 u_p(i,j)}{\partial r_{ij}^2} - \frac{3}{4}\beta \left(\frac{\partial u_p(i,j)}{\partial r_{ij}} \right)^2 \right] h_2^{hd}(i,j) \times \left(\frac{\lambda}{r_{ij}} \right)^2 \left[- \frac{\partial^2 u_p(i,j)}{\partial r_{ij}^2} + \frac{1}{r_{ij}} \frac{\partial u_p(i,j)}{\partial r_{ij}} + \frac{3}{4}\beta \left(\frac{\partial u_p(i,j)}{\partial r_{ij}} \right)^2 \right] P_2^{hd}(i,j) \right\}, \quad (2.18)$$

where

$$W_2^{hd}(i,j) = 2\lambda^4 \sum_x \psi_x^{0*}(i,j) e^{-\beta \hat{H}_2^0(i,j)} \psi_x^0(i,j) = 2\lambda^2 \int d\bar{k}\, e^{-\lambda^2 k^2/2\pi} \sum_l |\psi_{kl}^0(r_{ij},\theta)|^2, \quad (2.19)$$

$$h_2^{hd}(i,j) = 2\lambda^4 \sum_x \psi_x^{0*}(i,j) \left(- \frac{\lambda^2}{6\pi^2} \nabla_{ij}^2 \right) e^{-\beta \hat{H}_2^0(i,j)} \psi_x^0(i,j) = \frac{2\lambda^4}{6\pi^2} \int d\bar{k}\, k^2 e^{-\lambda^2 k^2/2\pi} \sum_l |\psi_{kl}^0(r_{ij},\theta)|^2, \quad (2.20a)$$

and

$$P_2^{hd}(i,j) = \frac{2\lambda^2}{6\pi^2} \int d\bar{k}\, e^{-\lambda^2 k^2/2\pi} \sum_l \psi_{kl}^{0*}(r_{ij},\theta) \frac{L^2}{\hbar^2} \psi_{kl}^0(r_{ij},\theta). \quad (2.20b)$$

Here $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and ψ_{kl}^0 is the eigenfunction of the relative hard-disk Hamiltonian $\hat{H}_{rel}^0$. L is the total angular momentum operator. It can be shown that

$$h_2^{hd}(i,j) = (1/3\pi) W_2^{hd}(i,j) + O(\lambda), \quad (2.21a)$$

$$P_2^{hd}(i,j) = (1/6\pi) W_2^{hd}(i,j) (r_{ij}/\lambda)^2 + O(\lambda^{-1}). \quad (2.21b)$$

Equations (2.21a, b) are derived in the Appendix. Substituting Eq. (2.21) in Eq. (2.18), we obtain

$$W_N^2(1,2,...,N) = \frac{\lambda^2\beta}{6\pi} e^{-\beta U_p} W_N^{hd}(1,2,...,N) \times \sum_{i<j} \left[\frac{\partial^2 u_p(i,j)}{\partial r_{ij}^2} + \frac{1}{r_{ij}} \frac{\partial u_p(i,j)}{\partial r_{ij}} - \frac{3}{4}\beta \left(\frac{\partial u_p(i,j)}{\partial r_{ij}} \right)^2 \right] + O(\lambda^3). \quad (2.22)$$

In the semiclassical limit, W_N^{hd} can be written as[6]

$$W_N^{hd}(1,2,...,N) = \exp\left[-\beta \sum_{i<j} u_{hd}(i,j) \right] \left[1 + \sum U_{hd}^m(i,j) + \sum U_{hd}^m(i,j,k) + \sum U_{hd}^m(i,j) U_{hd}^m(k,l) + ... \right], \quad (2.23)$$

where $U_{hd}^m(1,2,...,l)$ is the l-particle "modified" Ursell function for a hard-disk system. Explicit expressions for $U_{hd}^m(i,j)$ and $U_{hd}^m(i,j,k)$ have recently been obtained by Sinha and Singh.[6]

Substituting Eq. (2.11) in the expression of the grand partition function [Eq. (2.21a)] and integrating by parts, we obtain

$$\Xi^q = \sum_{N\geq 0} \frac{Z^N}{N!} \int\int \exp\left[-\beta \sum u(i,j) \right] \left[1 + \sum U_2^m(i,j) + \sum U_3^m(i,j,k) + \sum U_2^m(i,j) U_2^m(k,l) + ... \right] \prod_{i=1}^N d\mathbf{r}_i, \quad (2.24)$$

where

$$U_2^m(i,j) = U_{hd}^m(i,j) + [1 + U_{hd}^m(i,j)] U_p^m(i,j), \quad (2.25)$$

$$U_3^m(i,j,k) = U_{hd}^m(i,j,k) + [1 + U_{hd}^m(i,j,k)] U_p^m(i,j,k). \quad (2.26)$$

$U_p^m(i,j)$ and $U_p^m(i,j,k)$ are, respectively, two- and three-particle "modified" Ursell functions due to perturbation potential and are given by

$$U_p^m(i,j) = \frac{\lambda^2\beta}{6\pi} \left[\frac{\partial^2 u_p(i,j)}{\partial r_{ij}^2} + \frac{1}{r_{ij}} \frac{\partial u_p(i,j)}{\partial r_{ij}} - \frac{5}{4}\beta \left(\frac{\partial u_p(i,j)}{\partial r_{ij}} \right)^2 \right] + O(\lambda^3), \quad (2.27)$$

and

$$U_p^m(i,j,k) = - \frac{\lambda^2\beta^2}{24\pi} [\nabla_i u_p(i,j) \cdot \nabla_i u_p(i,k) + \nabla_j u_p(i,j) \cdot \nabla_j u_p(j,k) + \nabla_k u_p(i,k) \cdot \nabla_k u_p(i,k)] + O(\lambda^3). \quad (2.28)$$

Using Eq. (2.24), an expression for free energy can be obtained as

$$\frac{\beta A^q}{N} = \frac{\beta A^c}{N} - \frac{1}{2}\rho \int g^c(1,2) U_2^m(1,2)\, d\mathbf{r}_2 - \frac{1}{6}\rho^2 \int g^c(1,2,3) U_2^m(1,2,3)\, d\mathbf{r}_2\, d\mathbf{r}_3 - \frac{1}{8}\rho^3 \int [g^c(1,2,3,4) - g^c(1,2) g^c(3,4)] \times U_2^m(1,2) U_2^m(3,4)\, d\mathbf{r}_2\, d\mathbf{r}_3\, d\mathbf{r}_4 + \frac{\rho}{8\beta} K^c \left\{ \int \frac{\partial}{\partial \rho} [\rho^2 g^c(1,2)] U_2^m(1,2) d\mathbf{r}_2 \right\}^2 + O(\lambda^3), \quad (2.29)$$

where K^c is the isothermal compressibility for a classical fluid and is given by the relation[19]

$$\rho K^c/\beta = 1 + \rho \int [g^c - 1]\, d\mathbf{r}. \quad (2.30)$$

A^c and $g^c(1,2,...,l)$ are, respectively, the free energy and l-particle distribution function for a classical two-dimensional fluid. ρ is the number density.

The first-order quantum correction to the radial distri-

bution function (RDF) comes from W_N^0 only. W_N^1 and W_N^2 contribute to the order of λ^2. Thus, the expression for the RDF correct to the first-order correction is given as[6]

$$g^q(1,2) = [1 + U_{\rm hd}^m(1,2)]g^c(1,2) + \rho\int [U_{\rm hd}^m(1,2,3) + 2U_{\rm hd}^m(1,3)]g^c(1,2,3)d\mathbf{r}_3 + \frac{1}{2}\rho^2[1 + U_{\rm hd}^m(1,2)]\int U_{\rm hd}^m(3,4)[g^c(1,2,3,4) - g^c(1,2)g^c(3,4)]d\mathbf{r}_3\, d\mathbf{r}_4 - \frac{1}{2\beta}K^c[1 + U_{\rm hd}^m(1,2)]\left\{\frac{\partial}{\partial\rho}[\rho^2 g^c(1,2)] \times \int U_{\rm hd}^m(3,4)\frac{\partial}{\partial\rho}[\rho^2 g^c(3,4)]d\mathbf{r}_4\right\} + O(\lambda^2). \quad (2.31)$$

III. RADIAL DISTRIBUTION FUNCTION

A. Density independent radial distribution function

The density-independent RDF for a two-dimensional system may be written as

$$g_0^q(r) \equiv W_2(r) = 2\lambda^2\sum_x \psi_x^*(\mathbf{r})\exp(-\beta\hat{H}_{\rm rel})\psi_x(\mathbf{r}), \quad (3.1)$$

where the summation extends over all the eigenfunctions ψ_x of the relative Hamiltonian $\hat{H}_{\rm rel}$ of two particles, each of mass m

$$\hat{H}_{\rm rel} = -(\hbar^2/m)\nabla^2 + u(r).$$

For classical fluids, Eq. (3.1) reduces to

$$g_0^c(r) = \exp[-\beta u(r)]. \quad (3.2)$$

If we separate the intermolecular potential $u(r)$ as

$$u(r) = u_{\rm hd}(r) + u_p(r), \quad (3.3)$$

then, as discussed in Sec. II, we can solve Eq. (3.1) and write the solution as

$$g_0^q(r) = g_0^0(r) + g_0^1(r) + g_0^2(r) + \cdots, \quad (3.4)$$

where

$$g_0^0(r) = e^{-\beta u_p(r)}g_c^{\rm hd}(r), \quad (3.5)$$

$$g_0^1(r) = -\left(\frac{\lambda^2\beta}{2\pi}\right)e^{-\beta u_p(r)}\left[\frac{1}{2}\frac{\partial^2 u_p(r)}{\partial r^2} + \frac{1}{2r}\frac{\partial u_p(r)}{\partial r} - \frac{1}{3}\beta\left(\frac{\partial u_p(r)}{\partial r}\right)^2 + \frac{1}{2}\frac{\partial u_p(r)}{\partial r}\frac{\partial}{\partial r}\right]g_0^{\rm hd}(r), \quad (3.6)$$

$$g_0^2(r) = (\lambda^2\beta)e^{-\beta u_p(r)}\left\{\left[\frac{\partial^2 u_p(r)}{\partial r^2} - \frac{3}{4}\beta\left(\frac{\partial u_p}{\partial r}\right)^2\right]h_2^{\rm hd}(r) + \left(\frac{\lambda}{r}\right)^2\left[-\frac{\partial^2 u_p(r)}{\partial r^2} + \frac{1}{r}\frac{\partial u_p(r)}{\partial r} + \frac{3}{4}\beta\left(\frac{\partial u_p(r)}{\partial r}\right)^2\right]P_2^{\rm hd}(r)\right\}, \quad (3.7)$$

and $g_0^{\rm hd}(r)$ is the density-independent part of the RDF for a quantum mechanical hard-disk fluid. In the semiclassical limit, it is given by[6]

$$g_0^{\rm hd}(r) = \begin{cases} 1 + U_{\rm hd}^m(r), & \text{for } r > d \\ 0, & \text{for } r < d, \end{cases} \quad (3.8)$$

where

$$U_{\rm hd}^m(r) = \chi_0(r) + \chi_1(r) + \chi_2(r) + \ldots, \quad \text{for } r > d \quad (3.9)$$

with

$$\chi_0(r) = -\exp(-\xi^2), \quad (3.10a)$$

$$\chi_1(r) = (1/2\sqrt{2})(\lambda/d)\xi^2\,\mathrm{erfc}(\xi), \quad (3.10b)$$

$$\chi_2(r) = (1/8\pi)(\lambda/d)^2\xi^2[\xi^2 e^{-\xi^2} - \sqrt{\pi}\xi(2 + \xi^2)\mathrm{erfc}(\xi)]. \quad (3.10c)$$

Here $\xi = [(2\pi)^{1/2}/(\lambda/d)][(r/d) - 1]$ and $\mathrm{erfc}(\xi)$ is the complimentary error function. Expressions for $h_2^{\rm hd}(r)$ and $P_2^{\rm hd}(r)$ are derived in the Appendix. These are now inserted in Eqs. (3.5)–(3.7) and the resulting expressions are added to give $g_0^q(r)$

$$g_0^q(r^*) = e^{-\beta u_p(r^*)}[1 + \alpha_0(r^*) + \alpha_1(r^*) + O(\lambda/d)^3], \quad r^* > 1, \quad (3.11)$$

where

$$\alpha_0(r^*) = \chi_0(r^*), \quad (3.12a)$$

$$\alpha_1(r^*) = \chi_1(r^*) - \frac{1}{12\pi}\left(\frac{\lambda}{d}\right)^2\left[\beta\frac{\partial^2 u_p(r^*)}{\partial r^{*2}} + \frac{\beta}{r^*}\frac{\partial u_p(r^*)}{\partial r^*} - \frac{1}{2}\beta^2\left(\frac{\partial u_p(r^*)}{\partial r^*}\right)^2\right] - \frac{1}{4\pi}\left(\frac{\lambda}{d}\right)^2\beta\left(\frac{\partial u_p(r^*)}{\partial r^*}\right)\delta(r^* - 1), \quad (3.12b)$$

with

$$\frac{\partial}{\partial r^*}[g_0^{\rm hd}(r^*)] \equiv \delta(r^* - 1) + O(\lambda/d).$$

Here $r^* = r/d$ and δ is the Dirac δ function.

B. First-order density correction to the RDF

The l-particle distribution function can be expanded in powers of density ρ as[19]

$$g(1,2,\ldots,l) = \exp\left[-\beta\sum_{1<i<j<l}u(i,j)\right]\left[\sum_{n=0}^{\infty}a_n(1,2,\ldots,l)\rho^n\right], \quad (3.13)$$

where the coefficient $a_n(1,2,\ldots,l)$ is the cluster integral involving l-base points and n-field points. Equation (3.13) is valid for both classical and quantum systems. Substituting Eq. (3.13) in Eq. (2.31) we get the following expansion coefficients for $g^q(1,2)$:

$$a_0^q(1,2) = [1 + U_{\rm hd}^m(1,2)]a_0^c(1,2) + O(\lambda^2), \quad (3.14)$$

$$a_1^q(1,2) = [1 + U_{\rm hd}^m(1,2)]a_1^c(1,2)$$

$$- 2[1 + U^m_{hd}(1, 2)] \int \exp[-\beta u(1, 3)] U^m_{hd}(1, 3)\, d\mathbf{r}_3$$

$$+ \int \exp\{-\beta [u(1, 3) + u(2, 3)]\} [U^m_{hd}(1, 2, 3)$$

$$+ 2U^m_{hd}(1, 3)]\, d\mathbf{r}_3 + O(\lambda^2) \tag{3.15}$$

and so on, where

$$a^c_0(1, 2) = 1, \tag{3.16a}$$

$$a^c_1(1, 2) = \int f_{13} f_{23}\, d\mathbf{r}_3, \tag{3.16b}$$

and

$$f_{ij} = \exp[-\beta u(i, j)] - 1. \tag{3.17}$$

Equation (3.15) can be rewritten as

$$a^q_1(1, 2) = [1 + U^m_{hd}(1, 2)] a^c_1(1, 2) + \mathscr{L}(1, 2), \tag{3.18}$$

where

$$\mathscr{L}(1, 2)$$

$$= -2[1 + U^m_{hd}(1, 2)] \int \exp[-\beta u_p(1, 3)] U^m_{hd}(1, 3)\, d\mathbf{r}_3$$

$$+ \int \exp[-\beta \{u_p(1, 3) + u_p(2, 3)\}] [U^m_{hd}(1, 2, 3)$$

$$+ 2U^m_{hd}(1, 3)]\, d\mathbf{r}_3. \tag{3.19}$$

Correct to the first-order quantum correction, $\mathscr{L}(1, 2)$ can be evaluated by splitting the range of r_{12} into a number of intervals and considering $\mathscr{L}(1,2)$ in each interval.

(i) At $r_{12} = d$, $U^m_{hd}(1, 2, 3)$ can be written as

$$U^m_{hd}(1, 2, 3) = W^m_{hd}(1, 2, 3) - 1 - U^m_{hd}(1, 2)$$

$$- U^m_{hd}(1, 3) - U^m_{hd}(2, 3), \tag{3.20a}$$

where[6]

$$W^m_{hd}(r, \theta, \phi) = \frac{4\pi}{\theta} \sum_{n=1}^{\infty} \exp\left(-\frac{\pi r^2}{\lambda^2}\right) I_{n\pi/\theta}\left(\frac{\pi r^2}{\lambda^2}\right)$$

$$\times \sin^2\left(\frac{n\pi\phi}{\theta}\right), \tag{3.20b}$$

with

$$r_{13} = d + r \sin\phi,$$

$$r_{23} = d + r \sin(\theta - \phi), \tag{3.20c}$$

$$r_{12} = d(2 + 4\cos\theta)^{1/2}.$$

$W^m_{hd}(r, \theta, \phi)$ is the quantum mechanical spatial distribution function for the three hard disks lying in the plane. In Eq. (3.20b), I is the Bessel function of the imaginary argument.

Equation (3.20b) has been obtained by neglecting the curvature effect and is therefore correct to the order of λ^2.

At $r_{12} = d$, $U^m_{hd}(1,2) = -1$, and $W^m_{hd}(1, 2, 3) \to 0$. Thus

$$U^m_{hd}(1, 2, 3) = -U^m_{hd}(1, 3) - U^m_{hd}(2, 3). \tag{3.21}$$

This leads to

$$\mathscr{L}(1, 2) = 0$$

and

$$a^q_1(1, 2) = 0, \text{ at } r_{12} = d. \tag{3.22}$$

(ii) $d \leqslant r_{12} \leqslant d + \lambda$. In this region, the first-order contribution of $U^m_{hd}(1, 2, 3)$ comes only from the configuration in which either $r_{13} > d + \lambda$ or $r_{23} > d + \lambda$. Using the superposition approximation[17] we find

$$\mathscr{L}(1, 2) = 2[1 + U^m_{hd}(1, 2)] \int \exp[-\beta u_p(1, 3)]$$

$$\times f_p(2, 3) U^m_{hd}(1, 3)\, d\mathbf{r}_3$$

$$+ [1 + U^m_{hd}(1, 2)] \int \exp\{-\beta [u_p(1, 3)$$

$$+ u_p(2, 3)]\}$$

$$\times U^m_{hd}(1, 3) U^m_{hd}(2, 3) d\mathbf{r}_3. \tag{3.23}$$

Since $U^m_{hd}(r)$ correct to first-order correction is given as[6]

$$U^m_{hd}(r) \sim -\exp[-[2\pi/(\lambda/d)^2]\{(r/d) - 1\}^2], \tag{3.24}$$

we find that

$$\mathscr{L}(1, 2) = -[2/(r_{12}/d)](\lambda/d)[1 + U^m_{hd}(1, 2)]$$

$$\times e^{-\beta u_p(d)} \gamma(1, 2) + O(\lambda^2) \tag{3.25}$$

and

$$a^q_1(1, 2) = [1 + U^m_{hd}(1, 2)]$$

$$\times \{a^c_1(1, 2) - [\sqrt{2}/(r_{12}/d)](\lambda/d) e^{-\beta u_p(d)} \gamma(1, 2)\},$$

$$d < r_{12} < d + \lambda, \tag{3.26}$$

where

$$\gamma(1, 2) = \int_{|r_{12} - d|}^{r_{12} + d} f_p(2, 3) \frac{r_{23}}{\sin\alpha'_{23}} dr_{23}. \tag{3.27}$$

Here α'_{23} is the angle between the two vectors r_{12} and r_{13}. Thus

$$\cos(\alpha'_{23}) = (r^2_{12} + d^2 - r^2_{23})/2r_{12}d. \tag{3.28}$$

(iii) $r_{12} > d + \lambda$. For this configuration, $U^m_{hd}(r_{12}) \sim 0$ and the first-order contribution of $U^m_{hd}(1, 2, 3)$ comes from the loose cluster in which r_{12} and r_{13} (or r_{23}) are greater than $d + \lambda$ and r_{23} (or r_{13}) is less than $d + \lambda$. Using the superposition approximation, we obtain

$$\mathscr{L}(1, 2) = -[\sqrt{2}/(r_{12}/d)](\lambda/d) e^{-\beta u_p(d)} \gamma(1, 2) \tag{3.29}$$

and

$$a_1^q(1,2) = a_1^c(1,2) - [\sqrt{2}/(r_{12}/d)](\lambda/d)e^{-\beta u_p(d)}\gamma(1,2). \tag{3.30}$$

Thus the first-order density correction to the RDF, valid to the first-order quantum correction, is given by

$$a_1^q(1,2) = [1 + U_{\rm hd}^m(1,2)] \times \left\{a_1^c(1,2) - \frac{\sqrt{2}}{(r_{12}/d)}\left(\frac{\lambda}{d}\right)e^{-\beta u_p(d)}\gamma(1,2)\right\}. \tag{3.31}$$

Using the relation

$$f_{ij} = f_{\rm hd}(i,j) + [1 + f_{\rm hd}(i,j)]f_p(i,j), \tag{3.32}$$

Eq. (3.16b) can be written as

$$a_1^c(1,2) = [a_1^c(1,2)]_{\rm hd} - 4\pi\int_d^\infty f_p(1,3)r_{13}dr_{13} + A(1,2), \tag{3.33}$$

where

$$A(1,2) = \frac{2}{r_{12}}\int_d^\infty dr_{13}\int_{|r_{12}-r_{13}|}^{r_{12}+r_{13}} dr_{23}\frac{r_{23}}{\sin\alpha_{23}} \times [f_p(1,3)f_p(2,3) + 2f_p(1,3)], \tag{3.34}$$

with

$$\cos\alpha_{23} = (r_{12}^2 + r_{13}^2 - r_{23}^2)/2r_{12}r_{13}, \tag{3.35}$$

and $[a_1^c(1,2)]_{\rm hd}$ is the value of $a_1^c(1,2)$ for the hard-disk system and is given by[20]

$$[a_1^c(1,2)]_{\rm hd} = \begin{cases} \pi d^2\left[1 - \frac{2}{\pi}\sin^{-1}\left(\frac{r_{12}/d}{2}\right) - \left(\frac{r_{12}/d}{2}\right) \times\left(4 - \left|\frac{r_{12}}{d}\right|^2\right)^{1/2}\right], & \text{for } d \leqslant r_{12} \leqslant 2d, \\ 0, & \text{for } r_{12} > 2d. \end{cases} \tag{3.36}$$

Equation (3.31), which gives the first quantum correction to the first-order density-dependent part of the RDF, is a general expression for $a_1^q(1,2)$ of a two-dimensional hard-core fluid. The values of $a_1^c(1,2)$ and $\gamma(1,2)$ depend upon the nature of the perturbation potential. Here we evaluate $a_1^q(1,2)$ for a two-dimensional fluid, whose molecules interact via a square-well (SW) potential

$$u(r) = \begin{cases} \infty, & r < d \\ -\epsilon, & d < r < \eta d \\ 0, & r > \eta d. \end{cases} \tag{3.37}$$

For this potential model,

$$f_p(1,2) = \begin{cases} e^{\beta\epsilon} - 1 \equiv \Delta, & d < r < \eta d \\ 0, & r > \eta d. \end{cases} \tag{3.38}$$

Equations (3.33) and (3.34) are solved to give

$$\begin{aligned} a_1^c(r) = d^2\Bigg\{&\left[\pi - 2\sin^{-1}\left(\frac{r}{2d}\right) - \frac{r}{2d}\left[4 - \left(\frac{r}{d}\right)^2\right]^{1/2}\right] \\ &- \Delta\left[\pi(\eta^2-1) - 2\eta^2\sin^{-1}\left(\frac{r^2 + d^2(\eta^2-1)}{2r\eta d}\right)\right. \\ &\left. - 2\sin^{-1}\left(\frac{r^2 - d^2(\eta^2-1)}{2rd}\right) + 4\sin^{-1}\left(\frac{r}{2d}\right)\right. \\ &\left. + \left[-(\eta^2-1)^2 + 2(\eta^2+1)\left(\frac{r}{d}\right)^2 - \left(\frac{r}{d}\right)^4\right]^{1/2}\right. \\ &\left. - \frac{r}{d}\left[4 - \left(\frac{r}{d}\right)^2\right]^{1/2}\right] \\ &+ \Delta^2\left[2\eta^2\sin^{-1}\left(\frac{r^2 + d^2(\eta^2-1)}{2r\eta d}\right)\right. \\ &\left. - 2\eta^2\sin^{-1}\left(\frac{r}{2\eta d}\right)\right. \\ &\left. + 2\left[\sin^{-1}\left(\frac{r^2 - d^2(\eta^2-1)}{2rd}\right)\right]\right. \\ &\left. - 2\sin^{-1}\left(\frac{r}{2d}\right)\right. \\ &\left. + \left[-(\eta^2-1)^2 + 2(\eta^2+1)\left(\frac{r}{d}\right)^2 - \left(\frac{r}{d}\right)^4\right]^{1/2}\right. \\ &\left. - \frac{r}{d}\left[4 - \left(\frac{r}{d}\right)^2\right]^{1/2}\right]\Bigg\}, \end{aligned} \tag{3.39}$$

for $\eta < 2$.

From Eqs. (3.30) and (3.27) we get

$$a_1^q(r) = [1 + U_{\rm hd}^m(r)]\left[a_1^c(r) - 2\sqrt{2}d^2e^{\beta\epsilon}\Delta \times\left\{\cos^{-1}\left(\frac{r^2 - d^2(\eta^2-1)}{2rd}\right) - \cos^{-1}\left(\frac{r}{2d}\right)\right\}\left(\frac{\lambda}{d}\right)\right] + O((\lambda/d)^2), \tag{3.40}$$

for $\eta < 2$.

IV. VIRIAL COEFFICIENTS OF THE EQUATION OF STATE OF A DILUTE HARD-CORE FLUID

Using the relation[19]

$$P = \frac{\rho^2}{N}\left(\frac{\partial A}{\partial\rho}\right)_\beta, \tag{4.1}$$

and Eqs. (2.29) and (3.13), we obtain an expression for the equation of state in the form

$$\beta P^q = \rho + \sum_{n=2}^\infty B_n^q\rho^n, \tag{4.2}$$

where B_n^q is the nth virial coefficient for a semiclassical fluid. It can be written as

$$B_n^q = B_n^c + B_n^{qc}, \tag{4.3}$$

where B_n^c and B_n^{qc} are, respectively, the classical and quantum correction values of the nth virial coefficient. Thus, the quantum corrections to the second and third virial coefficients can be written as

$$B_2^{qc} = -\frac{1}{2}\int\exp[-\beta u(1,2)]U_2^m(1,2)d\mathbf{r}_2, \tag{4.4}$$

$$\begin{aligned} B_3^{qc} &= 4[B_2^{qc}]^2 - \int\exp[-\beta u(1,2)]a_1^c(1,2)U_2^m(1,2)d\mathbf{r}_2 \\ &\quad - \frac{1}{3}\int\exp\left[-\beta\sum_{i<j}^3 u(i,j)\right]U_3^m(1,2,3)\,d\mathbf{r}_2\,d\mathbf{r}_3. \end{aligned} \tag{4.5}$$

The classical values for the second and third virial coefficients are given by

$$B_2^c = -\frac{1}{2}\int f_{12}\, d\mathbf{r}_2 \,, \tag{4.6}$$

and

$$B_3^c = -\frac{1}{3}\int f_{12} f_{13} f_{23}\, d\mathbf{r}_2\, d\mathbf{r}_3. \tag{4.7}$$

A. Calculation of the second virial coefficient

The second virial coefficient for a two-dimensional fluid in the semiclassical limit is obtained from Eq. (4.3), i.e.,

$$B_2^q = B_2^c + B_2^{qc}. \tag{4.8}$$

Substituting Eq. (3.32) in Eq. (4.6), we find

$$B_2^c = \tfrac{1}{2}\pi d^2 + B_2^{pc}, \tag{4.9a}$$

where

$$B_2^{pc} = -\pi\int_d^\infty f_p(r) r\, dr. \tag{4.9b}$$

Substituting Eq. (2.25) in Eq. (4.4), the quantum correction to the second virial coefficient is given by

$$B_2^{qc} = -\pi\int_d^\infty \exp[-\beta u_p(r)]\, U_{\rm hd}^m(r) r\, dr - \pi\int_d^\infty \exp[-\beta u_p(r)]\, U_p^m(r)[1 + U_{\rm hd}^m(r)] r\, dr. \tag{4.10}$$

Since $U_{\rm hd}^m(r) \sim 0$ for $r > d + \lambda$, the main contribution of the first integral of Eq. (4.10) comes from the region $d < r < d + \lambda$. We make use of the Taylor expansion of $u_p(r)$ about d,

$$u_p(r) = \sum_{k=0}^{\infty} u_p^{(k)}(d)(r-d)^k/k!, \tag{4.11}$$

to evaluate the first integral of Eq. (4.10). The second integral of Eq. (4.10) can be evaluated using Eq. (2.27). Thus, the expression for a two-dimensional fluid in the semiclassical limit is given by

$$B_2^q = B_2^c + \frac{1}{2}\pi d^2\left[\frac{B_2^{\rm I}}{\sqrt{2}}\left(\frac{\lambda}{d}\right) + \frac{B_2^{\rm II}}{3\pi}\left(\frac{\lambda}{d}\right)^2 + \cdots\right], \tag{4.12}$$

where the coefficients $B_2^{\rm I}$ and $B_2^{\rm II}$ are given by

$$B_2^{\rm I} = e^{-\beta u_p(d)}, \tag{4.13}$$

$$B_2^{\rm II} = e^{-\beta u_p(d)}[1 - \tfrac{1}{2}\beta d u_p'(d)] + \frac{1}{4}\int_d^\infty dr\, r e^{-\beta u_p(r)}[\beta u_p'(r)]^2. \tag{4.14}$$

B. Calculation of the third virial coefficient

The third virial coefficient for a semiclassical fluid is given by

$$B_3^q = B_3^c + B_3^{qc}. \tag{4.15}$$

With the help of Eqs. (3.32) and (4.7), B_3^c for a two-dimensional hard-core fluid is given by

$$B_3^c = [B_3^c]_{\rm hd} + 4[B_2^{pc}]^2 - \int \exp[-\beta u_{\rm hd}(1,2)] f_p(1,2)[a_1^c(1,2)]_{\rm hd}\, d\mathbf{r}_2 - \frac{1}{3}\int \exp\Big[-\beta\sum_{i<j}^{3} u_{\rm hd}(i,j)\Big][3 f_p(1,3) f_p(2,3) + f_p(1,2) f_p(1,3) f_p(2,3)]\, d\mathbf{r}_2\, d\mathbf{r}_3, \tag{4.16}$$

where[21]

$$[B_3^c]_{\rm hd} = \tfrac{1}{4}\pi^2 d^4\left[\tfrac{4}{3} - \sqrt{3}/\pi\right]. \tag{4.17}$$

Substituting Eq. (3.33) in Eq. (4.5), we obtain

$$B_3^{qc} = 4[B_2^{qc}]^2 + 8 B_2^{qc} B_2^{pc} + [B_3^{qc}]_A + [B_3^{qc}]_D, \tag{4.18}$$

where

$$[B_3^{qc}]_A = -\int \exp[-\beta u_p(1,2)][a_1^c(1,2)]_{\rm hd}\, U_{\rm hd}^m(1,2) d\mathbf{r}_2 - \int \exp[-\beta u_p(1,2)] A(1,2) U_{\rm hd}^m(1,2) d\mathbf{r}_2 - \frac{1}{3}\int \exp\Big[-\beta\sum_{i<j}^{3} u_p(i,j)\Big] U_{\rm hd}^m(1,2,3)\, d\mathbf{r}_2\, d\mathbf{r}_3, \tag{4.19}$$

and

$$[B_3^{qc}]_D = -\int \exp[-\beta u_p(1,2)]\{[a_1^c(1,2)]_{\rm hd} + A(1,2)\} U_p^m(1,2)\, d\mathbf{r}_2 - \frac{1}{3}\int \times \exp\Big[-\beta\sum_{i<j}^{3} u_p(i,j)\Big] U_p^m(1,2,3)\, d\mathbf{r}_2\, d\mathbf{r}_3. \tag{4.20}$$

In order to evaluate the first integral of Eq. (4.19), we use Eq. (4.11) and the Taylor expansion of $[a_1^c(r)]_{\rm hd}$ about d,

$$[a_1^c(r)]_{\rm hd} = \tfrac{1}{2}\pi d^2\left[\tfrac{4}{3} - \sqrt{3}/\pi\right] - \sqrt{3} d(r-d). \tag{4.21}$$

The second integral of Eq. (4.19) can be evaluated after substituting the value of $A(1,2)$. The first-order correction is obtained from the loose cluster in which r_{13} and r_{23} are greater than $d + \lambda$ and $r_{12} < d + \lambda$, while the second-order correction comes from the configuration in which r_{12} and r_{13} (or r_{23}) lie between d and $d + \lambda$ and r_{23} (or r_{13}) is greater than $d + \lambda$. The leading contribution of third integral of Eq. (4.19), which is of the order of λ^2, comes from the cluster of three hard disks in a plane, in which two distances lie between d and $d + \lambda$ and the third distance is greater than $d + \lambda$. This can be chosen in three different ways. The integral can be evaluated following the method discussed elsewhere.[6]

After some algebra, we obtain,

$$[B_3^{qc}]_A = \frac{1}{4}\pi^2 d^4\left(\frac{4}{3} - \frac{\sqrt{3}}{\pi}\right)\left\{\sqrt{2}\left(\frac{\lambda}{d}\right) e^{-\beta u_p(d)}\left[1 + \frac{2}{\pi(\frac{4}{3} - \sqrt{3}/\pi)}\frac{A(d)}{d^2}\right]\right.$$

$$+\left(\frac{\lambda}{d}\right)^2\left[e^{-\beta u_p(d)}\left(\frac{2}{\pi}\left[\frac{1}{3}-\frac{\sqrt{3}}{\pi(\frac{4}{3}-\sqrt{3}/\pi)}\right]-\frac{1}{\pi}\beta d u_p'(d)\right)\right.$$

$$\left.+\frac{1}{(\frac{4}{3}-\sqrt{3}/\pi)}\left(e^{-\beta u_p(d)}C+e^{-2\beta u_p(d)}D\right)\right]+\cdots\Bigg\}, \tag{4.22}$$

where

$$C=\frac{2}{\pi^2}\left[(\sqrt{3})f_p(d)-\frac{1}{d}e^{-\beta u_p(d)}\int_d^{2d}f_p(1,2)\frac{[1-2(r_{12}/2d)^2]}{[1-(r_{12}/2d)^2]^{1/2}}\,dr_{12}\right], \tag{4.23}$$

and

$$D=\frac{8}{\pi}\left\{-0.05187+\frac{1}{d}\int_d^{2d}f_p(1,2)\left[\frac{1}{12}\left(\frac{\pi}{\theta}-\frac{\theta}{\pi}\right)\sin\theta-\frac{1}{2\pi}\cos\theta\right]\frac{dr_{12}}{(1-(r_{12}/2d)^2)^{1/2}}\right\}, \tag{4.24}$$

with

$$\cos\theta=\tfrac{1}{2}[\tfrac{1}{2}(r_{12}/d)^2-1]. \tag{4.25}$$

Substituting Eqs. (2.27) and (2.28) in Eq. (4.20), we get

$$[B_3^{qc}]_D=\frac{1}{4}\pi^2d^4[(\lambda/d)^2(E+F)+\cdots], \tag{4.26}$$

where

$$E=-\frac{8}{\pi d^2}\int_d^{\infty}e^{-\beta u_p(1,2)}\{[a_1^c(1,2)]_{\rm hd}+A(1,2)\}U_p^m(1,2)r_{12}\,dr_{12}\ , \tag{4.27}$$

and

$$F=\frac{2\beta^2}{3\pi^2d^2}\int_d^{\infty}dr_{12}\,e^{-\beta u_p(1,2)}\int_d^{\infty}dr_{13}e^{-\beta u_p(1,3)}\left(\frac{\partial u_p(1,3)}{\partial r_{13}}\right)\int_{|(r_{12}-r_{13})|}^{(r_{12}+r_{13})}dr_{23}\,\frac{r_{23}}{\tan\alpha_{23}}\,e^{-\beta u_p(2,3)}\left(\frac{\partial u_p(2,3)}{\partial r_{23}}\right). \tag{4.28}$$

Finally,

$$B_3^q=B_3^c+\tfrac{1}{4}\pi^2d^4(\tfrac{4}{3}-\sqrt{3}/\pi)[\sqrt{2}B_3^{\rm I}(\lambda/d)+2.15203\,B_3^{\rm II}(\lambda/d)^2+\cdots], \tag{4.29}$$

where

$$B_3^{\rm I}=e^{-\beta u_p(d)}\left\{1+\frac{2}{\pi(\frac{4}{3}-\sqrt{3}/\pi)}\frac{1}{d^2}\left[4B_2^{pc}+A(d)\right]\right\}, \tag{4.30}$$

$$B_3^{\rm II}=\frac{1}{2.15203}\left\{e^{-\beta u_p(d)}\left[\frac{2}{\pi}\left(\frac{1}{3}-\frac{2\sqrt{3}}{\pi(\frac{4}{3}-\sqrt{3}/\pi)}\right)-\frac{1}{\pi}\beta d u_p'(d)\right]\right.$$

$$+e^{-2\beta u_p(d)}\left[2+\frac{2\sqrt{3}}{\pi^2}-\frac{0.41496}{\pi}\right]\Big/\left[\frac{4}{3}-\frac{\sqrt{3}}{\pi}\right]$$

$$\left.+\frac{16}{3\pi^2(\frac{4}{3}-\sqrt{3}/\pi)d^2}B_2^{pc}B_2^{\rm II}+\frac{1}{(\frac{4}{3}-\sqrt{3}/\pi)}\mathscr{L}\right\}, \tag{4.31}$$

with

$$\mathscr{L}=\frac{8}{\pi d}e^{-2\beta u_p(d)}\int_d^{2d}f_p(1,2)\left[\frac{1}{12}\left(\frac{\pi}{\theta}-\frac{\theta}{\pi}\right)\sin\theta-\frac{1}{2\pi}\cos\theta\right]\frac{dr_{12}}{[1-(r_{12}/2d)^2]^{1/2}}$$

$$-\frac{2}{\pi^2d}e^{-\beta u_p(d)}\int_d^{2d}f_p(1,2)\frac{(1-2(r_{12}/2d)^2)}{[1-(r_{12}/2d)^2]^{1/2}}\,dr_{12}+E+F. \tag{4.32}$$

E and F are defined by Eqs. (4.27) and (4.28), respectively.

The classical third virial coefficient is obtained from Eq. (4.16),

$$B_3^c = \frac{1}{4}\pi^2 d^4\left[\left(\frac{4}{3} - \frac{\sqrt{3}}{\pi}\right) + 4\left(\frac{2B_2^{pc}}{\pi d^2}\right)^2 + \frac{4}{\pi^2 d^4}(G+H)\right], \tag{4.33}$$

where

$$G = -2\pi\int_d^\infty f_p(r)[a_1^c(r)]_{\rm hd} r\,dr, \tag{4.34}$$

$$H = -\int\int \exp\left[-\beta\sum_{i<j}^{3} u_{\rm hd}(i,j)\right][3f_p(1,3)f_p(2,3) + f_p(1,2)f_p(1,3)f_p(2,3)]\,d\mathbf{r}_2\,d\mathbf{r}_3. \tag{4.35}$$

From the study of the virial coefficients, we find that except for $B_2^{\rm I}$, which depends only on the potential at the core, the quantum corrections to the virial coefficients depend on the potential at the core as well as the shape of the potential well, provided only that it is bounded and continuous for $r > d$. The quantum coefficients B_2^I and B_3^I reduce to unity (i.e., the values of hard disks), when $u_p(r) \to 0$.

We now discuss the virial coefficients for some specific potential models.

V. VIRIAL COEFFICIENTS FOR SOME SPECIFIC POTENTIAL MODELS

A. Sutherland model

In the case of the Sutherland model, the perturbation potential is

$$u_p(r) = -\epsilon(d/r)^6, \quad r > d. \tag{5.1}$$

Then $B_2^{\rm I}$ and $B_2^{\rm II}$ are given by

$$B_2^{\rm I} = e^{\beta\epsilon}, \tag{5.2}$$

$$B_2^{\rm II} = e^{\beta\epsilon}[1 - 3\beta\epsilon] + \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{3}{2n+4}\right)(\beta\epsilon)^{n+2} \tag{5.3}$$

and the classical second virial coefficient is

$$B_2^c = -\frac{1}{2}\pi d^2\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{2}{6n-2}\right)(\beta\epsilon)^n. \tag{5.4}$$

The coefficients for the third virial coefficient are found to be

$$B_3^{\rm I} = e^{\beta\epsilon}\left[1 - \frac{2}{(\frac{4}{3} - \sqrt{3}/\pi)}\left\{\sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{4}{6n-2}\right)(\beta\epsilon)^n - \frac{1}{\pi d^2}A(d)\right\}\right], \tag{5.5}$$

$$B_3^{\rm II} = -e^{\beta\epsilon}[0.3185 + 0.8875(\beta\epsilon)] + 0.5044\,B_2^{\rm II}\left[\sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{2}{6n-2}\right)(\beta\epsilon)^n\right] + 0.5942\,\mathscr{L}. \tag{5.6}$$

The classical third virial coefficient for Sutherland model is obtained from Eq. (4.33).

B. Yukawa-tail model

For the Yukawa-tail model,

$$u_p(r) = -\epsilon\frac{\exp[-Z(r/d-1)]}{(r/d)}, \quad r > d, \tag{5.7}$$

where ϵ and Z are constants. Using Eq. (5.7), we obtain

$$B_2^{\rm I} = e^{\beta\epsilon}, \tag{5.8}$$

$$B_2^{\rm II} = e^{\beta\epsilon}\left[1 - \frac{1}{2}(1+Z)(\beta\epsilon)\right] + \frac{1}{4}\sum_{n=0}^{\infty}\frac{1}{n!}(\beta\epsilon)^{n+2}\left[Z + \frac{(n+2)}{(n+1)}Z^2 \times\left\{1 + (-1)^n\frac{(n+2)^n Z^n}{n!}e^{(n+2)Z} \times E_i(-(n+2)Z) + \sum_{k=0}^{n-1}\frac{(-1)^k(n+2)^k Z^{k+1}}{n(n-1)(n-2)\cdots(n-k)}\right\}\right]. \tag{5.9}$$

The classical second virial coefficient for a two-dimensional fluid with the Yukawa-tail potential is given by

$$B_2^c = \frac{1}{2}\pi d^2\left\{1 + 2(Z\beta\epsilon)(e^Z - 1) - 2\sum_{n=0}^{\infty}\frac{1}{n!}(nZ\beta\epsilon)^n e^{nZ} \times\left[(-1)^n\frac{E_1(nZ)}{(n-2)!} + \frac{e^{-nZ}}{(nZ)^{n-2}}\sum_{k=0}^{n-3}\frac{(-1)^k(nZ)^k}{(n-2)(n-3)\cdots(n-2-k)}\right]\right\}, \tag{5.10}$$

where

$$E_1(X) = -E_i(-X) = \int_X^\infty e^{-t}t^{-1}dt \tag{5.11}$$

is the exponential integral.

For this potential model, the coefficients for the third virial coefficient are

$$B_3^{\rm I} = e^{\beta\epsilon}\left\{1 + \frac{2}{(\frac{4}{3} - \sqrt{3}/\pi)}\left[4\left((Z\beta\epsilon)(e^Z - 1) - \sum_{n=2}^{\infty}\frac{1}{n!}(nZ\beta\epsilon)^n \times e^{nZ}\left[(-1)^{n-1}\frac{E_i(-nZ)}{(n-2)!} + \frac{e^{-nZ}}{(nZ)^{n-2}}\sum_{k=0}^{n-3}\frac{(-1)^k(nZ)^k}{(n-2)(n-3)\cdots(n-2-k)}\right]\right) + \frac{1}{\pi d^2}A(d)\right]\right\}, \tag{5.12}$$

$$B_3^{II} = -e^{\beta\epsilon}[0.3185 + 0.1479(\beta\epsilon)(1+Z)] + 1.3185e^{2\beta\epsilon} + 0.5044B_2^{II}(2B_2^{pc}/\pi d^2) + 0.5942\,\mathscr{L}. \tag{5.13}$$

The classical third virial coefficient is obtained from Eq. (4.33) using the relation

$$B_2^{pc} = B_2^c - \tfrac{1}{2}\pi d^2. \tag{5.14}$$

C. Wood–Saxan potential

In the case of the Wood–Saxan model,

$$u_p(r) = \frac{V_0}{1+\exp[Z(r/d-1)]}, \quad r > d, \tag{5.15}$$

where V_0 and Z are constants, we obtain expressions for B_2^I and B_2^{II} as

$$B_2^I = e^{-\beta V_0/2}, \tag{5.16}$$

$$B_2^{II} = e^{-\beta V_0/2}\left[1+\frac{1}{8}(Z\beta V_0)\right] + \frac{1}{4}\sum_{n=0}^{\infty}\frac{1}{n!}(-\beta V_0)^{n+2}\left[\frac{1}{Z}\frac{(n+4)}{2^{n+3}(n+2)(n+3)} + \frac{1}{Z^2}\sum_{k=1}^{\infty}\frac{1}{n+k+2}\left\{\frac{2}{(n+2)(n+k+1)} - \frac{1}{(n+3)(n+k+2)}\right\}\right]. \tag{5.17}$$

The classical second virial coefficient for a two-dimensional fluid with the Wood–Saxan potential is given by

$$B_2^c = \frac{1}{2}\pi d^2\left\{1 - 2\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}(\beta V_0)^n\sum_{k=1}^{\infty}\frac{1}{2^{n+k-1}(n+k-1)} \times\left[\frac{1}{Z}+\frac{1}{Z^2}\sum_{l=1}^{\infty}\frac{1}{2^{l-1}(n+k+l-2)}\right]\right\}. \tag{5.18}$$

For this model, the coefficients for the third virial coefficient are given by

$$B_3^I = e^{-\beta V_0/2}\left\{1 - \frac{2}{(\frac{4}{3}-\sqrt{3}/\pi)}\left[4\sum_{n=1}^{\infty}\frac{1}{n!}(-\beta V_0)^n \times\sum_{k=1}^{\infty}\frac{1}{2^{n+k-1}(n+k-1)}\left(\frac{1}{Z}+\frac{1}{Z^2} \times\sum_{l=1}^{\infty}\frac{1}{2^{l-1}(n+k+l-2)}\right) - \frac{1}{\pi d^2}A(d)\right]\right\}, \tag{5.19}$$

$$B_3^{II} = -e^{-\beta V_0/2}[0.3185 - 0.03700(\beta V_0)] + 1.3185\,e^{-\beta V_0} + 0.5044B_2^{II}(2B_2^{pc}/\pi d^2) + 0.5942\,\mathscr{L}. \tag{5.20}$$

The classical third virial coefficient is obtained from Eq. (4.33) using the value of B_2^{pc} given by Eq. (5.14).

D. Square-well model

In the case of the square-well (SW) model, the perturbation potential, given by

$$u_p(r) = \begin{cases} -\epsilon, & d < r < \eta d \\ 0, & r > \eta d \end{cases}, \tag{5.21}$$

has a singularity at $r = \eta d$. Since this method involves the derivatives of u_p, we express the perturbation potential in an analytic form[15]

$$u_p(r) = \frac{-\epsilon}{\exp[(r/d-\eta)/\alpha]-1}, \quad r > d, \tag{5.22}$$

where $\alpha \to 0$. Further the SW model has a potential cutoff $r = \eta d$. So in place of Eqs. (4.13)–(4.14) and (4.30)–(4.31), we use Eqs. (4.10) and (4.18) to obtain the coefficients of virial coefficients for the SW fluid. The integrals involving the perturbation potential u_p can be evaluated using the upper limit $\tau = \eta d$, while the integrals involving the derivatives of u_p can be evaluated following the method of Sinha and Singh.[15] Thus, for a two-dimensional SW fluid, the coefficients for the second virial coefficient are given by

$$B_2^I = 1 + \Delta\,\mathrm{erf}\,\delta \tag{5.23}$$

$$B_2^{II} = 1 + \Delta\,[1 - \tfrac{3}{4}e^{-\delta^2}] + [(\ln 2 - \tfrac{1}{4})/12]e^{\beta\epsilon}(\beta\epsilon)^2, \tag{5.24}$$

where

$$\Delta = e^{\beta\epsilon} - 1,$$

$$\delta = \sqrt{2\pi}\,(\eta-1)/(\lambda/d).$$

The classical second virial coefficient is

$$B_2^c = \tfrac{1}{2}\pi d^2[1 - \Delta(\eta^2-1)]. \tag{5.25}$$

The values of B_3^I and B_3^{II} for $\eta < 2$ are given below:

$$B_3^I = 1 - \frac{4}{(\frac{4}{3}-\sqrt{3}/\pi)}(\eta^2-1) + \Delta\left\{\left[1-\frac{4}{M}(\eta^2-1)\right]\mathrm{erf}\delta + \frac{2}{M}\left[\frac{\pi}{3}(3\eta^2-5) + 2\eta^2\sin^{-1}\left(\frac{\eta}{2}\right) + 2\sin^{-1}\left(\frac{2-\eta^2}{2}\right) + \eta(4-\eta^2)^{1/2} - \sqrt{3}\right]\right\} + \frac{2}{\pi M}\Delta^2\left[\pi(\eta^2-2) + 4\eta^2\sin^{-1}\left(\frac{\eta}{2}\right) - 2\eta^2\sin^{-1}\left(\frac{1}{2\eta}\right)\right.$$

$$+4\sin^{-1}\left(\frac{2-\eta^2}{2}\right)+2\eta(4-\eta^2)^{1/2}-2\sqrt{3}\Big]$$

$$+\frac{2}{\pi M}\Delta^3\Big[-\frac{\pi}{3}+2\eta^2\sin^{-1}\left(\frac{\eta}{2}\right)-2\eta^2\sin^{-1}\left(\frac{1}{2\eta}\right)+2\sin^{-1}\left(\frac{2-\eta^2}{2}\right)+\eta(4-\eta^2)^{1/2}-\sqrt{3}\Big], \tag{5.26}$$

$$B_3^{II}=1+\frac{\Delta}{2.15205}\left\{\frac{1}{M}\Big[\operatorname{erf}\delta+\frac{8}{3\pi}(\eta^2-1)+\frac{3\sqrt{3}}{\pi^2}-\frac{\eta}{\pi^2}\sqrt{4-\eta^2}\Big]+\frac{2}{\pi}\left(\frac{1}{3}-\frac{3}{\pi M}\right)(1-e^{-\delta^2})+\frac{1}{3\pi}e^{-\delta^2}\right\}$$

$$+\frac{\Delta^2}{2.15205}\frac{2}{M}\Big\{(\operatorname{erf}\delta)^2+\frac{4}{3\pi}(\eta^2-1)\left(1-\frac{3}{4}e^{-\delta^2}\right)-\frac{1}{\pi^2}\eta(4-\eta^2)^{1/2}+\frac{2\sqrt{3}}{\pi^2}-\frac{0.41496}{\pi}+\frac{8}{\pi}P\Big\}$$

$$+\frac{\Delta^3}{2.15205}\frac{1}{M}\left\{\frac{\sqrt{3}}{\pi^2}-\frac{1}{\pi^2}\eta(4-\eta^2)^{1/2}+\frac{8}{\pi}P\right\}$$

$$+\frac{(\ln 2-\frac{1}{4})}{2.15205}\frac{1}{9\pi M}e^{\beta\epsilon}(\beta\epsilon)^2\Big\{\Big[1-\frac{2}{\pi}\sin^{-1}\left(\frac{\eta}{2}\right)-\frac{3}{2\pi}\eta(4-\eta^2)^{1/2}\Big]$$

$$+\Delta\Big[7(\eta^2-1)+\frac{3}{\pi}[(4\eta^2-1)]^{1/2}-\frac{3}{\pi}\eta(4-\eta^2)^{1/2}+\frac{2}{\pi}\eta^2\sin^{-1}\left(\frac{2\eta^2-1}{2\eta^2}\right)$$

$$+\frac{2}{\pi}\sin^{-1}\left(\frac{1}{2\eta}\right)-\frac{4}{\pi}\sin^{-1}\left(\frac{\eta}{2}\right)\Big]+\Delta^2\Big[-\eta^2\left(\frac{1}{3}+\frac{2}{\pi\sqrt{3}}\right)+\frac{3}{\pi}(4\eta^2-1)^{1/2}$$

$$-\frac{3}{\pi}\eta(4-\eta^2)^{1/2}+\frac{2}{\pi}\frac{\eta}{(4-\eta^2)^{1/2}}+\frac{2}{\pi}\eta^2\sin^{-1}\left(\frac{2\eta^2-1}{2\eta^2}\right)+\frac{2}{\pi}\sin^{-1}(1/2\eta)-\frac{2}{\pi}\sin^{-1}(\eta/2)\Big]\Big\}, \tag{5.27}$$

where $M=(\frac{4}{3}-\sqrt{3}/\pi)$ and

$$P=\frac{1}{d}\int_d^{\eta d}\left[\frac{1}{12}\left(\frac{\pi}{\theta}-\frac{\theta}{\pi}\right)\sin\theta-\frac{1}{2\pi}\cos\theta\right]\frac{dr_{12}}{[1-(r_{12}/2d)^2]^{1/2}}. \tag{5.28}$$

The classical third virial coefficient can be obtained from Eq. (4.16). For $\eta<2$,

$$B_3^c=\tfrac{1}{4}\pi^2d^4\{M+\Delta[B_3^c]_1+\Delta^2[B_3^c]_2+\Delta^3[B_3^c]_3\}, \tag{5.29}$$

where

$$[B_3^c]_1=[3(\tfrac{4}{3}-\sqrt{3}/\pi)-4\eta^2+2(\eta^2-1)\sin^{-1}(\eta/2)+(1/\pi)\eta(\eta^2+2)], \tag{5.30}$$

$$[B_3^c]_2=2\Big[(\eta^2-1)^2-\frac{1}{\pi}\Big\{2\eta^4\sin^{-1}\left(\frac{2\eta^2-1}{2\eta^2}\right)+2\eta^2\Big[2\sin^{-1}\left(\frac{2\eta^2+1}{2\eta(2+2\eta^2)^{1/2}}\right)-2\sin^{-1}\left(\frac{3\eta}{2(2+2\eta^2)^{1/2}}\right)$$

$$+\sin^{-1}(1/2\eta^2)-3\sin^{-1}(\eta/2)]-\eta^3(4-\eta^2)^{1/2}+\frac{1}{2}(2\eta^2-1)(4\eta^2-1)^{1/2}+(2\eta^2+1)-\left(\frac{4\pi}{3}-\frac{5\sqrt{3}}{4}\right)$$

$$-2\Big[\sin^{-1}\left(\frac{2-\eta^2}{2\eta}\right)-2\sin^{-1}\left(\frac{\eta}{2}\right)\Big]\Big\}\Big], \tag{5.31}$$

and

$$[B_3^c]_3=\frac{4}{3}\Big[1-\frac{1}{\pi}\Big\{2\eta^4\Big[\left(\frac{\pi}{6}-\frac{\sqrt{3}}{2}\right)+\sin^{-1}\left(\frac{2\eta^2+1}{2\eta^2}\right)-2\sin^{-1}\left(\frac{1}{2\eta}\right)\Big]+2\eta^2\Big[2\sin^{-1}\left(\frac{2\eta^2+1}{2\eta(2+2\eta^2)^{1/2}}\right)$$

$$- 2\sin^{-1}\left(\frac{3\eta}{2(2+2\eta^2)^{1/2}}\right) - 2\sin^{-1}(\eta/2) + \sin^{-1}(1/2\eta)$$

$$+ \sin^{-1}\left(\frac{1}{2\eta^2}\right)\Big] - 2\sin^{-1}\left(\frac{1-\eta^2}{2\eta}\right) - \eta(\eta^2-1)\sqrt{4-\eta^2}$$

$$+ \frac{1}{2}(4\eta^2-1)^{3/2} + 2\eta^2 + 1 + 2\sqrt{3}\Big\}\Big]. \tag{5.32}$$

E. Application to the Lennard-Jones model

The method discussed in Secs. II and III can also be applied to a fluid, whose molecules interact via the Lennard-Jones (12-6) potential

$$u(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6], \tag{5.33}$$

where ϵ and σ are constants with units of energy and length, respectively. We divide the pair potential according to the Weeks, Chandler, and Andersen (WCA) scheme[22]

$$u(r) = u_r(r) + u_p(r), \tag{5.34}$$

where

$$u_r(r) = \begin{cases} u(r) + \epsilon, & r < 2^{1/6}\sigma \\ 0, & r > 2^{1/6}\sigma \end{cases}, \tag{5.35a}$$

and

$$u_p(r) = \begin{cases} -\epsilon, & r < 2^{1/6}\sigma \\ u(r), & r > 2^{1/6}\sigma. \end{cases} \tag{5.35b}$$

We reduce the fluid with the realistic repulsive forces into the hard-disk fluid with a suitable diameter 'd.' The value of d can be found from some variational method.[13] Then we get

$$B_2^{\mathrm{I}} = e^{\beta\epsilon}, \tag{5.36}$$

$$B_2^{\mathrm{II}} = e^{\beta\epsilon} + 3\sum_{n=0}^{\infty}\frac{1}{n!}(2\beta\epsilon)^{n+2}\sum_{k=0}^{n}\binom{n}{k} \times\frac{(-1)^k}{2^{k+1}}\left[\frac{1}{n+k+2} - \frac{2}{n+k+3} + \frac{1}{n+k+4}\right]. \tag{5.37}$$

The classical second virial coefficient is obtained from Eq. (4.9)

$$B_2^{c} = \frac{1}{2}\pi\sigma^2\left\{e^{\beta\epsilon}\left[\left(\frac{d}{\sigma}\right)^2 - 2^{1/3}\right] - 2^{1/3}\sum_{n=1}^{\infty}\frac{1}{n!}(\beta\epsilon)^n \times\sum_{k=0}^{n}\binom{n}{k}\frac{(-1)^k 2^{n-k}}{(3(n+k)-1)}\right\}. \tag{5.38}$$

The coefficients for the third virial coefficient in this case are given by

$$B_3^{\mathrm{I}} = e^{\beta\epsilon}\Big\{1 - \frac{2}{M}\Big(2\Big[1 - e^{\beta\epsilon}\Big(1 - \frac{2^{1/3}}{(d/\sigma)^2}\Big) + 2^{1/3}\sum_{n=1}^{\infty}\frac{1}{n!}\beta\epsilon)^n\sum_{k=0}^{n}\binom{n}{k}\frac{(-1)^k 2^{n-k}}{(3(n+k)-1)}\Big] - \frac{1}{\pi d^2}A(d)\Big)\Big\}, \tag{5.39}$$

$$B_3^{\mathrm{II}} = -0.3185e^{\beta\epsilon} + 1.3185e^{2\beta\epsilon} + 0.5044B_2^{\mathrm{II}}(2B_2^{pc}/\pi d^2) + 0.5942\mathscr{L}. \tag{5.40}$$

Here $\mathscr{L}$ is defined by Eq. (4.32) and B_2^{pc} is obtained using relation (5.14).

The classical third virial coefficient is obtained from Eq. (4.33) using the value of B_2^{pc} obtained from Eqs. (5.14) and (5.38).

VI. SUMMARY

The purpose of this paper has been to develop a theory for calculating the equilibrium properties of a two-dimensional semiclassical fluid, whose molecules interact via a hard-core plus an attractive tail potential. We have given explicit expressions for the density-independent part of the RDF $g_0^q(r)$ and the first-order density correction to it. The first-order quantum correction to the first-order density-dependent part of the RDF is calculated.

The quantum corrections to the second and third virial coefficients for some specific potential models (Sutherland, Yukawa-tail, Wood–Saxan, square-well, and the Lennard-Jones) have been evaluated. From the study, we find that the first-order quantum correction to the second virial coefficient depends only upon the potential at the core; the higher quantum corrections to the second virial coefficient and the quantum corrections to the third virial coefficient depend both on the potential at the core and the shape of the attractive well.

APPENDIX

In this Appendix we derive expansions of $h_2^{\mathrm{hd}}(r)$ and $P_2^{\mathrm{hd}}(r)$. With the help of Eqs. (2.19) and (2.20a), it can be shown that

$$h_2^{\mathrm{hd}}(r) = \begin{cases} -\dfrac{\lambda^3}{6\pi}\dfrac{\partial}{\partial\lambda}[\lambda^{-2}W_2^{\mathrm{hd}}(r)] \\ -\dfrac{\lambda^3}{6\pi}\dfrac{\partial}{\partial\lambda}[\lambda^{-2}g_0^{\mathrm{hd}}(r)]. \end{cases} \tag{A1}$$

Substituting Eq. (3.8), we immediately get

$$h_2^{hd}(r) = (1/3\pi)[1 - (1 - \xi^2)e^{-\xi^2}] + O(\lambda^2), \quad r > d. \tag{A2}$$

In order to derive $P_2^{hd}(r)$, we use Schrödinger's equation for a two-dimensional system in the form

$$\left[-\left\{\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right\} + \frac{L^2}{\hbar^2 r^2}\right]\psi_{kl} = k^2\psi_{kl}. \tag{A3}$$

This helps us develop the formula

$$6\pi^2[\lambda^2 P_2^{hd}(r) - r^2 h_2^{hd}(r)] = 2\lambda^4 r^2 \left\langle \mathbf{r}\left|\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right]e^{-\beta\hat{H}^0_{rel}}\right|\mathbf{r}\right\rangle, \tag{A4}$$

where $\hat{H}^0_{rel}$ is the Hamiltonian for the relative motion of two hard disks.

However, in evaluating the matrix element in (A4), we neglect the curvature effect and replace the hard disks by a hard wall.[23] Thus, we take the wave function to be

$$\psi = \begin{cases} 0, & r < d \\ \dfrac{1}{\sqrt{\pi}} \sin k_r(r - d), & r > d. \end{cases} \tag{A5}$$

Then, we obtain

$$\left\langle \mathbf{r}\left|\left[\frac{\partial^2}{\partial r^2} + \frac{\partial}{r\partial r}\right]e^{-\beta\hat{H}^0_{rel}}\right|\mathbf{r}\right\rangle = -\frac{\pi}{2\lambda^4}\theta(r - d) + O(\lambda^{-2}), \tag{A6}$$

where θ is the unit step function.

Substituting this in (A4) and using (A2), we obtain the expression for $P_2^{hd}(r)$

$$P_2^{hd}(r) = \frac{1}{6\pi}\left(\frac{r}{\lambda}\right)^2 - \frac{1}{3\pi}(1 - \xi^2)e^{-\xi^2}\left(\frac{r}{\lambda}\right)^2 + O(1). \tag{A7}$$

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Exact theory for the self-similarity and decay of homogeneous turbulence[a)]

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(Received 5 May 1982; accepted for publication 6 August 1982)

It is shown that space-time dilatation invariance ($\mathbf{x}\to\xi^{-1}\mathbf{x}$, $t\to\xi^{-2}t$, with concomitant transformations for dependent variables) and linearity of the Φ-equation engender an exact, time-explicit generic form for the solution applicable to freely-decaying homogeneous incompressible fluid turbulence. This solution features a summation over *mutually independent dynamical modes* labeled by the dilatation scaling-index $n(>1)$. Without the assumption of isotropy nor introduction of a closure approximation procedure, the theory provides an explanation for the experimentally observed self-similarity of the correlation tensors and the decay laws $\langle|\mathbf{u}(\mathbf{x},t)|^2\rangle\propto t^{-n}$ for the different types and decay stages of homogeneous turbulence.

PACS numbers: 47.25.Cg, 47.10. + g

Although a theory for homogeneous incompressible fluid turbulence should be based exclusively on the Navier–Stokes equation, classical statistical mechanics, and exact mathematical analysis, contemporary theoretical approaches[1–10] require *ad hoc* physicomathematical approximations to simplify and facilitate solution of the correlation tensor dynamical equations. The primary simplifying assumption of statistical spatial isotropy is usually made, notwithstanding the large-scale anisotropy evident even in the most controlled types of wind and water tunnel turbulence. Moreover, to obtain a solvable system of correlation tensor equations from the infinite hierarchy produced by Navier–Stokes nonlinearity, the assumption of isotropy must be supplemented by a closure approximation procedure.[1–10] Wyld[11] has shown that what is left out is not generally small compared to what is included by the various closure approximation procedures. Finally, it is difficult to assess the practical regime of applicability and the theoretical accuracy of the isotropic-closure approximation theories.

The functional differential Φ equation originally derived by Hopf[12] provides the proper starting point for a more rigorous theory, without the assumption of isotropy nor the introduction of a closure approximation procedure. I show in the following, that space-time dilatation invariance $\mathbf{x}\to\xi^{-1}\mathbf{x}, t\to\xi^{-2}t$, with concomitant transformations for dependent variables) and linearity of the Φ equation engender an exact, time-explicit generic form for the solution applicable to freely-decaying homogeneous turbulence. From this solution displayed below in (14), it follows that the quadratic velocity correlation tensor has the generic form shown in (16). In both (14) and (16) there appears a symbolic summation over discrete and/or continuous values of the dilatation scaling-index $n\ (>1)$; the latter constant parameter originates in the initial form of Φ at $t=0$ shown in (12), labels mutually independent dynamical modes, and serves as the decay exponent in (14) and (16). The decay law $u^2\propto t^{-n}$ and concomitant self-similarity of the velocity correlation tensors obtain for all $t>0$ if only a single dynamical mode is present, while $u^2\propto t^{-n}$ holds approximately if one dynamical mode is dominant in the summation during a stage of the decay.

[a)] This work was supported by the National Aeronautics and Space Administration grant NAG1-110.

Let $\mathbf{u}=(u_1(\mathbf{x},t), u_2(\mathbf{x},t), u_3(\mathbf{x},t))$ denote the velocity field of an incompressible fluid governed by the Navier–Stokes equation

$$\partial\mathbf{u}/\partial t = -\mathbf{u}\cdot\nabla\mathbf{u} + \nu\nabla^2\mathbf{u} - \rho^{-1}\nabla p, \tag{1}$$

in which ν,ρ are positive constants. For boundary-free flow with $\mathbf{x}=(x_1,x_2,x_3)$ in R_3, the incompressibility condition $\nabla\cdot\mathbf{u}=0$ can be used to eliminate the pressure term from (1); the resulting integro-differential equation

$$\partial\mathbf{u}/\partial t = -(\mathbf{u}\cdot\nabla\mathbf{u})^{\mathrm{tr}} + \nu\nabla^2\mathbf{u}, \tag{2}$$

features the transverse (solenoidal) part of the inertial term, where for any vector field in R_3,

$$\begin{aligned}\mathbf{v}^{\mathrm{tr}}(\mathbf{x}) &\equiv \mathbf{v}(\mathbf{x}) - \nabla(\nabla^{-2}\nabla\cdot\mathbf{v}(\mathbf{x}))\\ &\equiv \mathbf{v}(\mathbf{x}) + \frac{1}{4\pi}\nabla\int\frac{\nabla'\cdot\mathbf{v}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}d^3x'.\end{aligned} \tag{3}$$

A statistical state of incompressible fluid turbulence is described by an ensemble of solenoidal velocity fields that evolve dynamically according to (2). All equal-time multipoint velocity correlation tensors are contained in the complex-valued Fourier transform of the probability measure, the Hopf characteristic functional[12]

$$\begin{aligned}\Phi[\mathbf{y},t] \equiv 1 &+ i\int\langle u_j(\mathbf{x}',t)\rangle y_j(\mathbf{x}')d^3x'\\ &- \frac{1}{2}\int\langle u_j(\mathbf{x}',t)u_k(\mathbf{x}'',t)\rangle y_j(\mathbf{x}')y_k(\mathbf{x}'')d^3x'd^3x''\\ &- \frac{i}{6}\int\langle u_j(\mathbf{x}',t)u_k(\mathbf{x}'',t)u_l(\mathbf{x}''',t)\rangle\\ &\times y_j(\mathbf{x}')y_k(\mathbf{x}'')y_l(\mathbf{x}''')d^3x'd^3x''d^3x''' + \cdots.\end{aligned} \tag{4}$$

In (4), the real parameter field $\mathbf{y}=(y_1(\mathbf{x}), y_2(\mathbf{x}), y_3(\mathbf{x}))$ is required to be continuous, infinitely-differentiable, and of compact support, (i.e., a vector test function) but is otherwise unrestricted. Since the correlation tensors inherit the solenoidal quality of $\mathbf{u}$, the characteristic functional depends exclusively on the transverse part of $\mathbf{y}$: $\Phi[\mathbf{y},t]\equiv\Phi[\mathbf{y}^{\mathrm{tr}},t]$. The reality and nonnegativity of the normalized probability measure implies that $\Phi[\mathbf{y},t]^*\equiv\Phi[-\mathbf{y},t]$, $|\Phi[\mathbf{y},t]|\leqslant 1$, and several additional nonholonomic conditions.[13] Furthermore, since all $\mathbf{u}$ satisfy (2), it follows that Φ satisfies the time-evolution equation derived by Hopf[12]

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$$\partial\Phi/\partial t + \Omega\Phi = 0, \tag{5}$$

$$\Omega \equiv -i\int y_j^{\mathrm{tr}}(\mathbf{x})\frac{\delta}{\delta y_k(\mathbf{x})}\nabla_k\frac{\delta}{\delta y_j(\mathbf{x})}d^3x - \nu\int y_j(\mathbf{x})\nabla^2\frac{\delta}{\delta y_j(\mathbf{x})}d^3x, \tag{6}$$

in which $\delta/\delta y_j(\mathbf{x})$ denotes the Volterra functional derivative with respect to $y_j(\mathbf{x})$. The parameter field $\mathbf{y}$ is not required to be solenoidal in order for the three functional derivative operators $\delta/\delta y_j(\mathbf{x})$ to be unconstrained and mutually independent in (6).

In cases for which the turbulence is homogeneous, the probability measure over the ensemble is invariant under translations of the spatial coordinates, and the mean velocity $\langle \mathbf{u}(\mathbf{x}, t)\rangle$ is independent of $\mathbf{x}$. Since the expectation value of (1) then states that $\partial\langle \mathbf{u}(\mathbf{x}, t)\rangle/\partial t = 0$, one has $\langle \mathbf{u}(\mathbf{x}, t)\rangle = 0$ for all $t \geqslant 0$ in a Galilean frame for which $\langle \mathbf{u}(\mathbf{x}, 0)\rangle = 0$. The Hopf expression for the quadratic velocity correlation tensor follows from (4) as

$$\langle u_j(\mathbf{x}', t)u_k(\mathbf{x}'', t)\rangle = -\left.\frac{\delta^2\Phi}{\delta y_j(\mathbf{x}')\delta y_k(\mathbf{x}'')}\right|_{y=0} \equiv R_{jk}(\mathbf{r}, t), \tag{7}$$

with the spatial dependence exclusively upon $\mathbf{r} \equiv \mathbf{x}' - \mathbf{x}''$ for homogeneous turbulence; note that (7) is solenoidal, $\partial R_{jk}/\partial r_j = 0 = \partial R_{jk}/\partial r_k$, as a consequence of the incompressibility condition $\nabla\cdot\mathbf{u} = 0$. From (4) and (7) one obtains

$$\Phi[\mathbf{y}, t] = 1 - \frac{1}{2}\int R_{jk}(\mathbf{r}, t)\, y_j(\mathbf{x}') \times y_k(\mathbf{x}'')d^3x'd^3x'' + O(\mathbf{y}^3), \tag{8}$$

in a Galilean frame for which $\langle \mathbf{u}(\mathbf{x}, t)\rangle = 0$.

Let ξ denote a real positive disposable parameter. Under the dilatation transformation $\mathbf{y}(\mathbf{x}) \to \xi^2\mathbf{y}(\xi\mathbf{x})$, the functional derivative operators transform as $\delta/\delta y_j(\mathbf{x}) \to \xi\delta/\delta y_j(\xi\mathbf{x})$ to preserve the basic commutation relation $[\delta/\delta y_j(\mathbf{x}'), y_k(\mathbf{x}'')] = \delta_{jk}\delta^{(3)}(\mathbf{x}' - \mathbf{x}'')$ where $\delta^{(3)}$ is the three-dimensional Dirac distribution. Thus, under the transformation $\mathbf{y}(\mathbf{x}) \to \xi^2\mathbf{y}(\xi\mathbf{x})$, the operator (6) transforms

$$\Omega \to -i\xi^4\int y_j^{\mathrm{tr}}(\xi\mathbf{x})\frac{\delta}{\delta y_k(\xi\mathbf{x})}\nabla_k\frac{\delta}{\delta y_j(\xi\mathbf{x})}d^3x - \nu\xi^3\int y_j(\xi\mathbf{x})\nabla^2\frac{\delta}{\delta y_j(\xi\mathbf{x})}d^3x = \xi^2\Omega, \tag{9}$$

as seen by changing the dummy variable from $\mathbf{x}$ to $\xi^{-1}\mathbf{x}$ in the integrals shown in (9). Hence, Eq. (5) becomes

$$\left(\frac{\partial}{\partial t} + \xi^2\Omega\right)\Phi[\xi^2\mathbf{y}(\xi\mathbf{x}), t] = 0, \tag{10}$$

by replacement of the free parameter field $\mathbf{y}(\mathbf{x}) \to \xi^2\mathbf{y}(\xi\mathbf{x})$. With the additional transformation of the time variable $t \to \xi^{-2}t$, it follows from (10) that

$$\left(\frac{\partial}{\partial t} + \Omega\right)\Phi[\xi^2\mathbf{y}(\xi\mathbf{x}), \xi^{-2}t] = 0, \tag{11}$$

for all real $\xi > 0$ if $\Phi[\mathbf{y}(\mathbf{x}), t]$ satisfies (5). Equation (11) expresses the space-time dilatation invariance of the Φ Eq. (5).

Consider an initial statistical state at $t = 0$ such that

$$\Phi[\mathbf{y}, 0] = 1 - \mathop{\mathsf{S}}_{n(>1)} F_n[\mathbf{y}], \tag{12}$$

where the F_n's have definite homogeneity under the dilatation transformations,[14]

$$F_n[\xi^2\mathbf{y}(\xi\mathbf{x})] \equiv \xi^{2(n-1)}F_n[\mathbf{y}(\mathbf{x})], \tag{13}$$

for all real constant $\xi > 0$ and a certain fixed constant *scaling-index* n; the latter parameter must be greater than unity for (13) to be consistent in the limit $\xi \to 0+$ with $F_n[0] = 0$. It is understood that the *symbolic summation* S may embrace continuous values (by a weighted integration) as well as one or more discrete values of the scaling-index n. If (12) holds, the solution to (5) takes the form[15]

$$\Phi[\mathbf{y}(\mathbf{x}), t] = 1 - \mathop{\mathsf{S}}_{n(>1)} t^{-n+1}\mathscr{F}_n[t\mathbf{y}((t)^{1/2}\mathbf{x})] \tag{14}$$

for all $t \geqslant 0$, where the $\mathscr{F}_n$'s satisfy a structural equation[16] derived from (5) and consistent with $\mathscr{F}_n[0] = 0$,

$$\lim_{t\to 0} t^{-n+1}\mathscr{F}_n[t\mathbf{y}((t)^{1/2}\mathbf{x})] = F_n[\mathbf{y}(\mathbf{x})]. \tag{15}$$

The form (14) is an immediate consequence of Morgan's theorem[17] (commonly applied to obtain self-similar solutions to partial differential equations[18] invariant under one-parameter groups of transformations), the linearity of (5), the dilatation invariance expressed by (11), and the fact that (6) acts on a quantity independent of $\mathbf{y}$ to give zero. Thus, if the initial statistical state admits a linear decomposition of the form (12), the characteristic functional is given by the time-explicit generic form (14). The terms in the dilatation-index summation in (14) represent *mutually independent dynamical modes*, granted by the linearity and dilatation invariance of (5) for initial statistical states expressible in the form (12). The existence of mutually independent dynamical modes had not been conjectured previously for homogeneous turbulence governed by the essentially nonlinear Navier–Stokes equation; the form of the dynamical mode $\mathscr{F}_n[\mathbf{y}(\mathbf{x})]$ is fixed by a second-order functional differential equation[16] that involves n as an eigenvalue parameter if the asymptotic behavior of $\mathscr{F}_n$ is suitably prescribed for large $\mathbf{y}(\mathbf{x})$.

It follows from (14) and either (7) or (8) that

$$R_{jk}(\mathbf{r}, t) = \mathop{\mathsf{S}}_{n(>1)} t^{-n}\mathscr{A}_{jk}^{(n)}(\mathbf{r}/(t)^{1/2}), \tag{16}$$

for all $t \geqslant 0$, where

$$\mathscr{A}_{jk}^{(n)}(\mathbf{r}) \equiv \left.\frac{\delta^2\mathscr{F}_n[\mathbf{y}(\mathbf{x})]}{\delta y_j(\mathbf{x}')\delta y_k(\mathbf{x}'')}\right|_{y=0}. \tag{17}$$

The initial value of the quadratic correlation tensor (16) is

$$R_{jk}(\mathbf{r}, 0) = \mathop{\mathsf{S}}_{n(>1)} A_{jk}^{(n)}(\mathbf{r}), \tag{18}$$

where

$$A_{jk}^{(n)}(\mathbf{r}) \equiv \lim_{t\to 0} t^{-n}\mathscr{A}_{jk}^{(n)}(\mathbf{r}/(t)^{1/2}) \equiv \xi^{2n}A_{jk}^{(n)}(\xi\mathbf{r}) \tag{19}$$

for all $\xi > 0$; the final member of (19) is a consequence of (17), (15) and (13), or equivalently (8), (12) and (13). In the aca-

demic case for which the solenoidal tensor (19) is isotropic, its form is implied by the scaling relation in (19) to within a multiplying constant.[19] According to (16), the turbulence decays as

$$u^2 = u^2(t) \equiv \tfrac{1}{3}\langle |\mathbf{u}(\mathbf{x}, t)|^2 \rangle = \tfrac{1}{3} R_{jj}(0, t)$$

$$= \tfrac{1}{3} \sum_{n(>1)} t^{-n} \mathscr{A}_{jj}^{(n)}(0) \tag{20}$$

and the normalized tensor $R_{jk}(\mathbf{r}, t)/u^2$ is exclusively dependent upon $\mathbf{r}/(t)^{1/2}$ if only a single dynamical mode is present or if one dynamical mode is dominant in the scaling-index summation during the time-interval of interest.

Such single-dynamical-mode turbulence has been observed experimentally[20] with $n = 2.0$ (weak grid-generated) and $n = 3.3$ (strong waterfall-generated); in both cases self-similarity is evident in the normalized quadratic correlation tensor in terms of the variable $\mathbf{r}/(t)^{1/2}$, in precise agreement with the one-term specializations of (16) and (20). Strong grid-generated turbulence[21] features the decay law $u^2 \propto t^{-n}$ with $n = 1.2$ during the initial period of decay, and the associated normalized correlation tensors are again self-similar in $\mathbf{r}/(t)^{1/2}$ to within the accuracy of experimental measurement, for both the Taylor microscale and the Kolmogoroff similarity-length (which enters concurrently at very high Reynolds numbers) are approximately proportional to $(t)^{1/2}$ for n close to unity.[22] It is the scaling character of the initial statistical state at $t = 0$ that gives rise to these particular dynamical modes ($n = 2.0, 3.3, 1.2$) for different types of homogeneous turbulence. By employing the assumption of spatial isotropy and the eddy-damped quasi-normal approximation, Lesieur and Schertzer[10] arrived at the same theoretical conclusion: n is determined by the scaling character of the initial statistical state.

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[14] The prefactor $\xi^{2(n-1)}$ in (13) is the most general allowable and consistent with the group property of the dilatation transformations; the exponent appears as $2(n-1)$ in order to display the experimentally-determined constant n where it first enters theoretically.
[15] Units of time are understood to be based on a physical constant associated with the turbulence-generating mechanism, e.g., the time $M/U \equiv 1$ for grid-generated turbulence with M the mesh-spacing and U the constant upstream flow speed; hence, t is effectively a dimensionless variable in the scaling and other relations shown here.
[16] By substituting (14) into (5), performing the differentiations, and making a change of variabes, one obtains the equation for $\mathscr{F}_n = \mathscr{F}_n[\xi]$ with $\xi = \xi(\alpha)$:

$$(n-1)\mathscr{F}_n - \int \left(\xi_j + \frac{1}{2}\alpha_k \frac{\partial \xi_j}{\partial \alpha_k} - \nu \nabla_\alpha^2 \xi_j\right) \frac{\delta \mathscr{F}_n}{\delta \xi_j(\alpha)} d^3\alpha$$
$$+ i \int \xi_j^{1r} \frac{\delta}{\delta \xi_k(\alpha)} \frac{\partial}{\partial \alpha_k} \frac{\delta \mathscr{F}_n}{\delta \xi_j(\alpha)} d^3\alpha = 0.$$

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[18] See, for example, W. F. Ames, *Nonlinear Partial Differential Equations in Engineering*, (Academic, New York, 1972), Vol. II, p. 88.

[19] Because the solenoidal tensor (19) is homogeneous (of order $-2n$) in $\mathbf{r}$, the assumption of isotropy implies that it has the form

$$A_{jk}^{(n)}(\mathbf{r}) = a\left(\frac{\partial^2}{\partial r_j \partial r_k} - \delta_{jk}\nabla^2\right) r^{2-2n}$$
$$= 4(n-1)a\left[2\pi(\delta_{jk} - r^{-2} r_j r_k) r^{1-2n} \delta^{(3)}(\mathbf{r}) + n r_j r_k r^{-2n-2} - (n-1)\delta_{jk} r^{-2n}\right]$$

where use has been made of the elementary formula

$$\frac{\partial^2}{\partial r_j \partial r_k} r^{2-2n} = -8\pi(n-1) r_j r_k r^{1-2n} \delta^{(3)}(\mathbf{r}) - 2(n-1)(\delta_{jk} - 2n r^{-2} r_j r_k) r^{-2n},$$

and a is an arbitrary positive constant.

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[22] In terms of the dissipation rate $\epsilon = \epsilon(t) \equiv -d(\tfrac{3}{2}u^2)/dt$, the Kolmogoroff and Taylor lengths are defined respectively as[1] $\eta = \eta(t) \equiv (\nu^3/\epsilon)^{1/4}$ and $\lambda = \lambda(t) \equiv (15\nu u^2/\epsilon)^{1/2}$; the ratio of these characteristic lengths is $\eta/\lambda = 0.5081\, R_\lambda^{-1/2}$ where $R_\lambda \equiv u\lambda/\nu$ is the intrinsic Reynolds number, while the so-called integral scale $u^3/\epsilon = 0.01721\, \lambda^3/\eta^2$ is functionally dependent on η and λ. With a decay law $u^2 \propto t^{-n}$ one has $\eta \propto t^{(n+1)/4}$ and $\lambda = (10\nu t/n)^{1/2}$; in particular, the experimental value $n = 1.2$ gives $\eta \propto (t)^{0.55}$, making a dependence on $\mathbf{r}/\eta$ and $\mathbf{r}/\lambda$ practically indistinguishable from a dependence on the single variable $\mathbf{r}/(t)^{1/2}$ during the initial period of decay of strong grid-generated turbulence.

The electric double layer and electrohydrostatic surface deformation

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(Received 25 August 1981; accepted for publication 16 October 1981)

A study is made of the equilibrium configuration of a liquid surface under surface tension and gravity when additionally, the liquid is electrically conducting, is under a given electrostatic field, and has at the surface an electric double layer. The essential element here is the presence of the double layer, making the problem real in the sense of being distinct from what could be approached by the classical methods, and requiring the application of relatively recent considerations concerning electrostatic force in a continuum. From the point of view of applications, the significant feature is the prediction of a double-layer effect whose dependence upon the field is essentially linear, as compared with the quadratic, purely classical effect, and in specific problems that are solved, quantitative results in this respect are obtained, of possible use experimentally.

PACS numbers: 73.30 + y, 68.10. − m

1. INTRODUCTION

We are basically concerned with the following problem. An electrically conducting liquid, at rest and subject to given constraints, is under the influence of a given electrostatic field: to determine theoretically the shape of the surface of the liquid.

This might be thought of as a generalized Plateau problem, in which the surface is determined by, in addition to surface tension and gravity, the field, and the first question arising is how to include the field in the general hydrostatic equation that has to be solved. Classically, according to the Helmholtz theory of electrostatic force in a continuum (see, e.g., Jeans[1]), it would be considered that this was given by applying at the surface the Maxwell stress tensor. The Helmholtz theory has, however, long been a matter of controversy, one that goes back to the critique of Larmor[2] and was notably taken up by Livens[3] and Smith-White.[4] The opposing school considered that, contrary to the energy method of Helmholtz, the electric force in a continuum should be calculated on the basis of direct charge–charge, dipole–dipole, and charge–dipole interactions, and this point of view reached its fruition in the work of Brown.[5]

The main result of Brown's theory was, remarkably, to confirm the correctness of the Maxwell stress tensor. This was the case, however, for the purpose of calculating the *total* force and torque on a rigid body *in vacuo* or immersed in a fluid environment, a question of prime concern in electrostatics, but the question of what the correct stress tensor should be *locally*, as required for determining the action on a *deformable* body, such as a body of liquid, was still to be resolved. This was taken up by the present author,[6] and it was found yet again, that the Maxwell stress tensor was correct, *provided* that there is no electric double layer at the surface. If there is, then the stress tensor to be applied at the surface is, indeed, different from the Maxwell stress tensor.

This is clearly significant, for the presence of an electric double layer is a normal property of matter. It means, in the first place, that the deformation of a liquid surface under an applied field will be different from what would be predicted classically. In the second place, there is the implication of the presence of electrical stresses even in the *absence* of an applied field. This latter point was taken up[7] and led to a purely electrohydrostatic theory of surface tension. The former was investigated subsequently.[8,9]

The purpose of the present paper is to give a new theory of surface deformation. This is necessary since the early considerations just referred to[8,9] have been found completely invalid on account of deep-seated fluid-mechanical difficulties associated with the matching of stress systems at the liquid surface. A second, much shallower, error was the attachment of the wrong sign to the mean curvature of the surface. This also affected the surface-tension theory,[7] which has recently been corrected.[10]

The physical interest of the deformation theory, apart from the questions of principle involved, can be introduced by our pointing out that while the purely classical effect is quadratic in the sense of depending only on the square of a parameter describing the strength of the applied field, the contribution arising from the double layer is essentially linear. This means that, in a specific experiment, the deformation of the surface under the field will, on account of the double layer, be different if the field is reversed. Differential effects ascribed to the double layer have been known qualitatively for a long time (e.g., the differential vapor pressure for drop formation in the Wilson cloud chamber), and we venture to suggest that the surface-deformation theory might be the first to make quantitative predictions of this kind.

Now in our theory, surface tension T arises as a *consequence* of the general electrohydrostatic considerations, as has been pointed out above, instead of having to be introduced phenomenologically, as in the classical theory. In the same way, a second constant Φ appears, somewhat analogous to T. It is presumably, like T, characteristic of the materials present, but it differs in that it gauges the magnitude of the *interaction of applied fields* with the double layer. In a crude qualitative experiment it would perhaps be manifested as a "modification of surface tension" due to the field, but in a more refined, quantitative, sense this is not apt, for its effect is essentially linear, as we have said, and its mode of determining the surface is otherwise quite different in mathemat-

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ical detail from that of T. The point is that solutions of specific problems that we shall give open the possibility of the experimental determination of Φ. Thus, T and Φ having joint origin with the double layer, we have the prospect of a new line of approach or, at least, the reinforcement of established lines, to the physics of surface phenomena.

In the theoretical context, the classical Plateau problem is a well-known one in the calculus of variations or, formulated alternatively, leads to a nonlinear differential equation, and few exact solutions are known. The special difficulty of the present problem, however, even after the governing electrohydrostatic equations have been correctly formulated, will be made clear by the following remark. To determine the shape, one must know the electric field at the liquid surface; but the electric field is the solution of an electrostatic boundary-value problem whose data must include the shape of the surface. In fact, the formulation is in terms of simultaneous functional equations, prospects for the exact solution of which appear to be nil. Nonetheless, the equations can be attacked by perturbation theory, and an important part of the theory as a whole is to spell out this procedure.

In Sec. 2 we shall review very briefly the electrohydrostatic foundation of the deformation theory, and in Sec. 3 tackle the crucial and delicate stress-matching problem. In Sec. 4 we shall formulate in general terms a solution procedure. We shall find that situations have to be classified according to what we shall in due course call the zero-order surface. Once this is done, we shall have a general procedure for each such surface, and shall solve specific problems concerning cylindrical and spherical zero-order surfaces.

2. THE BOUNDARY-LAYER STRESSES

The methods of Brown's theory[5] being essentially continuum-mechanical, their adaptation[6] to the local analysis of effects at a surface require that the surface be "smoothed out." This is to say, the sharp boundary, representing a physical discontinuity between two phases, has to be replaced by a thin transition region in which quantities change abruptly but continuously from values characteristic of one phase to values characteristic of the other. This is, of course, more concordant with physical reality, and in any case, after obtaining certain results one can take limits if one so wishes. We refer to the thin transition region as the boundary layer.

The liquid we call A, and since it is electrically conducting, there is zero electrostatic field strength in its bulk. We call the environment, which is nonconducting, B, and this may be a liquid immiscible with A, a gas, or empty space. In any case, we assume that it can be treated as a uniform incompressible fluid dielectric with constant permittivity (dielectric constant) ϵ ($\geqslant 1$).

Insofar as A "has a surface," this must be taken as a mathematical surface S located in the boundary layer. We describe S by parametric equations $x = x(u,v)$, $y = y(u,v)$, $z = z(u,v)$. Then if $\xi^1 = u, \xi^2 = v, \xi^0 = \nu$, where ν is distance (positive or negative) in the direction normal to S at any point, zero on S, and increasing from A to B, ξ^λ ($\lambda = 0,1,2$) are curvilinear coordinates for describing the boundary layer. In fact, they are parallel-surface coordinates, any surface for $\xi^0 = \text{const}$ being parallel to S according to the definition of differential geometry (Eisenhart[11]). We regard the boundary layer as contained between surfaces $\xi^0 = c_A (< 0)$ and $\xi^0 = c_B (> 0)$, defining its thickness a as $c_B - c_A$. The ξ^λ are not in general orthogonal curvilinear coordinates; however, since ξ^0 is a pure (signed) distance normal to the directions of ξ^1 and ξ^2, their metric tensors $g_{\lambda\mu}$ and $g^{\lambda\mu}$ have the simplifying properties $g_{00} = g^{00} = 1$, $g_{0\mu} = g^{0\mu} (\mu \neq 0) = 0$. Parallel-surface coordinates with the tensor calculus are the essential mathematical apparatus of boundary-layer electrohydrostatics. They appear first to have been used in boundary problems of physics by Howarth.[12]

The electric double layer is contained in the boundary layer, and consistently with the classical, macroscopic spirit of the theory, we do not have to assume any particular model for it. We have only to make two general assumptions concerning its macroscopic character. These are (a) that, under no applied field, it is uniform with respect to position on the surface, and (b) that its structure (and hence uniformity) is undisturbed by the action of an applied field. While (a) will meet with little challenge, there may well be cases in which (b) is poor even as a first approximation (see Booth[13]) as, for example, that of mercury in contact with an electrolyte. However, ambient electrolytes are irrelevant here, B being a nonconductor, and it is our opinion that normally, the assumption will be good enough to provide a reliable working basis.

There is no field in the bulk of A but E_0, the outward-normal component of electric intensity E_λ, has some value when $\xi^0 = c_B$, E_B say, which is generally non-zero if there is an applied field, and then D_0, the outward-normal component of electric displacement D_λ, is ϵE_B, ϵ being, as we have said, the bulk permittivity of B. A decision has to be made as to suitable general expressions for E_0 and D_0 inside the boundary layer, and the simplest assumption which is consistent with the hypotheses (a) and (b) is that, as a first approximation in terms of a, the boundary-layer thickness,

$$\begin{aligned} E_0 &= \mathscr{E}(\xi^0) + f(\xi^0) E_B, \\ D_0 &= \mathscr{D}(\xi^0) + h(\xi^0) \epsilon E_B, \end{aligned} \qquad c_A \leqslant \xi^0 \leqslant c_B, \tag{1}$$

where $\mathscr{E}(\xi^0)$, $\mathscr{D}(\xi^0)$, $f(\xi^0)$, and $h(\xi^0)$ are independent of the applied field and satisfy the conditions $\mathscr{E}(c_A) = \mathscr{D}(c_A) = \mathscr{E}(c_B) = \mathscr{D}(c_B) = 0, f(c_A) = h(c_A) = 0, f(c_B) = h(c_B) = 1$. In fact, $\mathscr{E}(\xi^0)$ and $\mathscr{D}(\xi^0)$ represent the intrinsic double-layer field, very large if a is very small, while $f(\xi^0)$ and $h(\xi^0)$ represent the way the applied field is modified on crossing the boundary layer to the field-free interior of A.

The zero-applied-field surface tension [Cade,[10] Eq. (1)], which we can continue to call surface tension when there is an applied field, is given according to present notation by

$$T = -\frac{1}{4\pi} \int_{c_A}^{c_B} \mathscr{E}\mathscr{D}\, d\xi^0, \tag{2}$$

and we shall define the constant Φ by

$$\Phi = -\frac{1}{4\pi} \int_{c_A}^{c_B} (\mathscr{E} h + \mathscr{D} f)\, d\xi^0. \tag{3}$$

This definition of Φ differs from the previous one [Cade,[8] Eq.

(12)] through sign (a matter of pure convention) and by our avoiding the use of boundary-layer permittivity, using electric displacement instead.

We consider now in the boundary layer the stress tensor with respect to the coordinate system ξ^{λ} and in its mixed form $T^{\lambda}{}_{\mu}$, and shall be concerned with the components $T^{0}{}_{\mu}$. We shall take Cartesian coordinates with positive x axis vertically upward, and in keeping with usual convention (but contrary to Cade,[8,9] following Eisenhart[11]), shall define the mean curvature K_m of S as *half* the sum of the reciprocals of the principal radii of normal curvature. We correct the previous error in its sign[8,9] (see Sec. 1) by conforming to the convention appropriate to physical application, that a principal radius of normal curvature is positive if the corresponding curve is locally convex with respect to the liquid A.[14]

Now, with g the acceleration due to gravity and ω (a constant) the density of B, we can take over from the earlier work [Cade,[8] Eqs. (9) and (13)], but with the new conventions, the values of the stress components $T^{0}{}_{\mu}$ at the surface $\xi^{0} = c_A$:

$$
\begin{aligned}
T_A{}^{0}{}_{0} &= \frac{\epsilon E_B^2}{8\pi} - 2K_m(T + \Phi E_B) + g\omega x - \Gamma, \\
T_A{}^{0}{}_{1} &= \Phi \frac{\partial E_B}{\partial \xi^1}, \\
T_A{}^{0}{}_{2} &= \Phi \frac{\partial E_B}{\partial \xi^2},
\end{aligned}
\tag{4}
$$

where Γ is a constant. Under the new conventions K_m, T, and Φ have all had sign reversals, which is why the only apparent effect of correcting the sign of K_m has been to change the signs of the expressions for $T_A{}^{0}{}_{1}$ and $T_A{}^{0}{}_{2}$.

3. MATCHING OF THE INTERNAL STRESS SYSTEM

Let us for the time being denote the Cartesian coordinates by $x_i (i = 0,1,2)$, x_0 being the vertically upward one which in (4) is denoted by x. Then in the field-free bulk of A, where the density is ρ (a constant), the Cartesian stress tensor T_{ij} must satisfy the equations in Cartesian-tensor notation,

$$
\frac{\partial T_{ji}}{\partial x_j} = \begin{cases} g\rho & i = 0, \\ 0, & i \neq 0, \end{cases} \qquad T_{ji} = T_{ij}. \tag{5}
$$

Now in classical hydrostatics, it is normal to take T_{ij} as simply a multiple of the fundamental second-rank tensor δ_{ij} ($= 1$ when $i = j$, $= 0$ otherwise); to be precise, $T_{ij} = -p\delta_{ij}$, p being the hydrostatic pressure which, therefore, from (5), must satisfy

$$
\frac{\partial p}{\partial x_0} = -g\rho, \quad \frac{\partial p}{\partial x_1} = \frac{\partial p}{\partial x_2} = 0,
$$

leading at once to the familiar elementary result for the pressure in a liquid at rest. However, this form of T_{ij} will not do now, for by virtue of the tangential stresses $T_A{}^{0}{}_{1}$ and $T_A{}^{0}{}_{2}$ in (4), such a stress system will not at the surface $\xi^{0} = c_A$ join on continuously to the stresses $T_A{}^{0}{}_{\mu}$ (for transforming T_{ij} to the coordinates ξ^{λ}, we obtain $T^{0}{}_{0} = -p$, $T^{0}{}_{1} = T^{0}{}_{2} = 0$). We must therefore look for a system satisfying (5) but which is of a less simple form.

The problem of finding such a system does not appear to be soluble in general terms, and we have to specialize in two major respects. In the first place, we shall regard the effects of weight (expressed in terms of g, ρ, and ω) and of the applied field as small, the main factor in the determination of the surface being the surface tension T, and shall contemplate a perturbation procedure to the solution in which we can, in principle, work to any desired order in perturbation parameters which describe the weight and applied field. The zero-order approximation in this scheme is what we call the zero-order surface, the surface S without taking *any* account of the weight and applied-field effects. Our second specialization is to assume that this surface is a coordinate surface of some system of orthogonal curvilinear coordinates (including Cartesian coordinates as one particular possibility) which might be used to describe A.

Suppose that such a coordinate system is $X^i (i = 1,2,3)$, perhaps being x_i above if it happens to be Cartesian. We regard A as represented in this system, taking the stress tensor there in its mixed form $T^{i}{}_{j}$, whose covariant derivative (Eisenhart[11]) is

$$
T^{i}{}_{j,k} = \frac{\partial T^{i}{}_{j}}{\partial X^k} + T^{h}{}_{j} \begin{Bmatrix} i \\ h\ k \end{Bmatrix} - T^{i}{}_{h} \begin{Bmatrix} h \\ j\ k \end{Bmatrix},
$$

where the braced expressions are Christoffel symbols of the second kind. Contraction with respect to i and k gives the divergence of $T^{i}{}_{j}$, whence we find by simple rules of tensor analysis that the general form corresponding to (5) and which becomes (5) in the special case where the X^i are the x_i is, having relabelled some indices and put $x_0 = x$,

$$
\frac{\partial T^{j}{}_{i}}{\partial X^j} + T^{h}{}_{i} \begin{Bmatrix} j \\ h\ j \end{Bmatrix} - T^{j}{}_{h} \begin{Bmatrix} h \\ i\ j \end{Bmatrix} = \frac{\partial x}{\partial X^i} g\rho,
\tag{6}
$$

$(g_{ll}\, g^{mm})^{1/2} T^{l}{}_{m} = (g_{mm}\, g^{ll})^{1/2} T^{m}{}_{l}$ (l, m not summed).

At the surface $\xi^{0} = c_A$ we apply the transformation law for a mixed second-rank tensor in order to relate the components of $T^{i}{}_{j}$ to the right-hand members of (4):

$$
\begin{aligned}
&\frac{\epsilon E_B^2}{8\pi} - 2K_m(T + \Phi E_B) + g\omega x - \Gamma \\
&\qquad = \frac{\partial \xi^0}{\partial X^i} \frac{\partial X^j}{\partial \xi^0} T^{i}{}_{j},
\end{aligned}
\tag{7}
$$

$$
\begin{aligned}
\Phi \frac{\partial E_B}{\partial \xi^1} &= \frac{\partial \xi^0}{\partial X^i} \frac{\partial X^j}{\partial \xi^1} T^{i}{}_{j}, \\
\Phi \frac{\partial E_B}{\partial \xi^2} &= \frac{\partial \xi^0}{\partial X^i} \frac{\partial X^j}{\partial \xi^2} T^{i}{}_{j}.
\end{aligned}
$$

These are the stress-matching equations.

4. THE PERTURBATION METHOD

We can now outline verbally a solution procedure. We suppose that we can solve (6) to the extent of finding a general form of stress system containing at most two undetermined functions and which, taking these functions as zero, is a constant diagonal tensor $-p_0\delta_{ij}$. This last is the zero-order internal stress system, which we would assume if there were no weight and applied-field effects, when the surface S would be the zero-order one, say $X^0 = \text{const}$. We attempt to find a first-order surface S, that is, one correct to the first order in perturbation parameters representing the weight and the applied field. Our first step is to solve the electrostatic problem posed by the given applied field and the fact that the potential takes some prescribed constant value on the surface, taking the surface as the *zero-order* one. The solution is the first-order field, and to work with (7) with a view to finding the first-order surface, it is clearly sufficient to use this field, since it is that which, as represented in the equations, is correct to the first order in the perturbation parameters. Our ability to do this is the key to our method for now, knowing the left-hand members, we can use the second and third of Eqs. (7) to determine (to the first order) the unknown functions in the T^i_j, fixing for us the first-order stress system. Then the first of Eqs. (7) becomes an appropriate general formula for K_m, a differential equation for the first-order surface. Let us suppose that we have solved it.

Having thus calculated the first-order surface, we resolve the electrostatic problem, using now the boundary condition as applied to *this* surface. This gives us the second-order field, and now the description of the last paragraph is repeated but in terms of one order higher, ending with our having supposedly solved a differential equation for the second-order surface. In this way, we can in principle proceed to any order in the perturbation parameters.

In practice, a system that we study will be either two-dimensional or axisymmetric. Two-dimensionally, S is an infinite cylinder whose generators, on account of the role of gravity, are horizontal. In an axisymmetric system, S is a surface of revolution about an axis which, by the role of gravity in this case, is vertical, and which we take as coinciding with our vertically-upward x axis. In either case, we can obviously choose ξ^λ so that only one of ξ^1 and ξ^2 enters the discussion, the one which is the parameter t of a curve C which is the cross section of the cylinder in the two-dimensional case, and the section by a half-plane from the axis of revolution in the axisymmetric case.

Two-dimensionally, the mean curvature K_m of S is half the ordinary curvature κ of C,[15] and a function of t. Axisymmetrically, K_m does not so reduce, although of course, again, it is a function only of the parameter t of the curve C in this case.

In either case, we call C the profile and the problem of determining S reduces to that of finding the profile. Thus, in the perturbation procedure described above, the first stage is that of finding the first-order profile, the second that of finding the second-order profile, and so on. With $\nu = \xi^0$, and taking t as either ξ^1 or ξ^2, the stress-matching equations (7) reduce to the two equations

$$\begin{aligned}\frac{\epsilon E_B^{\,2}}{8\pi} - 2K_m(T + \Phi E_B) + g\omega x - \Gamma \\ = \frac{\partial \nu}{\partial X^i}\frac{\partial X^j}{\partial \nu} T^i_{\ j},\end{aligned} \tag{8}$$

$$\Phi \frac{dE_B}{dt} = \frac{\partial \nu}{\partial X^i}\frac{\partial X^j}{\partial t} T^i_{\ j},$$

and at each stage, subsequently to finding the stress system, the equation for finding the profile is a second-order ordinary, rather than partial, differential equation.

5. THE GENERAL CYLINDER PROBLEM

If we speak of, say, the general sphere problem, we are referring to the whole class of problems in which the zero-order surface is a sphere or part of a sphere, this dictating the choice of the curvilinear coordinate system X^i, which clearly should be spherical polar coordinates (r,θ,ϕ). If we have a drop of conducting liquid in a nonconducting liquid environment of the same density, it assumes, as we know, a spherical form under the action of surface tension. This is the simplest case of the Plateau problem. If the densities are unequal and there is an applied field, there is a departure from the spherical form, which it is the object of the present theory to be able to calculate, but clearly, according to the definitions in the theory, the zero-order surface is the sphere, so that the problem will be a particular case of the general sphere problem.

By "cylinder" in the present context, we mean a circular cylinder which (or part of which) is the zero-order surface, the class in this case being of two-dimensional problems. It also has physical significance, as we shall see in due course, although perhaps not obviously and only in problems involving parts of cylinders.

In this section we give a fairly detailed treatment of the general cylinder problem. It is tedious but rewarding, the result being quite remarkable from the theoretical standpoint, while giving us the basis for all specific cylinder problems.

We take the coordinate system X^i as cylindrical polar coordinates (r,θ,z), related to our Cartesian coordinates by $x = r\cos\theta, y = r\sin\theta, z = z$, and in which the zero-order profile is the circle (or a circular arc) $r = b$. Nothing concerning the z direction enters, and the general stress equations represented by (6), when we work out the Christoffel symbols with the use of the metric tensor $g_{00} = 1, g_{11} = r, g_{01} = g_{10} = 0$, assume the special form

$$\begin{aligned}&\frac{\partial T^r_{\ r}}{\partial r} + \frac{\partial T^\theta_{\ r}}{\partial \theta} + \frac{1}{r}(T^r_{\ r} - T^\theta_{\ \theta}) = g\rho\cos\theta,\\ &\frac{\partial T^r_{\ \theta}}{\partial r} + \frac{\partial T^\theta_{\ \theta}}{\partial \theta} + rT^\theta_{\ r} = -g\rho r\sin\theta,\\ &(1/r)T^r_{\ \theta} = rT^\theta_{\ r}.\end{aligned} \tag{9}$$

Let us look for a solution of the type

$$T^r{}_r = -p_0 + M(r)F(\theta),$$
$$T^\theta{}_r = G(\theta), \quad T^r{}_\theta = r^2 G(\theta), \tag{10}$$
$$T^\theta{}_\theta = -p_0 + N(r)H(\theta),$$

where p_0 is a constant, and whereby the third of Eqs. (9) is satisfied automatically. Substituting into the second, we find at once that $N(r) = r$ and that we can determine $H(\theta)$ in terms of $G(\theta)$. Then, substituting into the first, we obtain $M(r) = r$ and determine $F(\theta)$ in terms of $G(\theta)$. The result is

$$T^r{}_r = -p_0 + g\rho r\cos\theta - \tfrac{3}{2} r\int_{\theta_0}^{\theta} G(\tau)\,d\tau - \tfrac{1}{2} rG'(\theta),$$
$$T^\theta{}_r = G(\theta), \quad T^r{}_\theta = r^2 G(\theta), \tag{11}$$
$$T^\theta{}_\theta = -p_0 + g\rho r\cos\theta - 3r\int_{\theta_0}^{\theta} G(\tau)\,d\tau,$$

containing just the one undetermined function $G(\theta)$, and where θ_0 is an arbitrary constant. If $G(\theta) = 0$, we have simply, in polar coordinates, the ordinary hydrostatic stress tensor for a liquid of density ρ.

We can express the profile in polar form,

$$x = r(\theta)\cos\theta, \quad y = r(\theta)\sin\theta, \tag{12}$$

so that θ will be the parameter t. Since at zero order $r(\theta) = b$, we can write

$$r(\theta) = b\{1 + \lambda(\theta)\}, \tag{13}$$

and $\lambda(\theta)$ must be assumed small. The right members of Eqs. (8) when X^i are the present coordinates, become, respectively, written out in full,

$$\frac{\partial\nu}{\partial r}\frac{\partial r}{\partial\nu}T^r{}_r + \frac{\partial\nu}{\partial\theta}\frac{\partial r}{\partial\nu}T^\theta{}_r + \frac{\partial\nu}{\partial r}\frac{\partial\theta}{\partial\nu}T^r{}_\theta + \frac{\partial\nu}{\partial\theta}\frac{\partial\theta}{\partial\nu}T^\theta{}_\theta,$$

$$\frac{\partial\nu}{\partial r}\frac{\partial r}{\partial t}T^r{}_r + \frac{\partial\nu}{\partial\theta}\frac{\partial r}{\partial t}T^\theta{}_r + \frac{\partial\nu}{\partial r}\frac{\partial\theta}{\partial t}T^r{}_\theta + \frac{\partial\nu}{\partial\theta}\frac{\partial\theta}{\partial t}T^\theta{}_\theta, \tag{14}$$

and we have to calculate the partial derivatives on the profile C.

For (x,y) on C, $\theta = t$, so that $\partial\theta/\partial t = 1$ while, from (13), $\partial r/\partial t = b\lambda'(\theta)$. Since ν is the distance from (x,y) positive in the outward-normal direction, if ψ is the angle between this direction and the positive x direction (see Fig. 1) we have, for a point on the normal, $x(\nu) = x + \nu\cos\psi$, $y(\nu) = y + \nu\sin\psi$, so that

$$\{r(\nu)\}^2 = r^2 + 2(x\cos\psi + y\sin\psi)\nu + \nu^2,$$
$$\tan\theta(\nu) = \frac{y + \nu\sin\psi}{x + \nu\cos\psi},$$

and we can find $\partial r/\partial\nu$, $\partial\theta/\partial\nu$ on C in terms of x, y, and ψ. Then with (12), (13), and the fact that $\cos\psi = y'/(x'^2 + y'^2)^{1/2}$, $\sin\psi = -x'/(x'^2 + y'^2)^{1/2}$, derivatives being with respect to θ, we can express the results in terms of $\lambda(\theta)$. Having the four partial derivatives $\partial r/\partial\nu, \ldots,$ we obtain the $\partial\nu/\partial r, \ldots,$ in terms of them and the Jacobian $\partial(r,\theta)/\partial(\nu,t)$, according to the well-known rule of the calculus of two variables. All the derivatives are evaluated on the profile C, whereas we need them on the parallel curve for

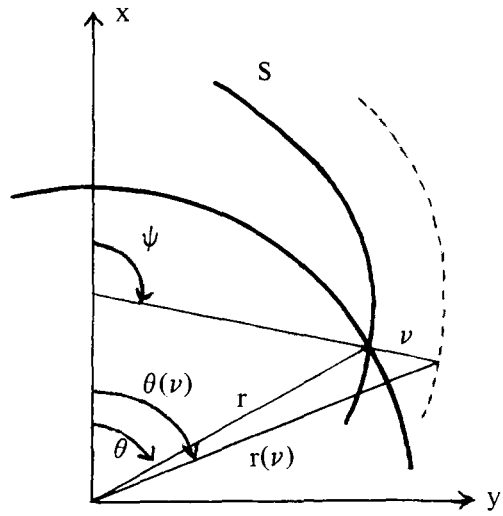

FIG. 1. The relationship of r,θ to ν,ψ.

$\nu = c_A$ (cf. Sec. 2), but the error is ignorable. Likewise, we can take dE_B/dt in (8) as $dE_B/d\theta$.

In this way and through (14), Eqs. (8) become the particular stress-matching equations appropriate to the general cylinder problem,

$$\frac{\epsilon E_B{}^2}{8\pi} - 2K_m(T + \Phi E_B) + g\omega x - \Gamma = \left(1 - \frac{\lambda'^2}{D^2}\right)T^r{}_r - \frac{b\lambda'(1+\lambda)^2}{D^2}T^\theta{}_r - \frac{\lambda'}{bD^2}T^r{}_\theta + \frac{\lambda'^2}{D^2}T^\theta{}_\theta,$$
$$\Phi\frac{dE_B}{d\theta} = \frac{b\lambda'(1+\lambda)}{D}T^r{}_r - \frac{b^2\lambda'^2(1+\lambda)}{D}T^\theta{}_r + \frac{1+\lambda}{D}T^r{}_\theta - \frac{b\lambda'(1+\lambda)}{D}T^\theta{}_\theta, \tag{15}$$
$$D = (1 + 2\lambda + \lambda^2 + \lambda'^2)^{1/2}.$$

We now proceed with the determination of $G(\theta)$ in (11), and understand clearly that we shall for the time being be working to the first power in whatever are the perturbation parameters, so that the result for $G(\theta)$ will be the first-order one. This means, expressing $\lambda(\theta)$ as

$$\lambda(\theta) = \eta(\theta) + \zeta(\theta) + \cdots, \tag{16}$$

where the nth term in the series is the contribution made to the solution at the nth stage of the perturbation process, that we require only $\eta(\theta)$. However, we cannot go wrong by retaining $\lambda(\theta)$ for the present, dropping powers and mutual products of this function and its derivatives, as they occur.

We approximate in this way, which involves taking into account (13) and the fact that $1/D$ in (15) can be expanded binomially, and also recognizing that there is nothing of zero order on the right of (11) except p_0, and hence find at once

from Eqs. (11) and the second of Eqs. (15) that, to the required order,

$$G(\theta)=\frac{\Phi}{b^2}\frac{dE_B}{d\theta}, \tag{17}$$

understanding, as explained in Sec. 4, that E_B comes from the solution of the field problem with the zero-order (cylindrical) profile. Now, substituting into the first of Eqs. (15) and approximating in exactly the same way, we obtain

$$\frac{\epsilon E_B{}^2}{8\pi}-2K_m(T+\Phi E_B)-g(\rho-\omega)b\cos\theta$$
$$=\Gamma^*-\frac{3}{2}\frac{\Phi}{b}E_B-\frac{1}{2}\frac{\Phi}{b}\frac{d^2E_B}{d\theta^2}, \tag{18}$$

where

$$\Gamma^*=\Gamma-p_0+\frac{3}{2}\frac{\Phi}{b}E_B(\theta_0), \tag{19}$$

and the problem of finding the first-order profile is reduced to finding λ satisfying, to this order, the single equation (18).

Now λ enters through the mean curvature K_m. We have seen that, two-dimensionally, $2K_m$ is the signed curvature κ of the profile, and this is given by the well-known polar formula

$$\kappa(\theta)=\frac{1}{r}\left\{1+\frac{2}{r^2}\left(\frac{dr}{d\theta}\right)^2-\frac{1}{r}\frac{d^2r}{d\theta^2}\right\}\left\{1+\frac{1}{r^2}\left(\frac{dr}{d\theta}\right)^2\right\}^{-3/2}. \tag{20}$$

We now go through again the kind of approximation procedure, in terms of λ, described above, and in this way, with some small algebraic manipulations and replacement of λ by η [Eq. (16)], (18) becomes

$$\frac{d^2\eta}{d\theta^2}+\eta=\Delta+\frac{g(\rho-\omega)b^2}{T}\cos\theta-\frac{\epsilon bE_B{}^2}{8\pi T}$$
$$-\frac{1}{2}\frac{\Phi}{T}E_B-\frac{1}{2}\frac{\Phi}{T}\frac{d^2E_B}{d\theta^2}, \tag{21}$$

in which

$$\Delta=b\Gamma^*/T+1, \tag{22}$$

and which is a simple differential equation for η.

If we were working to the order zero, we should have at this stage $\Delta=0$, with $\Gamma^*=\Gamma-p_0$ [from (19)] and Γ the external (constant) hydrostatic pressure p_1 in B, providing the well-known elementary formula (for a cylinder), $T/b=p_0-p_1$, relating surface tension to the pressure difference. Now, we cannot speak of Γ and p_0 as "pressures"; they are just constants in the actual stress system. On integrating (21), two constants will appear in addition to Δ, and then all three will be fixed, along with the first-order profile itself, by compliance with three given conditions, which we call end conditions, representing constraints upon the liquid A. The end conditions which we find useful in practice are that, for distinct values θ_1 and θ_2 of θ,

$$r'(\theta_1)=0,\quad r'(\theta_2)=0,\quad r(\theta_2)=b, \tag{23}$$

implying by (13) and (16), when we are working to the first order, that

$$\eta'(\theta_1)=\eta'(\theta_2)=\eta(\theta_2)=0. \tag{24}$$

This is, of course, but one of various possibilities.

Now suppose that we can solve (21) with $\Phi=0$, replacing Δ by Δ_0 obtained by taking $\Phi=0$ in (19). Let us call the result which satisfies the end conditions (24), η_0. Then this gives the first-order profile as determined just by surface tension, weight, and the "classical" electrostatic action, taking no account of the applied field acting upon the double layer. But we can write (21) as

$$\frac{d^2}{d\theta^2}\left\{\eta+\frac{1}{2}\frac{\Phi}{T}E_B(\theta)-\frac{3}{2}\frac{\Phi}{T}E_B(\theta_0)\right\}$$
$$+\left\{\eta+\frac{1}{2}\frac{\Phi}{T}E_B(\theta)-\frac{3}{2}\frac{\Phi}{T}E_B(\theta_0)\right\}$$
$$=\Delta_0+\frac{g(\rho-\omega)b^2}{T}\cos\theta-\frac{\epsilon b\{E_B(\theta)\}^2}{8\pi T}, \tag{25}$$

having used the fact that $\Delta=\Delta_0+\frac{3}{2}(\Phi/T)E_B(\theta_0)$,, and this is the same differential equation as for η_0 except for the replacement of η_0 by a new dependent variable. Thus immediately, the solution for η is

$$\eta=\eta_0-\frac{1}{2}\frac{\Phi}{T}E_B(\theta)+\frac{3}{2}\frac{\Phi}{T}E_B(\theta_0)$$
$$+C_1\cos\theta+C_2\sin\theta, \tag{26}$$

a complementary function with constants C_1 and C_2 appearing on the right. We have finally to ensure that η satisfies (24), and this gives us

$$E_B(\theta_0)=\tfrac{1}{3}\{E_B(\theta_2)-E_B'(\theta_1)\csc(\theta_2-\theta_1)$$
$$+E_B'(\theta_2)\cot(\theta_2-\theta_1)\},$$
$$C_1=\frac{1}{2}\frac{\Phi}{T}\{E_B'(\theta_1)\cos\theta_2-E_B'(\theta_2)\cos\theta_1\}$$
$$\times\csc(\theta_2-\theta_1), \tag{27}$$
$$C_2=\frac{1}{2}\frac{\Phi}{T}\{E_B'(\theta_1)\sin\theta_2-E_B'(\theta_2)\sin\theta_1\}$$
$$\times\csc(\theta_2-\theta_1).$$

We note that, with this determination of the constants, θ_0 is fixed,[16] representing determination of the first-order stress system (11) within the extent of the constant p_0.

Any specific problem presents a certain differential equation for η_0 whose prediction is, indeed, the same as it would be classically, and the remarkable result we have attained is (26), whose meaning is that the applied-field–double-layer effect is simply added on in a standard way, with no more equation solving. Still more remarkably, this phenomenon recurs at the second order (higher orders have not been tested). The second-order theory itself evolves by working to the second approximation in the theory above, with η known, so that we retain ζ [Eq. (16)], unknown and to be determined, along with known η^2, $\eta\eta'$, and η'^2. We consider no more description necessary.

6. THE GENERAL SPHERE PROBLEM

The theory of the general sphere problem is so closely parallel to that for the general cylinder problem that it will be sufficient to just write down analogs of formulas in Sec. 5 and

comment on points of significant difference. The reader who is more interested in applications could, with small sacrifice, proceed straight to Sec. 7.

The coordinate system X^i is spherical polar coordinates (r,θ,ϕ), related to our Cartesian system by $x = r\cos\theta$, $y = r\sin\theta\cos\phi$, $z = r\sin\theta\sin\phi$, and the zero-order profile is a circular arc $r = b$. A major difference, characteristic of stress theory, is that notwithstanding axial symmetry, we have to take into account the stress component $T^{\phi}{}_{\phi}$. We then find that the appropriate particular expression of (6) is

$$\begin{aligned}
&\frac{\partial T^{r}{}_{r}}{\partial r} + \frac{\partial T^{\theta}{}_{r}}{\partial \theta} + \frac{1}{r}(2T^{r}{}_{r} - T^{\theta}{}_{\theta} - T^{\phi}{}_{\phi}) \\
&\quad + T^{\theta}{}_{r}\cot\theta = g\rho\cos\theta, \\
&\frac{\partial T^{r}{}_{\theta}}{\partial r} + \frac{\partial T^{\theta}{}_{\theta}}{\partial \theta} + (T^{\theta}{}_{\theta} - T^{\phi}{}_{\phi})\cot\theta \\
&\quad + \frac{1}{r}T^{r}{}_{\theta} + rT^{\theta}{}_{r} = -g\rho r\sin\theta, \\
&(1/r)\,T^{r}{}_{\theta} = rT^{\theta}{}_{r}.
\end{aligned} \tag{28}$$

We assume now

$$T^{r}{}_{r} = -p_0 + M(r)F(\theta), \quad T^{\theta}{}_{r} = G(\theta), \quad T^{r}{}_{\theta} = r^2 G(\theta), \tag{29}$$

$$T^{\theta}{}_{\theta} = T^{\phi}{}_{\phi} = -p_0 + N(r)H(\theta)$$

and obtain, corresponding to (11), the solution

$$\begin{aligned}
T^{r}{}_{r} &= -p_0 + g\rho r\cos\theta - \tfrac{8}{3}r\int_{\theta_0}^{\theta} G(\tau)\,d\tau \\
&\quad - \tfrac{1}{3}rG'(\theta) - \tfrac{1}{3}rG(\theta)\cot\theta,
\end{aligned} \tag{30}$$

$$T^{\theta}{}_{r} = G(\theta), \quad T^{r}{}_{\theta} = r^2 G(\theta),$$

$$T^{\theta}{}_{\theta} = T^{\phi}{}_{\phi} = -p_0 + g\rho r\cos\theta - 4r\int_{\theta_0}^{\theta} G(\tau)\,d\tau.$$

The zero-order profile being a circular arc, we again have (13), leading to exactly the same particular stress-matching equations (15). We hence obtain the same first-order result (17) for $G(\theta)$, but because of the different formula for $T^{r}{}_{r}$, the analog of (18) is different. So is the expression for K_m which, as we have said, is not now half the ordinary curvature of the profile (cf. Eisenhart,[11] p. 227, example 4; the explicit expression is given by Cade[8]). Now the same derivation but with these differences leads to the analog of (21),

$$\begin{aligned}
&\frac{d^2\eta}{d\theta^2} + \cot\theta\frac{d\eta}{d\theta} + 2\eta \\
&\quad = \Delta + \frac{g(\rho-\omega)b^2}{T}\cos\theta - \frac{\epsilon b E_B{}^2}{8\pi T} \\
&\quad - \frac{2}{3}\frac{\Phi}{T}E_B - \frac{1}{3}\frac{\Phi}{T}\frac{d^2E_B}{d\theta^2} - \frac{1}{3}\frac{\Phi}{T}\frac{dE_B}{d\theta}\cot\theta,
\end{aligned} \tag{31}$$

$$\Delta = \frac{b\Gamma^*}{T} + 2, \quad \Gamma^* = \Gamma - p_0 + \frac{8}{3}\frac{\Phi}{b}E_B(\theta_0).$$

From this point, and with the same end conditions (24), the same procedure, with only differences of detail, goes through as led from (21) to (26). If η_0 is the solution of (31) when $\Phi = 0$, the actual solution of (31) is

$$\begin{aligned}
\eta &= \eta_0 - \frac{1}{3}\frac{\Phi}{T}E_B(\theta) + \frac{8}{3}\frac{\Phi}{T}E_B(\theta_0) \\
&\quad + C_1\cos\theta + C_2 Q_1(\cos\theta),
\end{aligned} \tag{32}$$

where Q_1 is the Legendre function of the second kind, of order 1, and the constants C_1, C_2, and θ_0 are given by

$$\begin{aligned}
E_B(\theta_0) &= \frac{1}{8}\left\{E_B(\theta_2) - \frac{E'_B(\theta_1)}{\delta}\right. \\
&\quad \times [Q'_1(\cos\theta_2)\cos\theta_2 + Q_1(\cos\theta_2)\sin\theta_2] \\
&\quad \left. + \frac{E'_B(\theta_2)}{\delta}[Q'_1(\cos\theta_1)\cos\theta_2 + Q_1(\cos\theta_2)\sin\theta_1]\right\}, \\
C_1 &= \frac{1}{3}\frac{\Phi}{T}\{E'_B(\theta_1)Q'_1(\cos\theta_2) - E'_B(\theta_2)Q'_1(\cos\theta_1)\}\frac{1}{\delta}, \\
C_2 &= \frac{1}{3}\frac{\Phi}{T}\{E'_B(\theta_1)\sin\theta_2 - E'_B(\theta_2)\sin\theta_1\}\frac{1}{\delta}, \\
\delta &= Q'_1(\cos\theta_1)\sin\theta_2 - Q'_1(\cos\theta_2)\sin\theta_1.
\end{aligned} \tag{33}$$

7. SOME SPECIFIC FIRST-ORDER SPHERE AND CYLINDER PROBLEMS

Consider the upward-facing horizontal plane surface of a solid conductor, having a straight groove of uniform width $2b$, and in the groove conducting liquid bulging above to an extent controllable by a pressure head, as shown sectionally in Fig. 2. Let this liquid be the liquid A, of density ρ, and above A is B, which is empty space or a nonconducting fluid of density $\omega \leqslant \rho$. By adjusting the pressure head we can force a situation in which the interface meets the conducting plane perpendicularly (see Fig. 2), and if $\omega = \rho$ and no electric field is applied, we have a two-dimensional case in which the surface is half a cylinder, that is to say, the profile a semicircle. With these special conditions, the actual profile coincides with what would otherwise be the zero-order profile. The corresponding axisymmetric arrangement, in which the zero-order surface is a hemisphere, is one in which, instead of a groove, we have a circular notch of radius b.

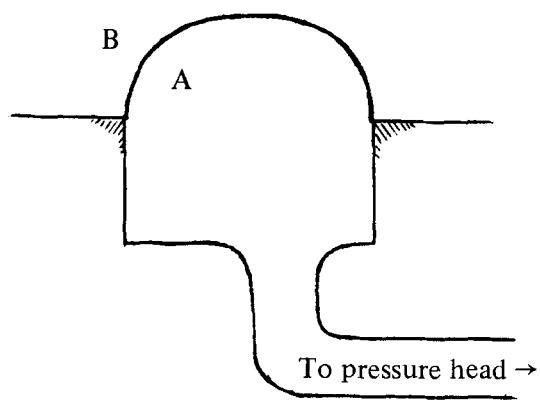

FIG. 2. The practical realization of a quasicircular-cylindrical (or quasi-spherical) liquid surface.

The above description is of what were previously called sessile-drop problems (Cade[8,9]), the experimental arrangement being that conceived for the practical realization of two- and three-dimensional sessile drops with fixed base dimension $2b$ and contact angle $\frac{1}{2}\pi$. Suppose that, in either case, the solid conductor and liquid A are at zero potential, and that the system is subjected to a uniform applied field which is vertical and of strength F, reckoned positive if the direction is upward (i.e., of x increasing). This could be realized (approximately) if the solid conductor were the lower member of a pair of condenser plates. The first-order electrostatic problems, whose solutions will give E_B for the first-order theory of the last two sections are: two-dimensionally, that of a conducting plane with semicylindrical prominence and three-dimensionally, that of a conducting plane with hemispherical boss, the external influence in each case being the said uniform field and the boundary condition, potential zero.[17] Solution of these problems by the method of electrical images is elementary (see Jeans[1]), giving in the respective two- and three-dimensional cases

$$E_B = 2F\cos\theta, \quad E_B = 3F\cos\theta. \tag{34}$$

The conditions of the "contact angle" of $\frac{1}{2}\pi$ and base dimension $2b$, along with symmetry and smoothness about the intersecting x axis, imply end conditions which are (23) with $\theta_1 = 0$, $\theta_2 = \frac{1}{2}\pi$.

With (34) and these end conditions, we find at once from (27) and (33) that $E_B(\theta_0) = 0$, $C_2 = 0$, while in (26) and (32), the C_1 term exactly cancels the $E_B(\theta)$ term. Thus in both cases $\eta = \eta_0$, representing that there is no Φ effect.

We introduce the perturbation parameters

$$\alpha = \frac{g(\rho-\omega)b^2}{T}, \quad \beta = \frac{F\Phi}{T}, \quad \gamma = \frac{\epsilon F^2 b}{2\pi T} \tag{35}$$

(we do not, according to what has just been said, need β at present), and then, from (21) and (31), putting $\Phi = 0$ and using subscript 0, we obtain as the respective equations for η_0

$$\frac{d^2\eta_0}{d\theta^2} + \eta_0 = \Delta_0 + \alpha\cos\theta - \gamma\cos^2\theta, \tag{36}$$

$$\frac{d^2\eta_0}{d\theta^2} + \cot\theta\frac{d\eta_0}{d\theta} + 2\eta_0 = \Delta_0 + \alpha\cos\theta - \tfrac{9}{4}\gamma\cos^2\theta. \tag{37}$$

The method of solution particularly suitable for these equations is variation of parameters (see any text on ordinary differential equations, e.g., Ince[18]). Carrying out the solution with use of the end conditions, and then (13) with η replaced by η_0, we obtain as the first-order profiles for the respective two- and three-dimensional cases,

$$r = b\{1 + \tfrac{1}{2}\alpha(\theta\sin\theta + \cos\theta - \tfrac{1}{2}\pi) + \tfrac{1}{3}\gamma\cos^2\theta\}, \tag{38}$$

$$r = b\{1 - \tfrac{1}{3}\alpha\cos\theta\ln(1+\cos\theta) + \tfrac{9}{16}\gamma\cos^2\theta\}. \tag{39}$$

These solutions are exactly as would be obtained classically, there being, as we have said, no Φ effect.

The conclusion is different for the cylinder problem in which everything is the same except that we have a different applied field. Instead of a field given to be uniform, we shall have that due to a uniform line charge of amount f per centimeter, parallel to the generators of the cylinder and passing through the point $(c,0)$ $(c > b)$ of the xy plane.

We shall not burden this exposition with the solution of the first-order electrostatic problem. It is obtained quite quickly by simple cylindrical harmonics, and still more quickly using the two-dimensional form of Robin's integral equation (see Durand[19]). In fact, the solution of Robin's equation is the surface-charge density, and a rule of elementary electrostatics (Coulomb's theorem) gives us at once E_B,

$$E_B(\theta) = \frac{8f}{\epsilon}\frac{c(b^2-c^2)\cos\theta}{(b^2+c^2)^2 - 4b^2c^2\cos^2\theta}. \tag{40}$$

We use the same perturbation parameter α as in (35), but replace β and γ there by

$$\tilde{\beta} = \frac{2f\Phi}{\epsilon bT}, \quad \tilde{\gamma} = \frac{2f^2}{\pi\epsilon bT}, \tag{41}$$

and it is convenient to introduce the dimensionless constants

$$a = \frac{b^2+c^2}{2bc}, \quad a' = \frac{b^2-c^2}{2bc}, \tag{42}$$

noting that

$$a'^2 = a^2 - 1. \tag{43}$$

Then the equation for η_0, η without the Φ effect, is

$$\frac{d^2\eta_0}{d\theta^2} + \eta_0 = \Delta_0 + \alpha\cos\theta - \frac{\tilde{\gamma}a'^2\cos^2\theta}{(a^2-\cos^2\theta)^2}, \tag{44}$$

which is solvable by variation of parameters, while the Φ effect is brought in by using (40) with (26) and (27), our having, as before, that $\theta_1 = 0$, $\theta_2 = \frac{1}{2}\pi$. The solution for η, used in place of λ in (13), gives by that equation the first-order profile, which is

$$\begin{aligned} r = b\Big\{1 &+ \tfrac{1}{2}\alpha(\theta\sin\theta + \cos\theta - \tfrac{1}{2}\pi) \\ &+ \tilde{\beta}a'\cos\theta\left(\frac{1}{a^2} - \frac{1}{a^2-\cos^2\theta}\right) \\ &+ \frac{1}{2}\tilde{\gamma}a'\left[\frac{a'}{2a}\left(\cos\theta\ln\frac{a+\cos\theta}{a-\cos\theta}\right.\right. \\ &+ \left.\left.\left(1 - \frac{1}{a'^2}\right)\sin\theta\arctan(\sin\theta/a') - \arctan\frac{1}{a'}\right)\right]\Big\}. \end{aligned} \tag{45}$$

8. THE SECOND-ORDER CYLINDER AND UNIFORM FIELD PROBLEM

Returning to the two-dimensional uniform-field situation, the condition that the potential should vanish on the line $x = 0$ and on the first-order profile (38), is the boundary condition for the second-order field problem for the electrohydrostatic problem as a whole. If we calculate this field (to the extent of E_B), there is no difficulty in principle in calculating the second-order profile, according to the procedure indicated briefly at the end of Sec. 5.

In fact, the electrostatic problem is not an elementary one, but we can nevertheless find E_B to the first order in α and γ (which is all we require) by applying a perturbation process to Robin's integral equation. This has been done before (Cade[9]), but the result was wrong on account of the first-order profile obtained by the early considerations being wrong. However, the difference is only a question of values of constant factors, and using the correct profile (38), the

previous second-order field solution can be corrected at once by a mere change of a constant, to give

$$E_B(\theta) = F\Big\{2\cos\theta - \alpha[(\theta\sin\theta + \cos\theta - 6/\pi)\cos\theta + (1/\pi)\sin 2\theta \ln(\sec\theta + \tan\theta) + (2/\pi)\cos 2\theta\Psi(\theta)] \times \tfrac{1}{3}\gamma\cos 3\theta\Big\}, \tag{46}$$

where

$$\Psi(\theta) = \int_\theta^{\pi/2} \ln(\sec t + \tan t)dt. \tag{47}$$

This function is related to Clausen's integral,

$$\mathrm{Cl}(\theta) = -\int_0^\theta \ln(2\sin\tfrac{1}{2}t)dt, \tag{48}$$

by

$$\Psi(\theta) = 2\mathrm{Cl}(\tfrac{1}{2}\pi + \theta) + \tfrac{1}{2}\mathrm{Cl}(\pi - 2\theta), \tag{49}$$

and tables of $\mathrm{Cl}(\theta)$ have been given by, among others, Ashour and Sabri[20] and Lewin.[21]

The process outlined at the end of Sec. 5 leads to a differential equation with the same left member as (21) but with the replacement of η by ζ [Eq. (16)], and a right member which is very much more complicated, and as we said, the situation is one in which we solve for ζ_0, ζ with no Φ effect, and simply add on the Φ effect afterwards, now using the end conditions $\zeta'(0) = \zeta'(\frac{1}{2}\pi) = \zeta(\frac{1}{2}\pi) = 0$. The solution process for ζ_0, by variation of parameters, is laborious in the extreme, but once complete, complementing it with the Φ terms is relatively easy.

The final result for the second-order profile, in terms of the perturbation parameters (35), is

$$r = b\{1 + \tfrac{1}{2}\alpha(\theta\sin\theta + \cos\theta - \tfrac{1}{2}\pi) + \tfrac{1}{3}\gamma\cos^2\theta - \tfrac{1}{2}\alpha^2 f_1(\theta) + \tfrac{1}{45}\gamma^2 f_2(\theta) + \tfrac{1}{2}\alpha\beta f_3(\theta) - \tfrac{1}{6}\beta\gamma f_4(\theta) + \gamma\alpha f_5(\theta)\},$$

$$f_1(\theta) = \tfrac{3}{4}\pi(\theta\sin\theta + \cos\theta - \tfrac{1}{2}\pi) + (1 + \tfrac{1}{4}\theta^2)\cos^2\theta,$$

$$f_2(\theta) = 10 - 17\sin^2\theta + 7\sin^4\theta,$$

$$f_3(\theta) = \left(\theta\sin\theta + \cos\theta + \frac{2}{\pi} - \frac{\pi}{2}\right)\cos\theta + \frac{1}{\pi}\sin 2\theta\ln(\sec\theta + \tan\theta) + \frac{2}{\pi}\cos 2\theta\Psi(\theta),$$

$$f_4(\theta) = 3\cos\theta + \cos 3\theta,$$

$$f_5(\theta) = (\pi^2/32 + \tfrac{2}{3} + \tfrac{1}{48}\sin^2\theta)\cos\theta - (\pi/6 - 9/8\pi)\cos^2\theta + \tfrac{11}{16}(\theta\sin\theta - \tfrac{1}{2}\pi) + \tfrac{1}{24}(\sin 2\theta - 3\theta)\theta\cos\theta - \frac{5}{8\pi}\sin\theta\cos^2\theta\ln(\sec\theta + \tan\theta) + \frac{1}{8\pi}(3 + 4\sin^2\theta)\cos\theta\Psi(\theta) + \frac{1}{2\pi}\{\sin\theta\Omega(\theta) - \Omega(\tfrac{1}{2}\pi)\}, \tag{50}$$

where

$$\Omega(\theta) = \int_0^\theta \Psi(t)dt. \tag{51}$$

This function, which was tabulated by the present author,[9] is also, like Ψ, related in a simple way to one tabulated by Lewin.[21]

9. DISCUSSION

We anticipated in Sec. 1 the fact that the Φ terms in a profile solution will predict a differential effect upon the profile on field reversal. Clearly, this differential effect would be the property to use in an experiment aimed at the measurement of Φ, as it separates off qualitatively the Φ effect from the weight effect and the "classical" electrostatic deformation. In fact, the differential maximum height h_d is what, no doubt, one would measure. Denoting the solution (45) by $r(f,\theta)$ and (50) by $r(F,\theta)$, we shall have $h_d = r(f,0) - r(-f,0)$ in the former case, and $h_d = r(F,0) - r(-F,0)$ in the latter. Thus, referring to the definitions (35) and (41) of the perturbation parameters, we find at once for the former, first-order line-charge profile,

$$h_d = -2\tilde{\beta}/a'a^2 \tag{52}$$

[having used (43)], while for the latter, second-order uniform-field profile,

$$h_d = \beta\left\{\alpha\left[1 - \frac{\pi}{2} + \frac{2}{\pi}(1 + \Psi(0))\right] - \tfrac{4}{3}\gamma\right\}. \tag{53}$$

Taking an experimental arrangement as described in Sec. 7 one would, presumably, choose for the liquid A a weak electrolyte. For we require only that A be a conductor, and in this way we have the best chance of avoiding difficulties which might arise with strong electrolytes or liquid metals (distortion of the double layer v, Sec. 2). In the second place, using for A an aqueous solution, it would be easy to obtain a nonconducting liquid B which was transparent and of *nearly the same density*, which should allow the half-width b of the groove to be relatively large, facilitating measurement.

The absence of Φ effects from the first-order uniform-field profiles (38) and (39) might be seen as a distant consequence of the elementary fact that a dipole experiences no force in a uniform field, although this facile observation is not in itself sufficient without some elaboration. There are practical implications. For, expecting effects to be generally small, one would, experimentally, wish to use a large field. But in the line-charge case, where the field would presumably be provided by a thin wire, its largeness at the liquid surface would be limited by considerations of dielectric breakdown, since it would be so much larger close to the wire. In the uniform-field case one could, indeed, have a very large field. But then the effect itself, being of second order, would, for a given order of field, be much smaller.

The optimum theoretical basis for an experiment would be a first-order profile which contains a Φ effect but for which the applied field, although no doubt nonuniform, does not, in the theory, become infinite anywhere. But it is precisely here that one meets the greatest obstacle to finding specific profile solutions, namely, in the difficulty of solving the electrostatic problems involved. Further progress from the quantitative physical point of view would seem to lie with seeking and solving a problem such as we have just described.

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[14]In other words, the medium whose bulk is regarded as the interior region. Previously (Ref. 10), the criterion "higher-density" was used instead of "interior." For practical purposes the conventions are equivalent except for the present one having the advantage of fixing the sign even when the densities are equal.
[15]But retaining the correct sign; for it is the convention of differential geometry to define the curvature of a curve as a nonnegative.
[16]Provided that the first of Eqs. (27), as an equation for θ_0, has only one solution. In any case, it is seen by applying (17) to (11) that the inference to follow is still true.
[17]Consistently with the presence of double layers at the liquid A and plane-conductor surfaces, there must be phase-boundary potentials (contact potentials), and these destroy the zero-potential boundary condition. However, the E_B that we require is by superposition of the classical solution with the pure double-layer field *outside the double layer*, and the latter is normally very small in relation to the applied field used in an electrostatic experiment. On these grounds, there seems to be little doubt that our procedure is justified.
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Erratum: Structure and representations of the symmetry group of the four-dimensional cube [J. Math. Phys. 23, 944 (1982)]

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(Received 3 August 1982; accepted for publication 11 August 1982)

PACS numbers: 02.20.Qs, 02.20.Rt, 99.10. + g

(1) Page 944, in the middle of the left column: Delete

$$e_4 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix},$$

and replace it by

$$e_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

(2) Page 946, left column, line 14: Delete the comma before $\sim_{W_4}$, i.e., write "Then $(\mathbf{a},\pi) \sim_{W_4} (\mathbf{b},\sigma)\cdots$."

(3) Page 946, right column, line 11: Replace $T_{ij}(\mathbf{a},\pi)$ by $T_{ji}(\mathbf{a},\pi)$.

(4) Page 946, right column, between lines 28 and 29: Insert

$(\mathbf{a},\pi) \mapsto \operatorname{sgn}[\Phi(\mathbf{a},\pi)]$ ("signum S_8").

(5) Page 946, left column, line 22: Delete $1 \leqslant n \leqslant \operatorname{ord} \pi$ and replace it by $1 \leqslant n < \operatorname{ord} \pi$.