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A Perturbation Method for the Classical Time-Dependent Pair Correlation Function

RAPHAEL ARONSON
Department of Nuclear Engineering, New York University, New York, New York
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A perturbation technique useful for computing many-time thermal averages of classical quantities is developed. The canonical distribution function for the system is shown to evolve isothermally from that for a free-particle system as the interaction is switched on slowly. This permits convenient use of an interaction picture in which to perform thermal averaging. The technique is applied to the calculation of the time-dependent pair correlation function in position for a uniform gas. The correlation function is shown to be a sum of two components, one the solution of a kinetic equation and essentially a generalization of the autocorrelation in equilibrium, the other a generalization of the mutual correlation function in equilibrium. The equations arise as sums over diagrams. The equations resulting from the random phase approximation, valid for the short-time behavior, are solved exactly. It is shown directly that the generalized dielectric function given in terms of the correlation function is identical with that found by solution of the kinetic equation in the random phase approximation for all frequencies.

I. INTRODUCTION

IT has been shown by many authors[1-3] that transport coefficients can be given in terms of time-dependent pair correlation functions determined in equilibrium. More generally, the two-particle correlation functions describe a large number of macroscopic properties and serve as links between the microscopic and macroscopic worlds.

This paper describes a perturbation approach to the calculation of time- and space-dependent pair correlation functions in equilibrium. We consider classical systems with velocity-independent pair interactions. The basic formalism is introduced in Sec. II.

Since we are interested in two-time (or more generally, many-time) averages, we do not wish to give any particular emphasis to time zero. For that reason we consider in Sec. III the motion of the system in purely dynamical terms. All correlations including those initially present in the actual system are regarded as resulting from an initial free-particle distribution when the interactions are turned on slowly. The point of view corresponds to that of an interaction picture.

The resulting expression for the pair correlation function can be pictured in terms of the diagrams introduced by Prigogine.[4] It turns out that in the thermodynamic limit as the volume and the number of particles go to infinity, with the density remaining finite, only two types of diagrams contribute. The correlation functions are found in terms of the solutions of the corresponding integral equations. These equations are obtained in Sec. IV.

In Sec. V the equations are solved in the random

[1] M. S. Green, J. Chem. Phys. **22**, 398 (1954).
[2] R. Kubo, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience Publishers, Inc., New York, 1960) Vol. I; J. Phys. Soc. Japan **12**, 570 (1957).
[3] P. Mazur, in *Fundamental Problems in Statistical Mechanics*, edited by E. G. D. Cohen (Interscience Publishers, Inc., New York, 1962).
[4] I. Prigogine, *Non-Equilibrium Statistical Mechanics*, (Interscience Publishers, Inc., New York, 1962).

phase approximation (RPA).[5] The well-known result that in the RPA the generalized dielectric function[6] obtained from the kinetic equation is the same as that found by a response function method for all frequencies[7] is domonstrated directly for classical systems.

The relation of the time-dependent theory to the equilibrium theory is discussed in Sec. VI.

II. BASIC FORMALISM

Consider a classical system of N particles with Hamiltonian H. The Liouville equation for the distribution function φ_S can be written[4]

$$i\,\partial\varphi_S(t)/\partial t = L\varphi_S(t), \tag{2.1}$$

where the Liouville operator L is defined as

$$L = -i\sum_{i=1}^{N} \partial_i H\cdot\nabla_i + i\sum_{i=1}^{N}\nabla_i H\cdot\partial_i. \tag{2.2}$$

Here ∂_i is the gradient with respect to the momentum of the ith particle. In terms of the Poisson bracket $\{\ \}$,

$$L\varphi = i\{H, \varphi\}. \tag{2.3}$$

We will be concerned with averages over the distribution function of functions of the positions and momenta of the N particles. If $f(\Gamma) = f(\{\mathbf{r}_i\}, \{\mathbf{p}_i\})$ is such a function, its average at time t is

$$\langle f(t)\rangle_S = \int d\Gamma\, f(\Gamma)\varphi_S(t), \tag{2.4}$$

where $\varphi_S(t)$ is a solution of (2.1).[8] Here Γ represents a point in phase space.

Since L is Hermitian, as can be shown quite easily, (2.1) is similar in form to the Schrödinger equation, which is why we have used the subscript S. The major difference is that L is not positive-definite, but its eigenvalues appear in pairs $\pm\lambda_i$. The solution to (2.1) can be written

$$\varphi_S(t) = e^{-iLt}\varphi_S(0). \tag{2.5}$$

The equilibrium distribution is stationary, so it is given by

$$L\varphi_S = 0. \tag{2.6}$$

On the other hand we can introduce a "Heisenberg" picture too. A function $f_H(t) = f[\Gamma(t)]$ changes in time with the motion of the system. Since $\partial f_H(t)/\partial t = 0$,

$$\frac{Df_H(t)}{Dt} = -\{H, f_H\} = iLf_H(t), \tag{2.7}$$

with the solution

$$f_H(t) = e^{iLt}f_H e^{-iLt}. \tag{2.8}$$

The factor $\exp(-iLt)$ is inserted after f because $f(t)$ will be used in expressions multiplied by something on the right and the exponential factor is supposed to act on f only. Here $f = f(0) = f_S = f_H(0)$. We identify also $\varphi_H = \varphi_S(0) = \varphi(0)$. In terms of $f_H(t)$, the average at time t is given by

$$\langle f(t)\rangle_H = \int d\Gamma\, f_H(t)\varphi_H. \tag{2.9}$$

By virtue of (2.5), (2.8), and the easily verifiable fact that

$$\int d\Gamma\, LF = 0 \tag{2.10}$$

for any function F of interest (assuming periodic boundary conditions in configuration space) and for any Hamiltonian, the average (2.9) gives a result identical to (2.4). We have equivalent "Schrödinger" and "Heisenberg" pictures. The latter is, however, more useful because it enables us to define many-time averages. Thus

$$\langle f_1(t_1)\cdots f_n(t_n)\rangle_H = \int d\Gamma\, f_{1H}(t_1)\cdots f_{nH}(t_n)\varphi(0). \tag{2.11}$$

It is important to note that by (2.7) *any* constant of the motion is a solution of (2.6). In most quantum mechanical problems the ground state is assumed nondegenerate. Here the "ground state," given by $L = 0$, is highly degenerate.

For our purposes it is most convenient to work in an interaction picture.[9] Interaction picture variables will be written without subscripts. We break the Hamiltonian into an unperturbed part H_0 and a perturbation H'. Correspondingly, we have $L = L_0 + L'$. We define

$$f(t) = \exp(iL_0t)f\exp(-iL_0t). \tag{2.12}$$

L' is also assumed to develop in time according to

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[5] D. Bohm and D. Pines, Phys. Rev. **82**, 625 (1951); Phys. Rev. **85**, 338 (1952).

[6] That is, with the Coulomb potential replaced by an arbitrary potential $v(\mathbf{r})$.

[7] D. Pines, J. Nucl. Energy **2**, Part C, 5 (1961).

[8] The expectation value $\langle f(t)\rangle$ given by (2.4) can be put in symmetric form to resemble a quantum mechanical expectation value. Since φ_s is positive-definite, we may define $\psi_s(t) = [\varphi_s(t)]^{\frac{1}{2}}$. Then $\langle f(t)\rangle = \langle\psi_s(t)|\, f\,|\psi_s(t)\rangle$. The form (2.4), though, seems more useful.

[9] See, for instance, S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson and Company, Evanston, Illinois, 1961), Chap. 11.

(2.12). The Liouville equation becomes

$$i(\partial\varphi(t)/\partial t) = L'(t)\varphi(t). \tag{2.13}$$

The solution can be written

$$\varphi(t) = U(t, t')\varphi(t'), \tag{2.14}$$

where $U(t, t')$ is the unitary time-development operator

$$U(t, t') = \left[\exp\left(-i\int_{t'}^{t} L'(t'')\,dt''\right)\right]_+. \tag{2.15}$$

The symbol $[\ ]_+$ will be used to indicate that non-commuting factors in the bracket are to be ordered from right to left according to increasing time of their arguments. Then the average $\langle f(t)\rangle$ is given by

$$\langle f(t)\rangle = \int d\Gamma\, f(t)\varphi(t). \tag{2.16}$$

Since (2.10) holds for both L_0 and L' and

$$[\exp(-iL_0t)]U(t, 0) = \exp(-iLt),$$

Eq. (2.16) gives the same result as (2.4) and (2.9). The unitarity of U follows also; that is, for any F of interest,

$$\int d\Gamma\, U(t, t')F = \int d\Gamma\, F. \tag{2.17}$$

In particular,

$$\langle U(t, t')\rangle = 1. \tag{2.18}$$

The unperturbed motion is just the free-particle motion of the system, so H_0 is the kinetic energy. Then

$$L_0 = -i\sum_{i=1}^{N} \mathbf{v}_i\cdot\nabla_i \tag{2.19}$$

and

$$f(t) = f(\{\mathbf{r}_i + \mathbf{v}_it\}, \{\mathbf{p}_i\}), \tag{2.20}$$

where $\mathbf{v}_i$ is the velocity of the ith particle.

III. DEVELOPMENT OF THE DISTRIBUTION FUNCTION AS PERTURBATION IS TURNED ON

The two-particle correlation functions are averages of the form (2.11). The equilibrium distribution $\varphi = \varphi(0)$ is canonical. Then

$$\langle f_1(t_1)f_2(t_2)\rangle_H = \int d\Gamma\, f_1 \times \exp[iL(t_1 - t_2)]f_2e^{-\beta H}/(d\Gamma\, e^{-\beta H}), \tag{3.1}$$

where $\beta = 1/k_BT$. The correlations at time t_2 are included in $e^{-\beta H}/(d\Gamma e^{-\beta H})$, and the subsequent motion of the system is described by the propagator $\exp[-iL(t_1 - t_2)]$.

In order to avoid this rather awkward singling out of time zero (or t_2), we want to adopt the quantum mechanical procedure of turning on the perturbation slowly, starting from a free-particle system, and taking interaction picture averages. It is not *a priori* clear that the procedure can be carried out with the Liouville operator. It requires, first, that there exists a stationary solution of the free-particle Liouville equation that develops into the canonical distribution over which we wish to average as the interaction is turned on; and second, that this solution can be written down explicitly out of the infinity of stationary solutions of the Liouville equation. It will be shown that this procedure is in fact possible for perturbations which depend on position only.

In order to point up the differences from the usual quantum mechanical situation, we will proceed in the standard way.[9] Let φ_0 be an arbitrary stationary distribution for the unperturbed system. Then

$$L_0\varphi_0 = 0. \tag{3.2}$$

The interaction part of the Hamiltonian is written as $H'\exp(-\epsilon t)$ with $\epsilon > 0$. The expansion of U from (2.15) gives

$$U_\epsilon(0, -\infty) = 1 + \sum_{n=1}^{\infty}(-i)^n\int_{-\infty}^{0} dt_1\cdots\int_{-\infty}^{t_{n-1}} dt_n \times \exp[\epsilon(t_1 + \cdots + t_n)]L'(t_1)\cdots L'(t_n). \tag{3.3}$$

Let us define

$$\varphi = \lim_{\epsilon\to 0}\frac{U_\epsilon(0, -\infty)\varphi_0}{\int d\Gamma\, U_\epsilon(0, -\infty)\varphi_0} = U(0, -\infty)\varphi_0, \tag{3.4}$$

where $U(0, -\infty) = \lim_{\epsilon\to 0} U_\epsilon(0, -\infty)$. The last equality in (3.4) follows from (2.17).[10] Then the adiabatic theorem of Gell-Mann and Low states that φ is an eigenfunction of the total Liouville operator L with eigenvalue zero. Thus φ too is stationary. The theorem does *not* say which stationary state is obtained. One expects, of course, that the result of such a long, slow process will be a canonical distribution, but that does not say yet how φ and φ_0 are related.

Assume that φ_0 is a canonical distribution at some temperature $T = 1/k_B\beta$ (k_B = Boltzmann's constant) for free particles, i.e., a Maxwellian. Then the process described by (3.4) is reversible in the thermodynamic sense. The question is then what kind of

[10] In distinction to the usual quantum mechanical case, the denominator in (3.4) does not give an infinite phase factor.

process is being described. It is shown in Appendix A that Eq. (3.4) is a dynamical description of an isothermal process. The final canonical distribution is appropriate to the same temperature as the initial one. That is,

$$\varphi = \varphi(\beta) = U(0, -\infty)\varphi_0(\beta), \tag{3.5}$$

where φ_0 is Maxwellian and $\varphi(\beta)$ is the canonical distribution function for the actual system at the temperature given by β. The normalization of φ implied by (3.4) is automatically correct, so that the partition function need not be computed.

The result is true in a perturbative sense. That is, the equality (3.5) holds term-by-term in the expansion in $\beta(H' - \langle H' \rangle)$ where H' is a velocity-independent perturbation. Equation (3.5) is ultimately used in computing reduced distributions. For these, each term in the perturbation series gives a perfectly finite result for any number of particles, no matter how large, so long as the density is finite.

The question of the convergence of the perturbation series for the reduced distributions is not answered. The starting point is a gas of noninteracting particles. We do not expect convergence if the isothermal process described by (3.4) takes the system through a phase transition. Thus, the perturbation procedure, when valid, holds for gases and in general may not describe a liquid phase.

Henin, Résibois, and Andrews[11] and Andrews[12] have obtained an expression for a uniform medium that is identical to (3.5) with φ given by (3.4). The interpretation is different from ours and does not make clear the difficulties in applying the perturbation expansion to liquids. Their calculation has an error,[13] which can be rectified, however, by the arguments of Appendix A, and their final result is correct. They did not consider external fields.

We have, finally, using (3.4)

$$\langle [f_1(t_1) \cdots f_n(t_n)]_+ \rangle_H = \langle [f_1(t_1) \cdots f_n(t_n) U(\infty, -\infty)]_+ \rangle. \tag{3.6}$$

The right-hand side of (3.6) is evaluated in the interaction picture. By virtue of (2.17), $U(\infty, -\infty)$ can be replaced by $U(t', -\infty)$, where t' is the largest of the t_i. We will be concerned from here on with expressions such as (3.6). All correlations on the right-hand side are taken into account by the dynamical operator U. The average is over the distribution for free particles, so L_0 is given by (2.19). The interaction Liouville operator is

$$L' = i \sum_i \nabla_i H' \cdot \partial_i, \tag{3.7}$$

where H' is assumed to depend on the relative particle coordinates only.

Having established this general result, we now specialize to uniform systems of N identical particles.

IV. THE TWO-PARTICLE CORRELATION FUNCTION

Consider a homogeneous system of N identical particles in a volume Ω. The particle density is

$$\rho(\mathbf{r}, t) = \sum_{i=1}^{n} \delta[\mathbf{r} - \mathbf{r}_i(t)] \tag{4.1}$$

and the mean density of the system is

$$n = N/\Omega = \langle \rho(\mathbf{r}, t) \rangle_H. \tag{4.2}$$

We are concerned with the two-particle correlation function S which describes correlations of density fluctuations. In a uniform medium, S can depend only on differences in position and time, so it is given by

$$S(\mathbf{r} - \mathbf{r}', t - t') = \langle [\rho(\mathbf{r}, t) - n][\rho(\mathbf{r}', t') - n] \rangle_H. \tag{4.3}$$

Using the Fourier expansion

$$F(\mathbf{r}) = \Omega^{-1} \sum_{\mathbf{k}} F(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \tag{4.4}$$

to transform to the more convenient wavenumber space, Eq. (4.3) becomes

$$S(\mathbf{k}, t) = \Omega^{-1} \langle \rho_{\mathbf{k}}(t) \rho_{-\mathbf{k}}(0) \rangle_H = \Omega^{-1} \langle \rho_{\mathbf{k}} e^{-iLt} \rho_{-\mathbf{k}} \rangle_H \quad \text{for} \quad \mathbf{k} \neq 0, \quad = 0 \quad \text{for} \quad \mathbf{k} = 0, \tag{4.5}$$

using (2.10). Here

$$\rho_{\mathbf{k}} = \sum_i \exp(-i\mathbf{k}\cdot\mathbf{r}_i) \tag{4.6}$$

is the Fourier expansion coefficient obtained from (4.1). S is symmetric in both $\mathbf{k}$ and t.

Applying (3.6) to (4.5) gives for $\mathbf{k} \neq 0$ and $t > 0$ (which we shall assume from now on)

$$S(\mathbf{k}, t) = \Omega^{-1} \langle [\rho_{\mathbf{k}}(t) \rho_{-\mathbf{k}}(0) U(t, -\infty)]_+ \rangle. \tag{4.7}$$

We have made use of the fact that $U(\infty, t)$ can be removed from the time-ordered product (3.6) without changing the result, because of (2.17). Ex-

[11] F. Henin, P. Résibois, and F. Andrews, J. Math. Phys. **2**, 68 (1961).

[12] F. Andrews, Physica **27**, 1054 (1961).

[13] Henin, Résibois, and Andrews (Ref. 11) and Andrews (Ref. 12) assumed in effect that $\lim_{\epsilon \to 0} (L_0 - i\epsilon)^{-1} L_0 = 1$. See also I. Prigogine, Ref. 4, Chap. 12. The correct expression is $\lim_{\epsilon \to 0} (L_0 - i\epsilon)^{-1} L_0 = 1 - P_0$. (See Appendix A.)

panding U, we obtain

$$S(\mathbf{k}, t) = \Omega^{-1} \sum_{n=0}^{\infty} (-i)^n \int_{-\infty}^{t} dt_1 \cdots \int_{-\infty}^{t_{n-1}} dt_n \times \langle [\rho_{\mathbf{k}}(t)\rho_{-\mathbf{k}}(0)L'(t_1) \cdots L'(t_n)]_+ \rangle. \quad (4.8)$$

The unperturbed state is a free-particle state. The perturbation is assumed due to two-body interactions, so the Hamiltonian is

$$H = \sum_i (p_i^2/2m) + \tfrac{1}{2} \sum_{i,j}{}' v(|\mathbf{r}_i - \mathbf{r}_j|). \quad (4.9)$$

The prime indicates that the term $i = j$ is missing. In wavenumber space,

$$L_0 = m^{-1} \sum_i \mathbf{p}_i \cdot \mathbf{k}_i,$$

$$L' = -1/(2\Omega) \sum_{\mathbf{k}} v(\mathbf{k}) \times \sum_{i,j} \exp [i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)]\mathbf{k}\cdot(\partial_i - \partial_j). \quad (4.10)$$

Eq. (4.8) can be represented diagrammatically by the method of Prigogine,[4] summarized in Appendix B. A vertex describing the transfer of wavenumber $\mathbf{k}$ from particle β to particle α is associated with a factor[14]

$$-iL_{\alpha\beta}(\mathbf{k}) = i\Omega^{-1}v(\mathbf{k})\mathbf{k}\cdot(\partial_\alpha - \partial_\beta), \quad (4.11)$$

where $v(\mathbf{k})$ is the transform of $v(\mathbf{r})$ and is not to be confused with a velocity $\mathbf{v}_i$. A free propagator line for a particle α with wavenumber $\mathbf{k}$ between times t and t' $(t > t')$ corresponds to a factor

$$\Gamma_\alpha(\mathbf{k}, t - t') = \exp [-i\mathbf{k}\cdot\mathbf{v}_\alpha(t - t')]. \quad (4.12)$$

Because of (3.4), only connected diagrams contribute to $S(\mathbf{k}, t)$. Each term exp $-i\mathbf{k}\cdot\mathbf{r}_i(t)$ in $\rho_{\mathbf{k}}(t)$ corresponds to the addition of a wavenumber $\mathbf{k}$ to the propagator for particle i at time t and can be represented by a directed vertical line carrying wavenumber $\mathbf{k}$. Each such vertical line can be regarded as an end of the diagram. The vertical line can be omitted if either just before or just after the transfer of wavenumber $\mathbf{k}$, particle i has zero wavenumber. In that case the diagram evidently ends with a free propagator. Thus $S(\mathbf{k}, t)$ is represented by the sum of all connected diagrams with two ends a time t apart.

It is convenient to define an irreducible correlation part (ICP) of a diagram as a part all of whose vertices are at least doubly connected to each other. They are equivalent to the irreducible clusters discussed by Weinstock.[15]

[14] Note that the factor $\frac{1}{2}$ in (4.10) does not appear in (4.11) because α and β are fixed.

[15] J. Weinstock, Phys. Rev. **132**, 454 (1963).

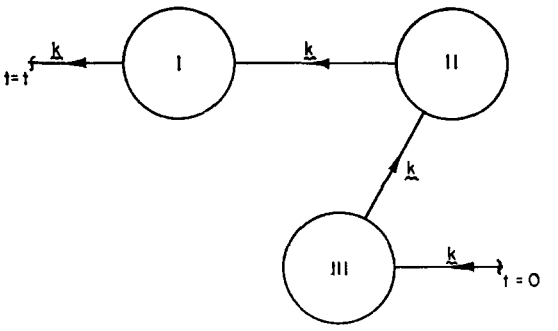

FIG. 1. Schematic reduced diagram for a two-particle correlation function.

The most general diagram contributing to S consists of a number of ICP's (or possibly none) alternating with free propagators of wavenumber $\mathbf{k}$ to form a linear (i.e., nonbranching) chain with two ends. One end of the chain is at a time τ and the other end at a time $t + \tau$. We can, in all generality, put $\tau = 0$. The other vertices may be arranged in any temporal order, though as we show, most of these arrangements give no contribution. A typical diagram for S is shown in Fig. 1. The ICP's are represented by numbered circles. Each linking propagator bears wavenumber $\mathbf{k}$ because conservation of wave number at every vertex implies conservation of $\mathbf{k}$ in the large. A vector $\mathbf{k}$ going backward in time is equivalent to $-\mathbf{k}$ going forward in time. The ordering is important because the vertices represent operators in momentum space.

An ICP is characterized by the particle labels associated with the two free propagators attached to it; by $\mathbf{k}$; by the time difference $t_1 - t_2$ of the two vertices at which the free propagators are attached; and, of course, by its internal structure.

The significance of the reduction is that ICP's are local in space and time, at least for short-range forces. The times are short because typical wavenumbers k' transferred in an interaction are of the order of r_0^{-1}, the reciprocal of the range of the interaction. The free-particle propagator between two successive vertices in the ICP behaves something like exp $(-i\mathbf{k}'\cdot\mathbf{v}_i\Delta t)$. The exponent oscillates rapidly to produce cancellation for time intervals much larger than about $(k'v)^{-1} \sim r_0 v^{-1}$, which is the collision time. For times of the order of the collision time, the particles involved must all be in a region whose dimensions are of the order r_0 if they are to interact in any manner except sequentially.[16]

[16] We pass over the potentially troublesome question of the extent to which ICP's of infinite order in λ, as for instance when the individual vertices are replaced by binary collision vertices (see Sec. VI), are still short-time quantities.

We will be concerned with the limit $N, \Omega \to \infty$ with $n = N/\Omega$ finite. The diagrams which contribute in this limit can be inferred from the following rules which give the order of magnitude of the diagrams.

(1) Every vertex contributes a factor λ/Ω, where λ is a measure of the interaction strength.

(2) Every closed loop gives a factor Ω because it involves a sum over $\mathbf{k}'$, and $\sum_{\mathbf{k}'} \to (\Omega/8\pi^3) \int d\mathbf{k}'$ when $\Omega \to \infty$.

(3) If there are r different particle indices there is a factor $N!/(N-r)! \sim N^r$ when N is large.

(4) Thus, if there are n vertices, m closed loops, and r particle indices, the diagram goes as $\lambda^n N^r/\Omega^{n-m}$.

(5) Consider particle indices being assigned to lines in a diagram according to decreasing time, that is, in going from left to right in the diagram. No new indices can be assigned at a creation vertex.

(6) Two new indices cannot be assigned at a destruction vertex. Such a vertex corresponds to an operator L_{ij}, the Liouville operator describing an interaction between the new particles i and j. An expression involving L_{ij} vanishes on being averaged if i and j are new particles, so such a diagram gives no contribution.

(7) Thus at most one new index can be assigned at any vertex. It follows that $r \leq n - m$. Therefore in the thermodynamic limit there are no infinite terms in the expansion of a statistical average.

(8) In the limit the only nonvanishing diagrams are those with $r = n - m$. Thus, in assigning particle indices, one must assign a new index whenever possible.

(9) It follows that no particle can appear in two disjoint particle lines, with the possible exception of semiconnected parts (defined in Appendix C). In particular, the only particle that two ICP's can have in common is the particle linking them.

(10) Any diagram with a destruction vertex (except possibly in a semiconnected part) vanishes. This follows from Rules 6 and 9.

(11) This eliminates all ICP's of form III in Fig. 1, in which both connecting propagators go out toward the right.

(12) It also implies that the leftmost (latest) vertex of an ICP must have a free propagation line attached to it.

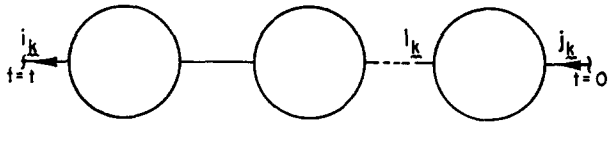

FIG. 2. Diagram for $M_{ij}(\mathbf{k}, t)$.

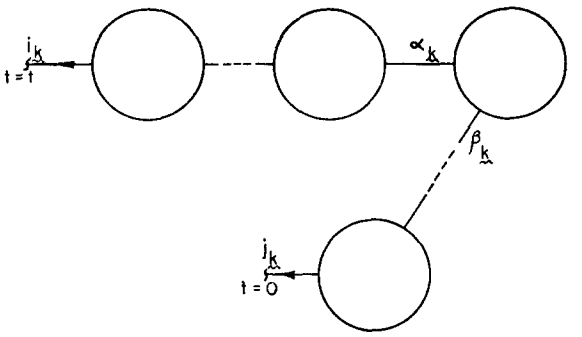

FIG. 3. Diagram for $C_{ij}(\mathbf{k}, t)$.

(13) Diagrams with semiconnected parts give no contribution, as shown in Appendix C.

With these rules[17] it is easy to show the general diagrammatic structure of $S(\mathbf{k}, t)$. By Rule 12, each diagram must end in a free propagator at time t. Let the end of $t = 0$ be a free propagator going to the left. Then the only allowable type of structure is of the form shown in Fig. 2, with ICP's of type I (one propagator going out to the right, one to the left) only. If the propagator starts out from $t = 0$ by going to the right, the only allowable type of structure is of the form shown in Fig. 3, with one ICP of type II (both propagators going out to the left). These results follow from Rule 11, which prohibits zig-zag structures.

A third possibility is that the end at $t = 0$ is not a free propagator, but a vertical line attached to the rightmost ICP. The corresponding diagrams are in all other respects of the form shown in Fig. 2.

Note that while by Rule 12, the latest vertex of an ICP must have a free propagation line at-

[17] Rules 10, 11, and 12 depend on the direction of time and not alone on the topology of the diagrams. They depend on our definition of a thermal average as

$$\langle f(t) \rangle = \int d\Gamma\, f_H(t)\varphi = \int d\Gamma\, f(t) U(t, -\infty)\varphi_0,$$

with the distribution function written on the right. This corresponds to the purely mechanical development of the system from a system of noninteracting particles in the remote past, where, however, an assumption of molecular chaos has been used at $t = -\infty$. An initial molecular-chaos assumption accords with the usual way of thinking about statistical mechanics. However, the same numerical values for thermal averages can equally well be computed from

$$\langle f(t) \rangle = \int d\Gamma\, \varphi f_H(t) = \int d\Gamma\, \varphi_0 U(\infty, t) f(t)$$

in which the interaction is slowly turned off in the future and molecular chaos assumed at $t = +\infty$. In that case, Rules 10, 11, and 12 would refer to creation vertices, ICP's of the second form, and the rightmost vertex, respectively. If we had chosen a symmetric description such as is used in quantum mechanics, i.e.,

$$\langle f(t) \rangle = \int d\Gamma\, \varphi^{\frac{1}{2}} f_H(t) \varphi^{\frac{1}{2}} = \int d\Gamma\, (\varphi_0)^{\frac{1}{2}} [U(\infty, -\infty) f(t)]_+ (\varphi_0)^{\frac{1}{2}},$$

then the three rules would not hold in any form.

tached, the other free propagator is not necessarily attached at the earliest vertex, which may in fact go back in time to $-\infty$.

The integral equations corresponding to the three types of structure can be written down immediately. Corresponding to Fig. 2 we have the operator $M_{ij}(\mathbf{k}, t)$ with

$$M_{ij}(\mathbf{k}, t) = \Gamma_i(\mathbf{k}, t)\delta_{ij} + \int_0^t dt' \int_0^{t'} dt'' \, \Gamma_i(\mathbf{k}, t - t') \times \sum_l R_{il}(\mathbf{k}, t' - t'')M_{lj}(\mathbf{k}, t''). \quad (4.13)$$

Here $R_{il}(\mathbf{k}, t)$ is the sum of all ICP's of type I (Fig. 1) characterized by a vertex involving particle i at the left with the other external vertex occurring a time t earlier and involving particle l. The wave number $\mathbf{k}$ is associated with every part of the diagram. Corresponding to Fig. 3 plus the case with a vertical line at $t = 0$, we have the operator $C_{ij}(\mathbf{k}, t)$, with

$$C_{ij}(\mathbf{k}, t) = \sum_\alpha \int_{-\infty}^t dt' \, M_{i\alpha}(\mathbf{k}, t - t') \times \left\{ \sum_\beta \int_{-\infty}^0 dt'' \, M_{j\beta}(-\mathbf{k}, -t'') \times T_{\alpha\beta}(\mathbf{k}, t' - t'') + x_{\alpha j}(\mathbf{k}, t') \right\}. \quad (4.14)$$

Here $T_{\alpha\beta}(\mathbf{k}, t)$ is the sum of all ICP's of type II [Fig. 3] characterized by one external vertex involving particle α at t' and one involving particle β at t''. $X_{\alpha j}(\mathbf{k}, t')$ is the sum of all ICP's with a vertex involving particle α at t' and one corresponding to addition of wavenumber $\mathbf{k}$ to particle j at time zero. The latter vertex does not involve the interaction, and other than changing the wavenumber of particle j, has no effect on the contribution of the ICP. It should be noted that $X_{\alpha j}(\mathbf{k}, t) = 0$ for $t \leq 0$.

In terms of M and C, the correlation function is

$$S(\mathbf{k}, t) = \Omega^{-1} \sum_{i,j} \langle M_{ij}(\mathbf{k}, t) + C_{ij}(\mathbf{k}, t) \rangle, \quad (4.15)$$

where the average is over the free particle distribution.

$M_{ij}(\mathbf{k}, t)$ takes into account correlations of particles i and j between 0 and t, although correlations between other particles that affect the motion of i and j indirectly may be involved into the remote past. $C_{ij}(\mathbf{k}, t)$ takes the correlations of i and j into account in the past, although modifications of the motion i at times between zero and t are included.[18]

Because (4.13) and (4.14) are convolutions, it is convenient to work with the frequency transforms. We define the two-sided transforms by the typical relation

$$S(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} e^{i\omega t} S(\mathbf{k}, t) \, dt \quad (4.16)$$

and one-sided transforms, identified by a bar, by the typical relation

$$\bar{S}(\mathbf{k}, \omega) = \int_0^{\infty} e^{i\omega t} S(\mathbf{k}, t) \, dt. \quad (4.17)$$

The transforms of (4.13) and (4.14) are

$$\bar{M}_{ij}(\mathbf{k}, \omega) = \bar{\Gamma}_i(\mathbf{k}, \omega)\delta_{ij} + \sum_l \bar{\Gamma}_i(\mathbf{k}, \omega)\bar{R}_{il}(\mathbf{k}, \omega)\bar{M}_{lj}(\mathbf{k}, \omega), \quad (4.18)$$

$$C_{ij}(\mathbf{k}, \omega) = \sum_\alpha \bar{M}_{i\alpha}(\mathbf{k}, \omega) \times \{ \sum_\beta \bar{M}^*_{j\beta}(\mathbf{k}, \omega)T_{\alpha\beta}(\mathbf{k}, \omega) + \bar{x}_{\alpha j}(\mathbf{k}, \omega) \}. \quad (4.19)$$

The symmetry properties can be seen from the fact that

$$\bar{\Gamma}_i(\mathbf{k}, \omega, \{\mathbf{p}_i\}) = \bar{\Gamma}_i(-\mathbf{k}, \omega, -\{\mathbf{p}_i\}) = \bar{\Gamma}^*_i(-\mathbf{k}, -\omega, \{\mathbf{p}_i\}) \quad (4.20)$$

and

$$L_{ij}(\mathbf{k}, \mathbf{p}_i, \mathbf{p}_j) = L_{ij}(-\mathbf{k}, -\mathbf{p}_i, -\mathbf{p}_j) = -L_{ij}(-\mathbf{k}, \mathbf{p}_i, \mathbf{p}_j). \quad (4.21)$$

It follows that $\bar{R}_{ij}$, T_{ij}, $\bar{M}_{ij}$, and C_{ij} have the same symmetry properties in $\mathbf{k}$, ω, and $\{\mathbf{p}_i\}$ as $\bar{\Gamma}_i$. These properties are given by (4.20). Since the averaging is symmetric in $\{\mathbf{p}_i\}$,

$$\langle M_{ij}(\mathbf{k}, \omega) \rangle = 2 \, \mathrm{Re} \, \langle \bar{M}_{ij}(\mathbf{k}, \omega) \rangle. \quad (4.22)$$

Symbolically, (4.18) can be written

$$\bar{\mathbf{M}} = \boldsymbol{\Gamma} + \bar{\boldsymbol{\Gamma}}\bar{\mathbf{R}}\bar{\mathbf{M}}, \quad (4.23)$$

where $\bar{\boldsymbol{\Gamma}}$ is diagonal. Equation (4.23) has the solution

$$\bar{\mathbf{M}} = (\mathbf{I} - \bar{\boldsymbol{\Gamma}}\bar{\mathbf{R}})^{-1}\bar{\boldsymbol{\Gamma}}, \quad (4.24)$$

with $\mathbf{I}$ the unit operator.

By Rule 9, if $j = i$ in (4.18), then $l = i$. We define the diagonal matrix $\mathbf{G}$ by

$$G_i = \bar{M}_{ii} = \bar{\Gamma}_i + \bar{\Gamma}_i\bar{R}_{ii}G_i, \quad (4.25)$$

[18] This decomposition resembles that used by Prigogine (Ref. 4, Chap. 11), in which a Fourier component ρ_γ of the distribution function at time t is decomposed into two classes. However, two-time quantities are being considered here and the two decompositions, while related, are not identical.

so that

$$G_i = (1 - \bar{\Gamma}_i \bar{R}_{ii})^{-1} \bar{\Gamma}_i. \tag{4.26}$$

Defining

$$\bar{\mathbf{R}}_{ij} = (1 - \delta_{ij}) \bar{R}_{ij} \tag{4.27}$$

and using (4.26) in (4.23), we get the matrix equation

$$\bar{\mathbf{M}} = \mathbf{G} + \mathbf{G}\bar{\mathbf{R}}\bar{\mathbf{M}}, \tag{4.28}$$

with the solution

$$\bar{\mathbf{M}} = (\mathbf{I} - \mathbf{G}\bar{\mathbf{R}})^{-1}\mathbf{G}. \tag{4.29}$$

If $\langle \Gamma_i \rangle$ describes the free-particle motion, then $\langle \sum_i M_{ij} \rangle$ describes motion in the actual system and may be identified with a quasiparticle. This identification becomes clearer in the context of the RPA discussed in the next section.

V. THE RANDOM PHASE APPROXIMATION

To solve the equations for **M** and **C**, one chooses some subclass of ICP's with which to approximate **R** on the basis of some argument as to why these ICP's are important. The simplest possible choice in which interactions are taken into account is to pick out those ICP's that consist of a single vertex, that is,

$$R_{ij}(\mathbf{k}, t) = T_{ij}(\mathbf{k}, t) = L_{ij}(\mathbf{k}) \delta(t). \tag{5.1}$$

One way of looking at the approximation is to observe that in each R_{ij} terms proportional to $n\lambda^q$ are neglected for $q > 1$ relative to terms proportional to $n\lambda$. Since the application of an R_{ij} operator is associated with a time integral in (4.13), the result is a function of $n\lambda t$ and is valid for times such that the $n\lambda^2 t$ contributions are small. The relaxation time is proportional to $(n\lambda^2)^{-1}$, so the approximation is valid for times short compared to the relaxation time, as pointed out by Balescu.[19]

With (5.1) and (4.11), Eqs. (4.18) and (4.19) become

$$\bar{M}_{ij}(\mathbf{k}, \omega) = \bar{\Gamma}_i(\mathbf{k}, \omega) \delta_{ij} + i\Omega^{-1} v(\mathbf{k}) \bar{\Gamma}_i(\mathbf{k}, \omega) \sum_l \mathbf{k} \cdot (\partial_i - \partial_l) \bar{M}_{lj}(\mathbf{k}, \omega), \tag{5.2}$$

$$C_{ij}(\mathbf{k}, \omega) = i\Omega^{-1} v(\mathbf{k}) \times \sum_{\alpha\beta} \bar{M}_{i\alpha}(\mathbf{k}, \omega) \bar{M}^*_{j\beta}(\mathbf{k}, \omega) \mathbf{k} \cdot (\partial_\alpha - \partial_\beta). \tag{5.3}$$

Evidently, (5.1) is the (RPA),[5] since there is no coupling between different **k** values in (5.2) and (5.3). In this approximation, the term in (4.14) involving $X_{\alpha j}$ vanishes.

When (5.2) is summed on j, multiplied by $\bar{\Gamma}_i^{-1}$, and averaged over the momentum of particle l, it becomes identical in form to the Fourier-transformed linearized Vlasov equation[19] for a one-component plasma with a uniform neutralizing background. The function $\langle \sum_i \bar{M}_{ij} \rangle$ is to be interpreted as a single-particle density. This result illustrates for a classical system the well-known result that the RPA and the self-consistent field approximation are equivalent.[20]

It is also well-known that the solution of the linearized Vlasov equation gives the same result for the dielectric function as does the response function method[2,3,21] in the RPA.[7,22] The equivalence has been shown for quantum mechanical plasmas and the classical result follows by a limiting argument. It is nevertheless of interest to demonstrate the equivalence by a completely classical argument. The result is important, because it points out explicitly one approximation which can be carried out consistently, so that a kinetic equation and a correlation function method give the same results for a transport coefficient, not only in the static case, but for all frequencies.

The evaluation of the dielectric function either way involves taking thermal averages of (5.2) and (5.3). The key observation is that the terms involving the momentum gradients uncouple on being thermally averaged. Thus

$$\langle \bar{\Gamma}_i \mathbf{k} \cdot (\partial_i - \partial_l) \bar{M}_{lj} \rangle = \langle \bar{\Gamma}_i \mathbf{k} \cdot \partial_i \rangle \langle \bar{M}_{lj} \rangle, \tag{5.4}$$

$$\langle \bar{M}_{i\alpha} \bar{M}^*_{j\beta} \mathbf{k} \cdot (\partial_\alpha - \partial_\beta) \rangle = \langle \bar{M}_{i\alpha} \mathbf{k} \cdot \partial_\alpha \rangle \langle \bar{M}_{j\beta} \rangle^* - \langle \bar{M}_{i\alpha} \rangle \langle \bar{M}_{j\beta} \mathbf{k} \cdot \partial_\beta \rangle^*. \tag{5.5}$$

Averaging (5.2), using (5.4), and summing on i, we find[23]

$$\sum \langle \bar{M}_{ij} \rangle = \langle \bar{\Gamma}_i \rangle / \epsilon_+(\mathbf{k}, \omega), \tag{5.6}$$

where

$$\epsilon_+(\mathbf{k}, \omega) = 1 - inv(\mathbf{k}) \langle \Gamma_i \mathbf{k} \cdot \partial_i \rangle. \tag{5.7}$$

The interpretation of $\bar{\mathbf{M}}$ and $\bar{\mathbf{\Gamma}}$ given above leads to the identification of ϵ_+ as a generalized dielectric function.[6]

From (4.11),

$$\bar{\Gamma}_i(\mathbf{k}, \omega) = -i(\mathbf{k} \cdot \mathbf{v}_i - \omega - i\delta)^{-1}, \tag{5.8}$$

where δ is a positive infinitesimal. Inserting (5.8)

[19] R. Balescu, *Statistical Mechanics of Charged Particles* (Interscience Publishers, Inc., New York, 1963).

[20] H. Ehrenreich and M. H. Cohen, Phys. Rev. **115**, 786 (1959).

[21] P. Nozières and D. Pines, Nuovo Cimento **9**, 470 (1958).

[22] S. Ichimaru, Ann. Phys. (N.Y.) **20**, 78 (1962).

[23] Most of the results involving ϵ_+ have been derived directly from the Vlasov equation by Balescu (Ref. 19) and by Ichimaru (Ref. 22).

into (5.7), one sees immediately that $\epsilon_+(\mathbf{k}, \omega)$ is analytic for Im $\omega \geq 0$ and that $\lim_{\epsilon\to 0} \epsilon_+(\mathbf{k}, \omega) = 1$.

We find from (5.8)

$$\langle \bar{\Gamma}_i \mathbf{k}\cdot\partial_i \rangle = -\beta\langle \bar{\Gamma}_i \mathbf{k}\cdot\mathbf{v}_i \rangle = i\beta(1 + i\omega\langle \bar{\Gamma}_i \rangle), \tag{5.9}$$

and for real ω,

$$\langle \bar{\Gamma}_i(\mathbf{k}, \omega)\rangle = \left(\frac{\pi m\beta}{2k^2}\right)^{\frac{1}{2}} \exp\left[-m\beta\omega^2/2k^2\right] \times \left\{1 + i\Phi\left[\left(\frac{m\beta}{2}\right)^{\frac{1}{2}}\frac{\omega}{k}\right]\right\}, \tag{5.10}$$

where $i\Phi$ is the error function of imaginary argument; that is

$$\Phi(x) = \left(2/\sqrt{\pi}\right)\int_0^x \exp(\xi^2)\, d\xi. \tag{5.11}$$

With (5.9) and (5.10), Eq. (5.7) becomes for real ω

$$\epsilon_+(\mathbf{k}, \omega) = 1 + n\beta v(\mathbf{k})\left\{1 - \left(\frac{\pi m\beta}{2}\right)^{\frac{1}{2}}\frac{\omega}{k} \times \exp(-m\beta\omega^2/2k^2)\Phi\left[\left(\frac{m\beta}{2}\right)^{\frac{1}{2}}\frac{\omega}{k}\right]\right\} + in\beta v(\mathbf{k})\left(\frac{\pi m\beta}{2}\right)^{\frac{1}{2}}\frac{\omega}{k}\exp(-m\beta\omega^2/2k^2). \tag{5.12}$$

It can be shown that $\epsilon_+(\mathbf{k}, \omega)$ has no zeros for Im $\omega \geq 0$ for any distribution[24] including a Maxwellian. More directly, inserting (5.9) into (5.7), one sees that $\epsilon_+(\mathbf{k}, \omega) = 0$ implies Re $\langle \bar{\Gamma}_i(\mathbf{k}, \omega)\rangle = 0$. But for $\omega = \omega_1 + i\omega_2$, with ω_1 real and $\omega_2 > 0$,

$$\text{Re}\,\langle \bar{\Gamma}_i(\mathbf{k}, \omega)\rangle = \omega_2\langle[(\mathbf{k}\cdot\mathbf{v}_i - \omega_1)^2 + \omega_2^2]^{-1}\rangle. \tag{5.13}$$

The average is certainly positive, so Re $\langle \bar{\Gamma}_i\rangle$ cannot vanish in the finite plane for Im $\omega > 0$. It does not vanish on the finite real axis either, by (5.10), so ϵ_+ has no zeros in the upper-half plane. It follows from (5.7), (5.8), and (5.9) that $[\epsilon_+(\mathbf{k}, \omega]^{-1} - 1$ approaches zero for $\omega \to \infty$ since it is analytic for Im $\omega \geq 0$, it satisfies the Kramers–Kronig relation

$$\text{Re}\,[\epsilon_+(\mathbf{k}, \omega)]^{-1} - 1 = (1/\pi)P\int_{-\infty}^{\infty} \text{Im}\,[\epsilon_+(\mathbf{k}, \omega')]^{-1} d\omega'/(\omega' - \omega). \tag{5.14}$$

Now multiplying (5.2) on the right by $\mathbf{k}\cdot\partial_j$ and averaging, we find in the same way as for (5.6),

$$\sum_i \langle \bar{M}_{ij}\mathbf{k}\cdot\partial_j\rangle = \frac{\langle \bar{\Gamma}_i\mathbf{k}\cdot\partial_i\rangle}{\epsilon_+(\mathbf{k}, \omega)}. \tag{5.15}$$

It follows from (5.3), (5.6), (5.8), (5.15), (4.15), and (4.22) that

$$S(\mathbf{k}, \omega) = 2n\,\text{Re}\,\frac{\langle \bar{\Gamma}_i\mathbf{k}\cdot\partial_i\rangle}{\epsilon_+(\mathbf{k}, \omega)} + 2n^2 v(\mathbf{k})\,\text{Im}\,\frac{\langle \bar{\Gamma}_i(\mathbf{k}, \omega)\rangle\langle \bar{\Gamma}_j\mathbf{k}\cdot\partial_j\rangle^*}{|\epsilon_+(\mathbf{k}, \omega)|^2}. \tag{5.16}$$

Equation (5.16) can be simplified with the aid of (5.7) to give

$$S(\mathbf{k}, \omega) = \frac{2n\,\text{Re}\,\langle \bar{\Gamma}_i(\mathbf{k}, \omega)\rangle}{|\epsilon_+(\mathbf{k}, \omega)|^2}. \tag{5.17}$$

It can be seen either by direct computation or by putting $v(\mathbf{k}) = 0$ into (5.7) that the correlation function for free particles is

$$S_0(\mathbf{k}, \omega) = 2n\,\text{Re}\,\langle \bar{\Gamma}_i(\mathbf{k}, \omega)\rangle = n(2\pi m\beta/k^2)^{\frac{1}{2}}\exp(-m\beta\omega^2/2k^2), \tag{5.18}$$

so that (5.17) can be written

$$S(\mathbf{k}, \omega) = S_0(\mathbf{k}, \omega)/|\epsilon_+(\mathbf{k}, \omega)|^2. \tag{5.19}$$

Eq. (5.19) is one expression of the conclusion of Nozières and Pines[21] that in the RPA the dressed particles can be regarded as having their strength modified by a frequency and wavenumber dependent factor $[\epsilon_+(\mathbf{k}, \omega)]^{-1}$, but otherwise behave like free particles.

Inserting (5.9) into (5.7), taking the imaginary part, and using (5.17), we find

$$\text{Im}\,[\epsilon_+(\mathbf{k}, \omega)]^{-1} = -\tfrac{1}{2}\beta v(\mathbf{k})\omega S(\mathbf{k}, \omega). \tag{5.20}$$

But one can also compute a generalized dielectric function $\epsilon(\mathbf{k}, \omega)$ by considering the linear response to an external charge inserted into the system. One finds[25] that (5.14) and (5.20) are satisfied with ϵ_+ replaced by ϵ. It follows that ϵ and ϵ_+ are identical. Thus in the RPA the kinetic equation (in this approach, the **M** equation) and the response function method give the same dielectric function for all frequencies.

The absence of zeros of ϵ_+ implies that the plasma is stable. This is, of course, a necessary condition for a response function approach to give meaningful results.

VI. COMPARISON WITH EQUILIBRIUM CORRELATIONS

The correlation function in equilibrium is just $S(\mathbf{k}, t = 0)$. From (4.15),

[24] See, for instance, O. Penrose, Phys. Fluids 3, 258 (1960).

[25] The quantum mechanical calculation of the dielectric function by a response function method is given by Nozières and Pines, Ref. 21. The classical calculation can be done in the same way, with the Hamiltonian H replaced by the Liouville operator L. See P. Mazur, Ref. 3.

$$S(\mathbf{k}, 0) = \Omega^{-1} \sum_{i,j} \langle M_{ij}(\mathbf{k}, 0) + C_{ij}(\mathbf{k}, 0)\rangle. \quad (6.1)$$

From (4.13),

$$\Omega^{-1}\langle M_{ij}(\mathbf{k}, 0)\rangle = n\langle \Gamma_i(\mathbf{k}, 0)\rangle = n. \quad (6.2)$$

This is just the Fourier transform of the autocorrelation (a δ function) in equilibrium.

On the other hand, Eq. (4.14) evaluated for $t = 0$ says to sum all possible diagrams with two free ends at $t = 0$, and all other vertices at negative times. But this is just the Fourier transform of the expansion of $U(0, -\infty)$. That is,

$$C_{ij}(\mathbf{k}, 0) = \Omega^{-N} \int \{d\mathbf{r}_i\} \times \exp(-i\mathbf{k}\cdot\mathbf{r}_i) \exp(i\mathbf{k}\cdot\mathbf{r}_j) U(0, -\infty). \quad (6.3)$$

Since in C_{ij} the particles i and j must be different,

$$\begin{aligned}
&\Omega^{-1} \sum_{i,j} \langle C_{ij}(\mathbf{k}, 0)\rangle \\
&= \Omega^{-1} \sum_{i,j}{}' \int d\Gamma \exp[-i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)] U(0, -\infty)\varphi_0, \\
&= \Omega^{-1} \sum_{i,j}{}' \int d\Gamma \exp[-i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)]\varphi, \\
&= \Omega^{-1} \int d\mathbf{r}\, d\mathbf{r}' \exp[-i\mathbf{k}\cdot(\mathbf{r} - \mathbf{r}')] \\
&\quad \times \sum_{i,j}{}' \int d\Gamma\, \delta(\mathbf{r} - \mathbf{r}_i)\delta(\mathbf{r}' - \mathbf{r}_j)\varphi. \quad (6.4)
\end{aligned}$$

But[26]

$$\sum_{i,j}{}' \int d\Gamma\, \delta(\mathbf{r} - \mathbf{r}_i)\delta(\mathbf{r}' - \mathbf{r}_j)\varphi = n^2 g(\mathbf{r} - \mathbf{r}'), \quad (6.5)$$

where g is the radial distribution function.

From (6.2), (6.4), and (6.5), we find on transforming back to coordinate space

$$S(\mathbf{r}, 0) = n\delta(\mathbf{r}) + n^2[g(\mathbf{r}) - 1]. \quad (6.6)$$

The term $-n^2$ comes from putting in the condition $S(\mathbf{k} = 0, 0) = 0$. Thus $S(\mathbf{r}, 0)$ is just the correlation function in equilibrium.

The reduction of S in Sec. IV has an analog in equilibrium statistical mechanics. An ICP corresponds to an irreducible equilibrium cluster,[27-29] with some essential (and some nonessential) differences.

In order to make a comparison, we sum ladders, i.e., diagrams with 1, 2, $\cdots$ successive interactions of each pair of interacting particles, the rest of the diagram structure remaining the same. One can draw new diagrams in which successive vertices cannot occur between the same two particles; each vertex is now interpreted as corresponding to $-if_{ij}$ (where f_{ij} is the binary collision operator) rather than to $-iL_{ij}$. The binary collision operator has been discussed in detail by Weinstock[15] and we do not go into it further here. It suffices to say that it is a generalization of the Mayer f function for equilibrium, given by $f_{ij} = \exp(-\beta V_{ij}) - 1$.

A Mayer diagram representing an irreducible cluster is characterized by having neither nodal points nor articulation points.[29] The Prigogine diagrams differ from the Mayer diagrams mainly in having interactions represented by points, and particles by lines, instead of the other way around. In a sense one type of diagram is the image of the other. Let us examine separately the ICP's entering into R_{ii} which involve a single unidentifiable particle i, and those entering into R_{ij} for $i \neq j$ which involve two identifiable particles. The second type of ICP by definition corresponds to equilibrium diagrams with no nodal points since the two defining particles are at least doubly connected. The first type of ICP just modifies the motion of particle i and, as we have pointed out, may be removed by replacing $\bar{\mathbf{\Gamma}}$ by $\mathbf{G}$. In a sense this corresponds to an equilibrium expansion in density rather than fugacity.[28,29]

A Mayer diagram is said to have an articulation point when the removal of one particle would cause a certain group or cluster of particles to be completely disconnected from the main cluster.[29] The given cluster of particles may be regarded as hanging on a single particle. That is, the particles in the cluster interact only with each other and with the one particle by which they are connected to the main part of the diagram. We can speak of a hanging cluster in nonequilibrium problems as well.

The replacement of $\bar{\mathbf{\Gamma}}$ by $\mathbf{G}$ removes certain hanging clusters, but not all of them. As an example, consider a situation in which a certain particle l interacts with particles i and j in an ICP contributing to R_{ij}. If there is a particle m which interacts twice with particle i, the two (i, m) vertices straddling the (i, l) vertex, then m cannot be removed from explicit consideration by renormalization.

One may now ask: If all hanging clusters cannot

[26] See, for instance, T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Company, Inc., New York, 1956), Sec. 29.

[27] J. E. Mayer and M. G. Mayer, *Statistical Mechanics* John Wiley & Sons, Inc., New York, 1940).

[28] G. E. Uhlenbeck and G. W. Ford in *Studies in Statistical Mechanics* (North-Holland Publishing Company, Amsterdam, 1962), Vol. 1.

[29] G. Stell in *The Equilibrium Theory of Classical Fluids*, edited by H. L. Frisch and J. L. Lebowitz (W. A. Benjamin, Inc., New York, 1964).

be removed, why then do they not contribute to the correlation function in equilibrium? The reason is that an equilibrium diagram containing interactions described by the pairs α, β, $\cdots$ (which need not all be different) corresponds to a sum of non-equilibrium diagrams with the same interacting pairs present, but taken over all possible time orderings, that is, permuted in all possible ways. This is apparent from the discussion in Appendix A in which a term in the expansion of $\exp(-\beta H')$ involves L' operators which are sums over all possible binary interaction operators. At equilibrium, the interactions in fact do take on all possible orderings, since there is a complete symmetry in the instants at which all the interactions are to take place, as shown by the expansion (3.3) of $U(0, -\infty)$. Away from equilibrium there are restrictions on the possible time orderings. For instance, in the terms of $C_{ij}(\mathbf{k}, t)$ involving an ICP of the form $\mathbf{T}$, no interactions of particle j can occur for positive times since particle j is not present in the diagram then. When there is symmetry in all the interaction times, the sum of all the diagrams with hanging clusters vanishes. The proof, given in Appendix C, is due in outline to Andrews.[12]

VII. SUMMARY

Classical many-time thermal averages can be conveniently computed for a gas in an interaction picture. The distribution over which the interaction picture average is to be taken is the free-particle distribution at the temperature of interest.

The diagrammatic representation of the operators whose interaction average gives the time-dependent two-particle correlation function is simply given for a uniform medium. Two distinct types of diagrams are seen to arise. One involves dynamical correlations only. The other involves statistical correlations in an intrinsic way. At equilibrium, the first type reduces to the autocorrelation function, and the second determines the radial distribution function. Integral equations can be written down in the time-dependent case for both types of diagrams.

The integral equations were solved in the random phase approximation. The dielectric constant computed from the kinetic equation (corresponding to dynamical correlations only) is seen to be identical to that found from the correlation function for all values of the frequency.

Some of the quantities that appear in the equations and diagrams can be identified as generalizations of quantities of interest in equilibrium. It is clear, however, that there are additional complications away from equilibrium that for sometimes subtle reasons disappear in the equilibrium limit.

VIII. ACKNOWLEDGMENT

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APPENDIX A.

Proof That $U(0, -\infty)$ Induces an Isothermal Process

Let φ_0 be the distribution function for a system of free particles. We want to prove (3.5) under the assumption that the perturbation depends on the particle positions only. The perturbation can be due to interactions or to external fields or both.

Applying (3.3) to φ_0 and carrying out the time integrations with the help of (3.2), we obtain the expansion

$$\varphi = \lim_{\epsilon \to 0} \sum_{n=0}^{\infty} \varphi_n(\epsilon), \tag{A1}$$

with

$$\varphi_n(\epsilon) = -(L_0 - in\epsilon)^{-1} L' \varphi_{n-1}(\epsilon) \tag{A2}$$

and

$$\varphi_0 = \exp(-\beta H_0) \Big/ \int d\Gamma \exp(-\beta H_0). \tag{A3}$$

Using the definition (2.3) of L, we find

$$\varphi_1(\epsilon) = \beta(L_0 - i\epsilon)^{-1}[L', H_0]\varphi_0 = i\beta(L_0 - i\epsilon)^{-1}\{H', H\}\varphi_0, \tag{A4}$$

where $[A, B]$ is the commutator of A and B. Then

$$\varphi_1 = -\beta \lim_{\epsilon \to 0} (L_0 - i\epsilon)^{-1} L_0 H' \varphi_0 = -\beta(1 - P_0)H'\varphi_0, \tag{A5}$$

where P_0 is the projection operator onto the space spanned by the zero-eigenvalue eigenfunctions of L_0.

Since H' depends on position only, Hamilton's equations give

$$\partial_i H = \partial_i H_0 = \mathbf{v}_i = \frac{\mathbf{p}_i}{m}. \tag{A6}$$

Consider the wavenumber representation of an arbitrary function f of the particle positions:

$$f(\{\mathbf{r}_i\}) = \Omega^{-1} \sum_{\{\mathbf{k}_i\}} f(\{\mathbf{k}_i\}) \exp(i\mathbf{k}_i \cdot \mathbf{r}_i), \tag{A7}$$

where $\{\mathbf{k}_i\}$ represents the $3N$-dimensional vector $\{\mathbf{k}_1, \cdots, \mathbf{k}_n\}$. From (2.19) and (A6),

$$L_0 f\varphi_0 = [L_0, f]\varphi_0 = \Omega^{-1} \sum_{\{\mathbf{k}_i\}} f(\{\mathbf{k}_i\}) \sum_i \mathbf{v}_i \cdot \mathbf{k}_i \exp(i\mathbf{k}_i \cdot \mathbf{r}_i)\varphi_0. \tag{A8}$$

The space defined by P_0 is characterized by $[L_0, f] = 0$, independent of the particle positions and the form of f. That is, it is given by the condition

$$\sum_i \mathbf{p}_i \cdot \mathbf{k}_i = 0. \tag{A9}$$

The phase space spanned by $\{\mathbf{p}_i\}$ is a $3N$-dimensional continuum in velocity. Consider a set $\{\mathbf{k}_i\} \neq (0, \cdots, 0)$. Equation (A9) defines a hyperplane in $\mathbf{p}$ space. For finite volume, there is a finite number of sets $\{\mathbf{k}_i\} \neq 0$. The union of all the planes defined by (A9) is of measure zero in $\mathbf{p}$ space, so gives no contribution to integrals over phase space.

The single point $\{\mathbf{k}_i\} = 0$ satisfies (A9) for all $\{\mathbf{p}_i\}$. But this point corresponds to a spatial average, which can be finite and must not be neglected. Thus

$$(1 - P_0)f(\{\mathbf{r}_i\})\varphi_0 = [f(\{\mathbf{r}_i\}) - \langle f(\{\mathbf{r}_i\})\rangle]\varphi_0, \tag{A10}$$

since the spatial average equals the average over the free-particle distribution.

When the volume becomes very large, the $\mathbf{k}$ space becomes a $3N$-dimensional continuum in the limit. So long as the Fourier components of $f(\{\mathbf{r}_i\})$ exist for $\{\mathbf{k}_i\} \neq 0$, the corresponding part of the space onto which P_0 projects is again of measure zero. Only the $\{\mathbf{k}_i\} = 0$ component contributes something finite. If the Fourier components diverge for $\{\mathbf{k}_i\} \to 0$, the calculation must be carried through for finite volume and the limit taken later. But since $f(\{\mathbf{r}_i\})$ will be a polynomial in the Hamiltonian, the limiting process could not be carried out at this stage of the calculation in any case. This occurs, for instance, for a Coulomb gas.

With (A10), Eq. (A5) becomes

$$\varphi_1 = -\beta \mathcal{H} \varphi_0, \tag{A11}$$

where

$$\mathcal{H} = H' - \langle H' \rangle. \tag{A12}$$

We now proceed by induction. Assume

$$\varphi_n = (n!)^{-1}(-\beta)^n \sum_{k=0}^{n} a_{nk} \mathcal{H}^k \varphi_0, \tag{A13}$$

where $\varphi_n = \lim_{\epsilon \to 0} \varphi_n(\epsilon)$. Then in the same way as for φ_1 we find, using (A2), that

$$\varphi_{n+1} = \frac{1}{(n+1)!}(-\beta)^{n+1}(1 - P_0) \times \sum_{k=0}^{n} \frac{n+1}{k+1} a_{nk} \mathcal{H}^{k+1} \varphi_0. \tag{A14}$$

It follows that φ_n is given by (A13) with $a_{00} = 1$ and the remaining a_{nk} determined by the recursion relations

$$\begin{aligned} a_{nk} &= (n/k) a_{n-1,k-1} \quad \text{for} \quad k > 0, \\ a_{n0} &= -P_0 \sum_{k=1}^{n} a_{nk} \mathcal{H}^k. \end{aligned} \tag{A15}$$

The direct expansion of $e^{-\beta \mathcal{H}}/\langle e^{-\beta \mathcal{H}} \rangle$ in powers of β gives

$$\begin{aligned} \varphi(\beta) &= \sum_{p=0}^{\infty} (-1)^p \sum_{k=0}^{\infty} \sum_{n_1=1}^{\infty} \cdots \\ &\quad \times \sum_{n_p=1}^{\infty} \frac{(-\beta)^{k+n_1+\cdots+n_p}}{k!\, n_1! \cdots n_p!} \langle \mathcal{H}^{n_1} \rangle \cdots \langle \mathcal{H}^{n_p} \rangle \mathcal{H}^k \varphi_0 \\ &= \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{p, k, \{n_i\}} (-1)^p \\ &\quad \times \frac{n!}{k!\, n_1! \cdots n_p!} \langle \mathcal{H}^{n_1} \rangle \cdots \langle \mathcal{H}^{n_p} \rangle \mathcal{H}^k \varphi_0, \end{aligned} \tag{A16}$$

where the inner summation in the last member is over values of $p, k, m, \cdots, n_p$ such that $k + n_1 + \cdots + n_p = n$. If we define α_{nk} by

$$\varphi(\beta) = \sum_{n=0}^{\infty} \frac{1}{n!} (-\beta)^n \sum_{k=0}^{n} \alpha_{nk} \mathcal{H}^k, \tag{A17}$$

then

$$\alpha_{nk} = \sum_{p, \{n_i\}} (-1)^p \frac{n!}{k!\, n_1! \cdots n_p!} \langle \mathcal{H}^{n_1} \rangle \cdots \langle \mathcal{H}^{n_p} \rangle, \tag{A18}$$

where the summation is such that $n_1 + \cdots + n_p = n - k$. Stepping n and k by one gives the same terms in $n_1, \cdots, n_p$. It follows that

$$\alpha_{n+1,k+1} = [(n+1)/(k+1)]\alpha_{nk}. \tag{A19}$$

Now multiply (A18) by $\mathcal{H}^k$, sum on k from 1 to n, apply the operator P_0, and write $q = p + 1$ and $k = n_q$. Then

$$\begin{aligned} P_0 \sum_{k=1}^{n} \alpha_{nk} \mathcal{H}^k &= -\sum_{q, \{n_i\}} \frac{n!}{n_1! \cdots n_q!} \langle \mathcal{H}^{n_1} \rangle \cdots \langle \mathcal{H}^{n_q} \rangle, \end{aligned} \tag{A20}$$

where now $n_1 + \cdots + n_q = n$. Comparing with (A17), we see that

$$\alpha_{n0} = -P_0 \sum_{k=1}^{n} \alpha_{nk} \mathcal{H}^k. \tag{A21}$$

Equations (A19) and (A21) are identical to (A15). Since $a_{00} = \alpha_{00} = 1$, the two expansions are identical, so (3.5) is proved.

One can proceed one step further. Suppose there is no external field and the interaction Hamiltonian is written

$$H' = \sum_\alpha \lambda_\alpha H_\alpha, \tag{A22}$$

where α denotes a pair of particles and λ is a strength parameter for the interaction of the pair α. The sum is over all the M pairs. Then the coefficients of $\lambda_1^{n_1} \cdots \lambda_M^{n_M}$ are the same in the two expansions, (A1) and (A16), since the λ's are arbitrary. The equality can be written as

$$\int_{-\infty}^{0} dt_1 \cdots \int_{-\infty}^{0} dt_n \, [L_{\alpha_1}(t_1) \cdots L_{\alpha_n}(t_n)]_+ = P(\alpha_1, \cdots, \alpha_n)\varphi. \tag{A23}$$

The α_i need not be distinct pairs. The left-hand side comes from the expansion of $U(0, -\infty)\varphi_0$. On the right, the projection operator $P(\alpha_1 \cdots, \alpha_n)$ picks out the coefficient of $\lambda_{\alpha_1} \cdots \lambda_{\alpha_n}$ in the expansion of the full canonical distribution function. This result is used in Appendix C.

We note finally that if

$$H' = \tfrac{1}{2} \sum_{i,j}{}' v(\mathbf{r}_i - \mathbf{r}_j) = \frac{1}{2\Omega} \sum_{\mathbf{k}} v(\mathbf{k}) \sum_{i,j}{}' \exp[i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)], \tag{A24}$$

then

$$\mathcal{K} = \tfrac{1}{2} \sum_{i,j}{}' \left[v(\mathbf{r}_i - \mathbf{r}_j) - \frac{1}{\Omega} \int v(\mathbf{r})\, d\mathbf{r} \right] = \frac{1}{2\Omega} \sum_{\mathbf{k}\neq 0} v(\mathbf{k}) \sum_{i,j}{}' \exp[i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)], \tag{A25}$$

so that

$$\langle \mathcal{K} \rangle = 0. \tag{A26}$$

APPENDIX B.

Diagrammatic Representation

We summarize here the rules for constructing diagrams. A less condensed account can be found elsewhere.[4,19] Every diagram corresponds to a wavenumber representation of some expression. Time goes from right to left. Each vertex corresponds to an operator $-iL_{ij}$ defined in (4.11). A line labeled $i_{\mathbf{k}}$ corresponds to free propagation and gives a factor $\Gamma_i(\mathbf{k}, t - t')$, defined in (4.12). In general, then, two lines converge at a vertex from the right and two emerge to the left. Only two particles are involved at a vertex and wavenumber is conserved.

Figure 4 shows the situation at a typical vertex. Particle i enters with wavenumber $\mathbf{k}_1$, and particle j with $\mathbf{k}_2$. Wavenumber $\mathbf{k}$ is transferred from j to i at the vertex.

A line corresponding to $\mathbf{k} = 0$ is omitted in drawing diagrams so if, for instance, $\mathbf{k} = \mathbf{k}_2$, then the $j_{\mathbf{k}_2-\mathbf{k}}$ line is omitted. If in addition $\mathbf{k}_1 = -\mathbf{k}_2$, the $i_{\mathbf{k}_1+\mathbf{k}}$ line is also omitted and we have a destruction vertex. If, on the other hand, $\mathbf{k}_1 = \mathbf{k}_2 = 0$, the two lines on the right are omitted and we have a creation vertex. If $\mathbf{k}_1 = 0$ and $\mathbf{k} = \mathbf{k}_2$, the vertex corresponds to the transfer of wavenumber $\mathbf{k}_2$ from j to i.

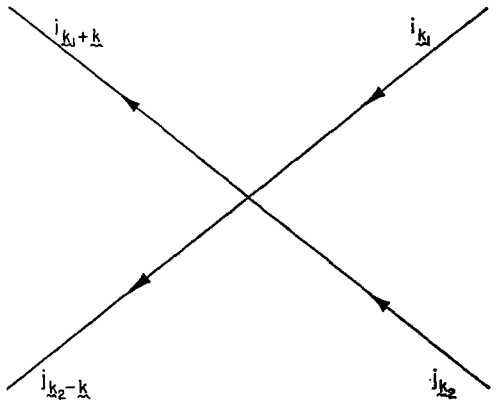

FIG. 4. Typical vertex.

APPENDIX C

Proof That Semiconnected Parts and Certain Hanging Clusters Do Not Contribute to Thermal Averages

We now prove that semiconnected parts and certain hanging clusters do not contribute to thermal averages. The proof involves a symmetry argument due to Andrews[12] who considered hanging clusters in equilibrium. We prove the theorem first for the simpler case of semiconnected parts, then extend the proof to hanging clusters in equilibrium and certain kinds of hanging cluster diagrams out of equilibrium. Andrews' argument is made complete by supplementing it with the results of Appendix A.

A semiconnected part (SCP) is a part of a diagram disconnected from the main part (the part with external lines), but which has one or more particles in common with it. It can be thought of as being connected to the main diagram by a $\mathbf{k} = 0$ line of the common particles. In the limit $N, \Omega \to \infty$ and N/Ω finite, Rule 8 of Sec. IV eliminates SCP's connected to the main diagram by more than a single particle. Rule 6 implies that the common particle is involved in the latest vertex of the SCP and at some later time in the main part. It cannot appear at an earlier time in the main part as well or Rule 8 would be violated. It follows that the interactions in the SCP precede all other interactions of the connecting particle, but there is no constraint on the earliest time involved.

Consider diagrams involving vertices for the pairs $\alpha_1, \cdots, \alpha_n$ in an SCP, and $\beta_1, \cdots, \beta_m$ in the remainder of the diagram. By the argument just given, one can write

$$[L_{\alpha_1}(t_1) \cdots L_{\alpha_n}(t_n)L_{\beta_1}(t_1') \cdots L_{\beta_m}(t_m')]_+ = [L_{\beta_1}(t_1') \cdots L_{\beta_m}(t_m')]_+[L_{\alpha_1}(t_1) \cdots L_{\alpha_n}(t_n)]_+. \quad \text{(C1)}$$

That is, the ordered product factorizes. Consider all such diagrams in which t_1 is the latest time in the semiconnected part. Then α_1 represents the particle pair (i, j), where i is the connecting particle and j is some other particle in the SCP. The ordered product is to be multiplied by functions of the coordinates and momenta of particles in the main part, integrated over the times, and averaged over the entire phase space. The averaging over the particles in the semiconnected part, except for particle i, can be done directly on the last ordered product in (C1). The integrations over the t_l can also be carried out. Thus one has to compute

$$\int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_1} dt_n \langle [L_{\alpha_1}(t_1) \cdots L_{\alpha_n}(t_n)]_+ \rangle_\alpha = \int d\Gamma_\alpha \, L_{ij}(t_1) \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_1} dt_n \times [L_{\alpha_2}(t_2) \cdots L_{\alpha_n}(t_n)]_+ \varphi_{0\alpha}. \quad \text{(C2)}$$

Here $\varphi_{0\alpha}$ is the part of φ_0 involving all particles in the semiconnected part except i, and $d\Gamma_\alpha$ is an element of the phase space of these particles. Now

$$\exp(-iL_0t_1) \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_1} dt_n \times [L_{\alpha_2}(t_2) \cdots L_{\alpha_n}(t_n)]_+ \varphi_0 = \int_{-\infty}^{0} dt_2 \cdots \int_{-\infty}^{0} dt_n \, [L_{\alpha_2}(t_2) \cdots L_{\alpha_n}(t_n)]_+ \varphi_0. \quad \text{(C3)}$$

Inserting (C3) and (A23) into (C2), we find that

$$\frac{1}{n!} \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_1} dt_n \langle [L_{\alpha_1}(t_1) \cdots L_{\alpha_n}(t_n)]_+ \rangle_\alpha = \int d\Gamma_\alpha \exp[i\mathbf{v}_i \cdot \nabla_i t_1] L_{ij} P(\alpha_1, \cdots, \alpha_n)\varphi_\alpha, \quad \text{(C4)}$$

where φ_α is the part of φ involving only particles in the SCP. Here $\exp(i\mathbf{v}_i \cdot \nabla_i t_1)$ is the only part of $\exp(iL_0t_1)$ that remains after integration over Γ_α. In terms of the interactions, $P(\alpha_1, \cdots, \alpha_n)$ involves only $H_{\alpha_1}, \cdots, H_{\alpha_n}$ and the momentum distribution function $\varphi_{0\alpha}$.

We are dealing with interactions symmetric in the two particles. Let

$$\mathbf{r}_l \to 2\mathbf{r}_i - \mathbf{r}_l \quad \text{(C5)}$$

for all particles l in the SCP other than i. Both sides of (C4) are invariant under the transformation (C5) since the only position dependence is on $\mathbf{r}_i - \mathbf{r}_l \to \mathbf{r}_l - \mathbf{r}_i$ for $l \neq i, j$ and on $\mathbf{r}_k - \mathbf{r}_l \to \mathbf{r}_l - \mathbf{r}_k$ for $k \neq i, j$, and the interactions are symmetric. On the other hand, under (C5),

$$L_{ij} = i\nabla_i H'(\mathbf{r}_i - \mathbf{r}_j) \cdot (\partial_i - \partial_j) \to -i\nabla_i H(\mathbf{r}_i - \mathbf{r}_j) \cdot (\partial_i - \partial_j) = -L_{ij}. \quad \text{(C6)}$$

It follows that the integrand of the right-hand side of (C4) is odd, so the integral vanishes. Thus semiconnected parts cannot contribute to thermal averages.

To extend the result to hanging clusters, assume that the factorization (C1) holds in the more general situation when the vertices involving particles in the hanging cluster correspond to some, but not necessarily all, of the α_i. That is, the interacting pairs in the hanging cluster form a subset of the α_i. Assume also that the time integrations over all the t_i in (C1) extend to some maximum time t_0. Then the symmetry argument above holds and hanging clusters which disappear before t_0 cannot contribute.

In equilibrium, $t_0 = 0$ and all the interacting pairs are among the α_i, so the result holds trivially. More generally, the conditions mean that at any time $t_0' < t_0$, the part of the diagram involving the α_i is detached from the main part. It is a component of $U(t_0', -\infty)\varphi_0$, which is itself an equilibrium distribution.

Asymptotic Renormalizability Conditions on Field Propagators

J. F. BOYCE*
International Center for Theoretical Physics, Trieste, Italy
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High-energy boundary conditions upon the basic Green's functions which limit the types of divergence arising in any approximational method of solution of a field theory are derived and shown to be related to the recently defined stability criterion.

I. AN ANALYSIS OF THE STABILITY CRITERION

IN order to solve a set of field equations in a nonperturbative manner it is necessary to have some criterion which may aid the choice of a particular method. Apart from using the general symmetries of the theory to in part determine an approximate solution,[1] the requirement that such a solution be susceptible to renormalization may be applied to impose further conditions. We establish conditions, in the form of bounds on the asymptotic behavior of certain products of the basic Green's functions of the theory, which are sufficient to ensure the above requirement. Given a theory having an n-point vertex whose Green's function in momentum space is $\Gamma(p_1, \cdots, p_n)$ and whose attached propagators are $\Delta(p_i)$, $(i = 1, \cdots, n)$, then the relevant product is

$$\Delta^{\frac{1}{2}}(p_1) \cdots \Delta^{\frac{1}{2}}(p_n)\Gamma(p_1, \cdots, p_n),$$

where summation over spin and internal indices is implied. This product is the stability complex associated with the vertex. Using the concept of asymptotic coefficients,[2] the limiting behavior of such an expression may be strictly defined. Stated roughly the derived conditions are

$$\Delta^{\frac{1}{2}}(p_1) \cdots \Delta^{\frac{1}{2}}(p_n)\Gamma(p_1, \cdots, p_n) \leq O(1/p^{2n-4}) \quad (1.1)$$

whenever all the momenta p_i become large, while

$$\Delta^{\frac{1}{2}}(p_1) \cdots \Delta^{\frac{1}{2}}(p_n)\Gamma(p_1, \cdots, p_n) < O(1/p^{2(n-m)-4}) \quad (1.2)$$

whenever m of them are held finite.

Specifically, these conditions ensure that the number of types of divergence which occur in any relevant multiple integral constructed from the basic Green's function is finite. This property implies that the subtraction procedure formulated by Dyson[3] and Salam[4] is equivalent to a renormalization of the masses and coupling constants of the theory.[5] It is found that for the case of electrodynamics the above conditions become identical with the stability criterion[6] and hence, although based upon quite different grounds, may be regarded as a generalization of it.

In Sec. II, the case of a single field, interacting with itself via a three-point vertex, is used to illustrate the meaning of the renormalizability conditions. The general case of any number of fields and any number of vertices is dealt with in Sec. III, while the definition in terms of Weinberg's asymptotic coefficients forms the content of the Appendix.

II. THE MEANING OF THE RENORMALIZABILITY CONDITIONS

Consider a theory having one propagator $\Delta(q)$ and a three-point vertex $\Gamma(q, r, s)$, momenta being directed inwards. The perturbative approximations to these quantities have evident asymptotic behaviors which allow the possible divergences of the theory to be easily identified. We shall adopt the inverse procedure by assuming power-law asymptotic behaviors and then determining how limiting the divergences affects the powers. However, it is preferable to consider the stability complex

$$\Delta^{\frac{1}{2}}(q)\Delta^{\frac{1}{2}}(r)\Delta^{\frac{1}{2}}(s)\Gamma(q, r, s),$$

rather than the individual Green's functions. Since the amplitude corresponding to a general two-particle connected diagram having l loops and E external lines is expressible in the form

$$I = \int d^4p_1 \cdots d^4p_l(\Delta^{\frac{1}{2}}\Delta^{\frac{1}{2}}\Delta^{\frac{1}{2}}\Gamma)^{2(l-1)}(\Gamma\Delta^{\frac{1}{2}}\Delta^{\frac{1}{2}})^E, \quad (2.1)$$

it is sufficient to consider the stability complex alone.

* Present address: Imperial College of Science and Technology, London.

[1] This idea is the basis of the gauge method formulated by Abdus Salam and R. Delbourgo, Phys. Rev. **135**, B1398 (1964).

[2] S. Weinberg, Phys. Rev. **118**, 838 (1960).

[3] F. J. Dyson, Phys. Rev. **75**, 1736 (1949).

[4] Abdus Salam, Phys. Rev. **82**, 217 (1951); Phys. Rev. **84**, 426 (1951).

[5] P. T. Matthews and Abdus Salam, Phys. Rev. **94**, 185 (1954).

[6] See Ref. 1, Part 1, Sec. A.

We assume that for all momenta large

$$\Delta^{\frac{1}{2}}(q)\Delta^{\frac{1}{2}}(r)\Delta^{\frac{1}{2}}(s)\Gamma(q, r, s) = O(1/p^{\beta}), \quad (2.2)$$

while if one is held finite

$$\Delta^{\frac{1}{2}}(q)\Delta^{\frac{1}{2}}(r)\Delta^{\frac{1}{2}}(s)\Gamma(q, r, s) = O(1/p^{\alpha}). \quad (2.3)$$

A precise definition of the meanings of these equations is given in the Appendix. It follows rigorously from them, and in an intuitive manner directly from Eqs. (2.2) and (2.3), that since any internal line of a two-particle-connected diagram carries at least one loop momentum the overall degree of diverence[7] is

$$D = 4l - (N - E)\beta - E\alpha$$

where N is the number of vertices. An immediate advantage of its expression in this form is the avoidance of the overcounting of divergences when the terms responsible for them cancel between the propagators and the vertex, one example where this occurs being vector electrodynamics.

Since
$$l = \tfrac{1}{2}(N - E) + 1, \quad (2.4)$$

$$D = 4 - (\beta - 2)N - (2 - \beta + \alpha)E. \quad (2.5)$$

The requirement that the degree of divergence should not increase whenever the number of internal vertices is increased implies

$$\beta \geq 2, \quad (2.6)$$

where the inequality corresponds to super-renormalizability. The additional condition for the degree of divergence to decrease upon increasing the number of external lines is

$$\alpha > 0. \quad (2.7)$$

These two equations constitute the renormalizability conditions. They exist on two different levels which are characteristic of the general conditions.

In order to exhibit the meaning of Eq. (2.6) we consider a general two-particle-connected diagram from which all external lines have been removed. The result is a vacuum diagram having the same internal structure as the original. Now it follows from Eq. (2.4) that any single increase in the number of its loops requires an insertion of two vertices. This insertion between two of its lines must be of one of the three forms shown in Fig. 1. But Eq. (2.6) just ensures that such insertions do not increase the overall degree of divergence of the diagram. This

[7] The degree of divergence, obtained by a power count of the integration momenta, was first employed in Sec. 5 of Ref. 3.

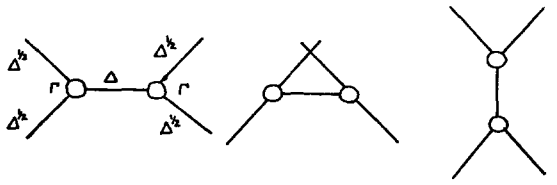

FIG. 1. Basic internal insertions.

implies by consistency, and it may be verified by a detailed analysis, that when $\beta = 2$, the degree of divergence of all such vacuum diagrams is four. It means that if the theory is just renormalizable, then the degree of divergence of any diagram may be characterized by its external line structure. For the general case $\beta \geq 2$, an upper bound on the degree of divergence may be so characterized. This is the necessary and sufficient condition for the primitively divergent diagrams[3] to be sufficient to characterize all the divergences of the theory.

The introduction of E external lines serves to reduce the degree of divergence by αE. Hence, given Eq. (2.6), the degree of divergence of any two-particle connected diagram satisfies

$$D \leq 4 - \alpha E. \quad (2.8)$$

Thus Eq. (2.7) ensures that the number of primitive divergents, and hence of types of divergence, is finite. In general, however, since α may be small, the number of primitive divergents may be very large.

In brief, the first of the renormalizability conditions ensures that the types of divergence contained within the theory are exhibited by the primitive divergents, while the second ensures that the number of such primitive divergents is finite.

III. THE GENERAL RENORMALIZABILITY CONDITIONS AND THEIR RELATION TO THE STABILITY CRITERION

Consider a theory composed of propagators Δ_i, $(i = 1, \cdots, \mathfrak{N})$ and vertices Γ_a, $(a = 1, \cdots, \mathfrak{A})$, the vertex Γ_a having n_a^i attached propagators of type i. The stability complex corresponding to this vertex is

$$\prod_i \Delta^{\frac{1}{2}n_a^i}\Gamma_a.$$

Let the asymptotic coefficient of this quantity whenever m^1 of the momenta of lines of type 1, m^2 of type 2, etc., are held fixed and all the remaining momenta tend independently to infinity be

$$\alpha(\{m^i\}) = \alpha(m^1, m^2, \cdots, m^{\mathfrak{N}}),$$

where

$$\{m^i\} = (m^1, \cdots, m^{\mathfrak{N}}).$$

Consider a two-particle connected diagram having E external lines, with I internal lines, of which I_i are of type i, and N vertices, of which N_a are of type a. Then

$$I = \sum_i I_i, \qquad 1 \leq i \leq \mathfrak{N};$$

$$N = \sum_a N_a, \qquad 1 \leq a \leq \mathfrak{A};$$

$$2I + E = \sum_i \sum_a n_a^i N_a;$$

while the number l of loops is given by

$$\begin{aligned} l &= I - N + 1, \\ &= \sum_a [\tfrac{1}{2} \sum_i n_a^i - 1] - \tfrac{1}{2}E + 1. \end{aligned} \tag{3.1}$$

Since $n_a = \sum_i n_a^i$ is the total number of lines emanating from the vertex Γ_a,

$$\tfrac{1}{2} \sum_i n_a^i - 1 > 0$$

for three- and higher-point vertices.

Let there be $A_a(\{m^i\})$ vertices Γ_a in the diagram which have the set $\{m^i\}$ as external lines. Thence

$$E = \sum_a \sum_{\mathcal{P}} (m^1 + m^2 + \cdots + m^{\mathfrak{N}}) A_a(\{m^i\}),$$

where $\sum_{\mathcal{P}}$ signifies summation over all sets $\{m^i\}$ which allow at least two lines of the vertex to be internal, except the case of all m^i zero, which occurs when none of the lines is external. More compactly,

$$E = \sum_a \sum_{\mathcal{P}} m A_a(\{m^i\}), \tag{3.2}$$

where

$$m = \sum_i m^i$$

and $\sum_{\mathcal{P}}$ signifies summation over all partitions of $1 \leq n \leq n_a - 2$ into sets $\{m^i\}$ having $\mathfrak{N}$ elements.

The total degree of divergence of the diagram is

$$D = 4l - \sum_a \sum_{\mathcal{P}} \alpha_a(\{m^i\}) A_a(\{m^i\}) - \sum_a \beta_a \{N_a - \sum_{\mathcal{P}} A_a(\{m^i\})\},$$

where $\beta_a = \alpha_a(\{m^i\})$, $m^i = 0$ for all i, viz., $-\beta_a$ is the asymptotic coefficient of the vertex whenever all the momenta tend to infinity.

Utilizing Eqs. (3.1) and (3.2)

$$D = 4 + \sum_a [2n_a - 4 - \beta_a] N_a - \sum_a \sum_{\mathcal{P}} [2m + \alpha_a(\{m^i\}) - \beta_a] A_a(\{m^i\}). \tag{3.3}$$

If D is not to increase whenever the number of any of the vertices increases

$$\beta_a \geq 2n_a - 4, \tag{3.4}$$

while, if the equality holds then

$$D = 4 - \sum_a \sum_{\mathcal{P}} [\alpha_a(\{m^i\}) - 2(n_a - m) + 4] A_a(\{m^i\}). \tag{3.5}$$

The additional condition for the number of primitive divergents to be finite is

$$\begin{aligned} &\alpha_a(\{m^i\}) > \beta_a - 2m, \\ \text{i.e.,}\quad &\alpha_a(\{m^i\}) > 2(n_a - m) - 4. \end{aligned} \tag{3.6}$$

Equations (3.4) and (3.6) may be identified with (1.1) and (1.2).

Their contents correspond exactly to those of Eqs. (2.6) and (2.7). They may be compared with the renormalization condition derived by Bogoliubov and Shirkov[8] by identifying the index of a vertex having all lines internal ω_a^{int}, with

$$\omega_a^{\text{int}} = \tfrac{1}{2} \sum_l (r_l + 2) - 4 = 2n_a - \beta_a - 4,$$

while

$$\tfrac{1}{2} \sum_{l,\text{ext}} (r_l + 2) = \sum_a \sum_{\mathcal{P}} [\alpha_a(\{m^i\}) + 2m - \beta_a] A_a(\{m^i\}).$$

Equations (3.4) and (3.6) have wider applicability since it has not been assumed that the asymptotic behavior of the vertices may be incorporated with the attached propagators, a restriction which makes the Bogoliubov and Shirkov condition inapplicable to the general case. They differ in that no positive-definite conditions have been imposed on the spectral functions, viz., $r_i > 0$ implying $\omega_i^{\text{int}} = \omega_i^{\max}$. Upon applying these additional conditions agreement is reached in all cases where both are applicable.

In the case of spinor electrodynamics, for approximations to which these conditions apply, Eq. (3.4) implies Eq. (3.6). It may then be identified with the stability criterion,[6] established as a necessary condition for the stability of any approximational method of solution of the Dyson–Schwinger equations. Due to the destructive interference which may occur between the divergent parts of separate contributions to an amplitude the conditions are in general too stringent. No general method for de-

[8] N. N. Bogoliubov and D. V. Shirkov, *Introduction to the Theory of Quantized Fields* (Interscience Publishers, Inc., New York, 1959), Sec. 28.

termining the allowed relaxation in response to a given over-all symmetry is known.

CONCLUSION

Since it may be shown that an extension of the Dyson–Salam subtraction procedure[9] is applicable to a general approximation scheme, the basic condition of renormalizability, that the number of types of divergence involved in the theory be finite, remains unaltered. Sufficient conditions for this to be satisfied are expressed by Eqs. (3.4) and (3.6) in the form of bounds upon the asymptotic behaviors of the products of Green's functions which form the stability complexes of the theory. They then have a form which is applicable to any approximational method of solution of any set of field equations which is expressed in terms of the Green's functions. It is conjectured that they have sufficient content as to be meaningful restrictions on the choice of approximation procedures. It is intended to give applications of them and to consider their consistency with the gauge invariance of the theory.

APPENDIX

The validity of the degree of divergence as a significant quantity is based upon Weinberg's asymptotic theorem.[2] This requires the concept of a special class of functions A defined as follows. A function $f(\mathbf{P})$ of n real variables $(p_1, \cdots, p_n)$ which are united to form a vector $\mathbf{P}$ in the n-dimensional space R is a member of the class of functions A_n if, given any subspace $S \subset R$ spanned by the m independent vectors $\{\mathbf{L}_1, \cdots, \mathbf{L}_m\}$ and finite region W, then

$$|f(\mathbf{L}_1\eta_1 \cdots \eta_m + \mathbf{L}_2\eta_2 \cdots \eta_m + \cdots + \mathbf{L}_m\eta_m + \mathbf{C})| \leq M\eta_1^{\alpha(\mathbf{L}_1)}(\ln \eta_1)^{\beta(\mathbf{L}_1)} \cdots (\eta_m)^{\alpha(\{\mathbf{L}_1,\cdots,\mathbf{L}_m\})} \times (\ln \eta_m)^{\beta(\mathbf{L}_1,\cdots,\mathbf{L}_m)}$$

provided that $\eta_1 \geq b_1, \cdots, \eta_m \geq b_m$ and $\mathbf{C} \in W$, where $b_1, \cdots, b_m$, and M are dependent only on $\mathbf{L}_1, \cdots, \mathbf{L}_m$, and W.

$$\alpha(S) = \alpha(\{\mathbf{L}_1, \cdots, \mathbf{L}_m\})$$

is the asymptotic coefficient which is characteristic of the subspace S, while the purpose of the lower bound conditions on the η's is to ensure that such characteristic behavior is indeed achieved.

Consider a general vertex Γ to which N propagators having momenta $(p_1, \cdots, p_N)$ may be attached. Let $(p_1, \cdots, p_n)$ be united to form a vector $\mathbf{P}$. If vectors $\mathbf{V}_i^\mu$ are defined such that

$$p_i^\mu = \mathbf{P}\cdot\mathbf{V}_i^\mu,$$

then the $\mathbf{V}_i^\mu$ form a basis in a real $4N$-dimensional space, R. The conservation of momenta may be expressed as

$$\mathbf{P}\cdot\mathbf{V}^\mu = 0,$$

where

$$\mathbf{V}^\mu = \sum_{i=1}^{N} \mathbf{V}_i^\mu,$$

and all momenta have been directed inwards. Hence $\mathbf{P}$ spans the space R' obtained by projecting V, the subspace spanned by the $\mathbf{V}^\mu$ along R, viz., $R' = \wedge(V)R$. The hypothesis that $\Gamma(\mathbf{P}) \in A_{4(N-1)}$ implies a direct correspondence between the asymptotic coefficients $\alpha(S)$ and the limiting behavior of Γ whenever a subset of its momenta tends to infinity. The statement that

$$\Gamma(p_1, \cdots, p_N) = O(p^\alpha) \quad \text{as} \quad (p_1, \cdots, p_i) \to \infty$$

means that α is the asymptotic coefficient associated with S, the subspace spanned by $\{\mathbf{V}_1, \cdots, \mathbf{V}_i\}$. This makes the statements concerning limits which are made in the text perfectly definite.

It should be noted that the hypothesis that the Green's functions belong to one of the classes A_n assumes that the contours of integration may be rotated in the energy plane so as to obtain a definite scalar product.

In order to state Weinberg's theorem we require several definitions. Any integral

$$f_I(\mathbf{P}) = \int \cdots \int d^4p_i \cdots d^4p_j\, f(p_1, \cdots, p_n),$$

where $(p_i, \cdots, p_j)$ is a subset of $(p_1, \cdots, p_n)$, may be expressed in the form

$$\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dy_1 \cdots dy_k\, f(\mathbf{P} + \mathbf{L}_1'y_1 + \cdots + \mathbf{L}_k'y_k),$$

where $(\mathbf{L}_1', \cdots, \mathbf{L}_k')$ are the unit vectors which correspond to the components of the set of four vectors $(p_i, \cdots, p_j)$. If

$$\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dy_1 \cdots dy_k\, |f(\mathbf{P} + \mathbf{L}_1'y_1 + \cdots + \mathbf{L}_k'y_k)|$$

is convergent, then the preceding integral is said to exist, and it follows that

$$f_I(\mathbf{P}) = \int_{P' \in I} d^k\mathbf{P}'\, f(\mathbf{P} + \mathbf{P}'),$$

[9] It can be shown, and is to be published elsewhere, that this procedure may be formulated in a manner which is applicable to the case of general approximations to the Green's functions, and that Weinberg's asymptotic theorem, upon which the efficacy of the procedure is based, still applies.

where $\mathbf{P} \in E = R \wedge I$, I being the subspace spanned by $\{\mathbf{L}_1', \cdots, \mathbf{L}_k'\}$. Upon defining the superficial divergence associated with the subspace S by

$$\mathfrak{D}(S) = \alpha(S) + \dim S,$$

where dim S is the dimension of S, then the asymptotic theorem takes the following form.

Given the function $f(P) \in A_n$ which is integrable over any finite region of R, then the condition

$$\max_{S \subset I} \mathfrak{D}(S) < 0$$

implies that (a) $f_I(\mathbf{P})$ exists and $\in A_{n-k}$; and (b) the asymptotic coefficient of $f_I(\mathbf{P})$ associated with $S \subset E$ is given by

$$\alpha_I(S) = \max_{\wedge(I)S'=S} \mathfrak{D}(S') - \dim S.$$

It may be shown that in the maximizing operations it is sufficient to consider those subspaces of R which are spanned by bases which correspond to subsets of the external and loop momenta, providing that all such subsets are considered. Hence, if the integral is superficially convergent with respect to all loop integrations for all possible choices of loop momenta, it is absolutely convergent. However, it is just these conditions which the Dyson–Salam subtraction procedure is designed to provide. Thus the asymptotic coefficients are meaningful in that they govern the number of subtractions to be made corresponding to a particular loop or set of loops and hence they provide a valid method for the identification of the divergences even in the general case.

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Empty Space-Times of Embedding Class Two

C. D. COLLINSON
Department of Applied Mathematics, The University of Hull, Hull, England.
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The null tetrad notation of Newman and Penrose is used to investigate empty space-times of embedding class two. Necessary conditions are found for algebraically special empty space-times to have this property.

1. INTRODUCTION

INTEREST has been renewed recently in the classical problem of embedding space-times in pseudo-Euclidean space. The motivation for this interest, together with several new results, is to be found in a series of papers appearing under the general title "Seminar on the Embedding problem"[1-6]. One of the few-known general results is that no empty space-time is of embedding class one (the embedding class of a space is the least number of extra dimensions required to perform the embedding).

In this paper, empty space-times are considered which can be embedded (locally and isometrically) in a pseudo-Euclidean space of six dimensions. The necessary and sufficient conditions for a space-time to be of embedding class two are that there exist two symmetric tensors a_{ij}, b_{ij}, and a vector s_i satisfying the following equations:[7]

Gauss equation:

$$R_{ijkl} = e_1(a_{ik}a_{jl} - a_{il}a_{jk}) + e_2(b_{ik}b_{jl} - b_{il}b_{jk});$$

Codazzi equations:

$$a_{ij;k} - a_{ik;j} = e_2(-s_k b_{ij} + s_j b_{ik}),$$
$$b_{ij;k} - b_{ik;j} = -e_1(-s_k a_{ij} + s_j a_{ik});$$

Ricci equation:

$$s_{i;j} - s_{j;i} + g^{kl}(a_{ki}b_{lj} - a_{kj}b_{li}) = 0.$$

In the above, g^{kl} and R_{ijkl} are the metric and curvature tensors of the space-time, and e_1 and e_2 are real constants of unit modulus.

Newman and Penrose[8] have introduced a formalism based on a tetrad of complex null vectors l^i, n^i, m^i, and $\bar{m}^i$. Algebraic manipulation within this formalism is comparable to manipulation in a local Minkowski coordinate system and the curvature tensor of an empty space-time is described concisely by five complex scalars $\psi_0, \cdots, \psi_4$. It seems reasonable, therefore, to expect the formalism to simplify, at least, the Gauss equation. The following two theorems are proved.

Theorem 1:
An empty space-time of embedding class two and type II or III (ie., having a nondegenerate algebraically special curvature tensor) must possess hypersurface orthogonal geodesic rays with zero shear and divergence.

Theorem 2:
An empty space-time of embedding class two and type N or D (ie., having a degenerate algebraically special curvature tensor) must possess hypersurface orthogonal geodesic rays with zero shear.

2. THE GAUSS-CODAZZI-RICCI EQUATIONS IN TETRAD NOTATION

All indices are now tetrad indices and γ_{mnp} are the complex Ricci rotation coefficients.[7,8] In tetrad notation the Gauss-Codazzi-Ricci equations are

$$R_{mnpq} = e_1(a_{mp}a_{nq} - a_{mq}a_{np}) + e_2(b_{mp}b_{nq} - b_{mq}b_{np}),$$

$$a_{mn;p} - a_{mp;n} - a_{mq}\gamma_n{}^q{}_p - a_{nq}\gamma_m{}^q{}_p + a_{mq}\gamma_p{}^q{}_n + a_{pq}\gamma_m{}^q{}_n = e_2(-s_p b_{mn} + s_n b_{mp}),$$

$$b_{mn;p} - b_{mp;n} - b_{mq}\gamma_n{}^q{}_p - b_{nq}\gamma_m{}^q{}_p + b_{mq}\gamma_p{}^q{}_n + b_{pq}\gamma_m{}^q{}_n = -e_1(-s_p a_{mn} + s_n a_{mp}),$$

and

$$s_{m;n} - s_{n;m} - s_q\gamma_m{}^q{}_n + s_q\gamma_n{}^q{}_m + a_{mq}b_n{}^q - a_{nq}b_m{}^q = 0,$$

where ; denotes the intrinsic derivative. On writing down each component of the Gauss equation explicitly, it proves useful to work not in terms of the a_{mn} and b_{mn} but rather in terms of certain quadratics of these arrays. The notation is now introduced.

[1] A. Friedman, Rev. Mod. Phys. **37**, 201 (1965).
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[8] E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).

3. USEFUL IDENTITIES

Consider a tensor T_{mnpq} which is proportional to the skew product of a symmetrical tensor t_{mn},

$$T_{mnpq} = \phi(t_{mp}t_{nq} - t_{mq}t_{np}).$$

The twelve scalars $T_0, \cdots, T_{11}$, defined by

$$\begin{aligned}
T_0 &= T_{1331} = \phi(t_{13}t_{13} - t_{11}t_{33}),\\
T_1 &= T_{1321} = \phi(t_{12}t_{13} - t_{11}t_{23}),\\
T_2 &= T_{1324} = \phi(t_{12}t_{34} - t_{14}t_{23}),\\
T_3 &= T_{2412} = \phi(t_{12}t_{24} - t_{22}t_{14}),\\
T_4 &= T_{2442} = \phi(t_{24}t_{24} - t_{22}t_{44}),\\
T_5 &= T_{1334} = \phi(t_{13}t_{34} - t_{14}t_{33}),\\
T_6 &= T_{1314} = \phi(t_{11}t_{34} - t_{13}t_{14}),\\
T_7 &= T_{1332} = \phi(t_{13}t_{23} - t_{12}t_{33}),\\
T_8 &= T_{2423} = \phi(t_{22}t_{34} - t_{23}t_{24}),\\
T_9 &= T_{2443} = \phi(t_{24}t_{34} - t_{23}t_{44}),\\
T_{10} &= T_{1212} = \phi(t_{11}t_{22} - t_{12}t_{12}),\\
T_{11} &= T_{3434} = \phi(t_{33}t_{44} - t_{34}t_{34}),
\end{aligned}$$

satisfy twelve quadratic identities, namely,

$$T_7(\bar{T}_2 - T_2) - T_5\bar{T}_3 + \bar{T}_9T_1 + \bar{T}_4T_6 - T_0\bar{T}_8 = 0, \tag{1a}$$

$$T_1\bar{T}_2 + T_6\bar{T}_3 + \bar{T}_1T_7 + T_{10}T_5 + T_0T_3 = 0, \tag{1b}$$

$$T_3\bar{T}_2 + T_8\bar{T}_1 + \bar{T}_{3\prime 7} + T_{10}T_9 + T_4T_1 = 0, \tag{1c}$$

$$T_5\bar{T}_2 - T_7\bar{T}_5 - \bar{T}_9T_6 + T_1T_{11} + T_0T_9 = 0, \tag{1d}$$

$$T_9\bar{T}_2 - \bar{T}_7\bar{T}_9 - \bar{T}_5T_8 + T_3T_{11} + T_4T_5 = 0, \tag{1e}$$

$$T_6(T_2 - \bar{T}_2) - T_1\bar{T}_5 + \bar{T}_1T_5 - \bar{T}_0T_7 + T_0\bar{T}_7 = 0, \tag{1f}$$

$$T_8(T_2 - \bar{T}_2) - T_3\bar{T}_9 + \bar{T}_3T_9 - \bar{T}_4\bar{T}_7 + T_4T_7 = 0, \tag{1g}$$

$$T_0T_2 - T_1T_5 - T_6T_7 = 0, \tag{1h}$$

$$T_4T_2 - T_3T_9 - T_8\bar{T}_7 = 0, \tag{1i}$$

$$-T_{10}(T_2 - \bar{T}_2) - T_1T_3 + {}_{\prime 1}\bar{T}_3 = 0, \tag{1j}$$

$$-T_{11}(T_2 - \bar{T}_2) - T_5T_9 + \bar{T}_5\bar{T}_9 = 0, \tag{1k}$$

$$T_{10}T_{11} - T_0T_4 + T_6T_8 - {}_{\prime 1}\bar{T}_9 + T_7\bar{T}_7 + \bar{T}_2^2 - \bar{T}_3\bar{T}_5 - 2T_2\bar{T}_2 = 0. \tag{1l}$$

These identities were found by inspection. Using each identity to eliminate a product of the T's it can be shown that no further independent quadratic identities exist.

The components of the Gauss equation can be written in empty space–time as

$$A_0 + B_0 = \psi_0, \tag{2a}$$

$$A_1 + B_1 = \psi_1, \tag{2b}$$

$$A_2 + B_2 = \psi_2, \tag{2c}$$

$$A_3 + B_3 = \psi_3, \tag{2d}$$

$$A_4 + B_4 = \psi_4, \tag{2e}$$

$$A_5 + B_5 = \psi_1, \tag{2f}$$

$$A_6 + B_6 = 0, \tag{2g}$$

$$A_7 + B_7 = 0, \tag{2h}$$

$$A_8 + B_8 = 0, \tag{2i}$$

$$A_9 + B_9 = \psi_3, \tag{2j}$$

$$A_{10} + B_{10} = -\psi_2 - \bar{\psi}_2, \tag{2k}$$

$$A_{11} + B_{11} = -\psi_2 - \bar{\psi}_2, \tag{2l}$$

where $\psi_0, \cdots, \psi_4$ are the tetrad components of the curvature tensor introduced by Newman and Penrose[8] and the scalars $A_0, A_1, \cdots$, and $B_0, B_1, \cdots$, are defined in terms of a_{mn} and b_{mn} in the same way as $T_0, T_1, \cdots$, are defined in terms of t_{mn}. Thus

$$\begin{aligned}
A_0 &= e_1(a_{13}a_{13} - a_{11}a_{33}),\\
B_0 &= e_2(b_{13}b_{13} - b_{11}b_{33}), \quad \text{etc.}
\end{aligned}$$

Substituting B for T in the quadratic identities (1a), $\cdots$, (1l) and using (2a), $\cdots$, (2l) to eliminate $B_0, B_1, \cdots$, in terms of $A_0, A_1, \cdots$, yields twelve equations linear in $A_0, A_1, \cdots$ (the terms quadratic in $A_0, A_1, \cdots$, are identically zero). These equations are

$$\psi_0A_8 - \psi_1(\bar{A}_9 - \bar{A}_3) + (\psi_2 - \bar{\psi}_2)A_7 + \bar{\psi}_3(A_5 - A_1) - \bar{\psi}_4A_6 = 0, \tag{3a}$$

$$\psi_0\psi_3 - \psi_1\psi_2 - \psi_0A_3 - \psi_1(A_{10} + \bar{A}_2) - \bar{\psi}_1A_7 - \bar{\psi}_2A_1 + (\psi_2 + \bar{\psi}_2)A_5 - \psi_3A_0 - \bar{\psi}_3A_6 = 0, \tag{3b}$$

$$\psi_1\psi_4 - \psi_3\psi_2 - \psi_4A_1 - \psi_3(A_{10} + \bar{A}_2) - \bar{\psi}_3\bar{A}_7 - \bar{\psi}_2A_3 + (\psi_2 + \bar{\psi}_2)A_9 - \psi_1A_4 - \bar{\psi}_1A_8 = 0, \tag{3c}$$

$$\psi_0\psi_3 - \psi_1\psi_2 - \psi_0A_9 - \psi_1(\bar{A}_2 + A_{11}) + \bar{\psi}_1A_7 - \bar{\psi}_2A_5 + (\psi_2 + \bar{\psi}_2)A_1 - \psi_3A_0 + \bar{\psi}_3A_6 = 0, \tag{3d}$$

$$\psi_1\psi_4 - \psi_3\psi_2 - \psi_4A_5 - \psi_3(\bar{A}_2 + A_{11}) + \bar{\psi}_3\bar{A}_7 - \bar{\psi}_2A_9 + (\psi_2 + \bar{\psi}_2)A_3 - \psi_1A_4 + \bar{\psi}_1A_8 = 0, \tag{3e}$$

$$-\psi_0\bar{A}_7 + \bar{\psi}_0A_7 + \psi_1(\bar{A}_5 - \bar{A}_1) - \bar{\psi}_1(A_5 - A_1) - (\psi_2 - \bar{\psi}_2)A_6 = 0, \tag{3f}$$

$$-\psi_4 A_7 + \bar{\psi}_4 \bar{A}_7 + \psi_3(\bar{A}_9 - \bar{A}_3) - \bar{\psi}_3(A_9 - A_3) - (\psi_2 - \bar{\psi}_2)A_8 = 0, \quad (3g)$$

$$\psi_0\psi_2 - \psi_1^2 - \psi_0 A_2 + \psi_1(A_1 + A_5) - \psi_2 A_0 = 0, \quad (3h)$$

$$\psi_4\psi_2 - \psi_3^2 - \psi_4 A_2 + \psi_3(A_3 + A_9) - \psi_2 A_4 = 0, \quad (3i)$$

$$\psi_2^2 - \bar{\psi}_2^2 - \psi_1\psi_3 + \bar{\psi}_1\bar{\psi}_3 + \psi_1 A_9 - \bar{\psi}_1\bar{A}_9 + (\psi_2 - \bar{\psi}_2)A_{11} + (\psi_2 + \bar{\psi}_2)(\bar{A}_2 - A_2) + \psi_3 A_5 - \bar{\psi}_3\bar{A}_5 = 0, \quad (3j)$$

$$\psi_2^2 - \bar{\psi}_2^2 - \psi_1\psi_3 + \bar{\psi}_1\bar{\psi}_3 + \psi_1 A_3 - \bar{\psi}_1\bar{A}_3 + (\psi_2 - \bar{\psi}_2)A_{10} + (\psi_2 + \bar{\psi}_2)(\bar{A}_2 - A_2) + \psi_3 A_1 - \psi_3\bar{A}_1 = 0, \quad (3k)$$

$$\psi_2^2 + 2\psi_2^2 - \psi_0\psi_4 - 2\bar{\psi}_1\bar{\psi}_3 + \psi_0 A_4 + \bar{\psi}_1(\bar{A}_9 + \bar{A}_3) + 2\psi_2\bar{A}_2 + 2\bar{\psi}_2(A_2 - \bar{A}_2) + (\psi_2 + \bar{\psi}_2)(A_{10} + A_{11}) + \bar{\psi}_3(\bar{A}_1 + \bar{A}_5) + \psi_4 A_0 = 0. \quad (3l)$$

The same equations hold with A replaced by B.

The usefulness of these equations can be demonstrated. The null tetrad can always be chosen so that $\psi_0 = 0$. If $a_{mn} = 0$ the equations yield, with $\psi_0 = 0$, $\psi_1 = \psi_2 = \psi_3 = \psi_4 = 0$. Hence the space–time is flat. This proves that no empty space–time is of embedding class one, since, for such space–times, a_{mn} and s_m could be put zero. Furthermore, if the determinant of the coefficients of $A_0, \cdots, A_{11}$ in the Eqs. (3) is nonzero, then $A_0, \cdots, A_{11}$ can be determined in terms of $\psi_0, \cdots, \psi_4$. By symmetry $B_0, \cdots, B_{11}$ can also be determined and will be equal to $A_0, \cdots, A_{11}$. Thus Eqs. (2a), $\cdots$, (2l), can be written with $A = 0$ and B replaced by $2B$. However, it has just been shown that such a system of equations is only possible in a flat space–time. Hence for embedding class two the determinant must be zero. This imposes a condition on the curvature tensor.

The two theorems stated in the Introduction can now be proven. Since these concern algebraically special space–times the null tetrad can be chosen so that $\psi_0 = \psi_1 = 0$. The converse of the Goldberg–Sachs theorem[8] gives $\gamma_{131} = \gamma_{133} = 0$. Geometrically this means that the tetrad vector $\mathbf{l}^i$ defines a congruence of geodesic rays with zero shear.[9] If $\gamma_{134} = \gamma_{143}$ the congruence is irrotational and therefore hypersurface-orthogonal.[10] If $\gamma_{134} = -\gamma_{143}$ the congruence is nondiverging. These results will all be used in proving the theorems.

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4. TYPE III

The null tetrad can be chosen so that ψ_3 is the only nonzero ψ and $\psi_3 = \bar{\psi}_3$. The Eqs. (3a), $\cdots$, (3l) yield $A_0 = A_1 = A_5 = A_6 = 0$, $A_{10} + \bar{A}_2 + \bar{A}_7 = A_{11} + \bar{A}_2 - \bar{A}_7 = 0$, $\psi_3 = A_3 + A_9$, with $A_3 = \bar{A}_3$, and $A_9 = \bar{A}_9$. These are consistent with the condition $\psi_3 \neq 0$ only if $a_{11} = a_{13} = 0$ and $a_{12} \neq 0$. In this case the following further equations are obtained, $a_{33} = a_{44}$, $a_{23} = a_{24}$, $a_{12} + a_{44} - a_{34} = 0$, and $\psi_3 = 2e_1 a_{12} a_{24}$. Similar results hold for b_{mn} and substituting into the Gauss equation gives $e_1 = -e_2$ (i.e., the embedding space is of signature 2), $a_{23} = -cb_{23}$, and $a_{mn} = cb_{mn}$ for all other choices of mn, where $c = \pm 1$.

Putting $mnp = 124$ in the Codazzi equations,

$$a_{12;4} + a_{12}\gamma_{412} - a_{44}\gamma_{132} - a_{34}\gamma_{142} + a_{24}\gamma_{134} = e_2(-s_4 b_{12}),$$

$$b_{12;4} + b_{12}\gamma_{412} - b_{44}\gamma_{132} - b_{34}\gamma_{142} + b_{24}\gamma_{134} = -e_1(-s_4 a_{12}).$$

Adding $-c$ times the first equation to the second leaves

$$a_{24}\gamma_{134} = 0.$$

Hence, since $a_{24} \neq 0$ ($\psi_3 \neq 0$), one has $\gamma_{134} = 0$ which proves Theorem 1 for type III space–times.

5. TYPE II

The null tetrad can be chosen so that ψ_2 and ψ_3 are the only nonzero ψ, and $\psi_3 = \bar{\psi}_3$. If $\psi_2 \neq \bar{\psi}_2$, the Eqs. (3a), $\cdots$, (3l) yield

$$A_0 = A_1 = A_4 = A_5 = A_6 = A_7 = A_8 = 0,$$

$$A_2 = \tfrac{1}{2}\psi_2,$$

$$A_{10} = A_{11} = -\tfrac{1}{2}(\psi_2 + \bar{\psi}_2) \quad \text{and} \quad A_9 = A_3 = \tfrac{1}{2}\psi_3.$$

Substituting these into the identity (1i) gives $\psi_3 = 0$ which contradicts the hypothesis. Hence, for embedding class two $\psi_2 = \bar{\psi}_2$. In this case the calculation proceeds as in Sec. 4 and it is found that

$$a_{11} = a_{13} = b_{11} = b_{13} = 0.$$

Equation (2k) then reads

$$2\psi_2 = e_1 a_{12}^2 + e_2 b_{12}^2.$$

Putting $mnp = 121$ in the Codazzi equations gives

$$a_{12;1} = -e_2 s_1 b_{12}$$

and

$$b_{12;1} = e_1 s_1 a_{12}.$$

Multiplying the first equation by e_1a_{12}, the second by e_2b_{12}, and adding yields

$$\tfrac{1}{2}(e_1a_{12}^2 + e_2b_{12}^2)_{;1} = 0.$$

Hence $\psi_{2;1} = 0$. However with the present choice of tetrad, one component of the Bianchi identities[8] becomes

$$\psi_{2;1} = 3\gamma_{134}\psi_2.$$

Thus $\gamma_{134} = 0$ which completes the proof of Theorem 1.

6. TYPE *N*.

The null tetrad can be chosen so that ψ_4 is the only nonzero ψ and $\psi_4 = \bar{\psi}_4$. Equations (3a), $\cdots$, (3l) yield

$$A_0 = A_1 = A_2 = A_5 = A_6 = 0 \quad \text{with} \quad A_7 = \bar{A}_7.$$

These and the Gauss equations are consistent only if $a_{11} = a_{13} = b_{11} = b_{13} = 0$. The calculation divides into three subcases.

(1) $a_{12} \neq 0$.

From Eq. (2k) $b_{12} \neq 0$, and so $A_2 = B_2 = 0$ imply $a_{34} = b_{34} = 0$. Putting $mnp = 314$ in the Codazzi equations gives

$$a_{12}\gamma_{134} = 0.$$

Hence

$$\gamma_{134} = 0.$$

(2) $a_{12} = 0$, not both a_{34}, b_{34} are zero.

From Eq. (2k) $b_{12} = 0$. Putting $mnp = 134$ in the Codazzi equations gives

$$a_{34}(\gamma_{134} - \gamma_{143}) = 0$$

and

$$b_{34}(\gamma_{134} - \gamma_{143}) = 0$$

Hence

$$\gamma_{134} = \gamma_{143}.$$

(3) $a_{12} = b_{12} = a_{34} = b_{34} = 0$.

Putting $mnp = 123, 324, 334$ in the first Codazzi equation gives

$$a_{23}\gamma_{143} - a_{33}\gamma_{142} = 0,$$

$$a_{23;4} - a_{23}\gamma_{214} - a_{22}\gamma_{314} + a_{32}\gamma_{412} + a_{42}\gamma_{312} + a_{33}\gamma_{244} - a_{23}\gamma_{344} = e_2(-s_4b_{23}),$$

$$a_{33;4} - 2a_{32}\gamma_{314} + a_{32}\gamma_{413} + 2a_{33}\gamma_{344} = e_2(-s_4b_{33}).$$

Taking γ_{142} times the last equation from γ_{143} times the second, using the first to eliminate derivatives of a_{mn}, and finally using the Newman–Penrose field equations[8] to eliminate derivatives of the γ's yields

$$-\gamma_{143}\gamma_{132}a_{24} + \gamma_{143}\gamma_{134}a_{22} - \gamma_{134}\gamma_{142}a_{23} = 0.$$

Suppose $\gamma_{134} \neq 0$. Then

$$a_{23} = Ua_{33}$$

and

$$a_{22} = U^2a_{33} + \bar{U}^2a_{44},$$

where $U = \gamma_{142}/\gamma_{143}$. Substituting these into (2e) gives

$$\psi_4 = -U^2[e_1a_{33}a_{44} + e_2b_{33}b_{44}],$$

which is zero because of (2l). Hence, since $\psi_4 \neq 0$, $\gamma_{134} = 0$ and this completes the proof of Theorem 2 for type-*N* space–times.

7. TYPE *D*.

The null tetrad can be chosen so that ψ_2 is the only nonzero ψ. As in type II space–times it is found that embedding is only possible if $\psi_2 = \bar{\psi}_2$. Using the Bianchi identity $\psi_{2;1} = 3\gamma_{134}\psi_2$ yields immediately $\gamma_{134} = \gamma_{143}$ which proves Theorem 2 for these space–times.

8. REMARKS

The metrics possessing hypersurface orthogonal geodesic rays with zero shear have been studied by Robinson and Trautman[11] and Kundt.[12] The Gauss–Codazzi–Ricci equations can be written explicitly for the metrics but are too difficult to solve. Further analysis of the type-*D* space–times for $\gamma_{134} \neq 0$ limits one to the *D*-*S* space–times of Robinson and Trautman. These include the Schwarzchild solution which is known to be of embedding class two.[13]

For space–times of type I the null tetrad can be chosen so that $\psi_0 = \psi_4 = 0$, $\psi_1 = \psi_3 \neq 0$ and $9\psi_2^2 \neq 16\psi_1^2$. Equations (3a), $\cdots$, (3l) possess solutions consistent with the identities (1a), $\cdots$, (1l) only if at least one of the expressions $\psi_2 - \bar{\psi}_2$, $2\psi_1^2 - \psi_2^2$, $4\psi_1^2 + 2\bar{\psi}_2^2 - \psi_2^2 - \psi_2\bar{\psi}_2$ is zero. The geometrical significance of this result is obscure. In each case the general solutions to (1a), $\cdots$, (1l) can be found but these contain several arbitrary scalars and the method becomes too unwieldy to yield further information.

The method depends on the simplicity of Eqs. (3a), $\cdots$, (3l). For space–times of higher embedding classes these equations will become multilinear equations in several sets of unknowns $A, B, C, \cdots$. These equations are unlikely to be of help in analyzing such space–times.

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Symmetry Properties of the 3j-Symbols for an Arbitrary Group*†

JEAN-ROBERT DEROME‡
Department of Mathematics, University of Toronto, Toronto, Ontario, Canada
(Received 20 September 1965)

The symmetry properties of the 3j-symbols are studied for an arbitrary compact group. It is shown that when the three j's are all inequivalent it is possible to choose 3j-symbols which are invariant under any permutation of the j's and of the corresponding m's (generalized magnetic quantum numbers). When two of the three j's are equivalent, the 3j-symbols can be chosen in such a way that at most a minus sign appears when the j's and m's are permuted. It is also shown that when the three j's are equivalent it is in general not possible to choose the 3j-symbol such that its absolute value is invariant under every permutation of the m's.

INTRODUCTION

In the development of Racah algebra for an arbitrary compact group it is possible to use 3j-symbols which are defined only up to a unitary transformation in the multiplicity variable.[1] In this paper we show how this arbitrariness in the definition of the 3j-symbol can be used to impose some simple symmetry relations among the various 3j-symbols.

It has been shown by Wigner[2] that the symmetry properties of the 3j-symbols for an arbitrary simply reducible (SR) group are essentially the same as for the rotation group in three dimensions. Hamermesh[3] has given the properties of the 3j-symbols of S_n, the symmetric group on n symbols, which is not SR if $n > 4$ and de Swart[4] has obtained the symmetry properties of the 3j-symbols for $SU(3)$. More recently Masuda[5] has given the symmetry properties of the 3j-symbols for an arbitrary (compact) group. For non-SR groups it is usually assumed that the 3j-symbol $(j_1j_2j_3)_{r,m_1m_2m_3}$ can be chosen such that its absolute value is invariant under any permutation of the j's and of the corresponding m's. However, as we will show, this assumption is in general valid only when at least two of the three j's are inequivalent.

THE TRANSPOSITION MATRICES

The matrix elements of the irreducible representation j of the group G are denoted by $j(R)^m{}_{m'}$, where $R \in G$. We write $j(R)_m{}^{m'}$ for the complex conjugate of $j(R)^m{}_{m'}$ and $[j]$ for the degree of j. Sums are implied over repeated m (generalized magnetic quantum number) and r (multiplicity) indices; the 3j-symbol is denoted by $(j_1j_2j_3)_{r,m_1m_2m_3}$ [by $(j_1j_2j_3)_r$ in shorthand form]. It is defined by

$$j_1(R)^{m_1}{}_{m_1'}j_2(R)^{m_2}{}_{m_2'} = \sum_{j_3}[j_3]\{(j_1j_2j_3)_{r,m_1m_2m_3}\}^* \times j_3(R)_{m_3}{}^{m_3'}(j_1j_2j_3)_{r,m_1'm_2'm_3'}, \quad (1)$$

where the indicated sum runs over all the equivalence classes of irreducible representations of G since $(j_1j_2j_3)_r$ is chosen to be zero whenever j_3^* is not a constituent of $j_1 \times j_2$ (i.e., whenever $j_1j_2j_3$ do not form a triad). The 1j-symbol $(j)_{mm'} = [j]^{\frac{1}{2}}(j0j^*)_{m0m'} = \{(j)^{mm'}\}^*$ can then be used as a metric tensor to define 3j-symbols with some of the m's contravariant. For instance

$$(j_1j_2j_3)_r{}^{m_1}{}_{m_2m_3} = (j_1)^{m_1m_1'}(j_1^*j_2j_3)_{r,m_1'm_2m_3}.$$

In shorthand notation $(j_1j_2j_3)_r{}^{m_1}{}_{m_2m_3}$ is written $(\mathbf{j}_1j_2j_3)_r$.[1] Similarly the unitary matrix

$$A(123)_{rs} = (j_1j_2j_3)_r(\mathbf{j}_1\mathbf{j}_2\mathbf{j}_3)_s$$

can be used as a multiplicity metric tensor to raise the multiplicity indices. It is then easy to show that[1]

$$(\mathbf{j}_1\mathbf{j}_2\mathbf{j}_3)^r = \{(j_1j_2j_3)_r\}^*.$$

We assume that for each representation space a definite choice of basis has been made. The 3j-symbol $(j_1j_2j_3)_r$ is then determined up to a unitary transformation in the multiplicity variable. We will say that two sets of 3j-symbols are U-equivalent if they

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‡ Present address: Laboratoire de Physique Théorique et Hautes Energies, Bâtiment 211, Faculté des Sciences, 91-Orsay, France.

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are related by a unitary transformation in the multiplicity variable and we write

$$\{(j_1j_2j_3)_{r,m_1m_2m_3}\}' = U(123)_r{}^{r'}(j_1j_2j_3)_{r',m_1m_2m_3}. \quad (2)$$

We now introduce the unitary matrices

$$M(a, bc)_r{}^{r'} = (j_aj_cj_b)_r(j_aj_bj_c)^{r'}, \quad (3)$$

and

$$M(ab, c)_r{}^{r'} = (j_bj_aj_c)_r(j_aj_bj_c)^{r'}, \quad (3')$$

where $j_aj_bj_c$ can be any permutation of the triad $j_1j_2j_3$. Using the unitarity of the $3j$-symbols[1] we obtain

$$(j_aj_cj_b)_r = M(a, bc)_r{}^{r'}(j_aj_bj_c)_{r'}, \quad (4)$$

and

$$(j_bj_aj_c)_r = M(ab, c)_r{}^{r'}(j_aj_bj_c)_{r'}. \quad (4')$$

In view of Eqs. (4) and (4') we call the matrices $M(a, bc)$ and $M(ab, c)$ transposition matrices. Given a triad $j_1j_2j_3$, there are at most twelve such transposition matrices: $M(1, 23)$, $M(2, 13)$, $M(3, 12)$, $M(12, 3)$, $M(13, 2)$, $M(23, 1)$, $M(1, 32)$, $M(2, 31)$, $M(3, 21)$, $M(21, 3)$, $M(31, 2)$, and $M(32, 1)$. There are six other unitary matrices which correspond to transpositions of the first and third j's in the $3j$-symbol, but these are not new because they are products of some of the above twelve. Similarly, the cyclic permutations of the j's and m's in a $3j$-symbol can be expressed as a product of transposition matrices. Moreover the twelve transposition matrices listed above are not all independent since

$$\begin{aligned} M(ab, c) &= M(ba, c)^{-1}, \\ M(a, bc) &= M(a, cb)^{-1}, \end{aligned} \quad (5)$$

and

$$M(23, 1)\, M(2, 13)\, M(12, 3) = M(3, 12)\, M(13, 2)\, M(1, 23). \quad (5')$$

Using Eqs. (5) and (5') we can express every transposition matrix in terms of five of them. We call such a set of five "independent" transposition matrices a fundamental set for the triad $j_1j_2j_3$. Without any loss in generality we choose $M(12, 3)$, $M(13, 2)$, $M(23, 1)$, $M(1, 23)$, and $M(2, 13)$ to be the fundamental transposition matrices (i.e., members of the fundamental set). Any permutation of the j's and m's in a $3j$-symbol can be obtained by applying successively a number of fundamental transpositions and their inverses.

According to Eqs. (3) and (3') the transposition matrices are completely determined by the $3j$-symbols and the transformations of the $3j$- symbols realized by the matrices $U(abc)$ induce the following transformations of the five fundamental transposition matrices:

$$\begin{aligned} M(12, 3)' &= U(213)\, M(12, 3)\, U(123)^{-1}, \\ M(13, 2)' &= U(312)\, M(13, 2)\, U(132)^{-1}, \\ M(23, 1)' &= U(321)\, M(23, 1)\, U(231)^{-1}, \\ M(1, 23)' &= U(132)\, M(1, 23)\, U(123)^{-1}, \\ M(2, 13)' &= U(231)\, M(2, 13)\, U(213)^{-1}. \end{aligned} \quad (6)$$

The transformation properties of the other permutation matrices are easily obtained from those of the fundamental set.

Let $j_1j_2j_3$ be three irreducible representations of a compact group G which form a triad, and suppose we are given a complete set of $3j$-symbols for this triad, i.e., we are given all $(j_aj_bj_c)_r$, where $j_aj_bj_c$ can be any permutation of $j_1j_2j_3$. We now wish to find a new complete set of $3j$-symbols which is U-equivalent to the given set and which yields the "simplest" permutation matrices, i.e., the simplest symmetry properties for the $3j$-symbols.[6]

For SR groups the usual choice of symmetry properties for the $3j$-symbols is that of Wigner.[2,7] It consists in taking[8]

$$M(a, bc) = M(ab, c) = (-1)^{j_a+j_b+j_c},$$

where $(-1)^j$ is a certain phase associated with j. For a general group such a simple choice is not possible.

Several authors assume that it is in general possible to diagonalize simultaneously all the fundamental transposition matrices of any triad. They then choose their $3j$-symbols such that the effect of a permutation of the j's and m's is at most a multiplicative phase. Below we give a counterexample which shows that this assumption is in general wrong.

In order to discuss the symmetry properties of the $3j$-symbols of a general group it is convenient to consider three different cases corresponding to three different types of triad.

CASE 1

If the three members of a triad are all inequivalent, i.e., $j_1 \neq j_2 \neq j_3 \neq j_1$, the five fundamental transposition matrices can be transformed to the

[6] It should be emphasized that this set is not necessarily unique, i.e., two U-equivalent but distinct sets of $3j$-symbols may satisfy the same symmetry relations.

[7] W. T. Sharp, "Racah Algebra and the Contraction of Groups." Report AECL-1098, Atomic Energy of Canada Ltd., Chalk River, Ontario, 1960.

[8] For SR groups the transposition matrices are just complex numbers of modulus one.

same unitary Hermitian matrix D by taking[9]

$$\begin{aligned} U(213) &= D, \\ U(123) &= M(12, 3), \\ U(132) &= D\,M(12, 3)\,M(1, 32), \\ U(312) &= M(12, 3)\,M(1, 32)\,M(31, 2), \\ U(321) &= D\,M(12, 3)\,M(1, 32)\,M(31, 2)\,M(3, 21), \\ U(231) &= M(12, 3)\,M(1, 32) \\ &\quad \times M(31, 2)\,M(3, 21)\,M(23, 1). \end{aligned} \tag{7}$$

This is easily checked by substituting Eq. (7) into Eq. (6).

It then follows that the transformed transposition matrices are all equal to D since every transposition corresponds to a product of an odd number of fundamental transpositions. A cyclic permutation corresponds to a product of an even number of transpositions and each new $3j$-symbol is therefore invariant under any cyclic permutation of its arguments.

Since one can always take $D = 1$ one can choose the $3j$-symbols to be invariant under any permutation of the j's and m's provided the three j's are inequivalent.

CASE 2

If exactly two of the three j's are equivalent, say $j_1 = j_2 \neq j_3$, Eqs. (6) become

$$\begin{aligned} M(11, 3)' &= U(113)\,M(11, 3)\,U(113)^{-1}, \\ M(13, 1)' &= U(311)\,M(13, 1)\,U(131)^{-1}, \\ M(1, 13)' &= U(131)\,M(1, 13)\,U(113)^{-1}. \end{aligned} \tag{8}$$

Clearly it may be possible to choose $M(11, 3)'$ equal to the unit matrix only if $M(11, 3)$ has no eigenvalue other than $+1$. Since $M(11, 3) = M(11, 3)^{-1}$ its possible eigenvalues are $+1$ and -1. Therefore, if $M(11, 3)$ has eigenvalues $+1$ and -1 with degeneracies S and A, respectively,[10] then by a suitable choice of $U(113)$ we can take

$$M(11, 3)' = \begin{bmatrix} 1_S & 0 \\ 0 & -1_A \end{bmatrix}. \tag{9}$$

If we now take

$$\begin{aligned} U(131) &= U(113)\,M(11, 3)\,M(1, 31), \\ U(311) &= U(113)\,M(1, 31)\,M(31, 1), \end{aligned}$$

we obtain

$$M(13, 1)' = M(1, 13)' = M(11, 3)' = \begin{bmatrix} 1_S & 0 \\ 0 & -1_A \end{bmatrix}.$$

Since $M(11, 3)' = (M(11, 3)')^{-1}$ it then follows that every new transposition matrix is equal to $M(11, 3)'$ and that every cyclic permutation leaves the $3j$-symbol invariant.

CASE 3

Finally if $j_1 = j_2 = j_3$ $(= j)$ the Eqs. (6) become

$$\begin{aligned} M(jj, j)' &= U(jjj)\,M(jj, j)\,U(jjj)^{-1}, \\ M(j, jj)' &= U(jjj)\,M(j, jj)\,U(jjj)^{-1}. \end{aligned} \tag{10}$$

Clearly the two fundamental transposition matrices $M(jj, j)$ and $M(j, jj)$ can be diagonalized simultaneously only if they commute, in which case

$$\int (\chi^j(R))^3\,dR = \int \chi^j(R^3)\,dR, \tag{11}$$

where $\chi^j(R)$ is the character of j and the integration is to be performed over the (compact) group. To prove this we use the fact that

$$(M(j, jj)\,M(jj, j))^2 = 1$$

which follows from the commutativity of the two Hermitian unitary matrices $M(j, jj)$ and $M(jj, j)$. This means that the $3j$-symbol $(jjj)_{r,mm'm''}$ is invariant under any cyclic permutation of the m's. It then follows from the properties[11] of the $3j$-symbols that

$$\int j(R)^m{}_n j(R)^{m'}{}_{n'} j(R)^{m''}{}_{n''}\,dR = \int j(R)^m{}_{n'} j(R)^{m'}{}_{n''} j(R)^{m''}{}_n\,dR.$$

Setting $m = n$, $m' = n'$, $m'' = n''$, and performing the sums we then obtain Eq. (11).[12]

We conclude by giving an example for which Eq. (11) does not hold. Consider S_6 the symmetric group on six symbols and let j be the irreducible representation of degree 16 usually denoted by the

[9] This matrix D must be unitary and Hermitan but it is otherwise arbitrary. For a non-SR group one usually takes $D = 1$. If the group is SR, $D = (-1)^{j_1+j_2+j_3}$ is the most convenient choice because it is then possible to consider the three different types of triad on the same footing.

[10] One easily shows that S and A are the multiplicities of $j_3{}^*$ in the symmetric and antisymmetric squares of j_1, respectively.

[11] See for instance Ref. 1, Eq. (2.5).

[12] Equation (11) can also be obtained as follows. We first observe that the matrices $M(jj, j)$ and $M(j, jj)$ generate a representation M of the group S_3. The transposition matrices can be taken in diagonal form only if M does not contain the irreducible representation [21] of S_3 and the multiplicity of [21] in M is easily found to be $\frac{1}{3}\int[(\chi^j(R))^3 - \chi^j(R^3)]\,dR/\int dR$.

Young diagram [321].[13] A simple calculation shows that

$$\sum_R (\chi^j(R))^3 - \sum_R \chi^j(R^3) = 2160.$$

Thus if j is the 16-dimensional irreducible representation of S_6 it is not possible to diagonalize simultaneously $M(jj, j)$ and $M(j, jj)$. In other words, it is not possible to choose the $3j$-symbols of S_6 in the "symmetric" form $(jjj)_{r,mm'm''} = \theta_r(jjj)_{r,m'mm''} = \theta_r'(jjj)_{r,mm''m'}$, where θ_r and θ_r' are just phase factors.[14] For $SU(3)$, although we could not find a similar counterexample, to our knowledge no proof has yet been given that the $3j$-symbols can all be chosen in diagonal form.

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ACKNOWLEDGMENTS

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[14] This statement contradicts Eq. (7.207b) of Hamermesh's book (Ref. 3). However this equation does not seem to follow from what precedes it.

Statistical Mechanics of High-Temperature Quantum Plasmas Beyond the Ring Approximation*

HUGH E. DEWITT
Lawrence Radiation Laboratory, University of California, Livermore, California
(Received 3 May 1965)

A quantum mechanical perturbation expansion of the partition function is used to evaluate the free energy of the electron gas and multicomponent plasmas to logarithmic accuracy in the particle number density, thus including the next important contribution beyond the ring approximation. The quantum generalization of Abe's work on the classical electron gas is given for the ladder interactions with the dynamic screened Coulomb potential, and each ladder is shown to be separately finite because of the finite size of the wave packets describing point electrons [of the order of the thermal de Broglie wavelength $\lambda = \hbar(\beta/2m)^{1/2}$]. The results show that quantum effects due to the uncertainty principle persist at high temperature, and that when $kT >$ Ryd plasmas are quantum systems, rather than classical, because λ is greater than the average distance of closest approach, βe^2. Results are also obtained for the Wigner–Kirkwood wave mechanical diffraction corrections to the classical electron-gas free energy which are valid for low temperature ($kT <$ Ryd). The connection between the high- and low-temperature formula is discussed, and it is shown how the logarithmic divergence in the free energy that is cut off at βe^2 in the low-temperature electron gas in the Abe theory is cut off at λ in the high-temperature case. Also it is shown that the quantum diffraction effects contained in the Montroll–Ward ring sum formula are valid only for $kT >$ Ryd, even though the quantum ring sum formula contains the classical Debye–Hückel result.

I. INTRODUCTION

IN this paper we consider the evaluation of the free energy of single-component and multicomponent plasmas at high temperature to logarithmic accuracy in the particle number density. The general method to be used is an evaluation of terms in the perturbation expansion of the partition function along the lines initiated by Montroll and Ward[1] some years ago. A quantum mechanical treatment is necessary from the beginning since quantum effects persist even at high temperature. These quantum effects, however, are primarily due to the uncertainty principle and not particle indistinguishability; thus in this paper we assume Maxwell–Boltzmann statistics. Over a very wide temperature and density regime the dominant contribution to the plasma free energy due to Coulombic interactions is given by the ring interactions, the equivalent of the Bohm and Pines random phase approximation (RPA).[2] The quantum mechanical ring sum formula obtained first by Montroll and Ward[1] has been evaluated for high-temperature plasmas and gives wave mechanical corrections[3] to the classical limit, the Debye–Hückel result. If these usually small wave mechanical corrections are retained, then it is also necessary to include additional corrections not in the RPA arising from a more accurate treatment of two-body interactions. The Feynman diagrams describing the higher-order contributions to the two-particle scattering amplitude are often described as ladders[4] and in this paper we will use this term to describe the analogous contributions to the free energy. The ladder diagrams were evaluated for the classical one-component plasma, a gas of point charges in a continuous neutralizing background, by Abe.[5] Here we give the quantum theory of the ladder diagrams.

It is helpful to consider the divergence difficulties that one finds with a simple perturbation expansion of the free energy of a system of point charges. These difficulties are simply illustrated by the classical electron gas. The Helmholtz free energy obtained from the first three terms of the expansion of the second virial coefficient in powers of e^2 is

$$\begin{aligned}\beta(F - F_0) &= -\frac{N^2}{2V}\int_0^\infty 4\pi r^2\,dr \\ &\quad\times\left[\frac{1}{2!}\left(\frac{\beta e^2}{r}\right)^2 - \frac{1}{3!}\left(\frac{\beta e^2}{r}\right)^3 + \cdots\right] \\ &= -4\pi N\rho\{\tfrac{1}{4}(\beta e^2)^2 L_{\max} - \tfrac{1}{12}(\beta e^2)^3 \\ &\quad\times\log(L_{\max}/L_{\min})\cdots\}, \qquad (1)\end{aligned}$$

where F_0 is the ideal-gas free energy, $\beta = 1/kT$, and $\rho = N/V$ is the number density for N particles

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in volume V. In the second line of Eq. (1) the cutoff lengths $L_{\max}$ and $L_{\min}$ indicate the linear and logarithmic divergencies which a correct theory should take care of automatically. Note that the first-order term in e^2 is removed by electrical neutrality. The summation of the ring diagrams replaces the second-order term in Eq. (1) with

$$-\frac{1}{2}\int_0^1 \frac{dg}{g}\int \frac{V\,d^3k}{(2\pi)^3}\frac{4\pi g e^2\beta\rho}{k^2}\frac{4\pi g e^2\beta\rho}{k^2+4\pi g e^2\beta\rho}$$
$$= -\frac{1}{2}\int \frac{V\,d^3k}{(2\pi)^3}\left\{\frac{1}{(k\lambda_D)^2}-\log\left[1+\frac{1}{(k\lambda_D)^2}\right]\right\} \quad (2)$$
$$= -4\pi N\rho\tfrac{1}{3}(\beta e^2)^2\lambda_D,$$

from which one sees that the cutoff of the linear divergence is the Debye length, $\lambda_D = (4\pi e^2\beta\rho)^{-\frac{1}{2}}$. Essentially the ring sum is a modification of second-order perturbation theory in which one Coulomb interaction is replaced by the screened Coulomb interaction:

$$u_s(r) = (e^2/r)e^{-r/\lambda_D}. \quad (3)$$

The logarithmic divergencies of the third-order term in Eq. (1) are removed following Abe[5] by replacing the simple third-order perturbation theory with

$$-\frac{N^2}{2V}\int_0^\infty 4\pi r^2\,dr\sum_{m=3}^{\infty}\frac{(-\beta u_s(r))^m}{m!}$$
$$= +4\pi N\rho\tfrac{1}{12}(\beta e^2)^3[\log(\lambda_D/\beta e^2) - D_c\cdots], \quad (4)$$
$$D_c = \log 3 + 2C - 11/6, \qquad C = 0.5772.$$

In the third-order term, the long-distance cutoff is again the Debye length, and the short-distance cutoff is the only other length in the classical problem, the average distance of closest approach, βe^2. Equation (4) is the first term of the nodal expansion developed independently by Abe,[5] Meeron,[6] and Friedman.[7] As applied to the electron gas, the nodal expansion is a rearrangement of the complete perturbation expansion of the free energy such that long- and short-distance divergencies are systematically cut off at λ_D and βe^2, respectively. Note that two steps are necessary to cut off the logarithmic divergencies in the third-order term of Eq. (1): (i) chains of Coulomb interactions are summed to give screened interactions, $u_s(r)$, between two particles, and (ii) the resulting ladder diagrams with screened interactions are summed from 3 to ∞. Step (i) gives $L_{\max} = \lambda_D$ and step (ii) gives $L_{\min} = \beta e^2$. The classical diagrams are shown in Fig. 1.

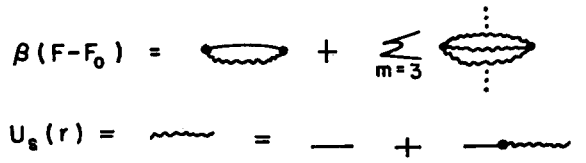

FIG. 1. Diagrammatic representation of the leading contribution to the free energy of the classical electron gas. Points represent charges, horizontal lines the Coulomb interaction, and wavy lines the screened interaction.

Wave mechanics introduces a third length, the thermal de Broglie wavelength, $\lambda\!\!\!^{-} = \hbar/(2mkT)^{\frac{1}{2}}$. The point charges of the classical problem must now be considered as interacting wave packets of spatial extension $\lambda\!\!\!^{-}$. This finite extension has the important consequence that each ladder term is separately finite. Thus the quantum theory of the third-order term in Eq. (1) gives $L_{\min} = \lambda\!\!\!^{-}$, and the mth-order term will be proportional to $(\beta e^2)^m/\lambda\!\!\!^{-m-3}$. It is important to realize that at high temperatures the thermal wavelength is larger than βe^2, i.e., $\lambda\!\!\!^{-} > \beta e^2$ when $kT >$ Ryd. Consequently the ladder interactions for $m \geq 4$ may be neglected in comparison with the $m = 3$ term at high enough temperatures. Thus the quantum theory of high-temperature plasmas is in one respect *simpler* than the theory of the classical electron gas, namely, step (ii), the summation of ladder diagrams, is not necessary. The uncertainty principle provides the necessary short-distance cutoff. The two diagrams required for the quantum treatment of the divergencies in Eq. (1) are shown in Fig. 2. Each particle is indicated by a bubble in which the downward line indicates the hole in the equilibrium Maxwellian momentum distribution after interaction and the upward line indicates the various excited states of the particle. The intermediate temperatures go from 0 to β, and indicate the "times" at which the interactions take place. In the classical limit, $\hbar = 0$, the bubbles shrink down to the points shown in Fig. 1.

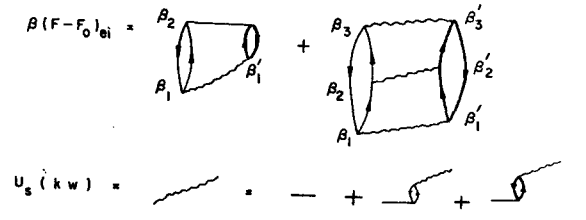

FIG. 2. Diagrams representing the leading contribution of electron–ion interactions to the free energy of a high-temperature plasma. Light bubbles represent electrons, and heavy bubbles, ions. The wavy lines indicate the dynamic screened interaction.

[6] E. Meeron, Phys. Fluids 1, 139 (1958).
[7] (a) H. F. Friedman, Mol. Phys. 2, 23 (1959); see also (b) H. F. Friedman, Mol. Phys. 2, 190, 436 (1959).

II. QUANTUM MECHANICAL FORMS OF THE LADDER INTERACTIONS

In this section we use the formalism of Bloch and de Dominicis[8] in conjunction with the Montroll and Ward procedure for summing chains of Coulomb interactions. Even with the neglect of quantum statistics the mathematical form of the ladder diagrams of Fig. 2 is vastly more complicated than the simple classical form appearing in Eq. (4). In place of the simple static screened interaction, $u_s(r)$, the quantum theory for the electron gas requires the nonstatic dynamic screened potential whose spatial Fourier transform is

$$\begin{aligned} &u_s(k_i, \beta_i - \beta_i') \\ &= \sum_{\substack{\nu=-\infty \\ (\nu=0,\pm1,\cdots,\pm\infty)}}^{\infty} \frac{u(k_i)\exp 2\pi i\nu(\beta_i - \beta_i')/\beta}{1 + \beta u(k_i)\lambda_2(\lambda k_i, 2\pi i\nu)} \\ &= \sum_{\nu} u_s(k_i, 2\pi i\nu)\exp\left[2\pi i\nu(\beta_i - \beta_i')/\beta\right] \\ &= u(k_i)\delta(\beta_i - \beta_i') + u_p(k_i, \beta_i - \beta_i'), \end{aligned} \tag{5}$$

with $u(k) = 4\pi e/k^2V$, and $u_s(k, 2\pi i\nu)$ is the four-dimensional Fourier transform:

$$u_s(k, 2\pi i\nu) = u(k)/[1 + \beta u(k)\lambda_2(\lambda k, 2\pi i\nu)]. \tag{6}$$

In the third line of Eq. (5) the screened potential is broken into the static Coulomb part and the nonstatic polarization potential whose four-dimensional Fourier transform is

$$u_p(k, 2\pi i\nu) = -\beta u(k)u_s(k, 2\pi i\nu)\lambda_2(\lambda k, 2\pi i\nu). \tag{7}$$

The function $\lambda_2(\lambda k, 2\pi i\nu)$ is the Fourier transform of the simplest charge density fluctuation, and has the form

$$\begin{aligned} \lambda_2(\lambda k, 2\pi i\nu) &= \int \frac{V\,d^3p\exp(\alpha - \beta p^2/2m)}{(2\pi\hbar)^3}\frac{1}{\beta}\int_0^\beta d\tau \\ &\times \exp\{2\pi i\tau/\beta - \tau[(\mathbf{p} + \hbar\mathbf{k})^2 - p^2]/2m\} \\ &= NL(z^2, 2\pi i\nu), \end{aligned} \tag{8}$$

where $z = \lambda k$, $\lambda = \hbar(\beta/2m)^{\frac{1}{2}}$, and $\alpha = \beta\mu$ is the chemical potential defined by

$$e^\alpha = (2\pi\hbar)^3\rho/(2\pi mkT)^{\frac{3}{2}}(2s + 1).$$

Explicit forms and various properties of the $L(z^2, 2\pi i\nu)$ functions are given in Ref. 3. Note that the quantity $1 + \beta u(k)\lambda_2(\lambda k, 2\pi i\nu)$ is the RPA expression for the plasma dielectric function for imaginary frequency values, $\beta\hbar\omega_\nu = 2\pi i\nu$.

The results for the ladder diagrams will be given for a two-component plasma composed of N_e electrons and N_i ions in a volume V. Electrical neutrality requires that $z_eN_e + z_iN_i = 0$, where z_e and z_i are the charge numbers of electron and ion, respectively. The electrons comprise a fraction $f_e = N_e/N$ and the ions $f_i = N_i/N$ of the total number of particles, $N = N_e + N_i$. The screened potential for the two-component system is the same as Eq. (5) except that the plasma dielectric function becomes

$$\begin{aligned} &\epsilon(k, 2\pi i\nu) \\ &= 1 + \beta u(k)[z_e^2\lambda_2(\lambda_e k, 2\pi i\nu) + z_i^2\lambda_2(\lambda_i k, 2\pi i\nu)] \\ &= 1 + (4\pi\beta e^2\rho)k^{-2}[z_e^2f_eL(\lambda_e^2k^2, 2\pi i\nu) \\ &\quad + z_i^2f_iL(\lambda_i^2k^2, 2\pi i\nu)] \underset{\nu=0}{\longrightarrow} 1 + 1/(k\lambda_D)^2, \end{aligned}$$

where $\lambda_D = (4\pi\beta\rho e^2\langle z^2\rangle)^{-\frac{1}{2}}$ is the multicomponent Debye length with $\langle z^2\rangle = z_e^2f_e + z_i^2f_i$.

The free energy will be denoted as

$$\beta(F - F_0) = -N\{S_{\text{ring}} + \sum_{m=3} S_{2,m}\cdots\},$$

where $S_{2,m}$ is the contribution of a ladder diagram with m dynamic screened interactions as given by Eq. (5). After the sum of all two-body interactions there will be similar contributions from clusters of n particles interacting via the dynamic screened potential, i.e., the complete quantum generalization of the Abe nodal expansion.[9] $S_{2,m}$ must include electron–electron interactions, electrons with ions, and ions with ions. The portion of $S_{2,m}$ arising from the temperature orderings shown in Fig. 2 is

$$\begin{aligned} &\frac{(-z_ez_i)^m}{2}\int\frac{V\,d^3p_e\exp(\alpha_e - \beta p_e^2/2m_e)}{(2\pi\hbar)^3} \\ &\times\int\frac{V\,d^3p_i\exp(\alpha_i - \beta p_i^2/2m_i)}{(2\pi\hbar)^3} \\ &\times\int\cdots\int\frac{V^{m-1}\,d^3k_1\cdots d^3k_m}{(2\pi)^{3(m-1)}}\,\delta\Big(\sum_{i=1}^m\mathbf{k}_i\Big) \\ &\times\int_0^{\beta>\beta_m>\cdots>\beta_1} d\beta_m\cdots\int_0^{\beta_2} d\beta_1\,\frac{1}{\beta^m} \\ &\times\int_0^{\beta>\beta_m'>\cdots>\beta_1'} d\beta_m'\cdots\int_0^{\beta_2'} d\beta_1' \\ &\times\exp\{-[(\beta_2 - \beta_1)(\mathbf{p}_{e,1}^2 - p_e^2) + \cdots \\ &+ (\beta_m - \beta_{m-1})(\mathbf{p}_{e,m-1}^2 - p_e^2)]/2m_e\} \\ &\times\exp\{-[(\beta_2' - \beta_1')(\mathbf{p}_{i,1}^2 - p_i^2) + \cdots \\ &+ (\beta_m' - \beta_{m-1}')(p_{i,m-1}^2 - p_e^2)]/2m_i\} \\ &\times u_s(k_1, \beta_1 - \beta_1')\cdots u_s(k_m, \beta_m - \beta_m'), \end{aligned} \tag{9}$$

[8] (a) C. Bloch and C. de Dominicis, Nucl. Phys. **7**, 459 (1958); see also (b) C. Bloch and C. de Dominicis, *ibid.* **10**, 181, 509 (1959).

[9] E. Meeron (Ref. 6) introduced the term "nodal expansion." A node is a particle with three or more interactions ending on it.

where

$$\mathbf{p}_{e,j} = \mathbf{p}_e + \hbar(\mathbf{k}_1 + \cdots + \mathbf{k}_j),$$
$$\mathbf{p}_{i,j} = \mathbf{p}_i - \hbar(\mathbf{k}_1 + \cdots + \mathbf{k}_j).$$

The other contributions come from the remaining $m!$ different orderings of the intermediate temperature variables. When all $m!$ time orderings are added together and the classical limit taken, the result is

$$NS_{2,m,ei} = \frac{(-\beta z_e z_i)^m}{2m!}\frac{N_e N_i}{V}\int\cdots\int\frac{d^3k_1\cdots d^3k_m}{(2\pi)^{3(m-1)}} \times \delta(\sum \mathbf{k}_i)\frac{4\pi e^2}{k_1^2 + 1/\lambda_D^2}\cdots\frac{4\pi e^2}{k_m^2 + 1/\lambda_D^2}$$
$$= Nf_e f_i \frac{(-\beta z_e z_i)^m}{2m!}\int d^3r\,(u_s(r))^m, \tag{10}$$

which gives the Abe result for the electron gas, Eq. (4).

For a static potential, $u(k)\delta(\beta_i - \beta_i')$, the expression (10) with each β_i' going from 0 to β is the entire quantum form of $S_{2,m}$ since the $\beta_i'\cdots\beta_m'$ integrations are removed by the $\delta(\beta_i - \beta_i')$ functions. For plasmas, however, the actual dynamic screened potential, Eq. (5), allows the m different interactions to cross. There are $m!$ possibilities corresponding to the different permutations of the intermediate temperature variables. As an example, if in Fig. 2 we have $\beta_2' < \beta_1'$, then the exponential in (10) containing p_i becomes

$$\exp[-((\beta_1' - \beta_2')[(\mathbf{p}_i - \hbar\mathbf{k}_2)^2 - p_e^2] + (\beta_3' - \beta_1')\{[\mathbf{p}_i - \hbar(\mathbf{k}_2 + \mathbf{k}_1)]^2 - p_e^2\})/2m_i].$$

Since we have assumed MB statistics the momenta $\mathbf{p}_e$ and $\mathbf{p}_i$ occur only in exponentials and can be easily integrated out. The complete result with all $m!$ time orderings is

$$NS_{2,m,ei} = \frac{(-z_e z_i)^m N_e N_i}{2m!V} \times \int\cdots\int\frac{V^{m-1}\,d^3k_1\cdots d^3k_m}{(2\pi)^{3(m-1)}} \times \delta(\sum\mathbf{k}_i)\int_0^\beta\cdots\int_0^\beta d\beta_m\cdots d\beta_1 \times \int_0^\beta\cdots\int_0^\beta d\beta_m'\cdots d\beta_1' \times G_m(\beta_1, \lambda_e\mathbf{k}_1, \cdots, \beta_m, \lambda_e\mathbf{k}_m) \times G_m(\beta_1', \lambda_i\mathbf{k}_i, \cdots, \beta_m', \lambda_i\mathbf{k}_m) \times u_s(k_1, \beta_1 - \beta_1')\cdots u_s(k_m, \beta_m - \beta_m'), \tag{11}$$

where $G_m(\beta_1, \lambda\mathbf{k}_1, \cdots)$ is the m interaction propagator defined by

$$G_m(\beta_1, \lambda\mathbf{k}_1, \cdots) = \sum_{\alpha=1}^{m!} G_{m,\alpha}(\beta_1, \lambda_e\mathbf{k}_1, \cdots), \tag{12}$$

where the summation over α gives the $m!$ permutations of the $\beta_1\cdots\beta_m$. For the ordering $\beta_m > \beta_{m-1} > \cdots > \beta_1$ the result with $\mathbf{k}_m = -(\mathbf{k}_1 + \cdots + \mathbf{k}_{m-1})$ is

$$G_{m,\beta>\beta_m>\cdots>\beta_1} = \exp(-\lambda^2\{[(\beta_2 - \beta_1)k_1^2 + \cdots + (\beta_m - \beta_{m-1})(\mathbf{k}_1 + \cdots + \mathbf{k}_{m-1})^2] - [(\beta_2 - \beta_1)\mathbf{k}_1 + \cdots + (\beta_m - \beta_{m-1}) \times (\mathbf{k}_1 + \cdots + \mathbf{k}_{m-1})]^2\}). \tag{13}$$

The propagators are periodic from 0 to β for each of the $m - 1$ intervals $\beta_m - \beta_i$ and thus may be expanded in Fourier series as

$$G_m(\beta_1, \lambda\mathbf{k}_1, \cdots) = \sum_{\nu_1\cdots\nu_m}\exp\left(\sum_{i=1}^m 2\pi i\nu_i\beta_i/\beta\right) \times L_m(\lambda\mathbf{k}_i, 2\pi i\nu_1, \cdots, \lambda k_{m-1}, 2\pi i\nu_{m-1}) \tag{14}$$
$$\nu_i = 0, \pm 1, \cdots, \pm\infty,$$
$$\nu_m = -\sum_{i=1}^{m-1}\nu_i,$$

where[10]

$$L_m(\lambda\mathbf{k}_1, 2\pi i\nu_1, \cdots, \lambda\mathbf{k}_{m-1}, 2\pi i\nu_{m-1}) = \sum_{\alpha=1}^{m!} L_{m,\alpha} = \frac{1}{\beta^m}\int_0^\beta\cdots\int_0^\beta d\beta_1\cdots d\beta_m \times \exp[2\pi i\nu_1(\beta_m - \beta_1) + \cdots + 2\pi i\nu_{m-1}(\beta_m - \beta_{m-1})]G_m(\beta_1, \lambda\mathbf{k}_1, \cdots). \tag{15}$$

By using the Fourier expansions for G_m and u_s, Eqs. (14) and (5), the temperature integrals in $S_{2,m}$ may be immediately performed to give

$$NS_{2,m,ei} = \frac{(-z_e z_i\beta)^m N_e N_i}{2m!\,V}\int\frac{V^{m-1}\,d^3k_1\cdots d^3k_m}{(2\pi)^{3(m-1)}} \times \delta(\sum_i\mathbf{k}_i)\sum_{\nu_1\cdots\nu_m}\delta_K(\sum\nu_i) \times L_m(\lambda_e\mathbf{k}_1, 2\pi i\nu_1, \cdots, \lambda_e\mathbf{k}_{m-1}, 2\pi i\nu_{m-1}) \times L(\lambda_i\mathbf{k}_1, 2\pi i\nu_1, \cdots, \lambda_i\mathbf{k}_{m-1}, 2\pi i\nu_{m-1}) \times u_s(k_1, 2\pi i\nu_1)\cdots u_s(k_m, 2\pi i\nu_m). \tag{16}$$

This result, Eq. (16), is the exact quantum form of the Abe theory. Unfortunately there is little hope

[10] E. W. Montroll, Les Houches Summer School lecture notes, in *La theorie des gaz neutres et ionises*, Hermann & Cie., Paris, 1960).

of evaluating it very far when $m > 2$ since there are $m - 1$ wave vectors (momentum transfers) to be integrated over, and $m - 1$ discrete frequencies $2\pi i\nu$ to be summed over, and the L_m functions are intractably complicated because of the $m!$ time orderings.

Equation (16) simplifies very much if there is a static potential $u(k)$ in place of $u_s(k, 2\pi i\nu)$ since then $\beta_i = \beta_i'$. One notes that, since the propagators G_m involve the thermal wavelength quadratically in an exponential [see Eq. (13)], we have

$$G_m(\beta_1, \lambda_e\mathbf{k}_1, \cdots)G_m(\beta_1, \lambda_i\mathbf{k}_1, \cdots) = G_m(\beta_1, \lambda_{ei}\mathbf{k}_1, \cdots), \quad (17)$$

since

$$\lambda_e^2 + \lambda_i^2 = \lambda_{ei}^2 = \frac{\hbar^2}{2\mu_{ei}kT}, \qquad \mu_{ei} = \frac{m_e m_i}{m_e + m_i}.$$

By using the Fourier expansion of G_m in Eq. (17) and integrating over the temperatures, one finds

$$\sum_{\nu_1 \cdots \nu_{m-1}} L_m(\lambda_e\mathbf{k}_1, 2\pi i\nu_1, \cdots, \lambda_e\mathbf{k}_{m-1}, 2\pi i\nu_{m-1}) \times L_m(\lambda_i\mathbf{k}_1, 2\pi i\nu_1, \cdots \lambda_i\mathbf{k}_{m-1}, 2\pi i\nu_{m-1}) = L_m(\lambda_{ei}\mathbf{k}_1, 0, \cdots, \lambda_{ei}\mathbf{k}_{m-1}, 0). \quad (18)$$

This relation holds only for Maxwell–Boltzmann statistics. For static potentials, the ν summations in the $S_{2,m}$ expression (16) disappear since all time orderings are equivalent, and we have

$$\begin{aligned} S_{2,m,ei}(\text{static}) = {} & \rho f_e f_i \frac{(-z_e z_i)^m}{2m!} \\ & \times \int \cdots \int \frac{V^{m-1}\, d^3k_1 \cdots d^3k_m}{(2\pi)^{3(m-1)}} \\ & \times \delta(\textstyle\sum \mathbf{k}_i) \int_0^{\beta > \beta_m > \cdots > \beta_1} d\beta_m \cdots \int d\beta_1 \\ & \times \exp\{-\lambda_{ei}^2 \{[(\beta_2 - \beta_1)k_1^2 + \cdots \\ & + (\beta_m - \beta_{m-1})(\mathbf{k}_1 + \cdots + \mathbf{k}_{m-1})^2] \\ & - [(\beta_2 - \beta_1)\mathbf{k}_1 + \cdots + (\beta_m - \beta_{m-1}) \\ & \times (\mathbf{k}_1 + \cdots + \mathbf{k}_{m-1})]^2\}) u(k_1) \cdots u(k_m). \end{aligned} \quad (19)$$

A ladder diagram with *two* screened interactions, $S_{2,2}$, in the present notation is not part of the Abe S_2 function since it is included in the ring diagrams. At this point, however, it is useful to discuss the ring diagrams in the same manner as $S_{2,m}$. Note that the ring diagrams as drawn in Fig. 2 appear to distinguish the electron and ion bubbles on the ends from the electron and ion bubbles in the screened interaction, as is actually the case in the ladder diagrams with $m \geq 3$. Since a ring diagram with n charges in the Montroll–Ward method is proportional to $(1/n)[\beta u(k)\lambda_2]^n$, it is convenient to replace the $1/n$ with an integration over the coupling constant, $e'^2 = ge^2$, so that

$$\int_0^1 \frac{dg}{g}\, g^n = \frac{1}{n}$$

as in Eq. (2). Thus the ring diagrams in Fig. 2 give[11]

$$\begin{aligned} NS_{\text{ring},ei} = {} & \frac{(z_e z_i)^2}{2} \int_0^1 \frac{dg}{g} \\ & \times \int \frac{V\, d^3p_e \exp(\alpha_e - \beta p_e^2/2m_e)}{(2\pi\hbar)^3} \\ & \times \int \frac{V\, d^3p_i \exp(\alpha_i - \beta p_i^2/2m_i)}{(2\pi\hbar)^3} \int \frac{V\, d^3k}{(2\pi)^3} \\ & \times 2 \int_0^{\beta} d\beta_2 \int_0^{\beta_2} d\beta_1 \frac{1}{\beta} \int_0^{\beta} d\beta_1' \\ & \times \exp(-\{(\beta_2 - \beta_1)[(\mathbf{p}_e + \hbar\mathbf{k})^2 - p_e^2]/2m_e \\ & + |\beta_2 - \beta_1'|\,[(\mathbf{p}_i - \hbar k)^2 - p_i^2]/2m_i\}) \\ & \times u_e(k) u_{s,e}(k, \beta_1 - \beta_1') \\ = {} & \frac{N_e N_i (z_e z_i \beta)^2}{2} \int_0^1 \frac{dg}{g} \sum_{\nu=-\infty}^{\infty} \int \frac{V\, d^3k}{(2\pi)^3} u_e(k) u_{s,e}(k, 2\pi i\nu) \\ & \times L_2(\lambda_e^2 k^2, 2\pi i\nu) L_2(\lambda_e^2 k^2, 2\pi i\nu). \end{aligned} \quad (20)$$

If we add together the results corresponding to Eq. (20) for $S_{\text{ring},ee}$ and $S_{\text{ring},ii}$ and perform the elementary g integration, then the complete ring sum becomes

$$\begin{aligned} NS_{\text{ring}} = {} & \frac{1}{2} \sum_{\nu=-\infty}^{\infty} \int \frac{V\, d^3k}{(2\pi)^3} \Big(\frac{4\pi\beta e^2 \rho}{k^2} \\ & \times [z_e^2 f_e L_2(\lambda_e^2 k^2, 2\pi i\nu) + z_i^2 f_i L_2(\lambda_i^2 k^2, 2\pi i\nu)] \\ & - \log\Big\{1 + \frac{4\pi\beta e^2 \rho}{k^2} [z_e^2 f_e L_2(\lambda_e^2 k^2, 2\pi i\nu) \\ & + z_i^2 f_i L_2(\lambda_i^2 k^2, 2\pi i\nu)]\Big\}\Big). \end{aligned} \quad (21)$$

This is the Montroll–Ward result for multicomponent plasmas.

It might appear at first sight that the separate evaluation of a part of the ring sum such as $S_{\text{ring},ei}$ is a meaningless exercise. In fact it will be shown

[11] The evaluation of $S_{2,2}$ and S_{ring} is simplified by the fact the 2! pieces of G_2 in Eq. (12) are identical so that we have

$$G_2(\beta_2, \lambda\mathbf{k}, \beta_2, -\lambda\mathbf{k}) = G(|\beta_2 - \beta_1|, \lambda k) = \exp\{-(\lambda k)^2[|\beta_2 - \beta_1| - |\beta_2 - \beta_1|^2]\}.$$

Similarly the two pieces of the Fourier transform, $L_2 = L_{2,\beta_2>\beta_1} + L_{2,\beta_1>\beta_2}$, are identical and one sees that L_2 as defined by Eq. (15) reduces to Eq. (8).

in the following sections that the quantum diffraction effects contained in the total ring sum, Eq. (21), are correct only when both $\lambda\!\!\!^{-}_e$ and $\lambda\!\!\!^{-}_i$ are greater than βe^2. If, as is usually the case, $\lambda\!\!\!^{-}_i < \beta e^2$ then the pieces of the ring sum must be evaluated separately. The result for $S_{\text{ring},ei}$ exact to $O(e^5)$ obtained using the method described in Ref. 3 is

$$S_{\text{ring},ei} = \tfrac{1}{3}z_e^2 z_i^2 f_e f_i \Lambda\{1 - (3\pi^{\frac{1}{2}}/2^4)\gamma_{ei} + \tfrac{3}{5}[\tfrac{1}{6}(\gamma_e^2 + \gamma_i^2) + \tfrac{1}{12}(z_e^2 f_e \gamma_e^2 + z_i^2 f_i \gamma_i^2)/\langle z^2\rangle] + \cdots\}, \tag{22}$$

where

$$\Lambda = \beta e^2\langle z^2\rangle/\lambda_D = 1/4\pi\rho\lambda_D^3,$$

$$\gamma_e = \lambda\!\!\!^{-}_e/\lambda_D, \qquad \gamma_i = \lambda\!\!\!^{-}_i/\lambda_D, \qquad \gamma_{ei} = \lambda\!\!\!^{-}_{ei}/\lambda_D.$$

III. EVALUATION OF THE THREE-RUNG LADDER

The complete form of $S_{2,m}$ as given by Eq. (16) is much too complicated to allow a complete analytical evaluation. Nevertheless, some useful comments may be made about it. For $m = 2$, i.e., essentially the ring sum, the complete quantum mechanical form can be evaluated to give a series expansion in powers of γ as indicated in Eq. (22). This exact evaluation is possible because there is only one wave vector to integrate, a simplification which is due to the fact that the ring integrals in configuration space are convolutions which become powers of $u(k)$ in k space. For $m \geq 3$ the reverse is true, i.e., in general one has $m - 1$**k**-vectors to integrate over, but in the classical form one gets powers of $u_s(r)$ in configuration space as shown in Eqs. (4) and (10). Thus it is expected that $S_{2,m}$ will be mathematically more tractable in configuration space than in k space. Unfortunately there seems to be no practical way to convert the exact expression for $S_{2,m}$ into a configuration-space integral. The reason is that we would have to find the Fourier transform of $u_s(k, \beta_i - \beta_i')$ in order to take into account the retardation effects that occur for $\beta_i \neq \beta_i'$. However, it should be further noted that the retardation effects [essentially the contributions from $u_s(k, 2\pi i\nu)$ for $\nu \neq 0$] play no role in cutting off the divergencies. Only the Debye screening length in the $\nu = 0$ is needed for the larger cutoff for $m = 3$, and only the pure Coulomb part of the screened potential is needed for $r < \lambda\!\!\!^{-}$. Thus to get the leading term of $S_{2,m}$ we can neglect retardation effects, and use the static approximation, Eq. (19). The ladder diagram integrals for static potentials *can* be written in configuration space; the result is

$$\begin{aligned} S_{2,m,ei}(\text{static}) = {} & \tfrac{1}{2}\rho f_e f_i(-z_e z_i\beta)^m \\ & \times \int \cdots \int d^3r, \cdots d^3r_m\, u(r) \cdots u(r_m) \\ & \times \int_0^{1>\nu_m>\cdots>\nu_1} d\nu_m \cdots \int_0 d\nu_1 \\ & \times \frac{\exp[-(\mathbf{r}_2 - \mathbf{r}_1)^2/4\lambda\!\!\!^{-2}_{ei}(\nu_2 - \nu_1)]}{[4\pi\lambda\!\!\!^{-2}_{ei}(\nu_2 - \nu_1)]^{\frac{3}{2}}} \\ & \cdot \frac{\exp[-(\mathbf{r}_3 - \mathbf{r}_2)^2/4\lambda\!\!\!^{-2}_{ei}(\nu_3 - \nu_2)]}{[4\pi\lambda\!\!\!^{-2}_{ei}(\nu_3 - \nu_2)]^{\frac{3}{2}}} \cdots \\ & \times \frac{\exp[-(\mathbf{r}_m - \mathbf{r}_1)^2/4\lambda\!\!\!^{-2}_{ei}(1 - \nu_m + \nu_1)]}{[4\pi\lambda\!\!\!^{-2}_{ei}(1 - \nu_m + \nu_1)]^{\frac{3}{2}}}. \end{aligned} \tag{23}$$

Equation (23) is the mth term of the perturbation expansion of the quantum mechanical second virial coefficient. By using $u(r) = (e^2/r)\exp(-r/\lambda_D)$ in (23) we have an approximation to the exact expression, Eq. (16), that is sufficient to give for $m = 3$ the logarithmic leading term and constant following it. For $r \gg \lambda\!\!\!^{-}_{ei}$ the integrand of (23) reduces to the classical form, $[u(r)]^m/m!$. After a change of variables in (23) for $m = 3$,

$$\mathbf{r}_1 = \mathbf{r}, \mathbf{r}_2 = \mathbf{r} + \lambda\!\!\!^{-}_{ei}\mathbf{x}_1, \mathbf{r}_3 = \mathbf{r} + \lambda\!\!\!^{-}_{ei}\mathbf{x}_2,$$

we have

$$\begin{aligned} S_{2,3,ei} \approx {} & \tfrac{1}{2}\rho f_e f_i(-z_e z_i\beta)^3 \int d^3r \int d^3x_1 \int d^3x_2 \int_0^1 d\nu_3 \int_0^{\nu_3} d\nu_2 \\ & \times \int_0^{\nu_3} d\nu_1\, u(r)u(|\mathbf{r} + \lambda\!\!\!^{-}_{ei}\mathbf{x}_1|)u(|\mathbf{r} + \lambda\!\!\!^{-}_{ei}\mathbf{x}_2|) \\ & \times \frac{\exp\{-[x_1^2/4(\nu_2 - \nu_1) + (\mathbf{x}_2 - \mathbf{x}_1)^2/4(\nu_3 - \nu_2) + x_2^2/4(1 - \nu_3 + \nu_1)]\}}{[(4\pi)^2(\nu_2 - \nu_1)(\nu_3 - \nu_2)(1 - \nu_3 + \nu_1)]^{\frac{3}{2}}}. \end{aligned} \tag{24}$$

In order to obtain the asymptotic form of this still difficult integral for the Debye potential we break the integration into two regions, $r < R$ and $r > R$ where R is any length such that $\lambda\!\!\!^{-}_{ei} < R < \lambda_D$. For $r > R$ the potentials are essentially independent of $\lambda\!\!\!^{-}_{ei}$ and the classical form may be worked out

to be

$$S_{2,3,ei}(r > R) = \frac{\rho f_e f_i (-\beta z_e z_i e^2)^3}{2 \cdot 3!} \times \int_R^\infty 4\pi r^2 \, dr \left(\frac{e^{-r/\lambda_D}}{r}\right)^3 = -\frac{z_e^3 z_i^3 f_e f_i}{\langle z^2 \rangle^3} \frac{\Lambda^2}{12} [-\log R/\lambda_D - \log 3 - C + O(R/\lambda_D) \cdots], \quad (25)$$

where Λ is defined as in Eq. (22).

For $r < R$ the simplest procedure seems to be to neglect the unnecessary screening factor, $\exp(-r/\lambda_D)$, since $R < \lambda_D$, and to make explicit use of the $1/r$ form of the potential. Thus we have

$$S_{2,3,ei}(r < R) = -\frac{z_e^3 z_i^3 f_e f_i}{\langle z^2 \rangle^3} \cdot \frac{\Lambda^2}{2} \int_0^1 dv_3 \int_0^{v_3} dv_2 \int_0^{v_3} dv_1 \int d^3x_1 \int_0^{R/\lambda_D} y^2 \, dy \times y^{-1}[y^2 + 2\gamma_{ei} y x_1 \cos\theta_1 + \gamma_{ei}^2 x_1^2]^{-\frac{1}{2}} [y^2 + 2\gamma_{ei} y x_2 \cos\theta_2 + \gamma_{ei}^2 x_2^2]^{-\frac{1}{2}} \times \frac{\exp\{-[x_1^2/4(v_2 - v_1) + (\mathbf{x}_2 - \mathbf{x}_1)^2/4(v_3 - v_2) + x_2^2/4(1 - v_3 + v_1)]\}}{[(4\pi)^2 (v_2 - v_1)(v_3 - v_2)(1 - v_3 + v_1)]^{\frac{3}{2}}}. \quad (26)$$

The r integration ($y = r/\lambda_D$) is done in three regions,

$$\gamma_{ei} x_1 < \gamma_{ei} x_2 < y, \gamma_{ei} x_1 < y < \gamma_{ei} x_2, y < \gamma_{ei} x_1 < \gamma_{ei} x_2,$$

with the result

$$\int_0^{R/\lambda_D} y^2 \, dy \frac{1}{y} \cdot \frac{1}{|\mathbf{y} + \gamma_{ei}\mathbf{x}_1|} \cdot \frac{1}{|\mathbf{y} + \gamma_{ei}\mathbf{x}_2|} = \log(R/\lambda_D)(1/\gamma_{ei}) + g(x_1, x_2, \cos\theta), \quad (27)$$

where $\cos\theta$ is the angle between $\mathbf{x}_1$ and $\mathbf{x}_2$, and

$$g(x_1, x_2, \cos\theta) = -\log x_2 + \sum_{n=1} \frac{(x_1/x_2)^n P_n(\cos\theta)}{2n(2n+1)} \left[1 - \left(\frac{\gamma_{ei} x_2}{R/\lambda_D}\right)^{2n}\right] + \frac{(x_2 - x_1)}{x_2} \sum_{n=1} \frac{(x_1/x_2)^n P_n(\cos\theta)}{(2n+1)} + \sum_{n=1} \frac{(x_1/x_2)^{n+1} P_n(\cos\theta)}{(2n+1)(2n+2)} \approx -\log x_2 + \frac{1}{2} \sum_{n=1} P_n(\cos\theta) \left[\frac{(x_1/x_n)^n}{n} - \frac{(x_1/x_2)^{n+1}}{n+1}\right] = -\log x_2 + \tfrac{1}{2}(x_1/x_2) + \tfrac{1}{2} \log \left(2(1 - \cos\theta) \left\{\left[1 - 2\frac{x_1}{x_2}\cos\theta + \left(\frac{x_1}{x_2}\right)^2\right]^{\frac{1}{2}} - \cos\theta + \frac{x_1}{x_2}\right\}^{-1} \times \left\{\left[1 - 2\frac{x_1}{x_2}\cos\theta + \left(\frac{x_1}{x_2}\right)^2\right]^{\frac{1}{2}} - \frac{x_1}{x_2}\cos\theta + 1\right\}^{-1}\right). \quad (28)$$

For $x_2 < x_1$ in expression (28), x_1 and x_2 are interchanged. Combining (26) with (25) removes the joining point R to logarithmic accuracy and one has

$$S_{2,3,ei} \approx -\frac{(z_e z_i)^3 f_e f_i}{\langle z^2 \rangle^3} \cdot \frac{\Lambda^2}{12} \left[\log\left(\frac{1}{\gamma_{ei}}\right) + D_q\right], \quad (29)$$

where

$$D_q = -\log 3 - C + I,$$

$$I = 3! \int_0^1 dv_3 \int_0^{v_3} dv_2 \int_0^{v_3} dv_1 \int d^3x_1 \, d^3x_2 \, g(x_1, x_2, \cos\theta) \times \frac{\exp\{-[x_1^2/4(v_2 - v_1) + (\mathbf{x}_2 - \mathbf{x}_1)^2/4(v_3 - v_2) + x_2^2/4(1 - v_3 + v_1)]\}}{[(4\pi)^2 (v_3 - v_2)(v_3 - v_2)(1 - v_3 + v_1)]^{\frac{3}{2}}}.$$

The constant D_c in the classical case can be evaluated exactly, and the result is given in Eq. (4). The quantum constant D_q has not proved tractable, but presumably is of the same order of magnitude as D_c.

IV. HIGH AND LOW FREE ENERGY OF THE ELECTRON GAS

We have seen from the results of the previous sections that when the fundamental lengths of an electron gas are ordered as $\beta e^2 < \lambda\!\!\!^{-} < \lambda_D$ then the appropriate dimensionless parameters for expressing the thermodynamic functions are the ratios $\Lambda = \beta e^2/\lambda_D$ and $\gamma_{ee} = \lambda\!\!\!^{-}_{ee}/\lambda_D$. The free energy has the form

$$\beta(F - F_0) = -N[\tfrac{1}{3}\Lambda g_2(\gamma_{ee}) + \tfrac{1}{12}\Lambda^2 g_3(\gamma_{ee}) + \Lambda^3 g_4(\gamma_{ee}) + \cdots], \quad (30)$$

where

$$\begin{aligned} g_2(\gamma) &= 1 - \tfrac{3}{16}\pi^{\frac{1}{2}}\gamma + \tfrac{1}{4}\gamma^2 - \cdots, \\ g_3(\gamma) &= \log\gamma + D_q + O(\gamma)\cdots, \\ &\vdots \qquad\qquad \vdots \\ g_m(\gamma) &= \frac{\mathfrak{a}_{m1}}{\gamma^{m-3}} + \frac{\mathfrak{a}_{m2}}{\gamma^{m-4}} + \cdots \\ &\quad + \mathfrak{a}_{m,m-2}(\log\gamma + D_m) + O(\gamma). \end{aligned} \quad (31)$$

The function $g_2(\gamma)$ from the ring sum may be worked out to all orders in γ (see Ref. 3). In Sec. III the $\log\gamma$ part of $g_3(\gamma)$ has been obtained, and the constant D_q appears as an intractable integral. The coefficients $\mathfrak{a}_{m1}$ of the leading term of $g_m(\gamma)$ may be reduced to integrals something like the expression for D_q, but no way has been found to evaluate them. The coefficient of γ in $g_2(\gamma)$ includes nonstatic effects.[12] For $m \geq 3$ the nonstatic effects also appear in the coefficient of the $O(\gamma)$.

The exact results that have been obtained so far are useful, though limited. One sees that the $O(\Lambda\gamma)$ term from the ring sum is the most important quantum correction, and this is followed by the $O(\Lambda^2 \log\gamma)$ term from the three-rung ladder. The pressure of the electron gas obtained from (30) and (31) is

$$\begin{aligned} \beta PV &= \rho\frac{\partial}{\partial\rho}\beta F \\ &= N[1 - \tfrac{1}{6}\Lambda(1 - \tfrac{3}{8}\pi^{\frac{1}{2}}\gamma_{ee} + \tfrac{3}{2}\gamma_{ee}^2 - \cdots) \\ &\quad - \tfrac{1}{12}\Lambda^2(\log\gamma_{ee} + D_q + \tfrac{1}{2})\cdots]. \end{aligned} \quad (32)$$

The $O(\Lambda\gamma^3)$ term in the ring sum is known, but there is little point in retaining it unless the $O(\Lambda^3/\gamma)$ term from the four-rung ladder is also retained.

We now compare the high-temperature quantum mechanical result, Eq. (30), with the result for a nearly classical electron gas. Nearly classical will be taken to mean $kT <$ Ryd so the $\lambda\!\!\!^{-} < \beta e^2$.[13] The classical limit ($\hbar = 0$) was obtained by Abe,[5] and small wave mechanical corrections may be calculated from the Wigner–Kirkwood (WK) expansion.[14] The appropriate dimensionless parameters are now $\Lambda = \beta e^2/\lambda_D$ and the WK expansion parameter $\eta_{ee} = \lambda\!\!\!^{-}_{ee}/\beta e^2 = \gamma_{ee}/\Lambda$. The free energy now has the form

$$\beta(F - F_0) = -N[S_{ring}(\Lambda) + \sum_{n=2} S_n(\Lambda) + \Lambda^2 G(\eta^2)], \quad (33)$$

and exact results for $\Lambda < 1$ and $\eta < 1$ as far as they are known at this time are

$$\begin{aligned} \beta(F - F_0) &= -N[\tfrac{1}{3}\Lambda + \tfrac{1}{12}\Lambda^2(\log\Lambda + D_c) \\ &\quad + \tfrac{1}{12}\Lambda^3\log\Lambda + \cdots \\ &\quad + \Lambda^2(-\tfrac{1}{24}\eta^2 + \tfrac{1}{120}\eta^4 + \tfrac{1}{126}\eta^6\cdots)]. \end{aligned} \quad (34)$$

The functions $S_n(\Lambda)$ are the terms of the nodal expansion[9] which describe a cluster of n particles interacting in all possible allowed ways via the Debye screened potential. The function $G(\eta^2)$ gives the residual wave mechanical effects as calculated from the terms of the WK expansion.[15] In Eq. (34) the terms of order $\Lambda^2 \log\Lambda$, Λ^2, and $\Lambda^3 \log\Lambda$ are the first terms in the expansion of $S_2(\Lambda)$. The three-node term, $S_3(\Lambda)$, was shown by Friedman to begin with $a\Lambda^3 + b\Lambda^4 \log\Lambda$, but the constants a and b are not yet evaluated. According to Friedman, $S_4(\Lambda)$ also begins with $O(\Lambda^3)$, while $S_5(\Lambda)$ and $S_6(\Lambda)$ begin with $O(\Lambda^4)$ and $S_7(\Lambda)$ with $O(\Lambda^5)$. It seems likely that the $S_n(\Lambda)$ functions become smaller than the beginning terms in a systematic way but there is no proof yet. The expansion does apparently converge.[16] The parameter Λ in the nodal expansion takes the place of the density when compared with the Mayer cluster expansion for ordinary nonideal gases. However, unlike the Mayer expansion for which the irreducible cluster integrals of order n form the coefficients of ρ^n, the nodal expansion is nonanalytic in Λ, as evidenced by the appearance of $\log\Lambda$. Equations (30) and (34) give exact results for the wave mechanical corrections in the respective limits $\beta e^2 < \lambda\!\!\!^{-}(kT >$ Ryd) and $\beta e^2 > \lambda\!\!\!^{-}$ ($kT <$ Ryd). In order for the two results to pass from one to the other when $kT \approx$ Ryd the function $G(\eta^2)$, for which only the first three terms of the series expansion are known, must have the form for $\eta > 1$:

[12] If the $\nu \neq 0$ contributions to the ring sum are neglected, the coefficient of the $O(\gamma)$ term is $(\pi^{\frac{1}{2}}/\sqrt{2}\cdot 8)(5 - 2\sqrt{2})$ which differs from the correct value $3\pi^{\frac{1}{2}}/16$ by only about 1.5%.

[13] Evidently since nearly classical means low temperature, there may be some question about the validity of assuming Maxwell–Boltzmann statistics. The importance of quantum statistics is measured by the size of the quantity $\rho\lambda\!\!\!^{-3}/(2s + 1)$, where s is the particle spin. Note that assuming an arbitrarily large spin s is a way of removing particle indistinguishability from the quantum mechanical problem.

[14] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1958), pp. 96–103. The author thanks Jan Grzesik for performing the extremely tedious calculations required for obtaining the $O(\eta^6)$ term in Eq. (34).

[15] H. E. DeWitt, J. Math. Phys. **3**, 1003 (1962). Equation (52) in this paper is incorrect since it gives the high-temperature form of $S_{2,2}$ and the WK expansion of the higher-order ladders.

[16] S. Brush, H. E. DeWitt, and J. Trulio, Nucl. Fusion **3**, 5 (1963).

$$G(\eta^2) \underset{\eta>1}{=} -\frac{\pi^{\frac{1}{2}}}{16}\eta + \tfrac{1}{12}(\log\eta + D_q - D_o) + a_{3,1}/\eta + \cdots . \quad (35)$$

It is reasonable to expect that $G(\eta^2)$ is a smooth function between the known limiting results (24) and (35), but at present it is not known how to calculate it when $\eta \approx 1$ ($kT \approx$ Ryd). To understand the two results it is helpful to draw on analogies with scattering theory. Note that the parameter η may be written as

$$1/\eta = e^2/\hbar\langle v\rangle,$$

where $\langle v\rangle$ is a thermal velocity. Thus $1/\eta$ is a measure of the validity of a scattering calculation in the near classical limit ($e^2/\hbar v \gg 1$) or scattering in the Born approximation ($e^2/\hbar v \ll 1$). In the quantum mechanical form of the free energy, Eq. (30), the RPA term is something like the calculation of the scattering amplitude with the dynamic screened potential in first Born approximation, the three-rung ladder giving the log γ is roughly equivalent to a second Born approximation of scattering in the static screened potential, and the evaluation of $g_m(\gamma) \approx a_{m1}/\gamma^{m-3}$ is equivalent to higher Born approximations with the *pure Coulomb* potential. The function $G(\eta^2)$ is shown in Fig. 3 with the region of uncertainty between the known limits shown as a dashed line. This region, $\eta \approx 1$, requires a complete quantum mechanical calculation, and no expansion procedure will help. Since, however, only the Coulomb potential is involved, it seems likely that this function can be exactly calculated because the Schrödinger equation can be solved exactly for the $1/r$ potential.

It is important to note that the quantum correction in the ring sum, $O(\Lambda\gamma)$, $O(\Lambda\gamma^2)$, etc., are valid only at high temperature, i.e., when $\Lambda < \gamma$. It is deceptive that these corrections apparently vanish as $\gamma \to 0$, since when $\gamma < \Lambda$, Eq. (34) is valid rather than (32). If one considers the ring sum alone, it is easy to come to the erroneous conclusion that the free energy is an analytic function of $\hbar$ in contradiction to the WK expansion.

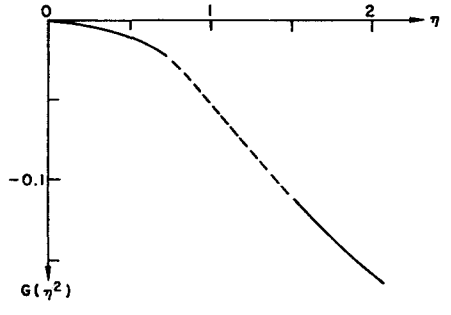

FIG. 3. Plot of $G(\eta^2)$ vs η. The solid portion for $\eta < 1$ is given by Eq. (34), and the solid portion for $\eta > 1$ is given by Eq. (35). The dashed line for $\eta \sim 1$ connecting the two solid pieces indicates the region of uncertainty which can presumably be calculated with the exact Coulomb wavefunctions.

V. THE MULTICOMPONENT PLASMA

Using the results of the previous sections we can now write down the free energy of a real plasma, such as fully ionized hydrogen. Because of the different particle masses, m_e and m_i, of a two-component plasma there will be three thermal wavelengths, λ_{ee}, λ_{ei}, and λ_{ii}, which must be compared with βe^2. Since protons and other ions are 2000 times and more heavier than electrons, the normal situation in a fully ionized plasma such as hydrogen with $kT >$ Ryd is that the lengths are ordered as

$$\lambda_{ii} < \beta e^2 < \lambda_{ei}, \lambda_{ee} < \lambda_D$$

and the appropriate dimensionless parameters are

$$\gamma_{ii} < \Lambda < \gamma_{ei}, \gamma_{ee} < 1.$$

Consequently the electron–electron and electron–ion interaction contributions to the free energy are given by the quantum mechanical limit, Eq. (30), while the ion–ion interactions are nearly classical and their contribution is given by Eq. (34). Note that in this situation the ring sum must be broken up into the various parts $S_{\text{ring},ee}$, $S_{\text{ring},ei}$, and $S_{\text{ring},ii}$ as given by Eq. (22), because the ion–ion quantum corrections in the complete ring sum are not valid when $\lambda_{ii} < \beta e^2$. The complete result for the multicomponent free energy to logarithmic accuracy is

$$\begin{aligned}\beta(F - F_0) = -N\Big\{&\frac{\Lambda}{3}\Big[1 - \frac{3\pi^{\frac{1}{2}}}{16}\\ &\times (z_e^4 f_e^2\gamma_{ee} + 2z_e^2 z_i^2 f_e f_i \gamma_{ei})/\langle z^2\rangle^2\\ &+ \frac{1}{4}\frac{z_e^2 f_e \gamma_e^2}{\langle z_i^2\rangle}\cdots\Big] + \frac{\Lambda^2}{12}\Big[z_e^6 f_e^2(\log\gamma_{ee} + D_q)\\ &+ 2z_e^3 z_i^3 f_e f_i(\log\gamma_{ei} + D_q)\\ &+ z_i^6 f_i^2\Big(\log\frac{z_i^2\beta e^2}{\lambda_D} + D_o\Big)\Big]\Big/\langle z^2\rangle^3 + \frac{z_i^6 f_i^2}{\langle z^2\rangle^3}\Lambda^2 G(\eta_{ii}^2)\Big\}.\end{aligned} \quad (36)$$

Equation (36) is valid for hydrogen for the temperature region Ryd $< kT < (m_i/m_e)$ Ryd. At much higher temperature when $\lambda_{ii} > z_i^2\beta e^2$ the ion–ion interaction must also be described quantum mechanically.

A low-temperature result for the free energy of a multicomponent plasma analogous to Eq. (34) is not possible since the multicomponent plasma has no classical limit. As the temperature is reduced below a rydberg, bound states between electrons

and ions begin to form. A rigorous calculation of the free energy of a partially ionized plasma including hydrogenic bound states has yet to be carried out.[17]

VI. DISCUSSION

The principal results of this paper, Eqs. (30) and (36), show that wave mechanical effects persist at high temperature. Thus plasmas with $kT >$ Ryd are *not* classical. In order to understand physically how this happens it is useful for a moment to consider a many-body system interacting with a more singular pair potential, $u(r) = g_p/r^p$. The average distance of closest approach defined by $\langle u(r) \rangle \approx kT$ is $l_c = (g_p/kT)^{1/p}$, while the thermal wave length is $\lambda\!\!\!^{-} = \hbar/(2mkT)^{\frac{1}{2}}$. At high temperature we see that $l_c > \lambda\!\!\!^{-}$ when $p > 2$. Thus the repulsive $1/r^p$ potential is sufficiently hard that the particle wave packets with extension $\lambda\!\!\!^{-}$ cannot intermingle at high temperature. Thus such a many-body system is evidently classical in the high-temperature limit, and the WK expansion may be used to give wave mechanical corrections since the WK expansion parameter $\eta = \lambda\!\!\!^{-}/l_c$ is indeed small for large $T(\eta \propto T^{\frac{1}{2}-1/p})$. In the plasma case, $p = 1$, the $1/r$ potential is sufficiently soft that the distance of closest approach becomes less than the de Broglie wavelength at high temperature, i.e., $e^2/kT < \lambda\!\!\!^{-}$ when $kT >$ Ryd, and consequently the particle wave packets overlap more at high temperature.

In this paper we have assumed Maxwell–Boltzmann statistics because we wished to focus attention on the quantum effects due to the uncertainty principle rather than effects due to particle indistinguishability. Nevertheless a complete accurate treatment of plasmas requires the inclusion of quantum statistics even at high temperature because exchange interactions are of the same order of magnitude as some of the wave mechanical effects. The first-order exchange term is of the order of $\gamma^2/(2s + 1)$ and seems to be safely negligible compared with Λ from the Debye–Hückel term. The second-order exchange term is also finite and is of order $\Lambda\gamma/(2s + 1)$, and hence is comparable to the first diffraction correction in the ring sum. The third-order exchange appears to be of order $\Lambda^2/(2s + 1)$ and thus contributes an additional constant to be added to D_q in Eq. (31). A complete discussion of statistic effects will be deferred to a later paper.

In view of the exact results now known for the plasma free energy it is worthwhile to comment on one approximation method used by various authors in recent years. This method is the attempt to find an effective or pseudo-potential replacing e^2/r in the classical calculation which is to include to some degree quantum effects. Such an effective potential must reduce to the pure Coulomb potential when $r \gg \lambda\!\!\!^{-}$ and be finite as $r \to 0$. One of the earliest forms and also the most tractable one for analytical evaluation is

$$u_{eff}(r) = \frac{z_e z_i e^2}{r}(1 - e^{-\alpha_{ei} r}), \tag{37}$$

which was used by Glauberman and Yukhnovskii.[18] In order to describe wave mechanical effects the quantity α_{ei} must be $a/\lambda\!\!\!^{-}_{ei}$ where a is a constant to be chosen by some suitable criterion. Recently Kelbg has proposed[19]

$$u_{eff}(r) = \frac{z_e z_i e^2}{r}\left\{(1 - e^{-r^2/2\lambda\!\!\!^{-2}_{ei}}) + \frac{\sqrt{2}\,\pi^{\frac{1}{2}} r}{\lambda\!\!\!^{-}_{ei}}[1 - \mathrm{Erf}\,(\sqrt{2}\,r/\lambda\!\!\!^{-}_{ei})]\right\}, \tag{38}$$

and a rather similar form has been obtained by Koppe and Hagenow[20] by approximating the Wigner distribution. These effective potentials may be put into classical expressions such as the ring sum, Eq. (2), and the ladder integrals, Eq. (4), and one can obtain quantum corrections of the same form as the exact results exhibited for the high-temperature electron gas in Eq. (30). Any such effective potential that is finite at $r = 0$ (usually proportional to $e^2/\lambda\!\!\!^{-}$) will cut off the short-range divergence of the three-rung ladder and give correctly the $\frac{1}{12}\Lambda^2 \log \gamma$ term in the free energy. Getting the exact value for the coefficient $\frac{1}{16}\pi^{\frac{1}{2}}$ of the $\Lambda\gamma$ term in the ring sum is harder since the region $r \approx \lambda\!\!\!^{-}$ contributes most. Kelbg's potential gives this result very closely and also the coefficient of $\Lambda\gamma^2$. The simpler form, Eq. (37), gives the coefficient of $\Lambda\gamma$ when a is chosen properly, but not the coefficient of $\Lambda\gamma^2$. Such effective potentials are interesting to try since the calculations of the free energy are much easier than the exact integrals of the quantum mechanical perturbation theory. For example, by using Eq. (37) one can obtain an approximate value for D_q and

[17] T. Nakayama and H. E. DeWitt, J. Quant. Spectr. Rad. Transfer 4, 623 (1964).

[18] (a) A. E. Glauberman and I. R. Yukhnovskii, Dokl. Akad. Nauk SSSR 93, 999 (1953); see also (b) translation, UCRL Trans. 668 (L).

[19] G. Kelbg, Ann. Phys. (N.Y.) 12, 354 (1954).

[20] K. Hagenow and H. Koppe, Proc. 5th Int. Conf. Ionization Phenomena in Gases, Paris 1963, p. 221.

the coefficients a_{m1} in Eq. (31) for the higher-order ladder terms. Nevertheless, in the opinion of this author, this semiclassical approach is of limited usefulness since the validity of the results obtained by using any u_{eff} can be tested only by comparison with exact results.

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Limiting Forms of the Screened Coulomb T Matrix

WILLIAM F. FORD
Lewis Research Center, Cleveland, Ohio
(Received 28 June 1965)

In the complex energy plane, the pure Coulomb T matrix possesses branch points which would not appear if the force were properly defined. This is demonstrated by a study of the screened Coulomb T matrix in the limit as the screening radius R tends to infinity. No branch points develop if the proper order of limiting processes is observed and the results agree with previous calculations; however, the T matrix is discontinuous in the limit. A formula for the screened Coulomb T matrix is given which is valid to order $1/R$ for all energies.

I. INTRODUCTION

THE T matrix for a system undergoing scattering is given by

$$T = V + V[1/(E + i\epsilon - K - V)]V. \quad (1)$$

Here K is the Hamiltonian for the system in the absence of interaction, and V is the interaction giving rise to the scattering. The total energy of the system is denoted by E; the small imaginary term $i\epsilon$ serves to make the Green's function

$$G = 1/(E + i\epsilon - K - V) \quad (2)$$

well defined.

We consider the T matrix in the momentum representation, with matrix elements denoted by $\langle \mathbf{k}_2|T|\mathbf{k}_1\rangle$. It is convenient to introduce a complex wavenumber k, which is related to the total energy by

$$E + i\epsilon = \hbar^2k^2/2m, \qquad 0 < \arg(k) < \pi;$$

thus the energy dependence of the T matrix may be indicated explicitly by $\langle \mathbf{k}_2|T(k)|\mathbf{k}_1\rangle$, or simply $T(k)$.

For most quantum-mechanical systems, the T matrix cannot be given in closed form. However, the case of a two-particle system with pure Coulomb interaction has been studied extensively, and recently Hostler and others[1] derived integral representations for the Coulomb Green's function which reduce to hypergeometric functions. From these the Coulomb T matrix can be obtained directly.

The resulting expression for $T(k)$, however, has the drawback that it does not approach a well-defined limit as $k^2 \to k_1^2$ or $k^2 \to k_2^2$, and indeed has branch points there. This behavior is certainly not correct, for one can show on very general grounds that the only singularities of $T(k)$ should be a branch point at $k = 0$ and simple poles on the imaginary k axis corresponding to the bound-state energies of $K + V$.

The correct form of the T matrix when $k^2 = k_1^2$ is given in Ref. 2, where a similar anomaly in the limiting process $|\mathbf{k}_2| \to |\mathbf{k}_1|$ was studied. The difficulty there was traced back to the long-range nature of the Coulomb force and disappeared when the effects of shielding were introduced.

In the present case the unphysical branch points are also due to neglect of shielding effects. The scattering of charged particles is caused by an interaction which is always screened at very large distances; the T matrix may therefore properly be regarded as depending on *two* parameters, ϵ and the screening radius R. To find the value of $T(k, R)$ for real k, one must take $\epsilon \to 0$ followed by $R \to \infty$. Usually, the ordering is unimportant, but the branch points at k_1^2 and k_2^2 occur in Hostler's expression because the limit $R \to \infty$ has been (implicitly) taken first.

[1] L. Hostler, J. Math. Phys. 5, 591 (1964); J. Schwinger, *ibid.* 5, 1606 (1964); E. H. Wichmann and C. H. Woo, *ibid.* 2, 178 (1961).

[2] W. F. Ford, Phys. Rev. B133, 1616 (1964).

the coefficients a_{m1} in Eq. (31) for the higher-order ladder terms. Nevertheless, in the opinion of this author, this semiclassical approach is of limited usefulness since the validity of the results obtained by using any u_{eff} can be tested only by comparison with exact results.

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Limiting Forms of the Screened Coulomb T Matrix

WILLIAM F. FORD
Lewis Research Center, Cleveland, Ohio
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In the complex energy plane, the pure Coulomb T matrix possesses branch points which would not appear if the force were properly defined. This is demonstrated by a study of the screened Coulomb T matrix in the limit as the screening radius R tends to infinity. No branch points develop if the proper order of limiting processes is observed and the results agree with previous calculations; however, the T matrix is discontinuous in the limit. A formula for the screened Coulomb T matrix is given which is valid to order $1/R$ for all energies.

I. INTRODUCTION

THE T matrix for a system undergoing scattering is given by

$$T = V + V[1/(E + i\epsilon - K - V)]V. \quad (1)$$

Here K is the Hamiltonian for the system in the absence of interaction, and V is the interaction giving rise to the scattering. The total energy of the system is denoted by E; the small imaginary term $i\epsilon$ serves to make the Green's function

$$G = 1/(E + i\epsilon - K - V) \quad (2)$$

well defined.

We consider the T matrix in the momentum representation, with matrix elements denoted by $\langle \mathbf{k}_2|T|\mathbf{k}_1\rangle$. It is convenient to introduce a complex wavenumber k, which is related to the total energy by

$$E + i\epsilon = \hbar^2k^2/2m, \qquad 0 < \arg(k) < \pi;$$

thus the energy dependence of the T matrix may be indicated explicitly by $\langle \mathbf{k}_2|T(k)|\mathbf{k}_1\rangle$, or simply $T(k)$.

For most quantum-mechanical systems, the T matrix cannot be given in closed form. However, the case of a two-particle system with pure Coulomb interaction has been studied extensively, and recently Hostler and others[1] derived integral representations for the Coulomb Green's function which reduce to hypergeometric functions. From these the Coulomb T matrix can be obtained directly.

The resulting expression for $T(k)$, however, has the drawback that it does not approach a well-defined limit as $k^2 \to k_1^2$ or $k^2 \to k_2^2$, and indeed has branch points there. This behavior is certainly not correct, for one can show on very general grounds that the only singularities of $T(k)$ should be a branch point at $k = 0$ and simple poles on the imaginary k axis corresponding to the bound-state energies of $K + V$.

The correct form of the T matrix when $k^2 = k_1^2$ is given in Ref. 2, where a similar anomaly in the limiting process $|\mathbf{k}_2| \to |\mathbf{k}_1|$ was studied. The difficulty there was traced back to the long-range nature of the Coulomb force and disappeared when the effects of shielding were introduced.

In the present case the unphysical branch points are also due to neglect of shielding effects. The scattering of charged particles is caused by an interaction which is always screened at very large distances; the T matrix may therefore properly be regarded as depending on *two* parameters, ϵ and the screening radius R. To find the value of $T(k, R)$ for real k, one must take $\epsilon \to 0$ followed by $R \to \infty$. Usually, the ordering is unimportant, but the branch points at k_1^2 and k_2^2 occur in Hostler's expression because the limit $R \to \infty$ has been (implicitly) taken first.

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The present work is intended to clarify the situation by studying the behavior of the screened Coulomb T matrix in the limit $R \to \infty$. In Sec. II the formalism is established and applied to the cutoff Coulomb potential. This interaction is chosen because it allows one to determine unambiguously the effects caused by extending the potential past the cutoff radius. In Sec. III these effects are isolated, and a general expression for the screened Coulomb T matrix is derived, which is valid to order $1/R$ for all k.

In Sec. IV the limits $\epsilon \to 0$ and $R \to \infty$ are taken. We find that branch points at k_1^2 and k_2^2 do not appear if the proper order of limits is used; furthermore, the resulting T matrix agrees with that obtained in Ref. 2. For other values of k, the screened and pure Coulomb T matrices are identical in the limit $R \to \infty$. Hence, the order of limiting processes is unimportant except in the vicinity of $k^2 = k_1^2$ and $k^2 = k_2^2$ or when $|\mathbf{k}_1| = |\mathbf{k}_2|$. (The last case requires special treatment and is not considered here; in the following sections it is assumed that $|\mathbf{k}_1| \neq |\mathbf{k}_2|$.) The branch points in the pure Coulomb T matrix are due to that part of the potential beyond the screening radius R; Sec. V treats the effects of this part of the potential on the plane wave part of the pure Coulomb wavefunction.

II. SCREENED COULOMB T MATRIX

We begin by making an expansion in Legendre polynomials of the T matrix for an arbitrary central potential $V(r)$:

$$\langle \mathbf{k}_2|\ T\ |\mathbf{k}_1\rangle = \frac{\hbar^2}{4\pi^2 m} \sum_{l=0}^{\infty} (2l+1) P_l(\hat{k}_1 \cdot \hat{k}_2) \langle k_2|\ T_l\ |k_1\rangle. \tag{3}$$

The coefficients $\langle k_2|T_l|k_1\rangle$ are given by[3]

$$\langle k_2|\ T_l\ |k_1\rangle = \frac{2\pi^2 m}{\hbar^2} \int_{-1}^{1} \langle \mathbf{k}_2|\ T\ |\mathbf{k}_1\rangle P_l(\mu)\, d\mu \qquad (\mu = \hat{k}_1 \cdot \hat{k}_2), \tag{4}$$

and may be obtained by using Eq. (1) if the Green's function is known. This is accomplished by making an expansion of the coordinate representation of the Green's function:

$$\langle \mathbf{r}|\ G\ |\mathbf{r}'\rangle = \frac{2m}{\hbar^2} \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\hat{r} \cdot \hat{r}') \langle r|\ G_l\ |r'\rangle. \tag{5}$$

After the angular integrations are carried out, we have

$$\langle k_2|\ T_l\ |k_1\rangle = B_l + M_l, \tag{6}$$

where

$$B_l = \int_0^{\infty} j_l(k_2 r) W(r) j_l(k_1 r) r^2\, dr, \tag{7}$$

and

$$M_l = \int_0^{\infty} r^2\, dr \int_0^{\infty} r'^2\, dr'\, j_l(k_2 r) W(r) \times \langle r|\ G_l\ |r'\rangle W(r') j_l(k_1 r') \tag{8}$$

with $W(r) = (2m/\hbar^2)V(r)$.

To obtain the partial wave Green's function $\langle r|G_l|r'\rangle$, we write the operator equation

$$(E + i\epsilon - K - V)G = 1$$

in the coordinate representation, which leads to

$$\left[\frac{1}{r}\frac{d^2}{dr^2} r + k^2 - \frac{l(l+1)}{r^2} - W(r)\right] \langle r|\ G_l\ |r'\rangle = \frac{\delta(r-r')}{r^2}. \tag{9}$$

The solution to this equation is easily shown to be

$$\langle r|\ G_l\ |r'\rangle = (1/ikrr') F_l(r_<) H_l(r_>), \tag{10}$$

where $r_<$ is the smaller and $r_>$ the larger of r, r', and where F_l and H_l are the regular and irregular solutions of

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - W(r)\right] f_l(r) = 0 \tag{11}$$

having the asymptotic forms

$$F_l(r) \sim \cos\left[kr - \tfrac{1}{2}\pi(l+1) + \delta_l\right], \qquad H_l(r) \sim e^{i[kr - \frac{1}{2}\pi(l+1) + \delta_l]}. \tag{12}$$

With this normalization the Wronskian of F_l and H_l is equal to ik.

We now apply these formulas to the cutoff Coulomb potential

$$V(r) = \begin{cases} V_0/r, & r < R, \\ 0, & r > R. \end{cases} \tag{13}$$

The solutions of Eq. (11) must in this case be proportional to pure Coulomb functions for $r < R$, and to free-particle functions for $r > R$. The Coulomb functions are normalized so that their Wronskian is equal to ik, and the free-particle functions are so chosen that the asymptotic forms of Eq. (12) are obtained for large r:

$$F_l(r) = \begin{cases} N_l F_l^c(r), & r < R, \\ \tfrac{1}{2}kr[e^{i\delta_l} h_l^{(1)}(kr) + e^{-i\delta_l} h_l^{(2)}(kr)], & r > R, \end{cases} \tag{14}$$

[3] The expansion here differs by a minus sign from that used in Ref. 2.

$$H_l(r) = \begin{cases} N_l^{-1} H_l^c(kr), & r < R, \\ kre^{i\delta_l} h_l^{(1)}(kr), & r > R. \end{cases} \tag{15}$$

Here $h_l^{(1)}$ and $h_l^{(2)}$ are spherical Hankel functions; the pure Coulomb functions F_l^c and H_l^c may be written[4]

$$F_l^c(r) = \tfrac{1}{2} C_l(\eta)(2kr)^{l+1} e^{ikr} \times \Phi(l + 1 + i\eta, 2l + 2; -2ikr), \tag{16}$$

$$H_l^c(r) = e^{\frac{1}{2}\pi\eta + i\sigma_l}(-2kr)^{l+1} e^{ikr} \times \Psi(l + 1 + i\eta, 2l + 2; -2ikr), \tag{17}$$

where

$$C_l(\eta) = e^{-\frac{1}{2}\pi\eta - i\sigma_l}[\Gamma(l + 1 + i\eta)/\Gamma(2l + 2)], \tag{18}$$

$$e^{2i\sigma_l} = \Gamma(l + 1 + i\eta)/\Gamma(l + 1 - i\eta), \tag{19}$$

and $\eta = mV_0/\hbar^2 k$. The quantities N_l and δ_l are determined by equating logarithmic derivatives of F_l at $r = R$, but to first order in $1/R$ this is equivalent to matching amplitudes and phases; accordingly,

$$N_l \sim 1, \qquad \delta_l(k) \sim \sigma_l - \eta \ln (2kR). \tag{20}$$

For brevity we introduce the functions

$$u_l(r, K) \equiv rj_l(Kr)W(r)F_l^c(r), \tag{21}$$

$$v_l(r, K) \equiv rj_l(Kr)W(r)H_l^c(r), \tag{22}$$

so that M_l may be written

$$M_l = \frac{1}{ik}\int_0^R u_l(r, k_2) \int_r^R v_l(r', k_1)\, dr'\, dr + \frac{1}{ik}\int_0^R v_l(r, k_2) \int_0^r u_l(r', k_1)\, dr'\, dr. \tag{23}$$

Now, by reversing the order of integration in the second term, we can show that

$$M_l = m_l(k_2, k_1) + m_l(k_1, k_2) = m_l + \tilde{m}_l, \tag{24}$$

where

$$m_l(k_2, k_1) = \frac{1}{ik}\int_0^R u_l(r, k_2) \int_r^R v_l(r', k_1)\, dr'\, dr. \tag{25}$$

In principle, therefore, evaluation of the cutoff Coulomb T matrix has been reduced to evaluation of $m_l(k_2, k_1)$ and the integral

$$B_l = 2\eta k \int_0^R j_l(k_2 r) j_l(k_1 r) r\, dr. \tag{26}$$

[A detailed study of the $l = 0$ terms $m_0(k_2, k_1)$ and B_0 is given in NASA TN D-2781.]

[4] Notation and formulas for the confluent hypergeometric functions Φ and Ψ are taken from Bateman Manuscript Project, *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill Book Company, Inc., New York, 1953), Vol. I, Chap. 6.

III. T MATRIX FOR LARGE R

The difficulty with the foregoing analysis is that it leads to expressions so complicated that the summation over l cannot be carried out in closed form. Since in practice the screening radius is always very large, one is then tempted to take limit $R \to \infty$ in the hope that the resulting series can be summed. This approach is successful, but care must be taken when $k^2 \to k_1^2$ or $k^2 \to k_2^2$ because the limiting process is nonuniform.

We begin by rewriting m_l in the form

$$ikm_l = \int_0^\infty u_l(r) \int_r^\infty v_l(r')\, dr'\, dr - \left[\int_0^R u_l(r)\, dr\right]\left[\int_R^\infty v_l(r)\, dr\right] - \int_R^\infty u_l(r) \int_r^\infty v_l(r')\, dr'\, dr, \tag{27}$$

which is possible if u_l and v_l are given some suitable definition for $r > R$. For the present purpose it is convenient to require that u_l and v_l have the *same functional form* for $r > R$ as for $r < R$; i.e., u_l and v_l are proportional to pure Coulomb functions times spherical Bessel functions for *all* r. With this definition, the first term in Eq. (27) is just what one would write for the pure Coulomb[5] T matrix, and to emphasize this we write

$$m_l(R) = m_l(\infty) - (1/ik)U_l(R)V_l(R) + \mathcal{O}(1/R), \tag{28}$$

where

$$U_l(R) = \int_0^R u_l(r)\, dr \tag{29}$$

and

$$V_l(R) = \int_R^\infty v_l(r)\, dr. \tag{30}$$

The third term in Eq. (27) has been dropped because, as shown in Appendix A, it is $\mathcal{O}(1/R)$ for all cases considered here.[6]

Generally speaking, the second term in Eq. (27) may also be neglected. To see this, consider the asymptotic forms of u_l and v_l,

$$u_l(r) \sim 2\eta k \frac{\sin(k_2 r - \frac{1}{2}\pi l)}{k_2 r} \times \sin[kr - \tfrac{1}{2}\pi l + \sigma_l - \eta \ln (2kr)], \tag{31}$$

[5] By "pure Coulomb" we mean a quantity obtained by assuming $R = \infty$ at the outset, as opposed to taking the limit $R \to \infty$ at the last.

[6] For simplicity, the symbol $\mathcal{O}(1/x)$ is used loosely throughout to denote any term which vanishes when $x \to \infty$.

$$v_l(r) \sim -2i\eta k \frac{\sin(k_1 r - \frac{1}{2}\pi l)}{k_1 r} \frac{e^{i(kr - \frac{1}{2}\pi l + \sigma_l)}}{(2kr)^{i\eta}}. \quad (32)$$

From Eq. (32) it follows, on integration by parts, that

$$V_l(R) = \frac{e^{ikR}}{(2kR)^{i\eta}} \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right]. \quad (33)$$

From Eq. (31) one can show that

$$[e^{ikR}/(2kR)^{i\eta}][ru_l(r)]$$

is a bounded function of r for $r \leq R$, $R \to \infty$; consequently, the quantity $e^{ikR}U_l(R)/(2kR)^{i\eta}$ has no worse than a logarithmic singularity as $R \to \infty$, and therefore

$$U_l(R)V_l(R) = \mathcal{O}[1/(k^2 - k_1^2)R]. \quad (34)$$

Equation (28) shows that $m_l(R)$ is given by its unscreened value $m_l(\infty)$ except when contributions to the latter from large r are important, and these occur only when $k^2 \to k_1^2$. Similar conclusions may be drawn for $\tilde{m}_l(R)$, the critical condition becoming $k^2 \to k_2^2$. Since $B_l(R) = B_l(\infty) + \mathcal{O}(1/R)$, we may write

$$\langle k_2|\, T_l(k, R)\, |k_1\rangle = \langle k_2|\, T_l(k, \infty)\, |k_1\rangle + \mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right] + \mathcal{O}\left[\frac{1}{(k^2 - k_2^2)R}\right], \quad (35)$$

or, after the summation over l has been performed,

$$\langle \mathbf{k}_2|\, T(k, R)\, |\mathbf{k}_1\rangle = \langle \mathbf{k}_2|\, T(k, \infty)\, |\mathbf{k}_1\rangle + \mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right] + \mathcal{O}\left[\frac{1}{(k^2 - k_2^2)R}\right]. \quad (36)$$

Now let us attempt to obtain a result more general than Eq. (36). This requires that we extract from the neglected terms and retain those parts which are important when

$$(k^2 - k_1^2)R \to 0 \text{ or } (k^2 - k_2^2)R \to 0.$$

For this purpose the quantity $U_l V_l$ must be examined in greater detail.

We begin with V_l, which is given asymptotically by

$$V_l(R) \sim \frac{\eta k}{k_1} e^{i\sigma_l} \int_R^\infty \frac{e^{ikr}}{(2kr)^{i\eta}} \times [e^{-ik_1 r} + (-1)^{l+1} e^{ik_1 r}] \frac{dr}{r}. \quad (37)$$

A change to $t = r/R$ as the variable of integration yields

$$V_l(R) \sim \frac{k}{ik_1} e^{i\delta_l(k)} \{f[(k - k_1)R] + (-1)^{l+1} f[(k + k_1)R]\}, \quad (38)$$

where

$$f(x) \equiv i\eta \int_1^\infty t^{-1-i\eta} e^{ixt}\, dt = i\eta e^{ix}\Psi(1, 1 - i\eta; -ix), \qquad |\arg(-ix)| < \tfrac{1}{2}\pi. \quad (39)$$

The asymptotic form of $f(x)$ is easily found to be $-\eta e^{ix}/x$, while for values of x approaching zero, the relation

$$i\eta e^{ix}\Psi(1, 1 - i\eta; -ix) = \Phi(-i\eta, 1 - i\eta; ix) - (-ix)^{i\eta}\Gamma(1 - i\eta) \quad (40)$$

yields

$$f(x) \underset{x \to 0}{\to} 1 - (-ix)^{i\eta}\Gamma(1 - i\eta). \quad (41)$$

When applied to $f[(k - k_1)R]$, Eq. (41) gives

$$f[(k - k_1)R] = 1 - C_0(\eta)e^{-i\sigma_0}[(k_1 - k)R]^{i\eta} + \mathcal{O}[(k - k_1)R] = 1 - C_0(\eta)e^{-i\delta_0(k)}[(k_1^2 - k^2)/4k_1^2]^{i\eta} + \mathcal{O}[(k - k_1)R], \quad (42)$$

where

$$-2\pi < \arg(k_1^2 - k^2) < 0. \quad (43)$$

The corresponding result for $f[(k + k_1)R]$ is exactly the same, except that the neglected terms are, of course, $\mathcal{O}[(k + k_1)R]$. Combining these results, we have for the behavior of $f[(k \pm k_1)R]$ as $R \to \infty$

$$f[(k \pm k_1)R] = \begin{cases} \dfrac{e^{ikR}}{(2kR)^{i\eta}} \mathcal{O}\left[\dfrac{1}{(k^2 - k_1^2)R}\right], & (44a) \\ 1 - C_0(\eta)e^{-i\delta_0(k)}\left(\dfrac{k^2 - k_1^2}{4k_1^2}\right)^{i\eta} + \mathcal{O}[(k^2 - k_1^2)R]. & (44b) \end{cases}$$

Before proceeding, let us note that to $\mathcal{O}(1/R)$ the product $U_l V_l$ can be written in the form

$$Af[(k - k_1)R] + Bf[(k + k_1)R] + \mathcal{O}(1/R),$$

where A and B are yet to be determined. We are, in fact, able to give exact expressions for A and B, valid for all k. However, since $f[(k - k_1)R]$ is already $\mathcal{O}(1/R)$ except when $k \to k_1$, an exact expression for A is really necessary only in the vicinity of $k = k_1$. Similarly, an exact expression for B is really necessary only in the vicinity of $k = -k_1$. For this reason we immediately put $k/k_1 = \pm 1$ in Eq. (38) and write

$$V_l(R) = -ie^{i\delta_l}\{f[(k - k_1)R] + (-1)^l f[(k + k_1)R]\} + \mathcal{O}(1/R). \quad (45)$$

Next we demonstrate that

$$\langle k_2|\, T_l(k, R)\, |k\rangle = (N_l e^{i\delta_l}/k)U_l(R), \quad (46)$$

i.e., U_l is proportional to $\langle k_2|T_l(k, R)|k_1\rangle$ for the special case where k_1 is complex and equal to k. The proof begins with the observation that Eqs. (6) to (8) may also be written as follows:

$$\langle k_2|\, T_l(k, R)\, |k\rangle = \int_0^\infty j_l(k_2 r)W(r)\psi_l(r)r^2\, dr, \quad (47)$$

where

$$\psi_l(r) = j_l(kr) + \int_0^\infty \langle r|\, G_l(k)\, |r'\rangle W(r')j_l(kr')r'^2\, dr', \quad (48)$$

and k_1 has been set equal to k.

Equation (48) is almost identical to one of the well-known integral equations for the radial wavefunction $F_l(r)$; it differs in that the wavenumbers in $j_l(kr)$ and $G_l(k)$ are exactly equal instead of equal in the limit $\epsilon \to 0$. This circumstance makes the integrand in Eq. (48) a perfect derivative, however, and, as shown in Appendix B, the result is what one might naively expect:

$$\psi_l(r) = e^{i\delta_l}[F_l(r)/kr]. \quad (49)$$

Equations (47) and (49) then lead directly to the desired expression for $U_l(R)$.

As mentioned above, in order to determine $U_l V_l$ to $\mathcal{O}(1/R)$, the coefficient of $f[(k - k_1)R]$ must be known exactly only when $k = k_1$; therefore,

$$\begin{aligned}(e^{i\delta_l}/k)U_l(R)f[(k - k_1)R] &= f[(k - k_1)R][(e^{i\delta_l}/k)U_l(R)]_{k=k_1} + \mathcal{O}(1/R) \\ &= f[(k - k_1)R]\langle k_2|\, T_l(k_1, R)\, |k_1\rangle + \mathcal{O}(1/R). \quad (50)\end{aligned}$$

In like manner we may write

$$\begin{aligned}(e^{i\delta_l}/k)U_l(R)f[(k + k_1)R] &= f[(k + k_1)R]\langle k_2|\, T_l(-k_1, R)\, |-k_1\rangle + \mathcal{O}(1/R) \\ &= (-1)^l f[(k + k_1)R]\langle k_2|\, T_l(-k_1, R)\, |k_1\rangle + \mathcal{O}(1/R). \quad (51)\end{aligned}$$

[The fact that $j_l(-x) = (-1)^l j_l(x)$ is used to obtain the final form of Eq. (51).] From Eqs. (45), (50), and (51) it follows that

$$\begin{aligned}m_l(R) &= m_l(\infty) + f[(k - k_1)R]\langle k_2|\, T_l(k_1, R)\, |k_1\rangle \\ &\quad + f[(k + k_1)R]\langle k_2|\, T_l(-k_1, R)\, |k_1\rangle + \mathcal{O}(1/R). \quad (52)\end{aligned}$$

The expression for $\tilde{m}_l(R)$ is similar, but with k_1 and k_2 interchanged. Using the symmetry property

$$\langle k_1|\, T_l(k)\, |k_2\rangle = \langle k_2|\, T_l(k)\, |k_1\rangle, \quad (53)$$

and its consequence

$$\langle \mathbf{k}_1|\, T(k)\, |\mathbf{k}_2\rangle = \langle \mathbf{k}_2|\, T(k)\, |\mathbf{k}_1\rangle, \quad (54)$$

which can be readily established from Eqs. (7) and (8), we may give a general expression for the screened Coulomb T matrix, correct to $\mathcal{O}(1/R)$ and valid for all k:

$$\begin{aligned}\langle \mathbf{k}_2|\, T(k, R)\, |\mathbf{k}_1\rangle &= \langle \mathbf{k}_2|\, T(k, \infty)\, |\mathbf{k}_1\rangle \\ &\quad + f[(k - k_1)R]\langle \mathbf{k}_2|\, T(k_1, R)\, |\mathbf{k}_1\rangle \\ &\quad + f[(k + k_1)R]\langle \mathbf{k}_2|\, T(-k_1, R)\, |\mathbf{k}_1\rangle \\ &\quad + f[(k - k_2)R]\langle \mathbf{k}_2|\, T(k_2, R)\, |\mathbf{k}_1\rangle \\ &\quad + f[(k + k_2)R]\langle \mathbf{k}_2|\, T(-k_2, R)\, |\mathbf{k}_1\rangle + \mathcal{O}(1/R). \quad (55)\end{aligned}$$

IV. LIMITING CASES

To complete the study of the screened Coulomb T matrix, we need closed-form expressions for the T matrices that appear on the right side of Eq. (55). The first is the pure Coulomb T matrix with complex k, which may be obtained from Hostler's work and written as follows:

$$\langle \mathbf{k}_2|\, T(k, \infty)\, |\mathbf{k}_1\rangle = \frac{V_0}{2\pi^2}\frac{1 + I(x)}{(\mathbf{k}_2 - \mathbf{k}_1)^2}, \quad (56)$$

where

$$I(x) = 2i\eta(1 - e^{-2\pi\eta})^{-1}\int_\infty^{(1+)} \left(\frac{s - 1}{s + 1}\right)^{i\eta}\frac{1}{s^2 - x^2}\, ds, \quad (57)$$

$$x^2 = 1 + [(k_2^2 - k^2)(k_1^2 - k^2)/k^2(\mathbf{k}_2 - \mathbf{k}_1)^2]. \quad (58)$$

The integral $I(x)$ may be evaluated by changing to

$$t = (s - 1)/(s + 1)$$

as the variable of integration, with the result

$$I(x) = \frac{1}{x}\left[{}_2F_1\left(1, i\eta; 1 + i\eta; \frac{x + 1}{x - 1}\right) - {}_2F_1\left(1, i\eta; 1 + i\eta; \frac{x - 1}{x + 1}\right)\right]. \quad (59)$$

Considered as a function of k, $I(x)$ has simple poles at $i\eta = -n (n = 1, 2, 3 \cdots)$ and branch points at $x^2 = 1$ and $x^2 = \infty$. These latter points correspond to $k^2 = k_1^2$, $k^2 = k_2^2$, $k^2 = 0$, and $k^2 = \infty$. The behavior of $I(x)$ as $x \to 1$ may be determined by analytic continuation of the hypergeometric series and is given by

$$I(x) \to C_0^2(\eta)\left(\frac{x - 1}{x + 1}\right)^{i\eta} - 1, \qquad -2\pi < \arg\left(\frac{x - 1}{x + 1}\right) < 0. \quad (60)$$

Applying this specifically to the case $k^2 \to k_1^2$, we can write

$$\langle \mathbf{k}_2 |\, T(k, \infty)\, | \mathbf{k}_1 \rangle \to \frac{V_0}{2\pi^2} C_0^2(\eta) \frac{(k_2^2 - k^2)^{i\eta}}{[(\mathbf{k}_2 - \mathbf{k}_1)^2]^{1+i\eta}} \left(\frac{k_1^2 - k^2}{4k_1^2}\right)^{i\eta}, \tag{61}$$

where

$$-\pi < \arg (k_2^2 - k^2) < \pi, \tag{62a}$$

$$-2\pi < \arg (k_1^2 - k^2) < 0. \tag{62b}$$

Next we consider the screened Coulomb T matrices appearing in Eq. (55). All these can be obtained in closed form from the basic result of Ref. 2,

$$\langle \mathbf{k}_2 |\, T(k, R)\, | \mathbf{k}_1 \rangle|_{k^2 = k_1^2} = \frac{V_0}{2\pi^2} C_0(\eta) e^{i\delta_0(k)} \frac{(k_2^2 - k^2)^{i\eta}}{[(\mathbf{k}_2 - \mathbf{k}_1)^2]^{1+i\eta}} + \mathcal{O}\left(\frac{1}{R}\right). \tag{63}$$

Although Eq. (63) was originally derived with the assumption that $k = k_1$, it also holds for $k = -k_1$. To show this, we note from Eq. (1) that $T(E - i\epsilon) = T(E + i\epsilon)^*$, if V and K are real. From this, in the limit $\epsilon \to 0$,

$$T(k \to k_1 e^{\pi i}) = [T(k \to k_1)]^*.$$

Equation (63) satisfies this relation and therefore holds for $k^2 = k_1^2$. The symmetry property (54) may be used to obtain the result for $k^2 = k_2^2$.

We can now see explicitly how the screened Coulomb T matrix behaves as $R \to \infty$. If k is complex, or is real but not equal to $\pm k_1$ or $\pm k_2$, all the f functions in Eq. (55) are $\mathcal{O}(1/R)$, and therefore

$$\lim_{R\to\infty} \langle \mathbf{k}_2 |\, T(k, R)\, | \mathbf{k}_1 \rangle = \langle \mathbf{k}_2 |\, T(k, \infty)\, | \mathbf{k}_1 \rangle = \frac{V_0}{2\pi^2} \frac{1 + I(x)}{(\mathbf{k}_2 - \mathbf{k}_1)^2}. \tag{64}$$

But when k approaches one of the critical values, say k_1, Eq. (55) reduces to

$$\langle \mathbf{k}_2 |\, T(k, R)\, | \mathbf{k}_1 \rangle = \langle \mathbf{k}_2 |\, T(k, \infty)\, | \mathbf{k}_1 \rangle + f[(k - k_1)R] \langle \mathbf{k}_2 |\, T(k_1, R)\, | \mathbf{k}_1 \rangle + \mathcal{O}(1/R). \tag{65}$$

The T matrix is thus represented by a combination of two terms, one correct for $R = \infty$, $k \neq k_1$, and the other correct for $k = k_1$, $R < \infty$; which term dominates is determined by $f[(k - k_1)R]$. If $R \to \infty$ faster than $k \to k_1$, the first term dominates, and we are led again to Eq. (64). As discussed previously, however, the limit $R \to \infty$ is actually a convenience and should be performed last, which corresponds to $(k - k_1)R \to 0$. Comparing Eq. (44b) to the T matrices as given in Eqs. (61) and (63) reveals that in this situation a cancellation takes place and yields

$$\langle \mathbf{k}_2 |\, T(k, R)\, | \mathbf{k}_1 \rangle = \langle \mathbf{k}_2 |\, T(k_1, R)\, | \mathbf{k}_1 \rangle + \mathcal{O}[(k - k_1)R] + \mathcal{O}\left(\frac{1}{R}\right) = \frac{V_0}{2\pi^2} C_0(\eta) e^{i\delta_0} \frac{(k_2^2 - k^2)^{i\eta}}{[(\mathbf{k}_2 - \mathbf{k}_1)^2]^{1+i\eta}} + \mathcal{O}[(k - k_1)R] + \mathcal{O}\left(\frac{1}{R}\right). \tag{66a}$$

In the general case, where $(k - k_1)R$ approaches some fixed value as $R \to \infty$, use of Eq. (40) leads to

$$\langle \mathbf{k}_2 |\, T(k, R)\, | \mathbf{k}_1 \rangle = \langle \mathbf{k}_2 |\, T(k_1, R)\, | \mathbf{k}_1 \rangle \times \Phi[-i\eta, 1 - i\eta; i(k - k_1)R] + \mathcal{O}(1/R). \tag{66b}$$

Obviously, similar results are obtained when k approaches any of the other critical values.

We may summarize our findings as follows: Generally, it makes no difference when the limit $R \to \infty$ is taken in the expression for the screened Coulomb T matrix; the result is identical to the pure Coulomb T matrix and does not depend on R. The exception to this generalization occurs when k^2 approaches k_1^2 or k_2^2. In this case the screened Coulomb T matrix admits of an asymptotic expansion, the leading term of which is a well-behaved function of k and depends on R through the logarithmic phase factor $e^{i\delta_0}$. In contrast, the pure Coulomb T matrix has branch points at k_1^2 and k_2^2, in addition to being independent of R.

Near these critical points, the difference between the pure and screened Coulomb T matrices is due to contributions to the former from $r' > R$. These contributions do not affect the angular dependence of the T matrix, but only its magnitude and phase. The effect on the magnitude is such as to make the T matrix discontinuous in the limit $R \to \infty$. This effect is strikingly displayed when k is on the real axis; near k_1, for instance, we have

$$\lim_{R\to\infty} |\langle \mathbf{k}_2 |\, T(k, R)\, | \mathbf{k}_1 \rangle| = \frac{V_0}{2\pi^2} \frac{1}{(\mathbf{k}_2 - \mathbf{k}_1)^2} \mathfrak{M}_1 \mathfrak{M}_2, \tag{67}$$

where

$$\mathfrak{M}_1 = \begin{cases} C_0(\eta), & k_1 > k, \\ 1, & k_1 = k, \\ e^{\pi\eta} C_0(\eta), & k_1 < k, \end{cases} \qquad \mathfrak{M}_2 = \begin{cases} C_0(\eta), & k_2 > k_1, \\ e^{\pi\eta} C_0(\eta), & k_2 < k_1. \end{cases} \tag{68}$$

V. WAVEFUNCTIONS

A remarkable finding of the preceding section is that when k^2 approaches k_1^2 or k_2^2, the entire contribution to the pure Coulomb T matrix comes from large values of r'. More precisely, the contribution from $r' > R$ consists of two parts identical except in normalization, one of which exactly cancels the contribution from $r' < R$. When screening is introduced, the cancellation is prevented. It is perhaps worth noting that this same phenomenon is responsible for the well-known distortion of the incident plane wave in a pure Coulomb field.

To see this, consider the wave operator $\Omega(k)$, which is related to the Green's function by the equation

$$\Omega(k) = 1 + G(k)V. \tag{69}$$

Suppose that $\Omega(k)$ operates on a plane wave of momentum $\hbar\mathbf{k}_1$, with $k \neq |\mathbf{k}_1|$. A partial wave expansion yields

$$\Omega(k)\phi_{\mathbf{k}_1} = (2\pi)^{-\frac{3}{2}} \sum_{l=0}^{\infty} i^l(2l+1)P_l(\hat{r}\cdot\hat{k}_1)R_l(r), \tag{70}$$

where

$$R_l(r) = j_l(k_1r) + \int_0^\infty \langle r|\, G_l(k)\, |r'\rangle W(r')j_l(k_1r')r'^2\, dr'. \tag{71}$$

[The radial function $R_l(r)$ is generally different from $\psi_l(r)$ of Sec. IV, because the wavenumbers in $j_l(k_1r)$ and $G_l(k)$ are different.] By making use of quantities defined in previous sections, we may develop the following exact expression for $R_l(r)$:

$$R_l(r) = j_l(k_1r) + \frac{1}{ikr}\{N_lH_l(r)U_l(r_<, k_1) + N_l^{-1}F_l(r)[V_l(r_<) - V_l(R)]\}, \tag{72}$$

where $r_<$ is the smaller of r and R. [We have written $U_l(r_<,k_1)$ to indicate explicitly that k_1 is involved, not k_2 as before.]

Now let us determine the asymptotic form of $R_l(r)$. Since $k^2 \neq k_1^2$, we have $V_l(r) = e^{ikr}\mathcal{O}(1/r)$ as before. Thus, if we suppose $r_<$ to be large enough that $N_l \sim 1$,

$$\begin{aligned} R_l(r) &\sim j_l(k_1r) + (1/ikr)[H_l(r)U_l(r_<, k_1) + \mathcal{O}(1/r_<)] \\ &\sim j_l(k_1r) - (e^{ikr}/r)(-i)^l\langle k|\, T_l(k, r_<)\, |k_1\rangle \\ &\quad + \mathcal{O}(1/r_<^2). \end{aligned} \tag{73}$$

This equation may be inserted into Eq. (70) and the summation over l performed, which yields

$$\Omega(k)\phi_{\mathbf{k}_1} \sim (2\pi)^{-\frac{3}{2}}\left[e^{i\mathbf{k}_1\cdot\mathbf{r}} - \frac{e^{ikr}}{r}\langle\mathbf{k}|\, T(k, r_<)\, |\mathbf{k}_1\rangle\right], \tag{74}$$

where $\mathbf{k} \equiv k\mathbf{r}/r$. The "scattering amplitude" $-\langle\mathbf{k}|T(k, r_<)|\mathbf{k}_1\rangle$ depends only weakly on $r_<$, through a logarithmic phase factor $e^{-i\eta\ln(2kr_<)}$; the plane wave $e^{i\mathbf{k}_1\cdot\mathbf{r}}$ is unaffected.

Although Eq. (74) has been derived assuming a cutoff Coulomb potential for $W(r)$, this restriction is not necessary. We can return to Eq. (72), set $R = \infty$, and proceed as before; now the only reference to a cutoff potential is to identify $U_l(r, k_1)$ as proportional to $\langle k|T_l(k, r)|k_1\rangle$. Thus we conclude that even in a pure Coulomb field, the incident plane wave is undistorted if $k^2 \neq k_1^2$.

However, if $k^2 \to k_1^2$, the result depends critically on when the limit $R \to \infty$ is taken. Equation (74) is still valid when $k^2 = k_1^2$ provided that $r \geq R$, i.e., the limit $R \to \infty$ is taken last. Here the factor $V_l(r_<) - V_l(R)$ in Eq. (72) prevents any cancellation due to contributions from $r' > R$. But if the limit $R \to \infty$ is taken first, the term $F_l(r)V_l(r)$ survives and becomes important as $k^2 \to k_1^2$. Now cancellation does take place, and after some rearrangement we find that

$$R_l(r) \sim C_0(\eta)\left(\frac{k_1^2 - k^2}{4k_1^2}\right)^{i\eta} e^{i\sigma_l}\frac{F_l^c(r)}{kr} + \mathcal{O}\left(\frac{1}{r_<^2}\right) \tag{75}$$

or

$$\Omega(k)\phi_{\mathbf{k}_1} \sim C_0(\eta)[(k_1^2 - k^2)/4k_1^2]^{i\eta}\psi_{\mathbf{k}_1}^c(\mathbf{r}), \tag{76}$$

where $\psi_{\mathbf{k}_1}^c(\mathbf{r})$ is the pure Coulomb wavefunction.[7] As is well known, $\psi_{\mathbf{k}_1}^c$ is given asymptotically by a scattered wave plus a distorted plane wave. We also note from Eq. (76) that $\Omega(k)\varphi_{\mathbf{k}_1}$ does not have unit amplitude for large r, a fact first pointed out by Mapleton.[8] Both these features which appear as $k^2 \to k_1^2$, the plane-wave distortion and the amplitude renormalization, are due to (unphysical) contributions from $r' > R$.

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APPENDIX A. ORDER OF MAGNITUDE OF $\int_R^\infty u_l V_l\, dr$

In the text, the third term in Eq. (27), which may be written

$$\int_R^\infty u_l(r)V_l(r)\, dr, \tag{A1}$$

[7] Equation (76) is actually an identity holding for all r, not an asymptotic equality. This can be proved by using the integral representation (56) in the relation $\Omega = 1 + (E + i\epsilon - K)^{-1}T$ and taking the limit $k^2 \to k_1^2$. The result is proportional to an integral representation for the pure Coulomb wavefunction.

[8] R. A. Mapleton, J. Math. Phys. 3, 297 (1962).

was neglected on the premise that it is always $\mathcal{O}(1/R)$ for cases of interest. To prove this, we first observe that (using the asymptotic form of u_l) the integral may be decomposed into four integrals of the type

$$\int_R^\infty \frac{e^{i\lambda r}}{r^{1+i\nu\eta}} V_l(r)\, dr, \tag{A2}$$

where λ and ν take on the values $\nu(k \pm k_2)$ and ± 1, respectively. From Eq. (33) for $V_l(r)$, we see immediately that $e^{i\lambda r}V_l(r)/r^{i\nu\eta} = \mathcal{O}(1/r)$ unless $k^2 \to k_1^2$; therefore

$$\int_R^\infty u_l V_l\, dr = \mathcal{O}\left[\frac{1}{(k^2 - k_1^2)R}\right]. \tag{A3}$$

To derive an expression valid when $k^2 \to k_1^2$, we integrate (A2) by parts and obtain

$$\frac{1}{i\lambda}\left\{\frac{e^{i\lambda r}}{r^{1+i\nu\eta}} V_l(r)\Big|_{r=R}^{r=\infty} + \int_R^\infty \frac{e^{i\lambda r}}{r^{1+i\nu\eta}}\left[\frac{1+i\nu\eta}{r} V_l(r) + v_l(r)\right] dr\right\}, \tag{A4}$$

since $dV_l/dr = -v_l$. From Eqs. (38)–(41) we can show that, for all values of k, $e^{i\lambda r}V_l(r)/r^{i\nu\eta}$ is bounded and $e^{i\lambda r}v_l(r)/r^{i\nu\eta}$ is $\mathcal{O}(1/r)$ as $r \to \infty$. Consequently, (A4) is $\mathcal{O}(1/\lambda R)$, which leads to

$$\int_R^\infty u_l V_l\, dr = \mathcal{O}\left[\frac{1}{(k^2 - k_2^2)R}\right]. \tag{A5}$$

Equations (A3) and (A5) indicate that the integral is negligible unless $k_1^2 = k_2^2$, which is excluded from the present discussion.

APPENDIX B. EVALUATION OF $\psi_l(kr)$

In Eq. (48) we encounter the integral

$$P = \int_0^\infty \langle r|\, G_l(k)\, |r'\rangle W(r') j_l(kr') r'^2\, dr',$$

which may be written explicitly as

$$P = \frac{1}{ik^2 r}\left[F_l(r)\int_r^\infty H_l(r')W(r')\mathfrak{F}_l(r')\, dr' + H_l(r)\int_0^r F_l(r')W(r')\mathfrak{F}_l(r')\, dr'\right],$$

where $\mathfrak{F}_l(r) \equiv krj_l(kr)$. Recalling that $F_l(r)$ and $H_l(r)$ are both solutions of

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - W(r)\right] f_l(r) = 0,$$

and observing that $\mathfrak{F}_l(r)$ satisfies a similar equation but with $W(r) \equiv 0$, we can readily verify that

$$f_l(r)W(r)\mathfrak{F}_l(r) = \frac{d}{dr}\left(\mathfrak{F}_l \frac{df_l}{dr} - f_l \frac{d\mathfrak{F}_l}{dr}\right) = \frac{d}{dr} W(\mathfrak{F}_l, f_l),$$

where $W(\mathfrak{F}_l, f_l)$ is the Wronskian of $\mathfrak{F}_l$ and f_l. Therefore,

$$P = \frac{1}{ik^2 r}\left[F_l(r)W(\mathfrak{F}_l, H_l)\Big|_{r'=r}^{r'=\infty} + H_l(r)W(\mathfrak{F}_l, F_l)\Big|_{r'=0}^{r'=r}\right],$$

and after some rearrangement,

$$P = \frac{1}{ik^2 r}\left[F_l(r)W(\mathfrak{F}_l, H_l)_{r'=\infty} - \mathfrak{F}_l(r)W(F_l, H_l)_{r'=r} - H_l W(\mathfrak{F}_l, F_l)_{r'=0}\right].$$

Since both F_l and $\mathfrak{F}_l$ vanish as $(kr)^{l+1}$ when $kr \to 0$, the last term is zero. The Wronskian of F_l and H_l is equal to ik, and from Eq. (12) one can establish that as $kr \to \infty$

$$W(\mathfrak{F}_l, H_l) \to ike^{i\delta_l(k,r)}.$$

For the cutoff Coulomb potential, the upper limit for the integral P should actually be $r' = R$, and thus finally

$$P = e^{i\delta_l(k,R)}[F_l(r)/kr] - j_l(kr).$$

This equation leads immediately to the result given in Eq. (49).

Multipole Theory in the Time Domain*

KENNETH D. GRANZOW
The Dikewood Corporation, Albuquerque, New Mexico
(Received 23 July 1965)

Spherical outgoing waves of arbitrary time dependence are first written in the usual way as a Fourier integral of a sinusoidally time-varying multipole expansion. It is then shown that the integrals over ω of the r- and t-dependent part of the multipole terms can be replaced by differential operators operating on arbitrary functions of retarded time. Thus a form of the multipole expansion is obtained that does not explicitly contain the frequency spectrum of the multipoles. Given the value of E_r (for electric multipoles, or B_r for magnetic multipoles) as a function of time on the surface of a sphere, expressions for the multipole expansions of all the spherical field components are derived. The method employs a convolution integral and is useful in problems involving a very broad frequency spectrum.

I. INTRODUCTION

THE classical treatment of spherical waves in terms of a multipole expansion is usually carried out with an assumed sinusoidal time variation. Since the frequency spectrum and phase are arbitrary, the actual time variation (after mathematically performing a Fourier integration) is also arbitrary. In this paper a multipole expansion is formulated that does not explicitly contain the frequency spectrum. The Fourier integral of the multipole spectrum multiplied by the spherical Hankel function, which appears in the classical formalism, is replaced in the present treatment by a differential operator and an arbitrary function of retarded time. Using the multipole expansion in this form, the problem of extrapolating to larger radii field values given on the surface of a sphere (which contains the source) can be solved in the time domain, i.e., without Fourier analysis. This is an advantage when dealing with electromagnetic fields consisting of a single (non-oscillatory) pulse. Numerically performing the Fourier transform of such a pulse requires integration of the product of the pulse function and a sinusoidal kernel; such numerical integration with a kernel which is periodic and whose sign oscillates necessarily involves much cancellation and hence buildup of roundoff error. Furthermore, two such integrals would be required if the result were to be obtained in the time domain by this method. The second such integration would be especially difficult because the frequency spectrum of such a pulse is necessarily broad. In the present treatment only one integration is involved and the kernel is not periodic.

The starting point is Jackson's form of the multipole expansion.[1] Only the electric multipole field will be considered; the magnetic multipoles can be treated in the identical manner with **E** replacing **B** and $-\mathbf{B}$ replacing **E**. Only outward moving waves will be treated in detail; the corresponding expressions for inward moving waves are only slightly different even though there are theoretical difficulties in applying them. Inward moving waves are discussed in the appendix. Some of the methods presented in this paper are generalizations of methods that have been applied to the dipole by Wicklund.[2]

II. MULTIPOLE EXPANSION TRANSFORMED TO THE TIME DOMAIN

The electric multipole field for outgoing waves can be written[1]

$$\mathbf{B} = \sum_{l,m} a_E(l, m) h_l^{(1)}(kr) \mathbf{X}_{lm}(\theta, \phi), \tag{1}$$

$$\mathbf{E} = \sum_{l,m} \frac{i}{k} a_E(l, m) \nabla \times h_l^{(1)}(kr) \mathbf{X}_{lm}(\theta, \phi), \tag{2}$$

where $\mathbf{X}_{lm}(\theta, \phi) = (1/[l(l+1)]^{\frac{1}{2}})\mathbf{L}Y_{lm}(\theta, \phi)$ (the vector spherical harmonic), the time dependence is $e^{-i\omega t}$, $h_l^{(1)}$ is the spherical Hankel function, and $a_E(l, m)$ is the amplitude of the multipoles. The coefficients $a_E(l, m)$ are arbitrary complex functions of ω. The spherical components of Eqs. (1) and (2) can be written

$$B_r = 0,$$

$$B_\theta = \sum_{l,m} \frac{a_E(l, m) h_l^{(1)}(kr)}{2[l(l+1)]^{\frac{1}{2}}} \left[\frac{l}{[(2l+1)(2l+3)]^{\frac{1}{2}}} \right.$$

$$\times \{[(l+m+1)(l+m+2)]^{\frac{1}{2}} e^{-i\phi} Y_{l+1,m+1}$$

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[1] J. D. Jackson, *Classical Electrodynamics* (John Wiley & Sons, Inc., New York, 1962), pp. 545, 546.

[2] J. S. Wicklund, "Extrapolation of the Electromagnetic Field," Diamond Ordnance Fuze Laboratories, TR-1058, 1962 (unpublished).

$$+ [(l - m + 1)(l - m + 2)]^{\frac{1}{2}} e^{i\phi} Y_{l+1,m-1}\}$$
$$+ \frac{l+1}{[(2l-1)(2l+1)]^{\frac{1}{2}}} \{[(l - m)$$
$$\times (l - m - 1)]^{\frac{1}{2}} e^{-i\phi} Y_{l-1,m+1}$$
$$+ [(l + m)(l + m - 1)]^{\frac{1}{2}} e^{i\phi} Y_{l-1,m-1}\}\Big],$$

$$B_\phi = \frac{i}{2} \sum_{l,m} \frac{a_E(l, m) h_l^{(1)}(kr)}{[l(l+1)]^{\frac{1}{2}}}$$
$$\times \{[(l + m)(l - m + 1)]^{\frac{1}{2}} e^{i\phi} Y_{l,m-1}$$
$$- [(l - m)(l + m + 1)]^{\frac{1}{2}} e^{-i\phi} Y_{l,m+1}\}, \quad (3)$$

and

$$E_r = \sum_{l,m} -a_E(l, m)[l(l+1)]^{\frac{1}{2}} \frac{h_l^{(1)}(kr)}{kr} Y_{lm},$$

$$E_\theta = \sum_{l,m} \frac{a_E(l, m)}{2[l(l+1)]^{\frac{1}{2}}} \frac{1}{(2l+1)}$$
$$\times [l h_{l+1}^{(1)}(kr) - (l+1) h_{l-1}^{(1)}(kr)]$$
$$\times ([(l - m)(l + m + 1)]^{\frac{1}{2}} e^{-i\phi} Y_{l,m+1}$$
$$- [(l + m)(l - m + 1)]^{\frac{1}{2}} e^{+i\phi} Y_{l,m-1}),$$

$$E_\phi = \frac{i}{2} \sum_{l,m} \frac{-a_E(l, m)}{[l(l+1)]^{\frac{1}{2}}} \Big\{ \frac{l h_{l+1}^{(1)}(kr)}{[(2l+1)(2l+3)]^{\frac{1}{2}}}$$
$$\times \{[(l + m + 1)(l + m + 2)]^{\frac{1}{2}} e^{-i\phi} Y_{l+1,m+1}$$
$$+ [(l - m + 1)(l - m + 2)]^{\frac{1}{2}} e^{+i\phi} Y_{l+1,m-1}\}$$
$$- \frac{(l+1) h_{l-1}^{(1)}(kr)}{[(2l-1)(2l+1)]^{\frac{1}{2}}} \{[(l - m)$$
$$\times (l - m - 1)]^{\frac{1}{2}} e^{-i\phi} Y_{l-1,m+1}$$
$$+ [(l + m)(l + m - 1)]^{\frac{1}{2}} e^{+i\phi} Y_{l-1,m-1}\}\Big\}. \quad (4)$$

A Fourier transform of Eqs. (3) and (4) can then be performed to yield multipole expansions of the field components in the time domain. Thus, in Eqs. (3), if $a_E(l, m) h_l^{(1)}(kr)$ is replaced by

$$\alpha_{EB}(l, m, r, t) = \int_{-\infty}^{+\infty} e^{-i\omega t} a_E(l, m) h_l^{(1)}(kr)\, d\omega, \quad (5)$$

and, in Eqs. (4), if

$$a_E(l, m) h_l^{(1)}(kr)/kr, \; a_E(l, m) h_{l+1}^{(1)}(kr)$$

and $a_E(l, m) h_{l-1}^{(1)}(kr)$ are replaced by

$$\alpha_{Er}(l, m, r, t) = \int_{-\infty}^{+\infty} e^{-i\omega t} a_E(l, m) \frac{h_l^{(1)}(kr)}{kr}\, d\omega, \quad (6)$$

$$\alpha_{E+}(l, m, r, t) = \int_{-\infty}^{+\infty} e^{-i\omega t} a_E(l, m) h_{l+1}^{(1)}(kr)\, d\omega, \quad (7)$$

and

$$\alpha_{E-}(l, m, r, t) = \int_{-\infty}^{+\infty} e^{-i\omega t} a_E(l, m) h_{l-1}^{(1)}(kr)\, d\omega, \quad (8)$$

respectively, the resultant multipole expansions are in the time domain. In the following, expressions will be found for α_{EB}, α_{Er}, α_{E+}, and α_{E-} that do not explicitly contain the frequency spectrum $a_E(l, m)$ of the multipoles, but instead contain arbitrary functions of retarded time $\alpha_E(l, m, t^*)$.

The spherical Hankel function can be written[3,4]

$$h_n^{(1)}(kr) = e^{i\omega t} \Xi_n(r) \{\exp[-i(\omega t^* + \pi/2)]/k^{n+1}\}, \quad (9)$$

where $t^* = t - r/c$ and $\Xi_n(r)$ is the differential operator

$$\Xi_n(r) = \sum_{i=0}^{n} \frac{\mu_{ni}}{r^{i+1} c^{n-i}} \frac{d^{n-i}}{dt^{*n-i}}, \quad (10)$$

where

$$\mu_{ni} = \frac{\prod_{k=0}^{i} (n + k)(n - k + 1)}{n(n+1) 2^i j!}.$$

The variable t is a dummy in Eq. (9). If, at a given *constant* radius r, a dimensionless retarded time τ is defined by the equation $\tau = ct^*/r$, the operator $\Xi_n(r)$ can be written in the simpler form

$$\Xi_n(r) = \frac{1}{r^{n+1}} \sum_{i=0}^{n} \mu_{ni} \frac{d^{n-i}}{d\tau^{n-i}}. \quad (11)$$

Substituting the expression for $h_n^{(1)}$ in Eq. (9) into Eq. (6), and associating the dummy t with time, one obtains

$$\alpha_{Er}(l, m, r, t) = \int_{-\infty}^{+\infty} a_E(l, m) \frac{1}{r} \Xi_l(r)$$
$$\times \frac{\exp[-i(\omega t^* + \pi/2)]}{k^{l+2}}\, d\omega. \quad (12)$$

The operator, $(1/r)\Xi_l(r)$, may be taken out from under the integral sign since it is not a function of ω [assuming that the coefficients $a_E(l, m)$ are well enough behaved functions of ω to allow the change in order of integration and differentiation]. The functions $\alpha_E(l, m, t^*)$ of retarded time are now defined by

$$\alpha_E(l, m, t^*) = \int_{-\infty}^{+\infty} [a_E(l, m)$$
$$\times \exp[-i(\omega t^* + \pi/2)]/k^{l+2}]\, d\omega. \quad (13)$$

[3] M. Abromowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Applied Mathematics Series 55, 1964), p. 439.

[4] J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill Book Company, Inc., New York, 1941), p. 405.

Equation (12) can then be written

$$\alpha_{Er}(l, m, r, t) = (1/r)\Xi_l(r)\alpha_E(l, m, t^*). \quad (14)$$

Since the functions $\alpha_E(l, m, t^*)$ are Fourier transforms of arbitrary functions of ω, they are arbitrary functions of retarded time. Similarly, one can write

$$\alpha_{EB}(l, m, r, t) = \frac{i}{c}\frac{\partial}{\partial t^*}\Xi_l(r)\alpha_E(l, m, t^*), \quad (15)$$

$$\alpha_{E+}(l, m, r, t) = \Xi_{l+1}(r)\alpha_E(l, m, t^*), \quad (16)$$

$$\alpha_{E-}(l, m, r, t) = \frac{-1}{c^2}\frac{\partial^2}{\partial t^{*2}}\Xi_{l-1}(r)\alpha_E(l, m, t^*). \quad (17)$$

The multipole expansion for the **B** field [Eqs. (3)] can now be written in the time domain as follows:

$$B_r = 0,$$

$$B_\theta = \sum_{l,m}\frac{1}{2[l(l+1)]^{\frac{1}{2}}}\frac{i}{c}\frac{\partial}{\partial t^*}\Xi_l(r)\alpha_E(l, m, t^*)$$
$$\times\left[\frac{l}{[(2l+1)(2l+3)]^{\frac{1}{2}}}\left\{[(l+m+1)\right.\right.$$
$$\times(l+m+2)]^{\frac{1}{2}}e^{-i\phi}Y_{l+1,m+1}$$
$$\left.\left.+[(l-m+1)(l-m+2)]^{\frac{1}{2}}e^{i\phi}Y_{l+1,m-1}\right\}\right.$$
$$+\frac{l+1}{[(2l-1)(2l+1)]^{\frac{1}{2}}}\left\{[(l-m)\right.$$
$$\times(l-m-1)]^{\frac{1}{2}}e^{-i\phi}Y_{l-1,m+1}$$
$$\left.\left.+[(l+m)(l+m-1)]^{\frac{1}{2}}e^{i\phi}Y_{l-1,m-1}\right\}\right],$$

$$B_\phi = \sum_{l,m}\frac{-1}{2[l(l+1)]^{\frac{1}{2}}}\frac{1}{c}\frac{\partial}{\partial t^*}\Xi_l(r)\alpha_E(l, m, t^*)$$
$$\times\{[(l+m)(l-m+1)]^{\frac{1}{2}}e^{i\phi}Y_{l,m-1}$$
$$-[(l-m)(l+m+1)]^{\frac{1}{2}}e^{-i\phi}Y_{l,m+1}\}. \quad (18)$$

Likewise, the multipole expansion for the **E** field [Eqs. (4)] can be written

$$E_r = \sum_{l,m}-[l(l+1)]^{\frac{1}{2}}\frac{1}{r}\Xi_l(r)\alpha_E(l, m, t^*)Y_{lm},$$

$$E_\theta = \sum_{l,m}\frac{1}{2[l(l+1)]^{\frac{1}{2}}}\frac{1}{(2l+1)}\left[l\Xi_{l+1}(r)\right.$$
$$\left.+\frac{(l+1)}{c^2}\frac{\partial^2}{\partial t^{*2}}\Xi_{l-1}(r)\right]\alpha_E(l, m, t^*)$$
$$\times\{[(l-m)(l+m+1)]^{\frac{1}{2}}e^{-i\phi}Y_{l,m+1}$$
$$-[(l+m)(l-m+1)]^{\frac{1}{2}}e^{+i\phi}Y_{l,m-1}\},$$

$$E_\phi = \frac{i}{2}\sum_{l,m}\frac{-1}{[l(l+1)]^{\frac{1}{2}}}$$
$$\times\left\{\frac{l}{[(2l+1)(2l+3)]^{\frac{1}{2}}}\Xi_{l+1}(r)\alpha_E(l, m, t^*)\right.$$
$$\times\{[(l+m+1)(l+m+2)]^{\frac{1}{2}}e^{-i\phi}Y_{l+1,m+1}$$
$$+[(l-m+1)(l-m+2)]^{\frac{1}{2}}e^{+i\phi}Y_{l+1,m-1}\}$$
$$+\frac{l+1}{[(2l-1)(2l+1)]^{\frac{1}{2}}}\frac{1}{c^2}\frac{\partial^2}{\partial t^{*2}}\Xi_{l-1}(r)\alpha_E(l, m, t^*)$$
$$\times\{[(l-m)(l-m-1)]^{\frac{1}{2}}e^{-i\phi}Y_{l-1,m+1}$$
$$\left.+[(l+m)(l+m-1)]^{\frac{1}{2}}e^{+i\phi}Y_{l-1,m-1}\}\right\}. \quad (19)$$

If the field to be described is independent of ϕ, then $m = 0$, and the multipole expansion reduces to

$$B_r = 0,$$

$$B_\theta = 0,$$

$$B_\phi = \frac{1}{(2\pi)^{\frac{1}{2}}}\sum_l\frac{1}{c}\frac{\partial}{\partial t^*}\Xi_l(r)\alpha_E(l, 0, t^*)\bar{P}_l^1,$$

$$E_r = \frac{1}{(2\pi)^{\frac{1}{2}}}\sum_l -[l(l+1)]^{\frac{1}{2}}\frac{1}{r}\Xi_l(r)\alpha_E(l, 0, t^*)\bar{P}_l^0,$$

$$E_\theta = \frac{1}{(2\pi)^{\frac{1}{2}}}\sum_l\frac{1}{(2l+1)}\left[l\Xi_{l+1}(r)\right.$$
$$\left.+\frac{(l+1)}{c^2}\frac{\partial^2}{\partial t^{*2}}\Xi_{l-1}(r)\right]\alpha_E(l, 0, t^*)\bar{P}_l^1,$$

$$E_\phi = 0, \quad (20)$$

where $\bar{P}_l^m$ is the normalized Legendre function.[5] Only in the special case of $m = 0$ are the field values real if $\alpha_E(l, 0, t^*)$ is real. For general values of m, the functions $\alpha_E(l, m, t^*)$ can be arbitrary complex functions of t^*. The real or imaginary parts of the expressions given in Eqs. (18) and (19) then represent the actual values of the field components. Since the operator $\Xi_l(r)$ plays a role similar to that of the Hankel function in the frequency domain expressions, it will be referred to as the Hankel operator.

III. SPHERICAL BOUNDARY-VALUE PROBLEM

Suppose electromagnetic field components are known as functions of time on the surface of a sphere that contains all the sources of the field of interest. Then (it will be shown that) the functions $\alpha_E(l, m, t^*)$ and $O_l(r)\alpha_E(l, m, t^*)$, where $O_l(r)$ is any of the operators in Eqs. (18) or (19), can be expressed as integrals of the given field.

[5] Reference 3, p. 332.

Only the components E_r will be used to obtain the functions $\alpha_E(l, m, t^*)$ and $O_l\alpha_E(l, m, t^*)$. The reason for this is twofold. First, the dependence of the terms of the expansion of E_r on the angle coordinates θ, ϕ is given simply by the spherical harmonic. Thus, on a sphere of radius r_0, E_r can be expressed in the form

$$E_r(t^*) = \sum_{l,m} -[l(l+1)]^{\frac{1}{2}} \frac{1}{r_0} \beta_E(l, m, t^*) Y_{l,m}, \quad (21)$$

where $\beta_E(l, m, t^*)$ is given by

$$\beta_E(l, m, t^*) = -\frac{r_0}{[l(l+1)]^{\frac{1}{2}}} \int_{\substack{\text{sphere of} \\ \text{radius } r_0}} E_r(t^*) Y^*_{l,m}\, d\Omega. \quad (22)$$

Second, the component E_r is due only to the electric multipole; even if a magnetic multipole is present, it does not contribute to E_r. Thus, if both types of multipole sources are assumed present simultaneously, the electric part will be selected from the total field if E_r is used to analyze the fields. The magnetic multipole part can be analyzed in an identical manner by replacing **E** by $-$**B** and **B** by **E**. Thus only B_r would be used to analyze the magnetic multipoles. All fields (and their derivatives) are assumed to be zero initially, i.e., at $t^* = 0$.

Equating the coefficients of $Y_{l,m}$ in Eq. (21) and the first of Eqs. (19) (with $r = r_0$), one obtains

$$\Xi_l(r_0)\alpha_E(l, m, t^*) = \beta_E(l, m, t^*). \quad (23)$$

Defining the dimensionless retarded time $\tau_0 = t^*c/r_0$, one can write Eq. (23) as

$$\Xi_l(r_0)\alpha'_E(l, m, \tau_0) = \beta'_E(l, m, \tau_0), \quad (24)$$

where

$$\alpha'_E(l, m, \tau_0) = a_E(l, m, \tau_0 r_0/c),$$

and

$$\beta'_E(l, m, \tau_0) = \beta_E(l, m, \tau_0 r_0/c).$$

To solve Eq. (24), Green's functions will be found that satisfy the equations

$$\Xi_l(r_0)G_l(\tau_0, \tau'_0) = \delta(\tau_0 - \tau'_0), \quad l = 0, \cdots, \infty, \quad (25)$$

with the initial conditions, $G_l(0, \tau'_0) = G_l^{(1)}(0, \tau'_0) = \cdots = G_l^{(l-1)}(0, \tau'_0) = 0$, where

$$G_l^{(i)}(0, \tau'_0) = d^i G_l(\tau_0, \tau'_0)/d\tau_0^i|_{\tau_0=0}.$$

The functions $\alpha'_E(l, m, \tau_0)$ will then be given by

$$\alpha'_E(l, m, \tau_0) = \int_0^{\tau_0} G_l(\tau_0, \tau'_0)\beta'_E(l, m, \tau'_0)\, d\tau'_0. \quad (26)$$

Due to the initial conditions below Eq. (25), $G_l(\tau_0, \tau'_0) \equiv 0$ for $0 \leq \tau_0 < \tau'_0$. For $0 < \tau'_0 < \tau_0$, the Green's functions are given by

$$G_l(\tau_0, \tau'_0) = r_0^{l+1}\left\{\sum_{i=1}^{\frac{1}{2}l,\, l \text{ even}\ \text{or}\ \frac{1}{2}(l-1),\, l \text{ odd}} \exp[p_{li}(\tau_0 - \tau'_0)] \times [c_{li} \sin q_{li}(\tau_0 - \tau'_0) + d_{li} \cos q_{li}(\tau_0 - \tau'_0)] + f_l \exp[p_{l,\frac{1}{2}(l+1)}(\tau_0 - \tau'_0)]\right\}, \quad (27)$$

where $f_l = 0$ if l is even and $(p_{li} \pm iq_{li})$ are roots of the polynomial equation

$$F_l(z) = 0, \quad (28)$$

where

$$F_l(z) = \sum_{i=0}^{l} \mu_{li} z^{l-i}.$$

The roots of $F_l(z)$ are the roots of $H^{(1)}_{l+\frac{1}{2}}(iz)$, the half-odd-integer-order Hankel function of the first kind. In Jahnke and Emde's notation,[6]

$$F_l(z) = z^l S_{l+\frac{1}{2}}(2z) = z^l(\tfrac{1}{2}\pi z)^{\frac{1}{2}} \exp(z)(i)^{l+\frac{1}{2}} H^{(1)}_{l+\frac{1}{2}}(iz).$$

Note that $H^{(1)}_{l+\frac{1}{2}}(iz)$ has a singular point at $z = 0$ which annihilates the zero and branch point in its coefficient; thus $F_l(z)$ is analytic and nonzero at $z = 0$. The general behavior of the roots of $H^{(1)}_{l+\frac{1}{2}}(iz)$ can be deduced from the graph on p. 243 of Jahnke and Emde (Ref. 6). It is found that for l odd, $F_l(z)$ has one real negative root and $(l-1)$ complex roots which appear in complex conjugate pairs and have negative real parts. For l even, all of the l roots of $F_l(z)$ are complex (appearing, of course, in complex conjugate pairs) and have negative real parts. Numerical values of the roots for $l \lesssim 16$ are given in the appendix. It is significant to note that all of the roots are distinct. Thus, $G_l(\tau_0, \tau'_0)$ can be written in the form of Eq. (27). The derivatives of $G_l(\tau_0, \tau'_0)$ for $0 < \tau'_0 < \tau_0$ can be written

$$\frac{d^k G_l(\tau_0, \tau'_0)}{d\tau_0^k} = r_0^{l+1}\left\{\sum_{i=1}^{\frac{1}{2}l,\, l \text{ even}\ \text{or}\ \frac{1}{2}(l-1),\, l \text{ odd}} r_{li}^k \exp[p_{li}(\tau_0 - \tau'_0)] \times [(d_{li} \cos k\theta_{li} + c_{li} \sin k\theta_{li}) \cos q_{li}(\tau_0 - \tau'_0) + (c_{li} \cos k\theta_{li} - d_{li} \sin k\theta_{li}) \sin q_{li}(\tau_0 - \tau'_0)] + f_l p^k_{l,\frac{1}{2}(l+1)} \exp[p_{l,\frac{1}{2}(l+1)}(\tau_0 - \tau'_0)]\right\}, \quad (29)$$

where $r_{li} \exp(i\theta_{li}) = p_{li} + iq_{li}$. Integration of both sides of Eq. (25) from $\tau'_0 - \epsilon$ to $\tau'_0 + \epsilon$ and taking the limit as $\epsilon \to 0$ reveals that $d^{l-1}G_l(\tau_0, \tau'_0)/d\tau_0^{l-1}$ must have a positive discontinuous jump of magnitude r_0^{l+1} at the point $\tau_0 = \tau'_0$. Thus

[6] E. Jahnke and F. Emde, *Table of Functions* (Dover Publications, Inc., New York, 1945), pp. 136–137.

$$\lim_{\epsilon \to 0} d^{l-1}G_l(\tau_0, \tau_0')/d\tau_0^{l-1}|_{\tau_0=\tau_0'+\epsilon} = r_0^{l+1}.$$

Since the lower-order derivatives must be continuous at $\tau_0 = \tau_0'$ to satisfy Eq. (25), the equations determining the constants c_{li}, d_{li}, and f_l in the Green's function for $0 < \tau_0' < \tau_0$ are

$$\sum_{i=1}^{\frac{1}{2}l,\, l \text{ even} \atop \frac{1}{2}(l-1),\, l \text{ odd}} r_{li}^k(d_{li} \cos k\theta_{li} + c_{li} \sin k\theta_{li})$$

$$+ f_l p_{l,\frac{1}{2}(l+1)}^k = \delta_{k,l-1}, \quad k = 0, 1, \cdots, l-1, \quad (30)$$

where δ_{ij} is the Kronecker delta.

Now that the Green's functions are determined, the next step is to find explicit expressions for $O_l(r)\alpha_E'(l, m, \tau_0)$, where, again, $O_l(r)$ is any of the operators appearing in Eqs. (18) and (19). Terms of the form

$$\frac{1}{r^{l+1}} \frac{d^k\alpha_E'(l, m, \tau_0)}{d\tau^k}, \qquad k = 1, 2, \cdots, l+1,$$

must be evaluated. By successive differentiations of Eq. (26) one obtains

$$\frac{d^k\alpha_E'(l, m, \tau_0)}{d\tau_0^k} = \int_0^{\tau_0} G_l^{(k)}(\tau_0, \tau_0')\beta_E'(l, m, \tau_0')\, d\tau_0', \qquad k = 1, \cdots, l-1,$$

$$\frac{d^l\alpha_E'(l, m, \tau_0)}{d\tau_0^l} = \int_0^{\tau_0} G_l^{(l)}(\tau_0, \tau_0')\beta_E'(l, m, \tau_0')\, d\tau_0' + r_0^{l+1}\beta_E'(l, m, \tau_0),$$

$$\frac{d^{l+1}\alpha_E'(l, m, \tau_0)}{d\tau_0^{l+1}} = \int_0^{\tau_0} G_l^{(l+1)}(\tau_0, \tau_0')\beta_E'(l, m, \tau_0')\, d\tau_0' + r_0^{l+1}\left[\frac{d\beta_E'(l, m, \tau_0)}{d\tau_0} - \tfrac{1}{2}l(l+1)\beta_E'(l, m, \tau_0)\right], \quad (31)$$

where $G_l^{(i)}(\tau_0, \tau_0') = d^iG_l(\tau_0, \tau_0')/d\tau_0^i$. Noting that $\tau_0 = \tau r/r_0$ and hence that

$$\frac{d^k}{d\tau^k} = \left(\frac{r}{r_0}\right)^k \frac{d^k}{d\tau_0^k},$$

one can write

$$\frac{1}{r^{l+1}} \frac{d^k\alpha_E'}{d\tau^k} = \frac{1}{r^{l-k+1}r_0^k} \times \left\{\int_0^{\tau r/r_0} G_l^{(k)}(\tau r/r_0, \tau_0')\beta_E'(l, m, \tau_0')\, d\tau_0' + \delta_{kl}r_0^{l+1}\beta_E'(l, m, \tau_0) + \delta_{k,l+1}r_0^{l+1} \times [d\beta_E'(l, m, \tau_0)/d\tau_0 - \tfrac{1}{2}l(l+1)\beta_E'(l, m, \tau_0)]\right\}, \qquad k = 1, 2, \cdots, l+1. \quad (32)$$

To obtain the final expression for the terms of $O_l(r)\alpha_E'$, the expression for $G_l^{(k)}$ given by Eq. (29) is substituted into Eq. (32) which yields

$$\frac{1}{r^{l+1}} \frac{d^k\alpha_E'}{d\tau^k} = \left(\frac{r_0}{r}\right)^{l-k+1} \times \left\{\int_0^{t^*c/r_0} \left[\sum_{i=1}^{\frac{1}{2}l,\, l \text{ even} \atop \frac{1}{2}(l-1),\, l \text{ odd}} r_{li}^k \exp\left[p_{li}\left(\frac{t^*c}{r_0} - \tau_0'\right)\right] \times [(d_{li} \cos k\theta_{li} + c_{li} \sin k\theta_{li}) \cos q_{li}(t^*c/r_0 - \tau_0') + (c_{li} \cos k\theta_{li} - d_{li} \sin k\theta_{li}) \sin q_{li}(t^*c/r_0 - \tau_0')] + f_l p_{l,\frac{1}{2}(l+1)}^k \exp[p_{l,\frac{1}{2}(l+1)}(t^*c/r_0 - \tau_0')]\right] \times \beta_E'(l, m, \tau_0')\, d\tau_0' + \delta_{kl}\beta_E'(l, m, \tau_0) + \delta_{k,l+1} \times [d\beta_E'(l, m, \tau_0)/d\tau_0 - \tfrac{1}{2}l(l+1)\beta_E'(l, m, \tau_0)]\right\}, \qquad k = 1, 2, \cdots, l+1. \quad (33)$$

The integrals in Eq. (33) are independent of r, that is, independent of the radius of observation of the field. Hence, for a given source, the integration need only be performed once to give field values everywhere outside the sphere.

The integrals required in Eq. (33) are

$$I_s(l, m, j, t^*) = \int_0^{t^*c/r_0} \sin q_{lj}\left(\frac{t^*c}{r_0} - \tau_0'\right) \times \exp\left[p_{lj}\left(\frac{t^*c}{r_0} - \tau_0'\right)\right]\beta_E'(l, m, \tau_0')\, d\tau_0', \quad (34)$$

$$I_c(l, m, j, t^*) = \int_0^{t^*c/r_0} \cos q_{lj}\left(\frac{t^*c}{r_0} - \tau_0'\right) \times \exp\left[p_{lj}\left(\frac{t^*c}{r_0} - \tau_0'\right)\right]\beta_E'(l, m, \tau_0')\, d\tau_0', \quad (35)$$

where $j = 1, 2, \cdots, \frac{1}{2}l$ if l is even. If l is odd, $j = 1, 2, \cdots, \frac{1}{2}(l+1)$ and $q_{l,\frac{1}{2}(l+1)}$ is taken to be zero. [The constant $p_{l,\frac{1}{2}(l+1)}$ is, of course, the real root of $F_l(z) = 0$.]

One can now write the expansions for B_θ, B_ϕ, E_r, E_θ, and E_ϕ at arbitrary radius r in terms of the integrals (34) and (35). Substituting the expressions for the derivatives of α_E' from Eq. (33) into Eq. (11) and using I_s and I_c to represent the integrals of Eqs. (34) and (35), one can write α_{EB}, α_{Er}, α_{E+}, and α_{E-} [as expressed in Eqs. (14) through (17)] as follows:

$$\alpha_{EB} = \frac{i}{r}\left[\tfrac{1}{2}l(l+1)\left(\frac{r_0}{r} - 1\right)\beta_E(l, m, t^*) + \frac{r_0}{c}\frac{d\beta_E(l, m, t^*)}{dt^*}\right] + \frac{i}{r}\sum_{i=0}^{l} \mu_{li}F_{lim}(r, t^*), \quad (36)$$

$$\alpha_{E_r} = \frac{r_0}{r^2}\beta_E(l, m, t^*) + \frac{1}{r}\sum_{i=0}^{l}\mu_{li}F_{l,i+1,m}(r, t^*), \quad (37)$$

$$\alpha_{E+} = \frac{(l+1)}{2r}\left[(l+2)\frac{r_0}{r} - l\right]\beta_E(l, m, t^*) + \frac{r_0}{rc}\frac{d\beta_E(l, m, t^*)}{dt^*} + \frac{1}{r}\sum_{i=0}^{l+1}\mu_{l+1,i}F_{lim}(r, t^*), \quad (38)$$

$$\alpha_{E-} = -\left\{\frac{l}{2r}\left[(l-1)\frac{r_0}{r} - l - 1\right]\beta_E(l, m, t^*) + \frac{r_0}{rc}\frac{d\beta_E(l, m, t^*)}{dt^*} + \frac{1}{r}\sum_{i=0}^{l-1}\mu_{l-1,i}F_{lim}(r, t^*)\right\}, \quad (39)$$

where

$$F_{lim}(r, t^*) = \left(\frac{r_0}{r}\right)^i\left\{\sum_{j=1}^{\frac{1}{2}l,\ l\text{ even}\atop\frac{1}{2}(l-1),\ l\text{ odd}} r_{lj}^{(l-i+1)} \times \{[d_{lj}\cos(l-i+1)\theta_{lj} + c_{lj}\sin(l-i+1)\theta_{lj}]I_c(l, m, j, t^*) + [c_{lj}\cos(l-i+1)\theta_{lj} - d_{lj}\sin(l-i+1)\theta_{lj}]I_s(l, m, j, t^*)\} + f_l p_{l,\frac{1}{2}(l+1)}^{(l-i+1)}I_c(l, m, \tfrac{1}{2}(l+1), t^*)\right\}.$$

The field components are then given by Eqs. (18) and (19) with α_{EB}, α_{Er}, α_{E+} and α_{E-} substituted for the quantities they represent.

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APPENDIX

A. Incoming Waves

If Eqs. (1) and (2) are rewritten with $h_l^{(2)}$ substituted for $h_l^{(1)}$, they then represent incoming waves. The equations in Sec. II involving $h_l^{(1)}$ can be rewritten with $h_l^{(2)}$ instead of $h_l^{(1)}$; they then apply to incoming waves. Since $h_l^{(2)}(kr)$ can be written

$$h_l^{(2)}(kr) = e^{i\omega t}\Xi_l^{(2)}(r)[\exp[-i(\omega t_a^* - \pi/2)]/k^{l+1}], \quad (40)$$

where

$$\Xi_l^{(2)}(r) = \Xi_l(r)|_{t^*=-t_a^*} = \sum_{i=0}^{l}\frac{\mu_{li}(-1)^{l-i}}{r^{j+1}c^{l-i}}\frac{d^{l-i}}{dt_a^{*l-i}},$$

$$t_a^* = t + r/c,$$

the equations involving $\Xi_l(r)$ can be written for incoming waves by substituting t_a^* for t^*, $\Xi_l^{(2)}(r)$ for $\Xi_l(r)$ [or equivalently $\mu_{li}(-1)^{l-i}$ for μ_{li}],

and

$$\left[\frac{\exp[-i(\omega t_a^* - \pi/2)]}{k^{l+1}}\right] \text{ for } \left[\frac{\exp[-i(\omega t^* + \pi/2)]}{k^{l+1}}\right].$$

In solving the boundary-value problem of Sec. III, the auxiliary Eq. (28) is the same except for a change in sign of the coefficients of the odd powers of z. The roots are the same as for outgoing waves except for a change of sign of the real parts. Thus the Green's function contains exponentials increasing in time instead of decreasing as in the outgoing-wave treatment. This comes about because incoming waves are related to outgoing waves basically by a time reversal. The Green's functions are not time reversals to

TABLE I. Roots of $H_{l+\frac{1}{2}}^{(1)}(iz) = 0$.

Order (l)	Real part of z	Imaginary part of z	Order (l)	Real part of z	Imaginary part of z
3	−2.322185	0.	12	−8.253457	0.867839
3	−1.838907	1.754381	12	−7.997204	2.608989
			12	−7.465614	4.370186
4	−2.896211	0.867234	12	−6.610991	6.171537
4	−2.103789	2.657418	12	−5.329710	8.052905
			12	−3.343023	10.124297
5	−3.646739	0.			
5	−3.351956	1.742661	13	−8.947802	0.
5	−2.324674	3.571023	13	−8.830184	1.736704
			13	−8.470615	3.483830
6	−4.248359	0.867510	13	−7.844380	5.254921
6	−3.735708	2.626272	13	−6.900370	7.070641
6	−2.515932	4.492673	13	−5.530681	8.972248
			13	−3.449867	11.073928
7	−4.971787	0.			
7	−4.758290	1.739286	14	−9.583335	0.868314
7	−4.070139	3.517174	14	−9.362826	2.607241
7	−2.685677	5.420694	14	−8.911220	4.361654
			14	−8.198775	6.143068
8	−5.587886	0.867614	14	−7.172405	7.973204
8	−5.204841	2.616175	14	−5.720353	9.894709
8	−4.368289	4.414442	14	−3.551087	12.025738
8	−2.838984	6.353911			
			15	−10.273503	0.
9	−6.297019	0.	15	−10.170628	1.736566
9	−6.129368	1.737848	15	−9.859659	3.480484
9	−5.604422	3.498157	15	−9.323611	5.242350
9	−4.638440	5.317272	15	−8.532440	7.034373
9	−2.979261	7.291464	15	−7.429402	8.878983
			15	−5.900151	10.819999
10	−6.922050	0.867690	15	−3.647357	12.979501
10	−6.615282	2.611555			
10	−5.967534	4.384950	16	−10.914145	0.875305
10	−4.886218	6.224985	16	−10.714492	2.602741
10	−3.108916	8.232699	16	−10.328305	4.356535
			16	−9.711228	6.126361
11	−7.622450	0.	16	−8.848105	7.928469
11	−7.484148	1.737140	16	−7.673256	9.787751
11	−7.057923	3.488977	16	−6.071237	11.747872
11	−6.301334	5.276207	16	−3.739232	13.935028
11	−5.115647	7.137018			
11	−3.229722	9.177112			

each other because the boundary conditions forced on them are not related by a time reversal. For outgoing waves, $G_l(\tau_0, \tau_0')$ was found to be zero for $\tau_0 \leqslant \tau_0'$; for $\tau_0 > \tau_0'$ it is nonzero, but exponentially decaying. For incoming waves the Green's functions $G_l^{(2)}(\tau_0, \tau_0')$ are again zero for $\tau_0 \leqslant \tau_0'$; for $\tau_0 > \tau_0'$, however, the functions $G_l^{(2)}$ exponentially rise.

B. Solutions of Scalar Wave Equation

Note that (rE_r) satisfies the scalar wave equation. It follows that the formalism and solution of the spherical boundary-value problem for (rE_r) can be applied to any quantity satisfying the scalar wave equation, i.e., the rectangular field components or vector potential components.[7]

C. Roots of the Hankel Function

Using double precision on an IBM 7044 computer, roots of Eq. (28) were obtained through the 16th order. Greater computer precision would be needed to obtain them beyond the 16th order. For $l = 1$, the root is -1, for $l = 2$, the roots are $-\frac{3}{2} \pm i\sqrt{3}$. Table I contains the roots that were found numerically.

[7] D. D. Babb and K. D. Granzow, "Extrapolating Electromagnetic Fields From Values in a Spherical Region," Air Force Weapons Laboratory, WL TR-64-179, 1965 (unpublished), Sec. II.

A Continuous Representation of an Indefinite Metric Space*

M. G. GUNDZIK†
Department of Physics, Syracuse University, Syracuse, New York
(Received 22 June 1965)

An overcomplete family of states (OFS) is constructed for a countably infinite linear vector space with an indefinite metric for the case that the metric is diagonal with eigenvalues $(-1)^n$, where n is an integer. A continuous representation is indicated and the properties of a semiclassical description of a quantum mechanical system (the pseudo oscillator whose creation and destruction operators $\bar{a}$ and $\bar{a}^+$ satisfy $[\bar{a}, \bar{a}^+] = -1$) defined in this vector space are studied. It is found that a consistent OFS $|z>$ can be constructed if the operator $G(z)$ which generates the state $|z>$ from the vacuum is unitary. Furthermore, with the statistical state of this system specified by a bounded pseudo-Hermitian density matrix $\bar{\rho}$, the related semiclassical complex function $\rho_A(z)$ for antinormal ordering of operators in the indefinite metric space is found to be bounded, with $\rho_A(z)$ and $[\rho_A(z)]^2$ integrable, continuous, and a boundary value of an entire analytic function of two complex variables. The semiclassical function $\rho_N(z)$ for normal ordering is associated with a sequence of functions $\rho_{N(\nu)}(z)$ whose square is integrable and related to a sequence of tempered distributions $\rho_{N(\nu)}$ such that the corresponding sequence of density matrices $\bar{\rho}_{(\nu)}$ converges to $\bar{\rho}$ in the norm.

I. INTRODUCTION

THE general properties of continuous representations of Hilbert spaces have been studied[1,2] and used to relate semiclassical and quantum phenomena in specific cases. In particular, the equivalence of the quantum and semiclassical descriptions of optical coherence has been shown by Sudarshan,[3] by Klauder, McKenna, and Currie,[4] and by Mehta and Sudarshan.[5] In this case, a positive-definite density matrix ϱ is used to specify the statistical state of the radiation field.

It is of interest to know whether continuous representations of linear vector spaces with an indefinite metric (IM) exist, and, if they do, how they are defined. Then, given such a continuous representation, does a well-defined semiclassical description of a quantum mechanical system defined in the IM space result? It is found, that, indeed, for the special case considered, such a continuous representation exists. Furthermore, the semiclassical description of the states of a simple pseudo oscillator defined in an IM space is a generalization of the description of the states of a normal simple oscillator defined in a Hilbert space.

In the following, Sec. II is devoted to the development of the overcomplete family of states (OFS) for the IM space defined by a simple pseudo oscillator, i.e., where the creation and destruction operators $\bar{a}^+$ and $\bar{a}$, respectively,[6] satisfy $[\bar{a}, \bar{a}^+] = -1$. In Sec. III, a quantum mechanical description of the statistical state of a simple pseudo oscillator is used along with the OFS of Sec. II to determine the corresponding semiclassical description. Section IV contains some conclusions.

II. AN OVERCOMPLETE FAMILY OF STATES FOR AN INDEFINITE METRIC SPACE

Here we will develop an OFS and then give some important properties of a continuous representation formed from it. This approach is parallel to that taken by R. J. Glauber[2] in his treatment of the continuous representation of the positive-definite metric (PDM) space, except for modifications introduced by the IM. A brief introduction to some of the important properties of IM spaces is given in Part A. In B, we introduce the IM space corresponding to the pseudo-harmonic oscillator. Then the OFS and a continuous representation of the IM space are considered in C and D, respectively.

A. Some Properties of Indefinite Metric Spaces

The properties of vector spaces with an IM have been discussed by L. K. Pandit.[7] In general, the norm squared[8] is $\langle u|u\rangle > 0, <0, = 0$. In particular,

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[1] See the following: J. R. Klauder, Ann. Phys. (N.Y.) 11, 123 (1960); J. Math. Phys. 4, 1055, 1058 (1963); *ibid.* 5, 177 (1964). Also see J. R. Klauder and J. McKenna, J. Math. Phys. 5, 878 (1964); *ibid.* 6, 68 (1965); S. S. Schweber, *ibid.* 3, 831 (1962).
[2] R. J. Glauber, Phys. Rev. 131, 2766 (1963).
[3] E. C. G. Sudarshan, Phys. Rev. Letters 10, 277 (1963).
[4] J. R. Klauder, J. McKenna, and D. G. Currie, J. Math. Phys. 6, 734 (1965).
[5] C. L. Mehta and E. C. G. Sudarshan, Phys. Rev. 138, B274 (1965).
[6] Henceforth, $\bar{A}$ will denote an operator defined in an IM space and **A** an operator defined in a positive-definite metric Hilbert space.
[7] L. K. Pandit, Nuovo Cimento, Suppl. 11, 157 (1959).
[8] In the following, we will denote vectors of a PDM space by $|v)$ and those of the IM space by $|u\rangle$. Further, we will refer to the norm squared simply as the norm.

if we choose an IM space to be in one-to-one correspondence with a PDM space, then[9]

$$\langle u \mid v\rangle = (u|\ \mathbf{n}\ |v), \tag{1}$$

where $\mathbf{n}$ is the usual Hermitian metric operator which is defined in the PDM space. Though it is customary to define a metric operator only in the PDM space, we will also define one, $\bar{\eta}$, in the IM space so that

$$\langle u|\ \bar{\eta}\ |u\rangle = (u \mid u).$$

This allows for added clarity in the following.

An operator $\bar{P}$ in the IM space is related to $\mathbf{P}$ by

$$\langle u|\ \bar{P}\ |v\rangle = (u|\ \mathbf{nP}\ |v).$$

The adjoint $\bar{P}^+$ is defined by

$$\langle v|\ \bar{P}\ |u\rangle^* = \langle u|\ \bar{P}^+\ |v\rangle = (u|\ \mathbf{nP}^+\ |v),$$

where the form of $\mathbf{P}^+$ is given by $\mathbf{P}^+ = \mathbf{n}^{-1}\mathbf{P}^H\mathbf{n}$, and $\mathbf{P}^H$ is the usual Hermitian adjoint. An operator which is invariant under the adjoint operation is said to be pseudo-Hermitian.

When a change of basis vectors is made in the IM space such that the operator $\bar{U}$ transforms the orthonormal base set $|u\rangle$ into the basis $|u'\rangle$, then

$$\langle u' \mid v'\rangle = \langle u|\ \bar{U}^+\bar{U}\ |v\rangle = (u|\ \mathbf{nU}^+\mathbf{U}\ |v).$$

In order that the metric be preserved, it is necessary that $\bar{U}^+\bar{U} = 1$. When the IM is preserved under a transformation $\bar{U}$ above, $\bar{U}$ is said to be pseudo-unitary. The corresponding pseudo-unitary operator in the PDM space satisfies $\mathbf{U}^+\mathbf{U} = 1$.

While Hermitian and unitary operators are diagonalizable and have real and unimodular eigenvalues, respectively, this is not always true for pseudo-Hermitian or pseudo-unitary operators. In fact, the difficulties arise because eigenvectors of zero norm may occur. In complete analogy with the Hermitian and unitary operators, however, one finds that the eigenvalues of the pseudo-Hermitian operators are real and those of the unitary operators unimodular for those eigenvectors with nonvanishing norm.

B. A Linear Space with an Indefinite Metric

We can construct a linear space with an IM using the usual procedure for constructing the Fock space for a single harmonic oscillator beginning, instead, with a single pseudo oscillator. The operators $\bar{a}$ and $\bar{a}^+$ of the pseudo oscillator are defined in the IM space by $\bar{a}\ |0\rangle = 0$, $\langle 0|\ \bar{a}^+ = 0$, and $[\bar{a}, \bar{a}^+] = -1$, where $|0\rangle$ is the vacuum state. One finds an orthonormal set of states $|n\rangle$ where n takes the values $0, 1, 2, \cdots$, which satisfy

$$\bar{a}^+\bar{a}\ |n\rangle = -n\ |n\rangle, \tag{2a}$$

$$\bar{a}\ |n\rangle = -n^{\frac{1}{2}}\ |n-1\rangle, \tag{2b}$$

$$\bar{a}^+\ |n\rangle = (n+1)^{\frac{1}{2}}\ |n+1\rangle, \tag{2c}$$

with

$$|n\rangle = [1/(n!)^{\frac{1}{2}}](\bar{a}^+)^n\ |0\rangle \tag{2d}$$

and

$$\langle m \mid n\rangle = (-1)^n\ \delta_{mn}. \tag{2e}$$

The corresponding PDM Hilbert space contains $|n)$ where $(m|n) = \delta_{mn}$, and the relation

$$\langle m \mid n\rangle = (m|\ \mathbf{n}\ |n) = (-1)^n\ \delta_{mn} \tag{3}$$

gives the form of the metric $\mathbf{n}$. It satisfies $\mathbf{n}^H = \mathbf{n}$ and $\mathbf{n}^2 = 1$.

The completeness relation in the IM space is

$$1 = \sum_n |n\rangle N_n\langle n|, \tag{4a}$$

where $N_n = (-1)^n$. The corresponding relation in the PDM space is

$$1 = \sum_n |n)(n|. \tag{4b}$$

A useful representation of the completeness relation is found by using $\mathbf{n}\ |n) = (-1)^n\ |n)$ and defining $\bar{\eta}\ |n\rangle = (-1)^n\ |n\rangle$ with $\bar{\eta}^+ = \bar{\eta}$ and $\bar{\eta}^2 = 1$. This then leads to

$$\langle m|\ \bar{\eta}\ |P\rangle = (m|\ \mathbf{nn}\ |P) = (m \mid P).$$

Now we can define an alternative form of (4a) and (4b), respectively, as

$$\bar{\eta} = \sum_n |n\rangle\langle n| \tag{5a}$$

and

$$\mathbf{n} = \sum_n |n)N_n(n|. \tag{5b}$$

The above formalism is sufficient to construct the OFS that is required.

C. Construction of an Overcomplete Family of States

In order to construct an OFS, we look for the complete set of states $|z\rangle$ which are eigenstates of $\bar{a}$ and, thus, satisfy $\bar{a}\ |z\rangle = z\ |z\rangle$; $|z\rangle$ is generated from the vacuum $|n = z = 0\rangle$ and z is a continuous parameter. Since $\bar{a}$ is not pseudo-Hermitian, the eigenvalues $z = x + iy = re^{i\theta}$ are, in general, complex. The state $|z\rangle$ can be expressed as a linear

[9] We are defining two different metrics on the same set of points. There is a one-to-one mapping of expectation values from one metric space to the other.

combination of the states $|n\rangle$ using the resolution of unity given in (4a); thus, we have

$$|z\rangle = \sum_n |n\rangle(-1)^n\langle n \mid z\rangle. \tag{6}$$

The recursion relation

$$z\langle n-1 \mid z\rangle = n^{\frac{1}{2}}\langle n \mid z\rangle \tag{7}$$

is found from the properties of the states $|n\rangle$ given above. This together with (6) yields

$$|z\rangle = \sum_n |n\rangle \frac{(-z)^n}{(n!)^{\frac{1}{2}}}\langle 0 \mid z\rangle \tag{8a}$$

and

$$\langle z| = \sum_n \frac{1}{(n!)^{\frac{1}{2}}}(-z^*)^n\langle z \mid 0\rangle\langle n|. \tag{8b}$$

Now the states $|z\rangle$ are specified except for the factor $\langle 0|z\rangle$. This factor is determined by requiring $|z\rangle$ to satisfy a normalization condition which would, at the same time, permit us to define a completeness relation in terms of $\int_{-\infty}^{\infty} |z\rangle\langle z|\, d^2z$ ($d^2z = dx\, dy = r\, dr\, d\theta$). The simplest normalization consistent with a well-defined completeness relation is

$$\langle z|\, \bar{\eta}\, |z\rangle = (z \mid z) = 1. \tag{9}$$

Using this with (8a) and (8b), we find that $|\langle 0 \mid z\rangle|^2 = e^{-|z|^2}$. With the phase chosen such that $\langle 0 \mid z\rangle = e^{-\frac{1}{2}|z|^2}$, (8a) becomes

$$|z\rangle = \sum_n |n\rangle \frac{(-z)^n}{(n!)^{\frac{1}{2}}} e^{-\frac{1}{2}|z|^2}. \tag{8c}$$

The form of the completeness relation can now be checked using (8c).

$$\begin{aligned}\int_{-\infty}^{\infty} |z\rangle\langle z|\, d^2z &= \int_0^{\infty}\int_0^{2\pi} \sum_{m,n} |m\rangle \frac{(-r)^{m+n}}{(m!\,n!)^{\frac{1}{2}}} e^{-i(n-m)\theta}\langle n|\, e^{-r^2} r\, dr\, d\theta,\\ &= \pi \sum |m\rangle\langle m|,\\ &= \pi\bar{\eta}.\end{aligned}$$

Thus, we have

$$\bar{\eta} = \frac{1}{\pi}\int_{-\infty}^{\infty} |z\rangle\langle z|\, d^2z, \tag{10a}$$

which is seen to correspond to

$$1 = \frac{1}{\pi}\int_{-\infty}^{\infty} |z\rangle(z|\, d^2z \tag{10b}$$

in the PDM space by using (9).

It is not possible to define a completeness relation if the normalization $\langle z \mid z\rangle = 1$ is assumed. In particular, this leads to the assignment of $e^{\frac{1}{2}|z|^2}$ to $\langle 0 \mid z\rangle$ which makes the integral, $\int |z\rangle\langle z|\, d^2z$, singular. This type of problem may arise in any treatment of countably infinite IM spaces if one attempts to define operations independently of any PDM space, since the concepts of continuity, convergence, and completeness may not be well defined.

The completeness relation (10a) restricts the form of $\bar{G}(z)$, where $|z\rangle = \bar{G}(z)\,|0\rangle$ and $|z_1 + z_2\rangle = \bar{G}(z_1)\,|z_2\rangle$. In fact, one can show that

$$\langle z|\, \bar{G}^+(z_0)\bar{\eta}\bar{G}(z_0)\, |z'\rangle = \langle z|\, \bar{\eta}\, |z'\rangle$$

follows from (10a) and the self-reproducing property which is discussed later and found in (32). This implies that

$$\bar{G}^+(z)\bar{\eta}\bar{G}(z) = \bar{\eta}, \tag{11}$$

and finally,

$$\mathbf{G}^H(z)\mathbf{G}(z) = 1.$$

in the PDM space. Therefore, $\mathbf{G}(z)$ must be unitary with respect to the PDM.

When we generate the state $|dz\rangle$ differing infinitesimally from the vacuum by the operator $\bar{G}(dz)$ with normalization $\bar{G}(0) = 1$, then by the requirement

$$\bar{a}\, \bar{G}(dz)\, |0\rangle = dz\, \bar{G}(dz)\, |0\rangle,$$

the commutation relation $[\bar{a}, \bar{a}^+] = -1$, and the unitarity of $\bar{G}(dz)$, we see that it is restricted to the form

$$\bar{G}(dz) = 1 - \bar{a}dz^* - \bar{a}^+dz. \tag{12}$$

Equation (12) satisfies (11) to first order using the fact that $\bar{\eta}$ anticommutes with $\bar{a}$ and $\bar{a}^+$ in this representation. The finite form corresponding to (12) is found by letting $z \to \lambda z$ and $dz \to zd\lambda$, where λ is a real parameter. This leads to

$$\begin{aligned}\frac{d\bar{G}(\lambda z)}{d\lambda} &= \lim_{\Delta\lambda\to 0} \frac{\bar{G}(z\lambda + z\Delta\lambda) - \bar{G}(z\lambda)}{\Delta\lambda}\\ &= (-\bar{a}z^* - \bar{a}^+z)\bar{G}(z\lambda).\end{aligned}$$

With a proper choice for λ, we find that

$$\bar{G}(z) = e^{(-\bar{a}z^* - \bar{a}^+z)}.$$

Using the well known identity

$$e^A e^B = e^{(A+B)+\frac{1}{2}[A,B]},$$

valid for all cases when the commutator $[A, B]$ is a number, we see that

$$\bar{G}(z) = e^{-\bar{a}^+z}e^{-\bar{a}z^*}e^{-\frac{1}{2}|z|^2} \tag{13}$$

leads to $|z\rangle$ in the form

$$|z\rangle = e^{-\bar{a}^+z}e^{-\frac{1}{2}|z|^2}\,|0\rangle. \tag{14}$$

This is just the form into which $|z\rangle$ given by (8c) reduces when (2d) is used.

D. A Continuous Representation of an Indefinite Metric Space

In the PDM case[2] there is a one-to-one mapping of the states of a harmonic oscillator onto the Hilbert space $\mathfrak{F}_n$ of entire analytic functions in which the scalar product is defined as $(f \mid g) = (1/\pi) \int f(z)^* g(z) e^{-|z|^2}\, dz$. Furthermore, it is known[10] that a unitary isomorphism exists between $\mathfrak{F}_n$ and the conventional Hilbert space of square-integrable functions. An analogous situation occurs for the continuous representation of an IM space. To see its exact form, let us make the transition from the states $|f\rangle$ of the pseudo oscillator to a space of entire analytic functions.

Let $|f\rangle$ represent some linear combination of the states $|n\rangle$ such that $\langle f| \bar{\eta} |f\rangle = (f \mid f) < \infty$. The projection of $|f\rangle$ onto the OFS $|z\rangle$ is

$$\begin{aligned} \langle z \mid f\rangle &= \langle z| f(\bar{a}^+) |0\rangle = f(z^*)\langle z \mid 0\rangle, \\ \langle z \mid f\rangle &= f(z^*) e^{-\frac{1}{2}|z|^2}; \end{aligned} \tag{15a}$$

and

$$\langle f \mid z\rangle = [f(z^*)]^* e^{-\frac{1}{2}|z|^2}. \tag{15b}$$

We can see that $f(z^*)$ is an entire analytic function in the following way. Let $|f\rangle$ be

$$|f\rangle = \sum_n b_n |n\rangle = \sum_n b_n \frac{1}{(n!)^{\frac{1}{2}}} (\bar{a}^+)^n |0\rangle.$$

Since boundedness requires that $\sum_n |b_n|^2 < \infty$, then $|b_n| \to 0$ as $n \to \infty$. Therefore,

$$f(z^*) = \sum_n b_n \frac{1}{(n!)^{\frac{1}{2}}} (z^*)^n$$

converges for finite $|z|$.

In order to calculate the form of the scalar product of two such states $\langle g|$ and $|f\rangle$, we make the transition to the corresponding PDM space and use the resolution of unity in terms of $|z\rangle$ given by (10b). Then $\langle g \mid f\rangle$ has the form

$$\langle g \mid f\rangle = (g| \mathfrak{n} |f) = \frac{1}{\pi} \int (g \mid z) f(z^*) e^{-\frac{1}{2}|z|^2}\, d^2z. \tag{16}$$

We return to the IM space to calculate $(g \mid z)$; it becomes

$$(g \mid z) = \langle g| \bar{\eta} |z\rangle = \frac{1}{\pi} \int \langle g \mid z'\rangle\langle z' \mid z\rangle\, d^2z', \tag{17}$$

where we have used the completeness relation in the form (10a). From (8c), we find that

$$\langle z' \mid z\rangle = e^{-z'^* z} e^{-\frac{1}{2}|z'|^2} e^{-\frac{1}{2}|z|^2}. \tag{18}$$

Using (15b) and (18), (17) becomes

$$(g \mid z) = \frac{1}{\pi} \int [g(z'^*)]^* e^{-z'^* z} e^{-|z|^2} e^{-|z'|^2}\, d^2z'.$$

When we express $g(z'^*)$ and $e^{-z'^* z}$ in terms of their expansions, integrate, and substitute into (16), we find that

$$\langle g \mid f\rangle = \frac{1}{\pi} \int g(-z)^* f(z) e^{-|z|^2}\, d^2z. \tag{19}$$

Therefore, in the IM case, there is a one-to-one mapping of the states of the pseudo oscillator with normalization $(f \mid f) < \infty$ into the generalized vector space $\mathfrak{F}_n'$ of entire analytic functions in which the scalar product is defined by (19). A similar form is encountered again in III where we consider the representation in $\mathfrak{F}_n'$ of the density matrix $\bar{\rho}$ for the pseudo oscillator.

III. STATISTICAL STATE OF A PSEUDO OSCILLATOR DEFINED IN AN INDEFINITE METRIC SPACE

Now we consider the properties of the semiclassical description of the statistical state of the quantum mechanical pseudo oscillator defined in an IM space using the OFS developed in II. A single state of the system is characterized by the destruction and creation operators $\bar{a}$ and $\bar{a}^+$, respectively, of the pseudo oscillator. We specify the statistical state of this system by a bounded pseudo-Hermitian density matrix $\bar{\rho}$ with certain trace properties such that the expectation value of an operator $\bar{O}$ in the IM space is given by $\mathrm{Tr}\,(\bar{\rho}\bar{O})$. Pseudo-Hermiticity is imposed to preserve linearity and in order that the projection of $\bar{\rho}$ to any nonzero norm state be real. The correspondence between the PDM and IM spaces used in II has the form

$$\langle m| \bar{\rho} |q\rangle = (m| \mathfrak{n}\varrho |q),$$

where ϱ is the PDM counterpart of $\bar{\rho}$.

In order to determine the semiclassical description of the given quantum mechanical system, we express the expectation value of some operator $\bar{G}(\bar{a}, \bar{a}^+)$ in a state described by $\bar{\rho}$, i.e., $\mathrm{Tr}\,[\bar{\rho}\bar{G}(\bar{a}, \bar{a}^+)]$, in terms of an integral over an appropriate distribution of states corresponding to the density matrix. This distribution will depend upon the ordering of the operators contained in $\bar{G}(\bar{a}, \bar{a}^+)$. Consider the case where $\bar{G}(\bar{a}, \bar{a}^+)$ is chosen to be

$$\bar{G}(\bar{a}, \bar{a}^+) = e^{+\beta\bar{a}^+} e^{-\alpha\bar{a}} \quad \text{or} \quad e^{-\alpha\bar{a}} e^{\beta\bar{a}^+}$$

where α and β are complex numbers.

[10] V. Bargmann, Commun. Pure Appl. Math. 14, 187 (1961).

The correspondence between Tr $(\bar{\rho}\bar{G})$ and an integral over a distribution is readily found for the case of antinormal ordering of the operators $\bar{a}$ and $\bar{a}^+$ by using the resolution of unity of the OFS $|z\rangle$ given by (10a); this leads to

$$\begin{aligned}\mathrm{Tr}\,(\bar{\rho}e^{-\alpha\bar{a}}e^{\beta\bar{a}^+}) &= \mathrm{Tr}\,(\bar{\rho}e^{-\alpha\bar{a}}\bar{\eta}\bar{\eta}e^{\beta\bar{a}^+}),\\ &= \mathrm{Tr}\left(\bar{\rho}e^{-\alpha\bar{a}}\frac{1}{\pi}\int d^2z\ |z\rangle\langle z|\ e^{-\beta\bar{a}^+}\bar{\eta}\right),\\ &= \frac{1}{\pi}\int \langle z|\ \bar{\eta}\bar{\rho}\ |z\rangle e^{-\alpha z}e^{-\beta z^*}\,d^2z.\end{aligned}$$

Now the correspondence is seen to be

$$\int \rho_A(z)e^{-\beta z^*}e^{-\alpha z}\,d^2z = \mathrm{Tr}\,(\bar{\rho}e^{-\alpha\bar{a}}e^{\beta\bar{a}^+}), \quad (20a)$$

where $\rho_A(z) = (1/\pi)\ \langle z|\ \bar{\eta}\bar{\rho}\ |z\rangle = (1/\pi)\ (z|\ \varrho\ |z)$. The correspondence is $\bar{\rho} \to \rho_A(z)$, $\bar{a} \to z$ and $\bar{a}^+ \to -z^*$ for antinormal ordering. The sign change that occurs here, i.e., $\bar{a}^+ \to -z^*$, is due to the fact that the metric $\bar{\eta}$ anticommutes with $\bar{a}^+$.

In complete analogy with (20a), we specify the correspondence for the normal ordered product to be

$$\int \rho_N(z)e^{-\beta z^*}e^{-\alpha z}\,dz^2 = \mathrm{Tr}\,(\bar{\rho}e^{\beta\bar{a}^+}e^{-\alpha\bar{a}}). \quad (20b)$$

If we denote the integrals (20a) and (20b) by $F_A(\alpha, \beta)$ and $F_N(\alpha, \beta)$, respectively, then for $F(\alpha, \beta)$ given by

$$F(\alpha, \beta) = \mathrm{Tr}\,(\bar{\rho}e^{-\alpha\bar{a}+\beta\bar{a}^+}),$$

we have

$$F_A(\alpha, \beta) = e^{\frac{1}{2}\alpha\beta}F(\alpha, \beta), \quad (20c)$$

and

$$F_N(\alpha, \beta) = e^{-\frac{1}{2}\alpha\beta}F(\alpha, \beta). \quad (20d)$$

The properties of $\bar{\rho}$ are considered in Part A. In B, the properties of $\rho_A(z)$ and its relation to physical systems are discussed. It is found that $\rho_A(z)$ is complex and that it is bounded, continuous, integrable, and its square is integrable. Furthermore, $\rho_A(z)$ is a boundary value of an entire analytic function of two complex variables which satisfies certain reproducing properties. The properties of $\rho_N(z)$ and its relation to $\rho_A(z)$ are discussed in C. While $\rho_N(z)$ is not bounded in the sense of $\rho_A(z)$, it is found that a sequence of tempered distributions $\rho_{N(\nu)}$ exists to which one can identify a sequence of functions $\rho_{N(\nu)}(x, y)$ whose square is integrable where the corresponding sequence of density matrices $\bar{\rho}_{(\nu)}$ converges to $\bar{\rho}$ in the norm.

The above properties are generalizations of the properties of the $\rho_A(z)$ and $\rho_N(z)$ that Mehta and Sudarshan defined[5] from the positive-definite Hermitian density matrix ϱ describing the statistical state of a normal oscillator in a Hilbert space.

A. Properties of ϱ

The density matrix $\bar{\rho}$ defined in the IM space is assumed to be a bounded pseudo-Hermitian operator which is a member of some trace class. In this case, the expectation value of finding the system in some particular state is positive or negative. In order that all of these expectation values be defined, we require that

$$\mathrm{Tr}\ \bar{\rho} = 1, \quad (21a)$$

$$\mathrm{Tr}\ \bar{\eta}\bar{\rho} = T, \quad (21b)$$

where $|T| < \infty$ and real. Further, we require that the PDM counterpart of $\bar{\eta}\bar{\rho}$, i.e., $\mathbf{n}\varrho$, which is Hermitian, be positive-definite; this implies that $T \geq 0$ since Tr $\bar{\eta}\bar{\rho}$ = Tr $\mathbf{n}\varrho$. This restriction is imposed so that, first of all, $\bar{\rho}$ reduces to the special case of the positive-definite Hermitian density matrix when $\mathbf{n} = 1$. Second, in the less restrictive case when $\mathbf{n}$ is nondegenerate and Hermitian with $\mathbf{n} \neq 1$ and $[\mathbf{n}, \varrho] = 0$, it requires that the corresponding $\bar{\rho}$ which is now also Hermitian, and thus, diagonalizable and which one can separate into positive and negative norm parts be such that its positive and negative norm eigenstates correspond to positive and negative eigenvalues, respectively.

The representation of $\bar{\rho}$ in the IM space defined by the pseudo oscillator is given by

$$\bar{\rho} = \sum_{m,n} \bar{\eta}\ |n\rangle\rho_{nm}\langle m|\ \bar{\eta},$$

where ρ_{nm} is given by

$$\rho_{nm} = \langle n|\ \bar{\rho}\ |m\rangle = (n|\ \mathbf{n}\varrho\ |m).$$

The trace conditions (21a) and (21b) require that

$$\sum_n (-1)^n\rho_{nn} = 1$$

and that

$$\sum_n \mathbb{I}\rho_{nn} = T. \quad (21c)$$

These together imply that $\lim_{n\to\infty} |\rho_{nm}| = 0$. Furthermore, since

$$|\rho_{nm}|^2 \leq |\rho_{nn}|\ |\rho_{mm}|,$$

then, $|\rho_{nm}| \to 0$ as $n \to \infty$ and $m \to \infty$, independently.

B. Properties of $\varrho_A(z)$

The explicit form which defines $\rho_A(z)$, i.e.,

$$\rho_A(z) = \frac{1}{\pi}\langle z|\ \bar{\eta}\bar{\rho}\ |z\rangle = \frac{1}{\pi}(z|\ \varrho\ |z) \quad (22a)$$

and the properties of $\bar{\rho}$ allow us to determine the properties of $\rho_A(z)$. It is immediately evident from (22a) that $\rho_A(z)$ is, in general, complex unless $[\bar{\eta}, \bar{\rho}] = [\eta, \rho] = 0$. The real and imaginary parts of $\rho_A(z)$ are given by

$$\text{Re } \rho_A(z) = (1/\pi)(z| \varrho_R |z), \tag{22b}$$

$$\text{Im } \rho_A(z) = (1/\pi)(z| \varrho_I |z), \tag{22c}$$

where

$$\varrho_R = \tfrac{1}{2}(\varrho + \varrho^{\mathrm{H}})$$

and

$$\varrho_I = \tfrac{1}{2}(\varrho - \varrho^{\mathrm{H}})$$

are the Hermitian and skew-Hermitian parts of ϱ, respectively.

We show that $\rho_A(z)$ has the following properties.

(1) $\rho_A(z)$ is bounded, $|\rho_A(z)| \leq |\text{Tr } (\bar{\eta}\bar{\rho})|/\pi = T/\pi$.

(2) The integral $|\int \rho_A(z) e^{-\beta z^*} e^{-\beta^* z}\, dz^2| \leq e^{\frac{1}{2}|\beta|^2}$ is bounded. Also, $\rho_A(z)$ is integrable since $\int \rho_A(z)\, d^2 z = 1$.

(3) The square of $\rho_A(z) \equiv \rho_A(x, y)$ is integrable. That is, $0 \leq \int [\rho_A(x, y)]^2\, dx\, dy \leq 1/\pi$. Also, we find that

$$\left|\int \rho_A(x, y)\, dx\right| \leq \frac{2}{\pi}; \qquad \left|\int \rho_A(x, y)\, dy\right| \leq \frac{2}{\pi}.$$

(4) $\rho_A(z) = \rho_A(x, y)$ is the boundary value of an entire analytic function of two complex variables.

We begin by showing the bound of $\rho_A(z)$. From our definition of $\rho_A(z)$ given in (22a), and the fact that $\bar{\eta}\,|z\rangle = |-z\rangle$ (see Sec. II.), we have

$$\rho_A(z) = \frac{1}{\pi}(-z| \mathbf{n}\varrho |z).$$

Since $\mathbf{n}\varrho$ is Hermitian, it may be diagonalized in the PDM space and expressed in terms of its eigenvalues ω_n and eigenvectors $|\xi_n)$ in the diagonal form

$$\mathbf{n}\varrho = \sum_n \omega_n |\xi_n)(\xi_n|.$$

Under the unitary transformation $\mathbf{S}$ which diagonalizes $\mathbf{n}\varrho$, the vectors $|z) \rightarrow \mathbf{S}\,|z) = |z')$. Thus, $\rho_A(z)$ is given by

$$\rho_A(z) = \sum_n \frac{\omega_n}{\pi}(-z' \mid \xi_n)(\xi_n \mid z').$$

Since $\mathbf{n}\varrho$ is defined to be positive-definite, then the ω_n are positive and $\omega_n \leq T$; this leads to

$$|\rho_A(z)| \leq \frac{T}{\pi} |\sum_n (-z' \mid \xi_n)(\xi_n \mid z')|,$$

$$= \frac{T}{\pi} |(-z'| (\sum_n |\xi_n)(\xi_n|)\, |z')|;$$

$$|\rho_A(z)| \leq \frac{T}{\pi} |(z| \mathbf{n}\, |z)|,$$

$$= \frac{T}{\pi} |e^{-2|z|^2}|.$$

Our final result is

$$|\rho_A(z)| \leq \frac{T}{\pi}. \tag{23}$$

The bound on the real part of $\rho_A(z)$ can also be found using (22b) directly. For the special case that $\varrho_R = \frac{1}{2}(\varrho + \varrho^H)$ is positive-definite and $\text{Tr } \varrho_R = 1 = T$, we find

$$0 \leq \text{Re } \rho_A(z) \leq 1/\pi.$$

This is the result which is obtained for $\rho_A(z)$ when ϱ is defined as the PDM density operator for a state described in terms of a normal oscillator defined on a Hilbert space.[5]

In order to consider the second point, we set $\alpha = \beta^*$ in (20a) and rewrite it as

$$\int \rho_A(z)\, e^{-\beta z^* - \beta^* z}\, dz^2 = e^{\frac{1}{2}|\beta|^2} \text{Tr } (\bar{\rho}\, e^{-\beta^* \bar{a} + \beta \bar{a}^+}). \tag{24}$$

Since the eigenvalues of a pseudo-unitary operator for nonzero norm eigenvectors have unit modulus, then the expectation value of $e^{-\beta^* \bar{a} + \beta \bar{a}^+}$ for a given state satisfies

$$|\langle e^{-\beta^* \bar{a} + \beta \bar{a}^+}\rangle| \leq 1.$$

The normalization $\text{Tr } (\bar{\rho}) = 1$, leads to

$$|\text{Tr } (\bar{\rho}\, e^{-\beta^* \bar{a} + \beta \bar{a}^+})| = |\langle e^{-\beta^* \bar{a} + \beta \bar{a}^+}\rangle| \leq 1. \tag{25}$$

Using (25), (24) can be written with the bound

$$\left|\int \rho_A(z)\, e^{-\beta z^* - \beta^* z}\, d^2 z\right| \leq e^{\frac{1}{2}|\beta|^2}. \tag{26}$$

By letting $\beta = \frac{1}{2}(s + it)$ and $z = x + iy$, the left side of Eq. (26) with $\rho_A(z) \equiv \rho_A(x, y)$ is written as

$$L(s, t) = \int \rho_A(x, y)\, e^{-(sx + ty)}\, dx\, dy, \tag{27}$$

and

$$|L(s, t)| \leq e^{+(s^2 + t^2)/8}. \tag{26a}$$

The function $L(s, t)$ can be identified with the bilateral Laplace transform[11] of $\rho_A(x, y)$, where the strip of convergence of (27) in the s and t complex

[11] An entire operational calculus based on the bilateral Laplace transform has been developed by B. Van der Pol and H. Bremmer. See B. Van der Pol and H. Bremmer, *Operational Calculus based on the Two Sided Laplace Transform* (Syndics of the Cambridge University Press, London, 1955).

planes must be specified. Certainly, (27) converges for $s = t = 0$ since (24) and (27) imply that

$$L(0, 0) = \int \rho_A(z)\, d^2z = 1.$$

The bilateral Laplace transform converges for finite values of real s and t by (26). The inverse of (27) is given by

$$\rho_A(x, y) = \frac{1}{(2\pi i)^2} \int_{c_1-i\infty}^{c_1+i\infty} ds \int_{c_2-i\infty}^{c_2+i\infty} dt\, L(s, t)\, e^{(sx+ty)}. \tag{28}$$

where $c_1 = \text{Re } s = s$ of (27) and $c_2 = \text{Re } t = t$ of (27) and the integration is performed in the complex s- and t-planes within the respective strips of convergence defined by (26) and (27). The bound of (26) in addition to the boundedness of $\bar{\rho}$ is sufficient to ensure that (28) exists. Furthermore, since $L(s, t)$ is found[11] to be analytic and free of singularities in s and t, then we can shift the contour defined in (28) to any region, i.e., any value of c_1 for the s plane and any c_2 for the t plane contained in the region of convergence.

In the case of the bilateral Laplace transform, one can show[11] that the product rule

$$\int_{-\infty}^{\infty} \rho_A^*(-x, -y)\rho_A(x, y)\, dx\, dy = \frac{1}{(2\pi i)^2} \int_{c_1-i\infty}^{c_1+i\infty} \int_{c_2-i\infty}^{c_2+i\infty} |L(s, t)|^2\, ds\, dt \tag{29a}$$

holds. However, from (22a) we note that $\rho_A^*(-z) = \rho_A(z)$. This condition implies that Re $\rho_A(z)$ is even and Im $\rho_A(z)$ is odd under the change from z to $-z$; i.e., we have Re $\rho_A(z) =$ Re $\rho_A(-z)$, and Im $\rho_A(z) =$ $-$Im $\rho_A(-z)$. This together with (29a) and (26a) leads us to an integrability condition on the square of the form

$$\int_{-\infty}^{\infty} [\rho_A(x, y)]^2\, dx\, dy = \int_{-\infty}^{\infty} \{[\text{Re } \rho_A(z)]^2 - [\text{Im } \rho_A(z)]^2\}\, dx\, dy \leq \frac{1}{(2\pi i)^2} \int_{c_1-i\infty}^{c_1+i\infty} \int_{c_2-i\infty}^{c_2+i\infty} e^{\frac{1}{2}(s^2+t^2)}\, ds\, dt.$$

The right side of the inequality can be evaluated for $c_1 = c_2 = 0$; making the change of variables, we have

$$\int_{-\infty}^{\infty} [\rho_A(x, y)]^2\, dx\, dy \leq \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} e^{-\frac{1}{2}(s^2+t^2)}\, dt.$$

The upper bound is seen to be

$$\int_{-\infty}^{\infty} [\rho_A(x, y)]^2\, dx\, dy \leq \frac{1}{\pi}.$$

The lower bound on the above integral is seen to be zero by applying the above change of variables directly to (29a). The final form is then

$$0 \leq \int [\rho_A(x, y)]^2\, dx\, dy \leq \frac{1}{\pi}, \tag{29b}$$

where the integral is real.

We can also show that $\rho_A(x, y)$ is integrable over each of its arguments separately. First, we integrate (28) over x,

$$\int_{-\infty}^{\infty} \rho_A(x, y)\, dx = \int_{-\infty}^{\infty} dx \frac{1}{(2\pi i)^2} \int_{c-i\infty}^{c+i\infty} L(s, t)\, e^{(sx+ty)}\, ds\, dt,$$
$$= \int_{-\infty}^{\infty} dx \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt\, L(is, it)\, e^{-i(sx+ty)},$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, L(0, it)\, e^{ity}.$$

But, this gives

$$\left| \int \rho_A(x, y)\, dx \right| \leq \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, |L(0, it)|, = \frac{1}{2\pi} \int dt\, e^{-t^2/8},$$

and the final form is

$$\left| \int_{-\infty}^{\infty} \rho_A(x, y)\, dx \right| \leq \left(\frac{2}{\pi}\right)^{\frac{1}{2}}. \tag{30a}$$

Similarly, we find that

$$\left| \int_{-\infty}^{\infty} \rho_A(x, y)\, dy \right| \leq \left(\frac{2}{\pi}\right)^{\frac{1}{2}}. \tag{30b}$$

In the case that Im $\rho_A(x, y) = 0$, (29b), (30a), and (30b) yield results similar to those obtained for the positive-definite density matrix ρ corresponding to the normal oscillator. The contribution of the negative norm states is contained in Im $\rho_A(x, y)$.

Now we show that $\rho_A(z)$ corresponding to the IM $\bar{\rho}$ is a boundary value of an entire analytic function of two complex variables. The derivation follows Mehta and Sudarshan.[5] We let

$$\rho(\delta, \gamma) = \frac{1}{\pi} \langle \delta^* |\, \bar{\eta}\bar{\rho}\, | \gamma \rangle\, e^{\frac{1}{2}|\delta|^2}\, e^{\frac{1}{2}|\gamma|^2}, \tag{31a}$$

where δ and γ are complex numbers. We introduce the vectors of the IM space defined by the pseudo oscillator.

$$\rho(\delta,\gamma) = \frac{1}{\pi}\sum_{m,n}\langle\delta^*\mid n\rangle\langle n\mid\bar{\rho}\mid m\rangle\langle m\mid\bar{\eta}\mid\gamma\rangle e^{\frac{1}{2}|\delta|^2}e^{\frac{1}{2}|\gamma|^2},$$

$$= \frac{1}{\pi}\sum_{m,n}\frac{(\delta)^n(-\gamma)^m}{(n!\,m!)^{\frac{1}{2}}}\langle n\mid\bar{\rho}\mid m\rangle,$$

$$\rho(\delta,\gamma) = \frac{1}{\pi}\sum_{m,n}\rho_{nm}\frac{(\delta)^n(-\gamma)^m}{(n!\,m!)^{\frac{1}{2}}}. \tag{31b}$$

Since $|\rho_{nm}| \to 0$ as $m \to \infty$ and $n \to \infty$, independently, we see that $\rho(\delta, \gamma)$ is finite and convergent for all finite values of δ and γ. Thus, $\rho(\delta, \gamma)$ is an entire analytic function of δ and γ. Using the definition (31a), we see that $\rho_A(z)$ is given by

$$\rho_A(z) = \rho(z^*, z)\, e^{-|z|^2}. \tag{31c}$$

If we now express δ and γ in terms of two independent complex variables, i.e., $\alpha = \frac{1}{2}(\delta + \gamma)$ and $\beta = \frac{1}{2}(\delta - \gamma)$, then the corresponding $\rho(\alpha, \beta)$ is an entire analytic function of α and β. By letting $\delta \to z$ and $\gamma \to z^*$, we approach the boundary of $\rho(\alpha, \beta)$ corresponding to $\alpha \to x$ and $\beta \to iy (z = x + iy)$. Thus, for $\alpha = x$ and $\beta = iy$, $\rho_A(z) = \rho_A(x, y)$ is the boundary value of an entire analytic function of two complex variables.

Now one can prove the following theorem which has its counterpart for the positive-definite metric case. If for any bounded operator $\bar{A}$, defined in the IM space

$$A(z) = \langle z\mid\bar{\eta}\bar{A}\mid z\rangle = 0$$

in any finite area over the complex z-plane, then $A(z) = 0$ over the whole complex z plane and, further, the operator $\bar{A}$ itself is identically zero. The proof goes through in the same way as for the positive-definite metric case.[5]

One has the same self-reproducing property for our $\rho(\delta, \gamma)$ as in the positive-definite metric case. Here we use the resolution of the identity for the IM, OFS $|z\rangle$ given by (10a). This leads to

$$\rho(\delta,\gamma) = \frac{1}{\pi^2}\int\langle\delta^*\mid\bar{\eta}\bar{\rho}\mid z\rangle\langle z\mid\bar{\eta}\mid\gamma\rangle\, e^{\frac{1}{2}|\gamma|^2}\, e^{\frac{1}{2}|\delta|^2}\, d^2z.$$

Using (8c), we find that

$$\langle z\mid\bar{\eta}\mid\gamma\rangle = e^{-\frac{1}{2}|z|^2}\, e^{-\frac{1}{2}|\gamma|^2}\, e^{z^*\gamma}.$$

This gives

$$\rho(\delta,\gamma) = \frac{1}{\pi}\int\rho(\delta, z)K(z,\gamma)\, d^2z, \tag{32}$$

where

$$K(z,\gamma) = e^{-|z|^2+z^*\gamma}.$$

C. Properties of $\varrho_N(z)$ and the Relation between $\varrho_N(z)$ and $\varrho_A(z)$.

We have already seen that $\rho_A(z)$ is well defined in the IM case. The properties of $\rho_N(z)$, however, are not so easily determined. In the following, we find that if $\rho_N(z)$ is given, then $\rho_A(z)$ is determined. The relation between $\rho_N(z)$ and $\rho_A(z)$ is the same as found in the PDM case.[5] We also show that there exists a sequence of tempered distributions $\rho_{N(\nu)}$ identified with functions whose square is integrable where the corresponding sequence of density matrices $\bar{\rho}_{(\nu)}$ converge to $\bar{\rho}$ in the norm.

The relation of $\rho_N(z)$ to $\rho_A(z)$ is found at once. If $\rho_N(z)$ is given, then we can construct a diagonal form for the density matrix $\bar{\rho}$ in terms of $\rho_N(z)$. This is found to be

$$\bar{\rho} = \int\rho_N(z)\mid z\rangle\langle z\mid\bar{\eta}\, d^2z. \tag{33a}$$

Then, we get back (20a), i.e.,

$$\mathrm{Tr}\,(\bar{\rho}\, e^{\beta\bar{a}^+}\, e^{-\alpha\bar{a}}) = \int\rho_N(z)\, e^{-\beta z^*}\, e^{-\alpha z}\, d^2z.$$

Now, using the fact that

$$\rho_A(z) = (1/\pi)\langle z\mid\bar{\eta}\bar{\rho}\mid z\rangle,$$

we arrive at

$$\rho_A(z) = \frac{1}{\pi}\int\rho_N(\gamma)\,|\langle z\mid\bar{\eta}\mid\gamma\rangle|^2\, d^2\gamma. \tag{33b}$$

This is independent of the operator $\bar{G}(\bar{a}, \bar{a}^+)$ and thus, completely general.

In order to study the properties of $\rho_N(z)$, we consider the form $F_N(\alpha, \beta)$ given above;

$$F_N(\alpha,\beta) = \int\rho_N(z)\, e^{-\beta z^*-\alpha z}\, d^2z.$$

This is rewritten in terms of $z = x + iy$, with

$$\alpha = \tfrac{1}{2}(p + iq) + \tfrac{1}{2}(v - iu),$$
$$\beta = \tfrac{1}{2}(p + iq) - \tfrac{1}{2}(v - iu).$$

Then,

$$F_N(\alpha,\beta) = F_N(\alpha',\beta') = \int\rho_N(x, y)\, e^{-\alpha' z-\beta' v}\, dx\, dy, \tag{34}$$

where $\alpha' = p + iq$ and $\beta' = u + iv$. If one could show that $F_N(\alpha', \beta')$ is at worse bounded by a polynomial as $|\alpha'|$ and $|\beta'| \to \infty$, then it is possible to identify ρ_N with a distribution that maps

$$e^{-\alpha' z-\beta' v} \xrightarrow{\rho_N} F_N(\alpha',\beta'),$$

or one could identify $\rho_N(x, y)e^{-(px+uy)}$ with a tempered distribution that maps

$$e^{i(qx+vy)} \rightarrow F_N(\alpha', \beta')$$

for p and u in a finite domain Γ. However, as in the PMD case, $F_N(\alpha', \beta')$ is not generally bounded in the manner required. Nevertheless, one can construct a sequence of distributions $\rho_{N(\nu)}$ where the corresponding $F_N(\alpha', \beta')$ is bounded for each member and such that the $\bar{\rho}_{(\nu)}$ converge to $\bar{\rho}$ as $\nu \rightarrow \infty$. Such a sequence is not unique.

First we will show that there exists a sequence of functions $\rho_{N(\nu)}(x, y)$ whose square is integrable such that the corresponding operators $\bar{\rho}_{(\nu)}$ converge to $\bar{\rho}$ in the norm. For this purpose we introduce the sequence of functions $\rho_{N(\nu)}(x, y)$ defined by[12,13]

$$\int \rho_{N(\nu)}(x, y)\, e^{-(px+uy)}\, e^{-i(qx+vy)}\, dx\, dy = \begin{cases} F_N(\alpha', \beta') & \text{for} \quad A \leq p, u \leq B, \\ & \text{and} \quad -\nu \leq q, v \leq \nu, \\ 0 & \text{otherwise,} \end{cases} \tag{35}$$

where A and B are real and finite. Since $F_A(\alpha, \beta) = e^{-\alpha\beta}F_N(\alpha, \beta)$, from (20c) and (20d), $F_N(\alpha, \beta)$ is bounded for bounded values α and β. This allows us to identify (35) with a bilateral Laplace transform and ensures that the inverse transform

$$\frac{1}{(2\pi i)^2} \int_{c_1-i\infty}^{c_1+i\infty} ds \int_{c_2-i\infty}^{c_2+i\infty} dt\, F_{N(\nu)}(s, t)\, e^{sx+ty} = \rho_{N(\nu)}(x, y) \tag{36}$$

exists for $p = c_1$, $u = c_2$ and $F_{N(\nu)}(s, t)$ equal to the right side of (35). Recalling the product rule (29a) for the bilateral Laplace transform, we are led to the condition

$$0 \leq \int \rho^*_{N(\nu)}(-x, -y)\rho_{N(\nu)}(x, y)\, dx\, dy < \infty \tag{36a}$$

for finite ν. However, from (33a) we see that the pseudo-Hermiticity of $\bar{\rho}$ implies

$$\bar{\rho} = \bar{\rho}^+ = \int \rho^*_N(z)\bar{\eta}\, |z\rangle\langle z|\, d^2z.$$

Using the fact that $\bar{\eta}\, |z\rangle = |-z\rangle$ and making a change of variables we find

$$\bar{\rho} = \int \rho^*_N(-z)\, |z\rangle\langle z|\, \bar{\eta}\, d^2z. \tag{36b}$$

Since $F_N(\alpha', \beta')$ is bounded for bounded values of α' and β', we see that $p = c_1 = 0$ and $u = c_2 = 0$ are in the region of convergence of (35). Thus we rewrite (36) as

$$\rho_{N(\nu)}(x, y) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt\, F_{N(\nu)}(is, it)\, e^{i(sx+ty)}. \tag{36c}$$

Furthermore, from (35) we see that

$$F_{N(\nu)}(is, it) = \int_{-\infty}^{\infty} \rho_{N(\nu)}(x, y)\, e^{-i(sx+ty)}\, dx\, dy.$$

Taking the complex conjugate of both sides and making a change of variables we have

$$F^*_{N(\nu)}(is, it) = \int_{-\infty}^{\infty} \rho^*_{N(\nu)}(-x, -y)\, e^{-i(sx+ty)}\, dx\, dy. \tag{36d}$$

The representation of $\bar{\rho}$ in the terms of ρ_N has been given by (33a) and (36b). Similarly, for each $\rho_{N(\nu)}$ there is a $\bar{\rho}_{(\nu)}$ given by

$$\bar{\rho}_{(\nu)} = \int \rho_{N(\nu)}(z)\, |z\rangle\langle z|\, \bar{\eta}\, d^2z = \int \rho^*_{N(\nu)}(-z)\, |z\rangle\langle z|\, \bar{\eta}\, d^2z, \tag{37a}$$

which leads to

$$F_{N(\nu)}(is, it) = \int_{-\infty}^{\infty} \rho^*_{N(\nu)}(-x, -y)\, e^{-i(sx+ty)}\, dx\, dy.$$

Comparing this with (36d) we see that

$$F^*_{N(\nu)}(is, it) = F_{N(\nu)}(is, it). \tag{37b}$$

However, from (36c) we find that

$$\rho^*_{N(\nu)}(-x, -y) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt\, F^*_{N(\nu)}(is, it)\, e^{i(sx+ty)}.$$

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[12] A sequence of square-integrable functions defined in terms of Fourier transforms was introduced for the positive-definite metric case by Klauder, McKenna, and Currie (see Ref. 4).

[13] It is also possible to define a sequence of distributions $\rho_{N(\nu)}$ which corresponds to the sequence of density matrices similar to that used by Mehta and Sudarshan. That is, a sequence defined by

$$\langle n|\, \bar{\rho}_{(\nu)}\, |m\rangle = \begin{cases} \rho_{n,m}, & 0 \leq m, n \leq \nu, \text{ not } m = n = 0; \\ \rho_{0,0} + \sum_{\mu=\nu+1}^{\infty} \rho_{\mu,\mu}, & n = m = 0; \\ 0 & \text{otherwise;} \end{cases}$$

where $|m\rangle$ is an eigenvector of the operator $\bar{a}^+\bar{a}$, i.e., a state in the IM space of the pseudo oscillator. One can show that this sequence $\bar{\rho}_{(\nu)}$ converges to $\bar{\rho}$ in the norm and is associated with a sequence of distributions $\rho_{N(\nu)}$ defined on the set of infinitely differentiable functions of compact support such that the mapping is

$$e^{-(px+uy)-(qx+vy)} \xrightarrow{\rho_{N(\nu)}} F_{N(\nu)}(\alpha', \beta').$$

This together with (36c) and (37b) shows that $\rho_{N(\nu)}(x, y) = \rho^*_{N(\nu)}(-x, -y)$. Now the "pseudo" square-integrability condition (36a) leads to an integrability condition on the square, i.e.,

$$0 \leq \int [\rho_{N(\nu)}(x, y)]^2 \, dx \, dy < \infty. \tag{37c}$$

As in the case of $\rho_A(z)$, since Re $\rho_{N(\nu)}(z)$ is an even function and Im $\rho_{N(\nu)}(z)$ is odd, the above integral in (37c) is real.

It should be noted that the pseudo-Hermiticity of $\bar{\rho}$ enabled us to restrict the large class of functions which includes a subclass of nonlinear functions[14] which satisfy condition (36a) to the more restrictive class of linear functions satisfying (37c). The same result was also found in the case of $\rho_A(z)$. Thus we see that the assumption of pseudo-Hermiticity for $\bar{\rho}$ in an IM space, in addition to imposing reality on the eigenvalues of nonzero norm states, is also necessary for linearity.

Now we show that $\bar{\rho}_{(\nu)}$ converges to $\bar{\rho}$ in the norm. The norm squared of $\bar{\rho}$ is given by

$$||\bar{\rho}||^2 = \text{Tr}\,(\bar{\rho}^+\bar{\rho}) = \text{Tr}\,(\bar{\rho}^2).$$

Using (33a) and (33b) this becomes

$$||\bar{\rho}||^2 = \pi \int d^2z \, \rho_N(z) \, \rho_A(z).$$

However, $\rho_A(z)$ is well defined and given in (28) by the inverse bilateral Laplace transform of $F_A(s, t)$, where s and t are complex. Thus we have

$$||\bar{\rho}||^2 = \frac{\pi}{(2\pi i)^2} \int d^2z \int_{c_1-i\infty}^{c_1+i\infty} ds \int_{c_2-i\infty}^{c_2+i\infty} dt \times F_A(s, t)\, e^{(sx+ty)} \rho_N(z).$$

But it was established above that $c_1 = c_2 = 0$ is in the region of convergence of $\rho_A(z)$. Making a change from $s \to +is$ and $t \to it$, the above becomes

$$||\bar{\rho}||^2 = \frac{\pi}{(2\pi)^2} \int d^2z \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \times F_A(is, it)\, e^{i(sx+ty)} \rho_N(z).$$

After the integration over z and using the fact that

$$F_A(\alpha, \beta) = e^{-\alpha\beta} F_N(\alpha, \beta), \tag{38a}$$

$$||\bar{\rho}||^2 = \frac{1}{4\pi} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \, |F_N(is, it)|^2 \, e^{st}.$$

In a completely similar manner the norm squared of $\bar{\rho}_{(\nu)}$ is

$$||\bar{\rho}_{(\nu)}||^2 = \frac{1}{4\pi} \int_{-\nu}^{\nu} ds \int_{-\nu}^{\nu} dt \, |F_N(is, it)|^2 \, e^{st}. \tag{38b}$$

In order that $\bar{\rho}_{(\nu)}$ converge to $\bar{\rho}$ in the norm it is necessary and sufficient that $||\bar{\rho}_{(\nu)} - \bar{\rho}_{(\nu')}|| \to 0$ as $\nu, \nu' \to \infty$. To show this we note that

$$||\bar{\rho}_{(\nu)} - \bar{\rho}_{(\nu')}||^2 = ||\bar{\rho}_{(\nu)}||^2 + ||\bar{\rho}_{(\nu')}||^2 - 2\,\text{Tr}\,(\bar{\rho}_{(\nu')}\bar{\rho}_{(\nu)}). \tag{38c}$$

From (37a) and (33b) we reduce the trace to the form

$$\text{Tr}\,(\bar{\rho}_{(\nu')}\bar{\rho}_{(\nu)}) = \pi \int d^2z \, \rho_{N(\nu')}(z) \, \rho_{A(\nu)}(z).$$

In the same way we arrived at (38a) we find that

$$\text{Tr}\,(\bar{\rho}_{(\nu')}\bar{\rho}_{(\nu)}) = \frac{1}{4\pi} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \, F_{N(\nu')}(is, it) \times F_{N(\nu)}(is, it)\, e^{st}.$$

Thus,

$$\text{Tr}\,(\bar{\rho}_{(\nu')}\bar{\rho}_{(\nu)}) = ||\bar{\rho}_{(\nu)}||^2 \quad \text{or} \quad ||\bar{\rho}_{(\nu')}||^2$$

depending upon whether ν or ν' is the smaller. Equation (38c) then becomes

$$||\bar{\rho}_{(\nu)} - \bar{\rho}_{(\nu')}||^2 = ||\bar{\rho}_{(\nu)}||^2 - ||\bar{\rho}_{(\nu')}||^2.$$

In the limit as $\nu, \nu' \to \infty$, the right side approaches zero since both terms approach $||\bar{\rho}||^2$. Thus $\bar{\rho}_{(\nu)}$ converges to $\bar{\rho}$ in the norm.

The relation of the sequence of functions $\rho_{N(\nu)}(x, y)$ above to a sequence of distributions is seen from (35). For each function of the sequence there is an associated distribution $\rho_{N(\nu)}$ which maps $e^{-(px+uv)}e^{-i(qx+vy)}$ to $F_{N(\nu)}(p, q, u, v)$. However, we can restrict $\rho_{N(\nu)}$ more than this immediately implies. Let the double, bilateral Laplace transform and double Fourier transform of a distribution T be defined by

$$\mathfrak{L}[T](p + iq, u + iv) = \int T\, e^{-(p+iq)x}\, e^{-(u+iv)y}\, dx\, dy$$

and

$$\mathfrak{F}[T](q, v) = \int T\, e^{-iqx}\, e^{-ivy}\, dx\, dy,$$

respectively. We further define the space L of test functions $f(q, v)$ which are infinitely different-

[14] Without the restriction of pseudo-Hermiticity on $\bar{\rho}$ the class of functions defined by (36a) admits functions of the following type.

$$f_1(x, y) = \begin{cases} e^{x^2+y^2}, & x, y \geq 0; \\ 0, & \text{otherwise}; \end{cases}$$

$$f_2(x, y) = \begin{cases} e^{x^2+y^2}, & x, y \leq 0; \\ 0, & \text{otherwise}; \end{cases}$$

The functions $f_1(x, y)$ and $f_2(x, y)$ are in the class of functions but their sum is not. I am indebted to the referee for pointing out this example.

iable and of rapid decrease, i.e.,

$$\lim_{\substack{|v|\to\infty \\ |q|\to\infty}} \left| q^j v^k \frac{\partial^m f(q, v)}{\partial q^m} \frac{\partial^n f(q, v)}{\partial v^n} \right| = 0$$

for all j, k, m, n. It can be shown[15] that if

$$\lim_{\substack{p\to 0 \\ u\to 0}} \int \mathfrak{L}[\rho_{N(\nu)}](p + iq, u + iv)\, f(q, v)\, dq\, dv = \int \mathfrak{F}[\rho_{N(\nu)}](q, v)\, f(q, v)\, dq\, dv, \qquad (39)$$

i.e., $\mathfrak{L}[\rho_{N(\nu)}]$ converges in the space of functionals defined on L to $\mathfrak{F}[\rho_{N(\nu)}]$ as $p, u \to 0$ in any domain Γ, then $\rho_{N(\nu)}$ is a tempered distribution. The condition of convergence (39) is easily satisfied by the $\rho_{N(\nu)}$ for any $f \in L$ and all operations indicated are well defined.

Thus, we have shown that there exists a sequence of tempered distributions $\rho_{N(\nu)}$ to which is associated a sequence of functions $\rho_{N(\nu)}(x, y)$ whose square is integrable where the corresponding sequence of density matrices $\bar{\rho}_{(\nu)}$ converges to $\bar{\rho}$ in the norm.

IV. CONCLUSIONS

We have used an OFS corresponding to a simple quantum mechanical system, the pseudo oscillator, defined in a linear space with an IM to derive a semiclassical form for describing the statistical state of such a system. The properties of this form, determined in Sec. III, were found to be a generalization of the semiclassical description of the corresponding quantum mechanical system defined in a Hilbert space; i.e., the normal harmonic oscillator. The semiclassical function $\rho_A(z)$ which corresponds to antinormal ordering of operators has the same properties in both cases when Im $\rho_A(z) = 0$. Thus, for antinormal ordering, there is a well-defined generalization from the semiclassical form of the simple oscillator of a Hilbert space to that of the pseudo oscillator of an IM space. On the other hand, for the semiclassical quantity $\rho_N(z)$ corresponding to normal ordering, all we can say is that in both cases there exists a sequence of tempered distributions for which the corresponding sequence of density operators $\rho_{(\nu)}$ converge to ρ in the norm.

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Leading Landau Curves of a Class of Feynman Diagrams*

JAMAL N. ISLAM
Department of Physics and Astronomy, University of Maryland, College Park, Maryland
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In a previous paper it was shown that the leading Landau curves of some Feynman diagrams do not give singularities on the physical sheet if some of the internal and external masses satisfy certain simple inequalities. In the present paper it is shown that a similar property is satisfied by a class of Feynman diagrams. The inequalities involve a fixed number of masses for the whole class.

I. INTRODUCTION

THE singularities corresponding to a given Feynman diagram lie on certain real algebraic curves whose implicit equations were given by Landau,[1] as follows

$$\sum \alpha_i q_i = 0,$$
$$\alpha_i(q_i^2 - m_i^2) = 0,$$

where q_i, α_i, and m_i refer, respectively, to the momentum, the Feynman parameter, and the mass associated with the jth internal line, and the sum is around each of a set of independent loops. The solution in which none of the α_i equals zero is known as the leading curve for the diagram. The solution obtained by setting some of the α_i equal to zero corresponds to the leading curve of the diagram obtained by contracting the appropriate lines. It is believed that as a consequence of unitarity the Landau singularities also appear in the complete amplitude, independent of perturbation theory.[2]

In a previous paper[3] (hereafter referred to as I) we studied the leading Landau curves of some Feynman diagrams. In the present paper we propose to extend this work to a class of diagrams and some other diagrams. We first recall some of the motivation for this work. For various reasons it is important to determine what singularities corresponding to a given diagram lie on the physical sheet as the latter is usually defined. In this connection the leading curves of only a few of the simplest diagrams have been analyzed in detail. These cases include the square,[4] the square with one diagonal,[5] the square with two nonintersecting diagonals,[6-8] and some other diagrams considered in I. In the first three cases, provided the external masses are not too large, the real section of the leading curve has parts singular on the physical sheet (with the attached complex surface nonsingular) and confined to the spectral regions. This implies that the Mandelstam representation is satisfied. The spectral regions for a given diagram are defined as the regions in the plane of the real invariants where the normal threshold cuts (given by the appropriate normal threshold contractions) in any two of the variables overlap. Now it is known[9] that as the external masses are increased, anomalous thresholds appear on the physical sheet for the square diagram before any higher-order diagram. It is pertinent to ask if a similar property holds for leading curves. In this connection, and also as a matter of intrinsic interest, it is important to discover if there exist any diagrams whose leading curves do not yield any parts singular on the physical sheet. In I it was shown that there are indeed some diagrams which yield no singularities on the physical sheet, if some of the external and internal masses satisfy certain simple inequalities, which are satisfied in the equal-mass case. For this it is necessary to assume the absence of singular acnodes.[5,8] In the present paper we study the leading curves of a class of diagrams and show that a similar property holds for the leading curves of this class. There is one difference in that one of the inequalities, which requires the square of a certain internal mass to be greater than the sum of the squares of two other internal masses, is not satisfied

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in the equal-mass case. Nevertheless it is remarkable that there is only one such inequality, and the number of masses involved in the inequalities is fixed, no matter how complicated a member of the class one considers. Also, it is not as if we consider a finite part of the diagrams, in fact, in the proof for the nth member of the class, the Feynman parameters associated with all the internal lines are involved. Further, we deal with completely general masses. It is interesting that something definite can be said about (a certain type of) diagrams of arbitrarily high order with quite general masses. In some special cases, such as the diagram of Fig. 2, the relevant inequalities are satisfied also in the equal-mass case, like the cases considered in I.

To explain the basic ideas, in Sec. 2 we consider two diagrams, the first of which is a member of the class of diagrams considered in Sec. 3. From the Landau equations we derive an equation involving the Feynman parameters and some of the masses, from which it is at once evident that if the masses satisfy certain simple inequalities, the Landau equations possess no solutions with all the Feynman parameters positive. This implies, as was shown in I, that in the assumed absence of singular acnodes the corresponding leading curve is nonsingular on the physical sheet. In Sec. 3 we apply these ideas to a class of diagrams and in Sec. 4 we consider some additional diagrams. In Sec. 5 we note that any diagram which has one of the diagrams under consideration embedded in it also satisfies a similar property. In Sec. 6 we discuss nonsingularity on the physical sheet.

II. TWO EXAMPLES

We first consider the diagram of Fig. 1. The momenta are as shown in the figure. The Feynman parameter and the mass associated with the momenta q, q_i, q_i', q_i'' are, respectively, α and m, α_i and m_i, α_i' and m_i', α_i'' and m_i''. We denote the external masses by m_a, m_b, m_c, and m_d, respectively. The labeling of the lines anticipates that of Sec. 3. The diagram of Fig. 1 has three independent loops, the loop equations for which are

$$\begin{aligned} \alpha_1 q_1 + \alpha_1' q_1' - \alpha_1'' q_1'' - \alpha_2'' q_2'' &= 0, \\ \alpha_2 q_2 + \alpha_2' q_2' - \alpha_2'' q_2'' - \alpha_3'' q_3'' &= 0, \\ \alpha q - \alpha_0 q_0 + \alpha_2 q_2 - \alpha_1 q_1 + \alpha_1'' q_1'' - \alpha_0' q_0' &= 0. \end{aligned} \tag{1}$$

We note that the diagram has vertices at which only three lines meet and that the arrows, which denote the direction of internal momenta, are drawn so that they are either coming into the vertex or

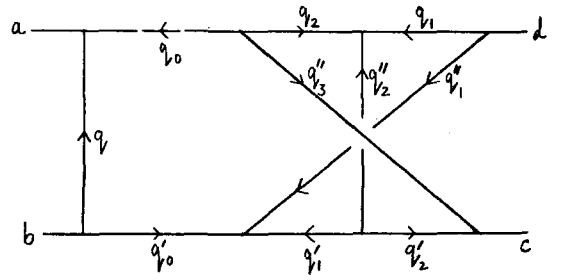

FIG. 1. One of the Feynman diagrams under consideration.

going away from it. This implies that the conservation law at the vertices is given by the vanishing of the sum of the three relevant momenta. From one of the vertices we get the conservation equation

$$q_0' + q_1' + q_1'' = 0, \tag{2}$$

Multiplying it by q_1, we get

$$q_1 q_0' + q_1 q_1' + q_1 q_1'' = 0. \tag{3}$$

We note that if k_i and k_j are any two internal momenta meeting at a vertex, then the scalar product $k_i k_j$ is a constant determined by the three relevant masses. For example, it is easily seen from the conservation equation (2) that

$$q_1' q_1'' = \tfrac{1}{2}(m_0'^2 - m_1'^2 - m_1''^2). \tag{4}$$

Thus in Eq. (3) $q_1 q_1''$ is a constant. Our aim in this section is to determine $q_1 q_0'$ and $q_1 q_1'$ in terms of the α's and the masses, and to substitute in Eq. (3) to get a certain relation involving only the α's and the masses. $q_1 q_1'$ can be obtained at once from the first of Eq. (1) by multiplying it by q_1'. We get

$$q_1 q_1' = (1/\alpha_1)(\alpha_1'' q_1' q_1'' + \alpha_2'' q_1' q_2'' - \alpha_1' m_1'^2). \tag{5}$$

The scalar products $q_1' q_1''$ and $q_1' q_2''$ depend only on the masses. We obtain $q_1 q_0'$ as follows. Apart from Eq. (2) there are three conservation equations involving only the internal momenta coming from three other internal vertices. We multiply these by q_0' to obtain

$$\begin{aligned} q q_0' + q_2 q_0' + q_3'' q_0' &= 0, \\ q_1 q_0' + q_2 q_0' + q_2'' q_0' &= 0, \\ q_1' q_0' + q_2' q_0' + q_2'' q_0' &= 0. \end{aligned} \tag{6}$$

Further, we obtain three other equations by multiplying the Eqs. (1), respectively, by q_0'. Together with Eq. (6), this gives six equations for the six unknowns $q q_0'$, $q_1 q_0'$, $q_2 q_0'$, $q_2' q_0'$, $q_2'' q_0'$, and $q_3'' q_0'$. We solve for $q_1 q_0'$ and substitute in Eq. (3) for $q_1 q_0'$ and

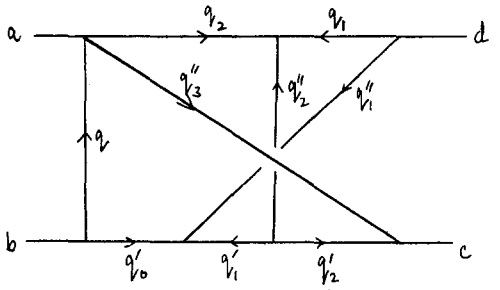

FIG. 2. A diagram obtained from that of Fig. 1 by contracting one of its lines.

q_1q_1' to obtain, after some manipulation, the equation

$$A(\alpha_1 q_1 q_1'' + \alpha_1'' q_1' q_1'' + \alpha_2'' q_1' q_2'' - \alpha_1' m_1'^2) - \alpha_1 B q_1' q_0' + \alpha C q_1'' q_0' + \alpha\alpha_1\alpha_2''\alpha_3'' q q_0' - \alpha_0'\alpha_1\alpha_2''\alpha_3'' m_0'^2 = 0, \quad (7)$$

where

$$A = \alpha_0[\alpha_1(\alpha_2 + \alpha_2' + \alpha_2'' + \alpha_3'') + \alpha_2''(\alpha_2 + \alpha_3'')] + \alpha_2\alpha_3''(\alpha_1 + \alpha_2'') + \alpha_1\alpha_2''\alpha_3'',$$

$$B = \alpha_0\alpha_1'(\alpha_2 + \alpha_2' + \alpha_2'' + \alpha_3'') + \alpha_1'\alpha_2\alpha_3'' + \alpha_0\alpha_2'\alpha_2'',$$

$$C = \alpha_0\alpha_1''(\alpha_2 + \alpha_2' + \alpha_2'' + \alpha_3'') + \alpha_1''\alpha_2\alpha_3'' + \alpha\alpha_2''\alpha_3''.$$

We note that the expressions A, B, and C are positive when the α's are. From Eq. (7) it is then clear that there can be no solution with all positive Feynman parameters if

$$q_1'q_0' > 0;\ q_1q_1'',\ q_1'q_1'',\ q_1''q_0',\ q_1'q_2'',\ qq_0' < 0, \quad (8)$$

i.e., if

$$m_1''^2 > m_1'^2 + m_0'^2,\quad m_d^2 < m_1^2 + m_1''^2,\quad m_2'^2 < m_1'^2 + m_2''^2,\quad m_b^2 < m_0'^2 + m^2. \quad (9)$$

We note that $q_1'q_1''$ and $q_1''q_0'$ automatically satisfy (8) when $q_1'q_0'$ satisfies it. The first inequality in (9) is not satisfied in the equal-mass case, but all the others are.

We now consider the diagram (Fig. 2) obtained from that of Fig. 1 by contracting the line associated with the momentum q_0. Following similar steps as before, we derive the relation corresponding to Eq. (7). This relation is obtained by setting $\alpha_0 = 0$ in Eq. (7). We then combine the $q_1'q_0'$ and $m_1'^2$ terms using the relation

$$q_1'q_1'' = -(q_1'q_0' + m_1'^2) \quad (10)$$

which is obtained by multiplying Eq. (2) by q_1'. We then get the relation

$$(\alpha_1\alpha_2 + \alpha_1\alpha_2'' + \alpha_2\alpha_2'')(\alpha_1 q_1 q_1'' + \alpha_2'' q_1' q_2'') + \{\alpha_1''(\alpha_1\alpha_2 + \alpha_1\alpha_2'' + \alpha_2\alpha_2'') + \alpha_1\alpha_1'\alpha_2\} q_1'q_1'' - (\alpha_1\alpha_2'' + \alpha_2\alpha_2'')\alpha_1' m_1'^2 + \alpha_1(\alpha_1''\alpha_2 + \alpha_1''\alpha_2'')q_1''q_0' + \alpha\alpha_1\alpha_2'' q q_0' - \alpha_0'\alpha_1\alpha_2'' m_0'^2 = 0. \quad (11)$$

From Eq. (11) it is clear that there is no solution corresponding to positive Feynman parameters if

$$q_1q_1'',\ q_1'q_2'',\ q_1'q_1'',\ q_1''q_0',\ qq_0' < 0,$$

i.e., if

$$m_d^2 < m_1^2 + m_1''^2,\quad m_2'^2 < m_1'^2 + m_2''^2,\quad m_0'^2 < m_1'^2 + m_1''^2,\quad m_1'^2 < m_0'^2 + m_1''^2,\quad m_b^2 < m^2 + m_0'^2. \quad (12)$$

We note that all the inequalities (12) are satisfied trivially in the equal-mass case. Further, the two sets of inequalities (9) and (12) involve only two of the external masses and not all the internal masses, so that if these inequalities are satisfied, the Landau equations possess no solution with positive α's independent of all the other external and internal masses. Equations containing the other masses can be obtained by considering a relation such as Eq. (3) at some different vertex.

III. A CLASS OF DIAGRAMS

In this section we consider a class of diagrams, the nth member of which is shown in Fig. 3. It is obtained by taking a ladder diagram with $(n + 1)$ straight rungs, twisting round one side of the ladder, and joining two of its ends to the two ends (the lines associated with the momenta q_0 and q_0') of a one-particle exchange diagram. In Fig. 3 the arrows are drawn assuming n to be even. To avoid considering a lot of $(-1)^n$ factors, we deal only with the cases where n is even. The other cases can be dealt with

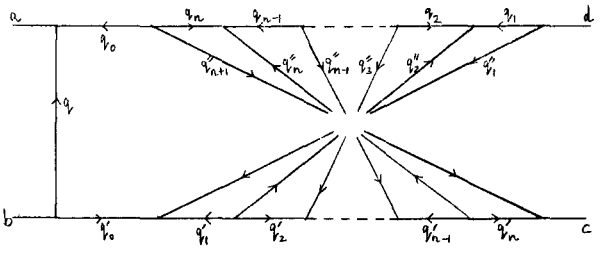

FIG. 3. A member of a class of diagrams considered in Sec. 3. The arrows are drawn assuming n to be even.

analogously. We note that in Fig. 3, too, the arrows are drawn so that they are all going away from a vertex, or coming into one. It is possible to draw the arrows this way when n is even. In the case where n is odd, the arrows can be drawn so that only at the vertex b are they not all going into or coming out of the vertex.

The momenta are as shown in Fig. 3. We denote the Feynman parameter and the mass associated with each momentum as in Sec. 2. Thus for example α_j' and m_j' are the Feynman parameter and the mass associated with the momentum q_j'. The diagram of Fig. 3 has $n+1$ independent loops, the loop equations for which are (throughout the following we assume n to be even)

$$\begin{aligned}
&\alpha_1 q_1 + \alpha_1' q_1' - \alpha_1'' q_1'' - \alpha_2'' q_2'' = 0,\\
&\alpha_2 q_2 + \alpha_2' q_2' - \alpha_2'' q_2'' - \alpha_3'' q_3'' = 0,\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&\alpha_n q_n + \alpha_n' q_n' - \alpha_n'' q_n'' - \alpha_{n+1}'' q_{n+1}'' = 0,\\
&\alpha q - \alpha_0 q_0 + \alpha_n q_n - \alpha_{n-1} q_{n-1} + \cdots\\
&\qquad + \alpha_2 q_2 - \alpha_1 q_1 + \alpha_1'' q_1'' - \alpha_0' q_0' = 0.
\end{aligned} \tag{13}$$

Exactly as in Sec. 2 we derive the Eqs. (2), (3), and (5), The difference in this case is in the solution of $q_1 q_0'$. To solve for $q_1 q_0'$, we proceed as follows. Apart from Eq. (2) there are the following $2n-1$ conservation equations at vertices.

$$\begin{aligned}
&q_0 + q_n + q_{n+1}'' = 0,\\
&q_{r-1} + q_r + q_r'' = 0, \qquad 2 \le r \le n;\\
&q_{r-1}' + q_r' + q_r'' = 0, \qquad 2 \le r \le n.
\end{aligned} \tag{14}$$

Solving for $q_2'', \cdots, q_{n+1}''$ and $q_2', \cdots, q_n'$, we get

$$\begin{aligned}
&q_{n+1}'' = -(q_0 + q_n),\\
&q_r'' = -(q_{r-1} + q_r), \qquad 2 \le r \le n;\\
&q_r' = (-1)^r (q_1 - q_1') + q_r, \qquad 2 \le r \le n.
\end{aligned} \tag{15}$$

We now multiply Eqs. (13) and (15) by q_0' to get $3n$ equations involving the $3n$ unknowns $q_0 q_0'$, $q_1 q_0'$, $\cdots, q_n q_0'$; $q_2' q_0', \cdots, q_n' q_0'$; $q_2'' q_0', \cdots, q_{n+1}'' q_0'$. We can eliminate $q_2' q_0', \cdots q_n' q_0'$; $q_2'' q_0', \cdots, q_{n+1}'' q_0'$ using Eqs. (15). We are then left with $n+1$ equations in the $n+1$ unknowns $q_0 q_0', \cdots, q_n q_0'$. These are the following:

$$\begin{aligned}
&(\alpha_1 + \alpha_2'') q_1 q_0' + \alpha_2'' q_2 q_0' = -\alpha_1' q_1' q_0' + \alpha_1'' q_1'' q_0',\\
&(\alpha_2' + \alpha_2'') q_1 q_0' + N_2 q_2 q_0' + \alpha_3'' q_3 q_0' = \alpha_2' q_1' q_0,\\
&-\alpha_3' q_1 q_0' + \alpha_3'' q_2 q_0' + N_3 q_3 q_0' + \alpha_4'' q_4 q_0' = -\alpha_3' q_1' q_0,\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&(-1)^r \alpha_r' q_1 q_0' + \alpha_r'' q_{r-1} q_0' + N_r q_r q_0'\\
&\qquad + \alpha_{r+1}'' q_{r+1} q_0' = (-1)^r \alpha_r' q_1' q_0',\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&\alpha_n' q_1 q_0' + \alpha_n'' q_{n-1} q_0' + N_n q_n q_0' + \alpha_{n+1}'' q_0 q_0' = \alpha_n' q_1' q_0',\\
&-\alpha_1 q_1 q_0' + \alpha_2 q_2 q_0' - \cdots - \alpha_{n-1} q_{n-1} q_0' + \alpha_n q_n q_0'\\
&\qquad - \alpha_0 q_0 q_0' = -\alpha_1'' q_1'' q_0' - \alpha q q_0' + \alpha_0' m_0'^2,
\end{aligned} \tag{16}$$

where $N_r = \alpha_r + \alpha_r' + \alpha_r'' + \alpha_{r+1}''$. We note that the scalar products appearing on the right-hand side of Eq. (16) are all constants determined by the masses. From Eq. (16) we get

$$q_1 q_0' = B_n / A_n \tag{17}$$

where

$$A_n = -\begin{vmatrix}
\alpha_1 + \alpha_2'' & \alpha_2'' & 0 & \cdots & \cdots & 0\\
\alpha_2' + \alpha_2'' & N_2 & \alpha_3'' & \ddots & & \vdots\\
-\alpha_3' & \alpha_3'' & N_3 & \alpha_4'' & \ddots & \vdots\\
\alpha_4' & 0 & \alpha_4'' & N_4 & \ddots & \vdots\\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots\\
\vdots & \vdots & & \ddots & \alpha_n'' & 0\\
\alpha_n' & 0 & \cdots & 0 & \alpha_n'' & N_n & \alpha_{n+1}''\\
-\alpha_1 & \alpha_2 & -\alpha_3 & \cdots & -\alpha_{n-1} & \alpha_n & -\alpha_0
\end{vmatrix} \tag{18}$$

and

$$B_n = -\begin{vmatrix} \alpha_2'' & 0 & \cdots & 0 & -\alpha_1' q_1' q_0' + \alpha_1'' q_1'' q_0' \\ N_2 & \alpha_3'' & & & \alpha_2' q_1' q_0' \\ \alpha_3'' & N_3 & \alpha_4'' & & -\alpha_3' q_1' q_0' \\ 0 & \alpha_4'' & N_4 & & \alpha_4' q_1' q_0' \\ \vdots & & \ddots & \alpha_n'' & \vdots \\ 0 & \cdots & 0 & \alpha_n'' \quad N_n \quad \alpha_{n+1}'' & \alpha_n' q_1' q_0' \\ \alpha_2 & -\alpha_3 & \alpha_4 \quad \cdots \quad -\alpha_{n-1} & \alpha_n & -\alpha_0 \quad -\alpha_1'' q_1'' q_0' - \alpha q q_0' + \alpha_0' m_0'^2 \end{vmatrix}$$

$$= -C_n q_1' q_0' + D_n q_1'' q_0' + E_n(\alpha q q_0' - \alpha_0' m_0'^2). \qquad (19)$$

We have a minus sign in front of the determinants for convenience. Substituting in Eq. (3) for $q_1 q_1'$ from Eq. (5), and for $q_1 q_0'$ from Eq. (17) and Eq. (19), we get

$$A_n(\alpha_1 q_1 q_1'' + \alpha_1'' q_1' q_1'' + \alpha_2'' q_1' q_2'' - \alpha_1' m_1'^2) - \alpha_1 C_n q_1' q_0' + \alpha_1 D_n q_1'' q_0' + \alpha_1 \alpha E_n q q_0' - \alpha_0' \alpha_1 E_n m_0'^2 = 0. \qquad (20)$$

It is shown in the Appendix that the expressions A_n, C_n, D_n, and E_n are positive when the α's are. It then follows at once from Eq. (20) that there is no solution with positive α's if

$$q_1' q_0' > 0;\ q_1 q_1'',\ q_1' q_1'',\ q_1'' q_0',\ q_1' q_2'',\ q q_1' < 0.$$

These are exactly the same inequalities as (8) and (9). One gets the same inequalities in the case where n is odd. Thus we have the remarkable result that if the inequalities (9) are satisfied, the diagram in Fig. 3 for all n have leading curves which are non-singular on the physical sheet, provided we assume the absence of singular acnodes (see Sec. 6). Equations similar to Eq. (20) containing the other masses can be obtained by considering an equation such as Eq. (3) at some different vertex.

IV. SOME OTHER DIAGRAMS

We now consider the diagram of Fig. 4. It is obtained by twisting the "square" diagram and the "double square" diagram and joining the two ends of one to the two ends of the other (the lines 5 and 6). We label the lines as in Fig. 4 and denote the momentum, the Feynman parameter, and the mass of the jth line by q_j, α_j, and m_j, respectively. The diagram of Fig. 4 has four independent loops, the loop equations for which can be taken as

$$\begin{aligned} \alpha_1 q_1 - \alpha_2 q_2 - \alpha_3 q_3 + \alpha_4 q_4 &= 0, \\ \alpha_7 q_7 - \alpha_8 q_8 - \alpha_{11} q_{11} + \alpha_{13} q_{13} &= 0, \\ \alpha_9 q_9 - \alpha_{10} q_{10} - \alpha_{11} q_{11} + \alpha_{12} q_{12} &= 0, \\ \alpha_3 q_3 - \alpha_4 q_4 + \alpha_5 q_5 - \alpha_6 q_6 + \alpha_7 q_7 & \\ - \alpha_{10} q_{10} - \alpha_{11} q_{11} &= 0. \end{aligned} \qquad (21)$$

From the (5, 9, 10) vertex we get a conservation equation which we multiply by q_{12} to obtain

$$q_5 q_{12} + q_9 q_{12} + q_{10} q_{12} = 0. \qquad (22)$$

We note that $q_9 q_{12}$ is a constant. We evaluate $q_{10} q_{12}$ and $q_8 q_{12}$ by methods similar to those of the previous sections. That is, we multiply the first of Eq. (21) by q_{10} to obtain $q_{10} q_{12}$, and multiply the Eqs. (21) and the rest of the conservation equations by q_5 to solve for $q_5 q_{12}$. We then substitute in Eq. (22) for $q_5 q_{12}$ and $q_{10} q_{12}$ to obtain, after some reduction, the equation

$$A'(-\alpha_9 q_9 q_{10} + \alpha_{12} q_9 q_{12} + \alpha_{11} q_{10} q_{11} + \alpha_{10} m_{10}^2) + \alpha_{12} B' q_5 q_{10} - \alpha_1 \alpha_4 \alpha_8 \alpha_{11} \alpha_{12} q_4 q_5 - \alpha_2 \alpha_3 \alpha_8 \alpha_{11} \alpha_{12} q_2 q_5 - \alpha_{12} C' q_5 q_9 + \alpha_3 \alpha_5 \alpha_8 \alpha_{11} \alpha_{12} m_5^2 = 0, \qquad (23)$$

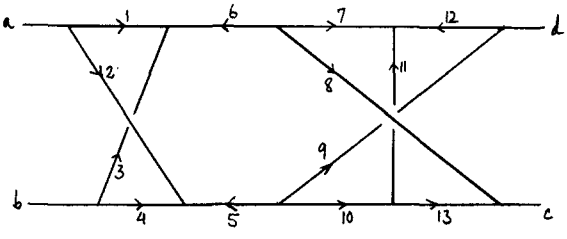

FIG. 4. Another of the Feynman diagrams under consideration.

where

$$A' = (\alpha_1\alpha_2 + \alpha_1\alpha_6 + \alpha_3\alpha_6)[\alpha_{11}(\alpha_7 + \alpha_8) + \alpha_{12}(\alpha_7 + \alpha_8 + \alpha_{11} + \alpha_{13})] + \alpha_8(\alpha_1 + \alpha_3)(\alpha_7\alpha_{11} + \alpha_7\alpha_{12} + \alpha_{11}\alpha_{12}),$$

$$B' = (\alpha_1\alpha_2 + \alpha_1\alpha_6 + \alpha_3\alpha_6)[\alpha_{10}(\alpha_7 + \alpha_8 + \alpha_{11} + \alpha_{13}) + \alpha_{11}\alpha_{13}] + \alpha_7\alpha_8\alpha_{10}(\alpha_1 + \alpha_3),$$

and

$$C' = \alpha_8\alpha_9(\alpha_1 + \alpha_3)(\alpha_7 + \alpha_{11}) + (\alpha_1\alpha_3 + \alpha_1\alpha_6 + \alpha_3\alpha_6)(\alpha_7 + \alpha_8 + \alpha_{11} + \alpha_{12}).$$

We note that the expressions A', B', and C' are positive when the α's are. It then follows that there is no solution corresponding to positive α's if

$$q_5q_{10},\ q_9q_{12},\ q_{10}q_{11} > 0;\ q_4q_5,\ q_2q_5,\ q_5q_9 < 0. \tag{24}$$

We note that at the vertices (10, 11, 13) and (9, 12, d) the momenta are not all going in or all coming out. This implies that q_9q_{12} is given by

$$q_9q_{12} = -\tfrac{1}{2}(m_d^2 - m_9^2 - m_{12}^2), \tag{25}$$

with a change of sign from Eq. (4), $q_{10}q_{11}$ also has this change of sign. The inequalities (24) then imply the following [noting that q_5q_9 automatically satisfies (24) when q_5q_{10} satisfies it]:

$$m_9^2 > m_5^2 + m_{10}^2,\quad m_d^2 < m_9^2 + m_{12}^2,$$
$$m_{13}^2 < m_{10}^2 + m_{11}^2,\quad m_2^2 < m_4^2 + m_5^2, \tag{26}$$
$$m_4^2 < m_2^2 + m_5^2.$$

All the inequalities in (26) except the first one are satisfied in the equal-mass case.

We now consider an equation such as Eq. (22) at the vertex (2, 4, 5), namely, the equation

$$q_1q_2 + q_1q_4 + q_1q_5 = 0. \tag{27}$$

We evaluate q_1q_4 and q_1q_5 using similar methods as before and substitute in (27) to obtain the equation

$$A'(\alpha_1q_1q_2 + \alpha_2q_2q_4 + \alpha_3q_3q_4) + \alpha_1\alpha_4B''q_2q_4 + \alpha_1\alpha_2C''q_2q_5 + \alpha_1\alpha_3\,Dq_5q_{10} - \alpha_1\alpha_3\alpha_9(\alpha_7\alpha_{13} - \alpha_8\alpha_{11})q_5q_9 - \alpha_4Em_4^2 - \alpha_1\alpha_3\alpha_5\{\alpha_{12}(\alpha_{11} + \alpha_{13}) + (\alpha_7 + \alpha_8)(\alpha_{11} + \alpha_{12})\}m_5^2 = 0, \tag{28}$$

where A' is given as above and

$$B'' = (\alpha_6\alpha_7 + \alpha_6\alpha_8 + \alpha_7\alpha_8)(\alpha_{11} + \alpha_{12}) + \alpha_6\alpha_{12}(\alpha_{11} + \alpha_{13}) + \alpha_8\alpha_{11}\alpha_{12},$$

$$C'' = B'' + \alpha_3\alpha_{12}(\alpha_{11} + \alpha_{13}) + \alpha_3(\alpha_7 + \alpha_8)(\alpha_{11} + \alpha_{12}),$$

$$D = \alpha_7\alpha_{10}\alpha_{11} + \alpha_{13}(\alpha_7\alpha_{10} + \alpha_7\alpha_{11} + \alpha_7\alpha_{12} + \alpha_{11}\alpha_{12}) + \alpha_{10}\alpha_{12}(\alpha_7 + \alpha_8 + \alpha_{11} + \alpha_{13}),$$

$$E = \alpha_3(\alpha_6\alpha_7 + \alpha_6\alpha_8 + \alpha_7\alpha_8)(\alpha_{11} + \alpha_{12}) + \alpha_3\alpha_6\alpha_{12}(\alpha_{11} + \alpha_{12}) + \alpha_8\alpha_{11}\alpha_{12}\alpha_{13}.$$

Since the coefficient of q_5q_9 in Eq. (28) can be either positive or negative, nothing can be said about the solution for positive α's. However, if $q_5q_9 = 0$, i.e., if

$$m_{10}^2 = m_5^2 + m_9^2, \tag{29}$$

then there is no solution for positive α if

$$q_1q_2,\ q_3q_4,\ q_2q_4,\ q_2q_5,\ q_5q_{10} < 0,$$

i.e., if

$$m_a^2 < m_1^2 + m_2^2,\quad m_b^2 < m_3^2 + m_4^2,$$
$$m_5^2 < m_2^2 + m_4^2,\quad m_4^2 < m_2^2 + m_5^2, \tag{30}$$
$$m_9^2 < m_5^2 + m_{10}^2.$$

We note that the last inequality in (30) follows from Eq. (29).

In Eq. (28) if α_{13} is put equal to zero, then the coefficient of q_5q_9 becomes an expression which is positive when the α's are, like the coefficients of the other scalar products in (28). This leads us to consider the diagram of Fig. 5, which is obtained from that of Fig. 4 by contracting the line 13. The equation corresponding to Eq. (28) for this diagram is obtained by setting α_{13} equal to zero in Eq. (28). From the resulting equation it follows that there is no solution with positive α's for the diagram of Fig. 5 if

$$q_1q_2,\ q_3q_4,\ q_2q_4,\ q_2q_5,\ q_5q_9,\ q_5q_{10} < 0,$$

i.e.,

$$m_a^2 < m_1^2 + m_2^2,\quad m_b^2 < m_3^2 + m_4^2,$$
$$m_5^2 < m_2^2 + m_4^2,\quad m_4^2 < m_2^2 + m_5^2, \tag{31}$$
$$m_9^2 < m_5^2 + m_{10}^2,\quad m_{10}^2 < m_5^2 + m_9^2.$$

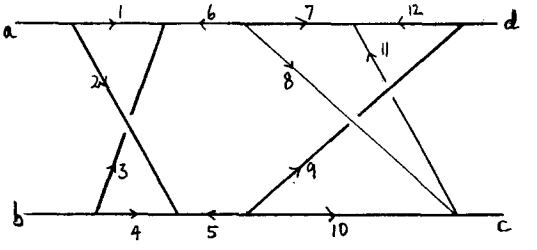

FIG. 5. A diagram obtained from that of Fig. 4 by contracting one of its lines.

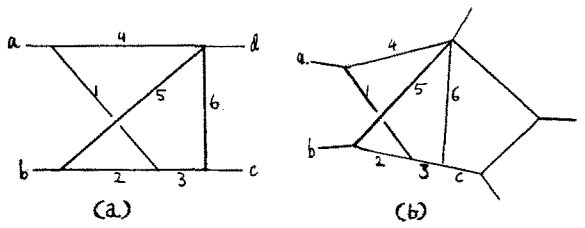

FIG. 6. An example of embedding. The leading curves of both diagrams (a) and (b) have no parts associated with positive Feynman parameters when the masses satisfy (32).

All the inequalities in (31) are satisfied in the equal-mass case. However, since the diagram of Fig. 5 contains a triangle diagram with two of the vertices of the triangle containing three lines each (the triangle with lines 7, 8, and 11), it is possible to get another condition for no solution with positive α's quite trivially. We obtain this condition by multiplying the loop equation for the loop (7, 8, 11) by q_7 to obtain

$$\alpha_7 m_7^2 - \alpha_8 q_7 q_8 - \alpha_{11} q_7 q_{11} = 0.$$

There is thus no solution with positive α's if

$$q_7 q_8,\ q_7 q_{11} < 0,$$

i.e., if

$$m_6^2 < m_7^2 + m_8^2, \quad m_{12}^2 < m_7^2 + m_{11}^2.$$

However, it is interesting that for this diagram there also exists the condition (31) involving the other masses.

It is clear that analyses similar to those of this section can be carried out for the following class of diagrams. Consider a ladder diagram with m straight rungs and another with n straight rungs. Now twist one side of each of these around and join the two ends of one to the two ends of the other, exactly in the manner that the diagram of Fig. 4 is obtained by joining a square diagram and a double square diagram. The class of diagrams considered in Sec. 3 is a subclass of this class. It is our belief that conditions similar to those in Eq. (26) can be obtained for no solutions with positive α's, for this larger class. However, we have not attempted to prove this.

V. EMBEDDING A DIAGRAM

Consider any of the diagrams studied in this paper or in I, some of whose masses satisfy inequalities which imply that there is no solution for the leading curve with positive α's. If such a diagram is embedded in a higher-order scattering or production diagram, then the leading curve of this higher-order diagram also possesses no solutions with positive α's. As was mentioned in I, this follows from the fact that the Feynman parameters of the original diagram satisfy an equation such as Eq. (7) independent of the rest of the diagram, so that if its masses satisfy the relevant inequalities, there will be no solution with the Feynman parameters of the subdiagram positive and hence none with all the Feynman parameters positive. An example of embedding is shown in Fig. 6. It can be easily shown, using the above methods, that the diagram of Fig. 6(a) (this diagram was considered in I) possesses no solution for the leading curve with positive α's if

$$\begin{gathered} m_a^2 < m_1^2 + m_4^2, \quad m_b^2 < m_2^2 + m_5^2, \\ m_c^2 < m_3^2 + m_6^2, \quad m_3^2 < m_1^2 + m_2^2, \\ m_2^2 < m_1^2 + m_3^2. \end{gathered} \tag{32}$$

It then follows by the above argument that the leading curve of Fig. 6(b) also possesses no solutions with positive α's if (32) is satisfied. We note that the vertex d of Fig. 6(a) can be connected to any number of other lines in the higher-order diagram.

VI. NONSINGULARITY ON THE PHYSICAL SHEET

In I we considered in detail to what extent the leading Landau curve possessing no parts corresponding to positive Feynman parameters implies nonsingularity of those parts on the physical sheet. It was shown that for scattering diagrams, i.e., for diagrams involving four external lines, to get nonsingularity on the physical sheet it is sufficient to assume the absence of singular acnodes.[5,8] We believe that for production diagrams, such as that of Fig. 6(b), the condition for no solution with positive α's also in some sense implies nonsingularity on some suitably defined physical sheet; but this is not clear.

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I am very grateful to Prof. J. S. Toll and other members of the physics department for their hospitality at the University of Maryland.

APPENDIX

In this Appendix we prove that the expressions A_n, C_n, D_n, and E_n of Sec. 3 are positive when the α's are.

Consider the determinant A_n. Expanding in terms of the last row, we have, after a slight simplification,

$$A_n = \sum_{r=1}^{n} \alpha_r A'_{r-1} \alpha''_{r+1} \cdots \alpha''_{n+1} + \alpha_0 A'_n, \tag{A1}$$

where

$$A_0' = 1, \quad A_1' = \alpha_1 + \alpha_2'',$$
$$A_2' = \begin{vmatrix} \alpha_1 + \alpha_2'' & \alpha_2'' \\ \alpha_2' + \alpha_2'' & N_2 \end{vmatrix},$$

and

$$A_r' = \begin{vmatrix} \alpha_1 + \alpha_2'' & \alpha_2'' & 0 & \cdots & \cdots & 0 \\ \alpha_2' + \alpha_2'' & N_2 & \alpha_3'' & \ddots & & \vdots \\ -\alpha_3' & \alpha_3'' & N_3 & \alpha_4'' & \ddots & \vdots \\ \alpha_4' & 0 & \alpha_4'' & N_4 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & \vdots & & \ddots & \ddots & \alpha_r'' \\ (-1)^r\alpha_r' & 0 & \cdots & 0 & \alpha_r'' & N_r \end{vmatrix}.$$

We now prove that determinants A_r' are positive when the α's are, for all r. To prove this we first expand A_r' in terms of the last row to get the following recurrence relation

$$A_r' = N_r A_{r-1}' - \alpha_r''^2 A_{r-2}' - \alpha_r'\alpha_2''\alpha_3'' \cdots \alpha_r''. \quad \text{(A2)}$$

We now use a process of induction. For this we assume that the expression A_{r-1}' is positive when the α's are, and that this expression has in it a term of the form $\alpha_r'' A_{r-2}'$ (which is also positive when the α's are). We further assume that the term $\alpha_r'' A_{r-2}'$ has in it a product of the form $\alpha_2''\alpha_3'' \cdots \alpha_r''$. We now show that these assumptions about A_{r-1}' imply similar properties of A_r', i.e., that A_r' is positive when the α's are, and that A_r' has in it a term of the form $\alpha_{r+1}'' A_{r-1}'$, which in turn has in it a product of the form $\alpha_2''\alpha_3'' \cdots \alpha_{r+1}''$. It is clear that the assumptions about A_{r-1}' imply that it can be written as

$$A_{r-1}' = \alpha_r'' A_{r-2}' + K_1 = \alpha_2''\alpha_3'' \cdots \alpha_r'' + K_2,$$

where K_1 and K_2 are positive when the α's are. Remembering the definition of N_r, we see that (A2) can be written as

$$\begin{aligned} A_r' &= (\alpha_r + \alpha_{r+1}'')A_{r-1}' + \alpha_r'(\alpha_2''\alpha_3'' \cdots \alpha_r'' + K_2) \\ &\quad + \alpha_r''(\alpha_r'' A_{r-2}' + K_1) \\ &\quad - \alpha_r''^2 A_{r-2}' - \alpha_r'\alpha_2''\alpha_3'' \cdots \alpha_r'' \\ &= (\alpha_r + \alpha_{r+1}'')A_{r-1}' + \alpha_r' K_2 + \alpha_r'' K_1. \quad \text{(A3)} \end{aligned}$$

Thus A_r' is positive when the α's are. Further, it is clear from the last form that A_r' has in it a term of the form $\alpha_{r+1}'' A_{r-1}$ which in turn has in it a product of the form $\alpha_2''\alpha_3'' \cdots \alpha_{r+1}''$ (since A_{r-1}' has the product $\alpha_2''\alpha_3'' \cdots \alpha_r''$ through the term $\alpha_r'' A_{r-2}'$). It is easy to verify that for the first few values of r, A_r' does indeed possess the properties assumed for the purpose of the induction. This completes the induction and proves that A_r' is positive when the α's are, for all values of r. It is then clear from (A1) that A_n is also positive when the α's are.

We now prove that the expressions C_n, D_n, and E_n are positive when the α's are. It can be seen easily that

$$E_n = \alpha_2''\alpha_3'' \cdots \alpha_{n+1}''. \quad \text{(A4)}$$

To get C_n and D_n, we expand the determinant B_n in terms of its last column. We then get

$$B_n = \sum_{r=1}^{n+1} I_r, \quad \text{(A5)}$$

where

$$I_r = \alpha_r'\alpha_2''\alpha_3'' \cdots \alpha_r'' I_r' q_1' q_0', \qquad 2 \le r \le n-1,$$
$$I_1 = (\alpha_1' q_1' q_0' - \alpha_1'' q_1'' q_0') I_1',$$
$$I_n = -\alpha_0\alpha_n'\alpha_2''\alpha_3'' \cdots \alpha_n'' q_1' q_0',$$
$$I_{n+1} = (\alpha q q_0' + \alpha_1'' q_1'' q_0' - \alpha_0' m_0'^2)\alpha_2''\alpha_3'' \cdots \alpha_{n+1}'',$$

and

$$I_r' = \begin{vmatrix} N_{r+1} & \alpha_{r+2}'' & 0 & \cdots & \cdots & 0 \\ \alpha_{r+2}'' & N_{r+2} & \alpha_{r+3}'' & \ddots & & \vdots \\ 0 & \alpha_{r+3}'' & N_{r+3} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \alpha_n'' & 0 \\ 0 & \cdots & 0 & \alpha_n'' & N_n & \alpha_{n+1}'' \\ (-1)^{r+1}\alpha_{r+1} & (-1)^{r+2}\alpha_{r+2} & \cdots & & -\alpha_{n+1} & \alpha_n & -\alpha_0 \end{vmatrix}.$$

Expanding in terms of the last row, we see after some simplification, that I_r' can be written as follows:

$$I_r' = -\alpha_0\Delta_{r+1,n} - \sum_{m=1}^{n-r} \alpha_{r+m}\alpha_{r+m+1}''\alpha_{r+m+2}'' \cdots \alpha_{n+1}''\Delta_{r+1,r+m-1}, \quad \text{(A6)}$$

where

$$\Delta_{r+1,r} = 1, \qquad \Delta_{r+1,r+1} = N_{r+1},$$

and

$$\Delta_{r,s} = \begin{vmatrix} N_r & \alpha_{r+1}'' & 0 & \cdots & \cdots & 0 \\ \alpha_{r+1}'' & N_{r+1} & \alpha_{r+2}'' & \ddots & & \vdots \\ 0 & \alpha_{r+2}'' & N_{r+2} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \alpha_s'' \\ 0 & \cdots & \cdots & 0 & \alpha_s'' & N_s \end{vmatrix}.$$

We now show that $\Delta_{r,s}$ is positive when the α's are. We first expand $\Delta_{r,s}$ in terms of the last row or column to get the following recurrence relation:

$$\Delta_{r,s} = N_s\Delta_{r,s-1} - \alpha_s''^2\Delta_{r,s-2}. \quad \text{(A7)}$$

As before we apply a process of induction. For this we assume that $\Delta_{r,s-1}$ is positive when the α's are and has in it an expression of the form $\alpha_s''\Delta_{r,s-2}$, which is also positive when the α's are. Thus we can write

$$\Delta_{r,s-1} = \alpha_s''\Delta_{r,s-2} + K,$$

where K is positive when the α's are. Substituting in Eq. (A7) for $\Delta_{r,s-1}$ and remembering the form of N_s, we have

$$\begin{aligned}\Delta_{r,s} &= (\alpha_s + \alpha_s' + \alpha_{s+1}'')\Delta_{r,s-1} \\ &\quad + \alpha_s''(\alpha_s''\Delta_{r,s-2} + K) - \alpha_s''^2\Delta_{r,s-2} \\ &= (\alpha_s + \alpha_s' + \alpha_{s+1}'')\Delta_{r,s-1} + \alpha_s''K. \end{aligned} \quad \text{(A8)}$$

Thus $\Delta_{r,s}$ is also positive when the α's are and has in it an expression of the form $\alpha_{s+1}''\Delta_{r,s-1}$. It is easy to verify that the properties assumed for $\Delta_{r,s-1}$ holds for the first few values of $s > r + 1$. This completes our induction and proves that $\Delta_{r,s}$ is positive when the α's are for all r, s. It then follows from Eq. (A6) that I_r' is negative when the α's are positive, for all r, $1 \leq r \leq n - 1$. Comparing the coefficients of $q_1'q_0'$, $q_1''q_0'$, qq_0', and $m_0'^2$ in B_n we see that

$$C_n = -\alpha_1'I_1' - \sum_{r=2}^{n-1} \alpha_r'\alpha_2''\alpha_3'' \cdots \alpha_r''I_r' + \alpha_0\alpha_n'\alpha_2''\alpha_3'' \cdots \alpha_n'',$$

$$D_n = -\alpha_1''I_1' + \alpha_1''\alpha_2'' \cdots \alpha_{n+1}'',$$

$$E_n = \alpha_2''\alpha_3'' \cdots \alpha_{n+1}''.$$

Since I_r' are negative when the α's are positive, for all r, $1 \leq r \leq n - 1$, it is clear that the expressions C_n, D_n, and E_n are positive when the α's are. This is what we set out to prove.

Effective Dielectric Constant, Permeability, and Conductivity of a Random Medium and the Velocity and Attenuation Coefficient of Coherent Waves*

JOSEPH B. KELLER AND FRANK C. KARAL, JR.
Courant Institute of Mathematical Sciences, New York University, New York, New York
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Random media are considered in which the dielectric constant, permeability, and conductivity are random functions of position. For them, the average electric field, electric current, dielectric displacement, magnetic field, and magnetic induction are determined, assuming that these average quantities are time-harmonic plane waves. The proportionality factors between appropriate pairs of these quantities are found and defined to be the effective dielectric constant, permeability, and conductivity of the random medium. These effective parameters depend upon the frequency and propagation constant of the field in addition to the two-point auto- and cross-correlation functions of the random dielectric constant, permeability, and conductivity. For transverse fields thay are all scalars. In addition the dispersion equation for the propagation constant of the average or coherent field, derived previously, is analyzed and solved for high- and low-frequency fields. From the propagation constant, the phase velocity and attenuation coefficient can be found.

1. INTRODUCTION

IN the experimental investigation of electromagnetic fields one always measures some sort of average field, such as the average over a small volume or over a short time interval, or both. For a slowly varying field in a uniform medium, this average field is practically equal to the instantaneous field at a point. However, in a very heterogeneous medium such as a turbulent gas or liquid, or a mixture of sands or powders, the average field may differ considerably from the instantaneous field at a point. Consequently the ratio of the average current to the average electric field, which ratio we may call the effective conductivity σ_{eff}, may differ appreciably from the actual conductivity σ at a given point. It may also differ from the average conductivity $\langle\sigma\rangle$. Therefore we consider the problem of calculating σ_{eff} as well as the effective dielectric constant ϵ'_{eff} and the effective magnetic permeability μ_{eff}. This problem is similar to that of determining the macroscopic parameters of matter from molecular properties.

To formulate the problem we introduce an ensemble of media, each with definite values of $\sigma(x)$, $\epsilon'(x)$, and $\mu(x)$, and a probability distribution over the ensemble. This ensemble with the associated probability distribution is what we call a random medium. By the average $\langle f(x, t)\rangle$ of a function $f(x, t)$ we shall mean the ensemble average, i.e., the average of $f(x, t)$ with respect to the probability distribution over the ensemble for fixed x, t. Then we define the effective parameters of the random medium by the equations

$$\langle \mathbf{D}\rangle = \epsilon'_{eff}\langle \mathbf{E}\rangle, \quad \langle \mathbf{B}\rangle = \mu_{eff}\langle \mathbf{H}\rangle, \quad \langle \mathbf{J}\rangle = \sigma_{eff}\langle \mathbf{E}\rangle. \quad (1.1)$$

Here $\mathbf{D}$ is the dielectric displacement, $\mathbf{B}$ the magnetic induction, $\mathbf{J}$ the electric current, $\mathbf{E}$ the electric field and $\mathbf{H}$ the magnetic field.

To compute the averages in (1.1) we must first determine the appropriate field in each medium of the ensemble. For this purpose we assume that $\epsilon'(x)$, $\mu(x)$, and $\sigma(x)$ are nearly constant so that we can determine the field by a perturbation method. To find the average field we assume that ϵ', μ, and σ are statistically homogeneous and isotropic. We also assume the field to be time-harmonic with angular frequency ω. Then we find that $\epsilon'_{eff}(\omega)$, $\sigma_{eff}(\omega)$, and $\mu_{eff}(\omega)$, which depend upon ω, are operators rather than scalar or tensor multipliers. When applied to a plane wave of wave-vector $\mathbf{k}$, these operators reduce to tensors which depend upon ω and $\mathbf{k}$. Therefore we denote them by $\epsilon'_{eff}(\omega, \mathbf{k})$, $\sigma_{eff}(\omega, \mathbf{k})$, and $\mu_{eff}(\omega, \mathbf{k})$. When applied to a transversely polarized plane wave they become scalars depending upon ω and $k = |\mathbf{k}|$, which we write as $\epsilon'_{eff}(\omega, k)$ $\sigma_{eff}(\omega, k)$, and $\mu_{eff}(\omega, k)$.

We obtain explicit expressions for these scalars in terms of the two-point auto- and cross-correlation functions of $\epsilon'(x)$, $\mu(x)$, and $\sigma(x)$. Although these expressions are somewhat complicated, we obtain expansions of them for both low and high frequencies. We also obtain similar expansions for k, the complex wavenumber or propagation constant of the coherent or average field for both low and high frequencies. They are obtained from the dispersion equation for k derived in our previous paper,[1] which was solved there only in a special case. Our method of analysis

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[1] F. C. Karal and J. B. Keller, J. Math. Phys. 5, 537 (1964).

is similar to that of Ref. 1, from which we shall also use some results.

Many authors have considered the problem of calculating the effective parameters of a random medium, but they have apparently treated only the static case $\omega = 0$. In addition, most treatments concern a mixture or suspension of particles of one homogeneous substance in another homogeneous substance. In this case it is possible to employ the methods usually used to derive the dielectric constant from molecular properties, since matter may be thought of as a suspension of particles in vacuum. Thus Brown[2] determined ϵ'_{eff} for a suspension at $\omega = 0$ by using the method of Yvon[3] and Kirkwood,[4] which had been devised for the calculation of static dielectric constants. This method is very similar to ours, which we have also applied to the dielectric constant problem for $\omega \neq 0$.[5] References to earlier work are given in Ref. 2.

For a continuous medium rather than a piecewise uniform one, Landau and Lifschitz[6] obtained a result for ϵ'_{eff} when $\omega = 0$ and $\sigma = 0$. Our result agrees with theirs when we specialize it to this case. Molyneux[7] has also treated this case and has obtained one term in ϵ'_{eff} beyond the result of Landau and Lifschitz. It is of third order in the magnitude of the random part of $\epsilon'(x)$ and involves the three-point correlation function of $\epsilon'(x)$. We have calculated only up to second-order terms, so we do not obtain this term. Hashin and Shtrikman[8] and Beran[9] have attempted to obtain bounds on ϵ'_{eff} for $\omega = 0$ by using variational principles.

2. FORMULATION

Let us consider a medium in which ϵ', μ, and σ differ from the constants ϵ'_0, μ_0, and σ_0 by small random amounts. To make this hypothesis explicit we introduce a small parameter η and assume that

$$\epsilon' = \epsilon'_0[1 + \eta\epsilon'_1(\mathbf{x})], \tag{2.1}$$

$$\mu = \mu_0[1 + \eta\mu_1(\mathbf{x})], \tag{2.2}$$

$$\sigma = \sigma_0[1 + \eta\sigma_1(\mathbf{x})]. \tag{2.3}$$

Since we shall consider time-harmonic fields of angular frequency ω, it will be convenient to introduce the complex dielectric constant $\epsilon = \epsilon' + i\omega^{-1}\sigma$ which may be written as

$$\begin{aligned}\epsilon &\equiv \epsilon_0[1 + \eta\epsilon_1(\mathbf{x})] \\ &= (\epsilon'_0 + i\omega^{-1}\sigma_0)\left(1 + \eta\,\frac{\epsilon'_0\epsilon'_1 + i\omega^{-1}\sigma_0\sigma_1}{\epsilon'_0 + i\omega^{-1}\sigma_0}\right).\end{aligned} \tag{2.4}$$

This equation defines ϵ_0 and $\epsilon_1(\mathbf{x})$.

From Maxwell's equations, by elimination, we can obtain an equation for $\mathbf{E}$. When the field is time-harmonic and the above expressions (2.1)–(2.4) are used in that equation, it can be written as [Ref. 1, Eq. (87)]

$$[L - \eta L_1 - \eta^2 L_2 + O(\eta^3)]\mathbf{E} = 0. \tag{2.5}$$

Here the operators L, L_1, and L_2 are defined by

$$L = \nabla\times\nabla\times - k_0^2, \tag{2.6}$$

$$L_1 = k_0^2(\mu_1 + \epsilon_1) + \nabla\mu_1\times\nabla\times, \tag{2.7}$$

$$L_2 = k_0^2\mu_1\epsilon_1 - \mu_1\nabla\mu_1\times\nabla\times. \tag{2.8}$$

The constant k_0 is defined by $k_0^2 = \omega^2\mu_0\epsilon_0$.

To solve (5) for $\mathbf{E}$ we begin with $\mathbf{E}_0(\mathbf{x})$, a non-random solution of (2.5) with $\eta = 0$. Then it follows from (2.5) that $\mathbf{E}$ is given by [Ref. 1, Eq. (5)]

$$\begin{aligned}\mathbf{E} &= \mathbf{E}_0 + \eta L^{-1}L_1\mathbf{E}_0 \\ &\quad + \eta^2[L^{-1}L_1L^{-1}L_1 + L^{-1}L_2]\mathbf{E}_0 + O(\eta^3).\end{aligned} \tag{2.9}$$

To obtain $\mathbf{D}$ we multiply (2.9) by ϵ' which is given by (2.1). Then we take the expectation value of each side of the resulting equation to obtain

$$\begin{aligned}\langle\mathbf{D}\rangle &= \epsilon'_0\mathbf{E}_0 + \eta\epsilon'_0[L^{-1}\langle L_1\rangle + \langle\epsilon'_1\rangle]\mathbf{E}_0 \\ &\quad + \eta^2\epsilon'_0[L^{-1}\langle L_1L^{-1}L_1\rangle + L^{-1}\langle L_2\rangle + \langle\epsilon'_1L^{-1}L_1\rangle]\mathbf{E}_0 \\ &\quad + O(\eta^3).\end{aligned} \tag{2.10}$$

In (2.10), $\langle\mathbf{D}\rangle$ is expressed in terms of $\mathbf{E}_0$, whereas in (1.1) $\langle\mathbf{D}\rangle$ is given in terms of $\langle\mathbf{E}\rangle$. Therefore we shall try to eliminate $\mathbf{E}_0$ from (2.10).

To this end we first average (2.9) to obtain $\langle\mathbf{E}\rangle$ in terms of $\mathbf{E}_0$. Then we solve the resulting equation for $\mathbf{E}_0$ by iteration or successive substitution. In this way we obtain [Ref. 1, Eq. (8)]

$$\begin{aligned}\mathbf{E}_0 &= \langle\mathbf{E}\rangle - \eta L^{-1}\langle L_1\rangle\langle\mathbf{E}\rangle \\ &\quad - \eta^2 L^{-1}[\langle L_1L^{-1}L_1\rangle - \langle L_1\rangle L^{-1}\langle L_1\rangle + \langle L_2\rangle]\langle\mathbf{E}\rangle \\ &\quad + O(\eta^3).\end{aligned} \tag{2.11}$$

Now we use (2.11) to eliminate $\mathbf{E}_0$ from (2.10) and

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[2] W. F. Brown, J. Chem. Phys. **23**, 1514 (1955).
[3] J. Yvon, Comp. Rend. Acad. Sci. (Paris) **202**, 35 (1936).
[4] J. Kirkwood, J. Chem. Phys. **4**, 592 (1936).
[5] D. J. Vezzetti and J. B. Keller, "Refractive Index, Attenuation, Dielectric Constant and Permeability for Waves in a Polarizable Medium" (to be published).
[6] L. Landau and E. Lifschitz, *Electrodynamics of Continuous Media* (Pergamon Press, London, 1960), p. 46.
[7] J. Molyneux, "Application of Perturbation Techniques to Problems in Statistical Continuum Theory" (Ph.D. dissertation, University of Pennsylvania, 1964).
[8] Z. Hashin and S. Shtrikman, J. Appl. Phys. **33**, 3125 (1962).
[9] M. Beran, "Use of the Variational Approach to Determine Bounds for the Effective Permittivity in Random Media" (unpublished).

obtain the following equation for $\langle \mathbf{D} \rangle$ in terms of $\langle \mathbf{E} \rangle$:

$$\langle \mathbf{D} \rangle = \epsilon_0' \langle \mathbf{E} \rangle + \eta \epsilon_0' \langle \epsilon_1' \rangle \langle \mathbf{E} \rangle + \eta^2 \epsilon_0' [\langle \epsilon_1' L^{-1} L_1 \rangle - \langle \epsilon_1' \rangle L^{-1} \langle L_1 \rangle] \langle \mathbf{E} \rangle + O(\eta^3). \quad (2.12)$$

Finally from (2.12) and the definition of $\epsilon_{eff}'(\omega)$ in (1.1) we obtain

$$\epsilon_{eff}'(\omega) = \epsilon_0' + \eta \epsilon_0' \langle \epsilon_1' \rangle + \eta^2 \epsilon_0' [\langle \epsilon_1' L^{-1} L_1 \rangle - \langle \epsilon_1' \rangle L^{-1} \langle L_1 \rangle] + O(\eta^3). \quad (2.13)$$

This is our first result for e_{eff}'. It simplifies somewhat when ϵ_1', μ_1, and σ_1 satisfy

$$\langle \epsilon_1' \rangle = 0, \qquad \langle \mu_1 \rangle = 0, \qquad \langle \sigma_1 \rangle = 0. \quad (2.14)$$

In this case (2.7) shows that $\langle L_1 \rangle = 0$ and (2.13) becomes

$$\epsilon_{eff}'(\omega) = \epsilon_0' + \eta^2 \epsilon_0' \langle \epsilon_1' L^{-1} L_1 \rangle + O(\eta^3). \quad (2.15)$$

Practically the same analysis leads to an expression for $\sigma_{eff}(\omega)$. We first multiply (2.9) by σ, given by (2.3), to obtain the current density $\mathbf{J}$. Then we average the resulting equation to obtain an expression for $\langle \mathbf{J} \rangle$. It is identical with the right side of (2.10) in which ϵ_0' and ϵ_1' are replaced by σ_0 and σ_1. Finally we eliminate $\mathbf{E}_0$ by means of (2.11) and find that

$$\sigma_{eff}(\omega) = \sigma_0 + \eta \sigma_0 \langle \sigma_1 \rangle + \eta^2 \sigma_0 [\langle \sigma_1 L^{-1} L_1 \rangle - \langle \sigma_1 \rangle L^{-1} \langle L_1 \rangle] + O(\eta^3). \quad (2.16)$$

When (2.14) is satisfied, (2.16) becomes

$$\sigma_{eff}(\omega) = \sigma_0 + \eta^2 \sigma_0 \langle \sigma_1 L^{-1} L_1 \rangle + O(\eta^3). \quad (2.17)$$

To determine $\mu_{eff}(\omega)$ we may repeat the above analysis using $\mathbf{H}$ and $\mathbf{H}_0$ instead of $\mathbf{E}$ and $\mathbf{E}_0$. Alternatively, we can utilize the fact that Maxwell's equations are invariant under the interchange of $\mathbf{E}$ with $\mathbf{H}$ and ϵ with $-\mu$. To apply this latter procedure to the result (2.13) we must also replace each ϵ' by the corresponding μ. In either way we obtain the following result for μ_{eff}:

$$\mu_{eff}(\omega) = \mu_0 + \eta \mu_0 \langle \mu_1 \rangle + \eta^2 \mu_0 [\langle \mu_1 L^{-1} \tilde{L}_1 \rangle - \langle \mu_1 \rangle L^{-1} \langle \tilde{L}_1 \rangle] + O(\eta^3). \quad (2.18)$$

In (2.18) $\tilde{L}_1$ is the operator obtained from L_1 by interchanging ϵ with μ,

$$\tilde{L}_1 = k_0^2(\epsilon_1 + \mu_1) + \nabla \epsilon_1 \times \nabla \times. \quad (2.19)$$

When (2.14) applies, (2.18) becomes

$$\mu_{eff}(\omega) = \mu_0 + \eta^2 \mu_0 \langle \mu_1 L^{-1} \tilde{L}_1 \rangle + O(\eta^3). \quad (2.20)$$

In the next section we shall evaluate the average in the expressions (2.15), (2.17), and (2.20) for $\epsilon_{eff}'(\omega)$, $\sigma_{eff}(\omega)$, and $\mu_{eff}(\omega)$. We choose these simplified expressions to evaluate because in applying the results we can pick ϵ_0', σ_0, and μ_0 to be the average values of ϵ', μ, and σ, and then (2.14) will hold. It is to be noted that our expressions for the effective parameters are operators. We shall see that they simplify to scalars when they are applied to a transversely polarized plane wave, provided the medium is statistically homogeneous and isotropic.

3. EVALUATION OF ϵ'_{eff}, σ_{eff}, AND μ_{eff}

To evaluate the average operator $\langle \epsilon_1' L^{-1} L_1 \rangle$ in (2.15) we first apply this operator to the plane wave $\mathbf{A} \exp(i\mathbf{k} \cdot \mathbf{x})$. Upon writing L^{-1} as an integral operator we obtain

$$\langle \epsilon_1' L^{-1} L_1 \rangle \mathbf{A} e^{i\mathbf{k} \cdot \mathbf{x}} = \left\langle \epsilon_1'(\mathbf{x}) \int G(\mathbf{x}, \mathbf{x}') L_1(\mathbf{x}') \mathbf{A} e^{i\mathbf{k} \cdot \mathbf{x}'} \, d\mathbf{x}' \right\rangle. \quad (3.1)$$

In (3.1) the Green's tensor $G(\mathbf{x}, \mathbf{x}')$ is given by

$$G(\mathbf{x}, \mathbf{x}') = G_1(r)\mathbf{I} + G_2(r)\hat{\mathbf{r}}\hat{\mathbf{r}}. \quad (3.2)$$

Here $\mathbf{r} = \mathbf{x} - \mathbf{x}'$, $r = |\mathbf{r}|$, $\hat{\mathbf{r}} = r^{-1}\mathbf{r}$, $\mathbf{I}$ is the unit dyadic and G_1 and G_2 are defined by

$$G_1(r) = (-1 + ik_0 r + k_0^2 r^2) e^{ik_0 r} (4\pi k_0^2 r^3)^{-1} - \delta(r)/12\pi k_0^2 r^2, \quad (3.3)$$

$$G_2(r) = (3 - 3ik_0 r - k_0^2 r^2) e^{ik_0 r}/4\pi k_0^2 r^3. \quad (3.4)$$

We now insert (3.2) and the expression (2.7) for L_1 into (3.1). Then the integrand in (3.1) becomes, after multiplication by $\epsilon_1'(x)$,

$$\begin{aligned} &\epsilon_1'(\mathbf{x}) G(\mathbf{x}, \mathbf{x}') L_1(\mathbf{x}') \mathbf{A} e^{i\mathbf{k} \cdot \mathbf{x}'} \\ &= [k_0^2 \{\epsilon_1'(\mathbf{x})\mu_1(\mathbf{x}') + \epsilon_1'(\mathbf{x})\epsilon_1(\mathbf{x}')\} G_1(r)\mathbf{A} \\ &\quad - i(\nabla'(\epsilon_1'(\mathbf{x})\mu_1(\mathbf{x}')) \cdot \mathbf{k}) G_1(r)\mathbf{A} \\ &\quad + iG_1(r)(\nabla'(\epsilon_1'(\mathbf{x})\mu_1(\mathbf{x}')) \cdot \mathbf{A})\mathbf{k} \\ &\quad + k_0^2 \{\epsilon_1'(\mathbf{x})\mu_1(\mathbf{x}') + \epsilon_1'(\mathbf{x})\epsilon_1(\mathbf{x}')\} G_2(r)(\mathbf{A} \cdot \hat{\mathbf{r}})\hat{\mathbf{r}} \\ &\quad - i(\nabla'(\epsilon_1'(\mathbf{x})\mu_1(\mathbf{x}')) \cdot \mathbf{k})(\mathbf{A} \cdot \hat{\mathbf{r}})\hat{\mathbf{r}} G_2(r) \\ &\quad + i(\nabla'(\epsilon_1'(\mathbf{x})\mu_1(\mathbf{x}')) \cdot \mathbf{A})(\mathbf{k} \cdot \hat{\mathbf{r}})\hat{\mathbf{r}} G_2(r)] e^{i\mathbf{k} \cdot \mathbf{x}'}. \end{aligned} \quad (3.5)$$

Next we take the expectation of each side of (3.5). Before writing the result we shall introduce the two-point auto- and cross-correlation functions $R_{\epsilon'\epsilon}(r)$, $R_{\epsilon'\mu}(r)$ and $R_{\mu\mu}(r)$ defined by

$$\begin{aligned} R_{\epsilon'\epsilon}(r) &= \langle \epsilon_1'(\mathbf{x})\epsilon_1(\mathbf{x}') \rangle, \\ R_{\epsilon'\mu}(r) &= \langle \epsilon_1'(\mathbf{x})\mu_1(\mathbf{x}') \rangle, \\ R_{\mu\mu}(r) &= \langle \mu_1(\mathbf{x})\mu_1(\mathbf{x}') \rangle. \end{aligned} \quad (3.6)$$

We have written the correlation functions as functions of r because we assume the medium to be statistically homogeneous and isotropic. Now the expectation of (5) becomes, after noting that $\nabla = \hat{\mathbf{r}}\partial/\partial r$, $\nabla' = -\hat{\mathbf{r}}\partial/\partial r$,

$$\langle \epsilon_1'(\mathbf{x})G(\mathbf{x},\mathbf{x}')L_1(\mathbf{x}')\rangle \mathbf{A}\, e^{ik\cdot\mathbf{x}'} = [k_0^2 G_1\{R_{\epsilon'\mu} + R_{\epsilon'\epsilon}\}\mathbf{A} + iG_1 R'_{\epsilon'\mu}(\hat{\mathbf{r}}\cdot\mathbf{k})\mathbf{A} - iG_1 R'_{\epsilon'\mu}(\hat{\mathbf{r}}\cdot\mathbf{A})\mathbf{k} + k_0^2 G_2\{R_{\epsilon'\mu} + R_{\epsilon'\epsilon}\}(\hat{\mathbf{r}}\cdot\mathbf{A})\hat{\mathbf{r}}]\, e^{ik\cdot\mathbf{x}'}. \tag{3.7}$$

Upon integrating (3.7) with respect to $\mathbf{x}'$ and using (3.1) we obtain

$$\langle \epsilon_1' L^{-1}L_1\rangle \mathbf{A}\, e^{ik\cdot\mathbf{x}} = k_0^2\mathbf{A}\int G_1\{R_{\epsilon'\mu} + R_{\epsilon'\epsilon}\}\, e^{ik\cdot\mathbf{x}'}\, d\mathbf{x}' + i\mathbf{A}\int G_1 R'_{\epsilon'\mu}(\hat{\mathbf{r}}\cdot\mathbf{k})\, e^{ik\cdot\mathbf{x}'}\, d\mathbf{x}' - i\mathbf{k}\int G_1 R'_{\epsilon'\mu}(\hat{\mathbf{r}}\cdot\mathbf{A})\, e^{ik\cdot\mathbf{x}'}\, d\mathbf{x}' + k_0^2\int G_2\{R_{\epsilon'\mu} + R_{\epsilon'\epsilon}\}(\hat{\mathbf{r}}\cdot\mathbf{A})\hat{\mathbf{r}}\, e^{ik\cdot\mathbf{x}'}\, d\mathbf{x}'. \tag{3.8}$$

The integrals in (3.8) can be simplified by setting $\mathbf{x}' = \mathbf{x} - \mathbf{r}$ and writing $d\mathbf{r} = dr\, dS$ where dS is the area element on a sphere of radius r centered at $\mathbf{x}$. It is also convenient to introduce $k = |\mathbf{k}|$ and $\hat{\mathbf{k}} = k^{-1}\mathbf{k}$. Then all the integrations over dS can be performed explicitly with the aid of the formulas in Appendix I of Ref. 1. As a result (3.8) can be written in the form

$$\langle \epsilon_1' L^{-1}L_1\rangle \mathbf{A}\, e^{ik\cdot\mathbf{x}} = [M_{\epsilon'\mu\epsilon} + N_{\epsilon'\mu\epsilon}\hat{\mathbf{k}}\hat{\mathbf{k}}]\mathbf{A}\, e^{ik\cdot\mathbf{x}}. \tag{3.9}$$

The scalars $M_{\epsilon'\mu\epsilon}$ and $N_{\epsilon'\mu\epsilon}$ in (3.9) are defined by setting $\alpha = \epsilon'$, $\beta = \mu$, and $\gamma = \epsilon$ in (3.10) and (3.11),

$$M_{\alpha\beta\gamma} = k_0^2\int_0^\infty \{R_{\alpha\gamma} + R_{\alpha\beta}\}\left\{G_1 f - G_2\frac{1}{r^2 k}\frac{\partial f}{\partial k}\right\} dr - k^2\int_0^\infty R'_{\alpha\beta}G_1\frac{1}{rk}\frac{\partial f}{\partial k}\, dr, \tag{3.10}$$

$$N_{\alpha\beta\gamma} = k^2\int_0^\infty R'_{\alpha\beta}G_1\frac{1}{rk}\frac{\partial f}{\partial k}\, dr - k_0^2\int_0^\infty \{R_{\alpha\gamma} + R_{\alpha\beta}\}G_2\frac{1}{r^2}\left(\frac{\partial^2 f}{\partial k^2} - \frac{1}{k}\frac{\partial f}{\partial k}\right) dr. \tag{3.11}$$

The function $f(k, r)$ in (3.10) and (3.11) is

$$f(k, r) = (4\pi r/k)\sin kr. \tag{3.12}$$

We now use (3.9) in (2.15) to obtain the following result for $\epsilon'_{eff}(\omega, \mathbf{k})$:

$$\epsilon'_{eff}(\omega, \mathbf{k}) = \epsilon_0'[1 + \eta^2\{M_{\epsilon'\mu\epsilon} + N_{\epsilon'\mu\epsilon}\hat{\mathbf{k}}\hat{\mathbf{k}}\}] + O(\eta^3). \tag{3.13}$$

Completely similar evaluations of the expectations of the operators in (2.17) and (2.20) lead to the following quite similar results for $\sigma_{eff}(\omega, \mathbf{k})$ and $\mu_{eff}(\omega, \mathbf{k})$:

$$\sigma_{eff}(\omega, \mathbf{k}) = \sigma_0[1 + \eta^2\{M_{\sigma\mu\epsilon} + N_{\sigma\mu\epsilon}\hat{\mathbf{k}}\hat{\mathbf{k}}\}] + O(\eta^3), \tag{3.14}$$

$$\mu_{eff}(\omega, \mathbf{k}) = \mu_0[1 + \eta^2\{M_{\mu\epsilon\mu} + N_{\mu\epsilon\mu}\hat{\mathbf{k}}\hat{\mathbf{k}}\}] + O(\eta^3). \tag{3.15}$$

Equations (3.13), (3.14), and (3.15) are our basic results for the effective parameters of a random medium.

We see from (3.13)–(3.15) that the effective parameters are tensors. They multiply transverse field components (i.e., those perpendicular to $\hat{\mathbf{k}}$) by one factor (e.g., $\epsilon_0'[1 + \eta^2 M_{\epsilon'\mu\epsilon}]$) and longitudinal field components by another factor (e.g., $\epsilon_0[1 + \eta^2\{M_{\epsilon'\mu\epsilon} + N_{\epsilon'\mu\epsilon}\}]$). Thus the $N_{\alpha\beta\gamma}$ terms may be omitted when applying the effective parameters to transverse waves. Since plane electromagnetic waves are strictly transverse in homogeneous media, it is to be expected that they will be practically transverse in a slightly inhomogeneous random medium. Therefore in such media, the $N_{\alpha\beta\gamma}$ terms may be unimportant and the effective parameters may practically be taken to be scalars. We investigate longitudinal waves further in Sec. 6.

To obtain numerical results for the effective parameters we must evaluate the Fourier-like integrals of the correlation functions in the expressions (3.10) and (3.11) which define $M_{\alpha\beta\gamma}$ and $N_{\alpha\beta\gamma}$. This evaluation is described in the next section.

4. EVALUATION OF $M_{\alpha\beta\gamma}$ AND $N_{\alpha\beta\gamma}$ FOR HIGH AND LOW FREQUENCIES

The integrals in (3.10) and (3.11) for $M_{\alpha\beta\gamma}$ and $N_{\alpha\beta\gamma}$ depend upon ω and k or equivalently upon $k_0 = \omega(\epsilon_0\mu_0)^{\frac{1}{2}}$ and k. In addition they involve various correlation functions which depend upon the particular random medium. Therefore we cannot evaluate these integrals until the correlation functions are specified. However we can evaluate them in general when the frequency ω is very high or very low. When ω is small then k_0 is small and we assume that k is also small and of the same order as k_0. Similarly when ω is large then k_0 is large and we assume that k is also large and of the same order as k_0. In dimensionless terms these hypotheses mean that $k_0 a$ and ka are both small or both large, where a is a typical correlation length of the medium.

The asymptotic evaluation of the integrals in (3.10) and (3.11) for k_0 and k large involves repeated integrations by parts, together with the explicit

evaluation of certain integrals and some other special procedures. The calculation is very lengthy, but the method is indicated in Appendix I. The first few terms in the final results are

$$M_{\alpha\beta\gamma} = [R_{\alpha\gamma}(0) + R_{\alpha\beta}(0)]\left[\frac{5k_0^2 - k^2}{4(k^2 - k_0^2)}\right] + \frac{R'_{\alpha\gamma}(0)}{2k_0}\left[-\frac{ik_0^2(k^2 + k_0^2)^2}{k^2(k^2 - k_0^2)^2} + \frac{k_0}{k}\left(1 + \frac{k_0^2}{k^2}\right)\cot^{-1}\frac{k_0}{ik}\right] + \frac{R''_{\alpha\gamma}(0)}{k_0^2}\left[\frac{k_0^2(k^4 - 3k^2k_0^2 - 2k_0^4)}{(k^2 - k_0^2)^3}\right] + \frac{R'_{\alpha\beta}(0)}{2k_0}\left[+\frac{i(k^2 + k_0^2)(k^4 - 2k_0^2k^2 - k_0^4)}{k^2(k^2 - k_0^2)^2} + \frac{k_0}{k}\left(2 + \frac{k_0^2}{k^2} - \frac{k^2}{k_0^2}\right)\cot^{-1}\frac{k_0}{ik}\right] + \frac{R''_{\alpha\beta}(0)}{k_0^2}\left[\frac{k_0^2(k^4 - 6k^2k_0^2 - 2k_0^4) - k^4(k^2 - 4k_0^2)}{(k^2 - k_0^2)^3}\right] + O\left(\frac{1}{k^3}\right), \tag{4.1}$$

$$N_{\alpha\beta\gamma} = -[R_{\alpha\gamma}(0) + R_{\alpha\beta}(0)]\left[\frac{k^2 + 3k_0^2}{4(k^2 - k_0^2)}\right] - \frac{R'_{\alpha\gamma}(0)}{2k_0}\left[-\frac{ik_0^2(3k^4 - 2k^2k_0^2 + 3k_0^4)}{k^2(k^2 - k_0^2)^2} + \frac{3k_0}{k}\left(1 + \frac{k_0^2}{k^2}\right)\cot^{-1}\frac{k_0}{ik}\right] - \frac{R''_{\alpha\gamma}(0)}{k_0^2}\left[\frac{k_0^2k^2(3k^2 - 7k_0^2)}{(k^2 - k_0^2)^3}\right] - \frac{R'_{\alpha\beta}(0)}{2k_0}\left[\frac{i(k^4 + k_0^4)(k^2 - 3k_0^2)}{k^2(k^2 - k_0^2)^2} + \frac{k_0}{k}\left(4 + 3\frac{k_0^2}{k^2} - \frac{k^2}{k_0^2}\right)\cot^{-1}\frac{k_0}{ik}\right] - \frac{R''_{\alpha\beta}(0)}{k_0^2}\left[\frac{-k^2(10k_0^4 + k^4 - 7k_0^2k^2)}{(k^2 - k_0^2)^3}\right] + O\left(\frac{1}{k^3}\right). \tag{4.2}$$

The evaluation of the integrals in (3.10) and (3.11) for k_0 and k small is quite straightforward. It merely involves the expansion of the integrand in powers of k_0 and k and term-by-term integration of the resulting series. The result of the calculation is

$$M_{\alpha\beta\gamma} = -\frac{1}{3}R_{\alpha\gamma}(0) - \frac{1}{3}\left(1 - \frac{k^2}{k_0^2}\right)R_{\alpha\beta}(0) + \frac{k^2}{15}\left(1 + 10\frac{k_0^2}{k^2}\right)\int_0^\infty rR_{\alpha\gamma}(r)\,dr + \frac{k^2}{15}\left[-4 - \frac{k^2}{k_0^2} + 10\frac{k_0^2}{k^2}\right]\int_0^\infty rR_{\alpha\beta}(r)\,dr + O(k^3), \tag{4.3}$$

$$N_{\alpha\beta\gamma} = -\frac{1}{3}\frac{k^2}{k_0^2}R_{\alpha\beta}(0) + \frac{1}{15}k^2\left(2 + \frac{k^2}{k_0^2}\right)\int_0^\infty rR_{\alpha\beta}(r)\,dr - \frac{k^2}{5}\int_0^\infty rR_{\alpha\gamma}(r)\,dr + O(k^3). \tag{4.4}$$

The expansions (4.1)–(4.4) can be used in (3.13)–(3.15) to obtain results for the effective parameters at high and low frequencies. In using them it is necessary to consider correlation functions involving ϵ. They can be expressed in terms of correlation functions involving ϵ' and σ by recalling the definition of ϵ_1 in (2.4). By using this definition in the definition (3.6) of the correlation functions we find

$$R_{\epsilon\alpha} = (1 + i\sigma_0/\omega\epsilon'_0)^{-1}\{R_{\epsilon'\alpha} + (i\sigma_0/\omega\epsilon'_0)R_{\sigma\alpha}\}. \tag{4.5}$$

For $\alpha = \epsilon$ this yields

$$R_{\epsilon\epsilon} = (1 + i\sigma_0/\omega\epsilon'_0)^{-2}\{R_{\epsilon'\epsilon'} + (2i\sigma_0/\omega\epsilon'_0)R_{\epsilon'\sigma} + (i\sigma_0/\omega\epsilon'_0)^2R_{\sigma\sigma}\}. \tag{4.6}$$

We shall now use the results of this section to discuss the effective parameters.

5. RESULTS FOR ϵ'_{eff}, σ_{eff}, AND μ_{eff}

Our results for the effective parameters are given by (3.13)–(3.15) in which $M_{\alpha\beta\gamma}$ and $N_{\alpha\beta\gamma}$ are given by the integrals (3.11) and (3.12). In Ref. 1, we have shown that plane waves in a random electromagnetic medium are either transverse or longitudinal, and we now consider only transverse waves. Then the $N_{\alpha\beta\gamma}$ terms in (3.13)–(3.15) drop out and we have for transverse waves

$$\epsilon'_{eff}(\omega, k)/\epsilon'_0 = 1 + \eta^2M_{\epsilon'\mu\epsilon} + O(\eta^3), \tag{5.1}$$

$$\sigma_{eff}(\omega, k)/\sigma_0 = 1 + \eta^2M_{\sigma\mu\epsilon} + O(\eta^3), \tag{5.2}$$

$$\mu_{eff}(\omega, k)/\mu_0 = 1 + \eta^2M_{\mu\epsilon\mu} + O(\eta^3). \tag{5.3}$$

The quantity $M_{\alpha\beta\gamma}$ is given explicitly by an integral in (3.11) as a function of k_0 and k. To use that

expression it is necessary to determine k as a function of k_0. The dispersion equation for k for both transverse and longitudinal waves was derived in Ref. 1 and is solved in the next section for high and low frequencies for any correlation functions. For intermediate frequencies the dispersion equation can be solved numerically for specific correlation functions. The solution for k can then be used in $M_{\alpha\beta\gamma}$ to yield the effective parameters as functions of frequency.

For low frequencies, $M_{\alpha\beta\gamma}$ is given by (4.3) in terms of k_0 and k, and for low-frequency transverse waves, k is given by (6.12). Upon using (6.12) in (4.3) we obtain $M_{\alpha\beta\gamma}$ as a function of k_0. The leading terms in $M_{\alpha\beta\gamma}$, which may be obtained by setting $k = k_0 + O(\eta^2)$ in (4.3), are

$$M_{\alpha\beta\gamma} = -\tfrac{1}{3}R_{\alpha\gamma}(0) + \frac{k_0^2}{15}\int_0^\infty (11R_{\alpha\gamma} + 5R_{\alpha\beta})r\,dr + O(k_0^3) + O(\eta^2). \quad (5.4)$$

By using (5.4) in (5.1)–(5.3) we obtain for low-frequency transverse waves

$$\epsilon'_{\text{eff}}(\omega)/\epsilon'_0 = 1 - \frac{\eta^2}{3}R_{\epsilon'\epsilon}(0) + \frac{\eta^2 k_0^2}{15}\int_0^\infty (11R_{\epsilon'\epsilon} + 5R_{\epsilon'\mu})r\,dr + O(k_0^3) + O(\eta^2), \quad (5.5)$$

$$\sigma_{\text{eff}}(\omega)/\sigma_0 = 1 - \frac{\eta^2}{3}R_{\sigma\epsilon}(0) + \frac{\eta^2 k_0^2}{15}\int_0^\infty (11R_{\sigma\epsilon} + 5R_{\sigma\mu})r\,dr + O(k_0^3) + O(\eta^2), \quad (5.6)$$

$$\mu_{\text{eff}}(\omega)/\mu_0 = 1 - \frac{\eta^2}{3}R_{\mu\mu}(0) + \frac{\eta^2 k_0^2}{15}\int_0^\infty (11R_{\mu\mu} + 5R_{\mu\epsilon})r\,dr + O(k_0^3) + O(\eta^2). \quad (5.7)$$

Correlation functions $R_{\alpha\epsilon}$ are given by (4.5) in terms of $R_{\alpha\epsilon'}$ and $R_{\alpha\sigma}$. When $\sigma_0 = 0$ and $k_0 = 0$, (5.5) reduces to the result given by Landau and Lifschitz.[6]

For high frequencies, $M_{\alpha\beta\mu}$ is given by (4.1) in terms of k_0 and k, and for high-frequency transverse waves, k is given by (6.11). In the derivation of (4.1) it has been assumed that $k - k_0$ is large. From (6.11) we see that this is the case when $(k_0\eta)^{\frac{1}{3}}$ is large. Upon using (6.11) in (4.1) we obtain $M_{\alpha\beta\gamma}$ as a function of k_0 for k_0 large. The leading terms in $M_{\alpha\beta\gamma}$ are, when $R'_{\alpha\gamma}(0) = R'_{\alpha\beta}(0) = 0$,

$$M_{\alpha\beta\gamma} = [R_{\alpha\gamma}(0) + R_{\alpha\beta}(0)][(k_0/2\eta)^{\frac{1}{3}}b - \tfrac{5}{16}] - (2k_0\eta^3)^{-\frac{1}{3}}b^3[R''_{\alpha\gamma}(0) + R''_{\alpha\beta}(0)] + \cdots. \quad (5.8)$$

Here b is given by

$$b = \{-R''_{\mu\mu}(0) - 2R''_{\mu\epsilon}(0) - R''_{\epsilon\epsilon}(0)\}^{-\frac{1}{3}}. \quad (5.9)$$

By using (8) in (5.1)–(5.3) we obtain the effective parameters for high-frequency transverse waves, when $R'_{\alpha\gamma}(0) = R'_{\alpha\beta}(0) = 0$. They are

$$\epsilon'_{\text{eff}}(\omega)/\epsilon'_0 = 1 + \eta^2[R_{\epsilon'\epsilon}(0) + R_{\epsilon'\mu}(0)][(k_0/2\eta)^{\frac{1}{3}}b - \tfrac{5}{16}] - (\eta/2k_0)^{\frac{1}{3}}b^3[R''_{\epsilon'\epsilon}(0) + R''_{\epsilon'\mu}(0)] + \cdots, \quad (5.10)$$

$$\sigma_{\text{eff}}(\omega)/\sigma_0 = 1 + \eta^2[R_{\sigma\epsilon}(0) + R_{\sigma\mu}(0)][(k_0/2\eta)^{\frac{1}{3}}b - \tfrac{5}{16}] - (\eta/2k_0)^{\frac{1}{3}}b^3[R''_{\sigma\epsilon}(0) + R''_{\sigma\mu}(0)] + \cdots, \quad (5.11)$$

$$\mu_{\text{eff}}(\omega)/\mu_0 = 1 + \eta^2[R_{\mu\mu}(0) + R_{\mu\epsilon}(0)][(k_0/2\eta)^{\frac{1}{3}}b - \tfrac{5}{16}] - (\eta/2k_0)^{\frac{1}{3}}b^3[R''_{\mu\mu}(0) + R''_{\mu\epsilon}(0)] + \cdots. \quad (5.12)$$

6. SOLUTION OF THE DISPERSION EQUATION FOR THE PROPAGATION CONSTANT AT HIGH AND LOW FREQUENCIES

In our earlier paper[1] we obtained the dispersion equation for the propagation constant k of a plane wave traveling in a random medium. For a transverse wave, the dispersion equation is [Ref. 1, Eq. (112)]

$$k^2 - k_0^2 - \eta^2[k_0^2R_{\mu\epsilon}(0) + D(k)] = 0. \quad (6.1)$$

For a longitudinal wave, it is instead [Ref. 1, Eq. (111)]

$$k_0^2 + \eta^2[k_0^2R_{\mu\epsilon}(0) + D(k) + M(k)] = 0. \quad (6.2)$$

The expressions for D and M in (6.1) and (6.2) can be written as

$$D(k) = k_0^4\int_0^\infty [R_{\mu\mu} + 2R_{\mu\epsilon} + R_{\epsilon\epsilon}]\left[G_1 f - G_2\frac{1}{r^2k}\frac{\partial f}{\partial k}\right]dr - k_0^2k^2\int_0^\infty [R'_{\mu\mu} + R'_{\mu\epsilon}]G_1\frac{1}{rk}\frac{\partial f}{\partial k}\,dr - k_0^2\int_0^\infty [R'_{\mu\mu} + R'_{\mu\epsilon}]\left[f + \frac{1}{r^2k}\frac{\partial f}{\partial k}\right]\left[G'_1 - \frac{1}{r}G_2\right]dr + k^2\int_0^\infty R''_{\mu\mu}\frac{1}{rk}\frac{\partial f}{\partial k}\left[G'_1 - \frac{1}{r}G_2\right]dr, \quad (6.3)$$

$$M(k) = -k_0^4\int_0^\infty [R_{\mu\mu} + 2R_{\mu\epsilon} + R_{\epsilon\epsilon}] \times \frac{1}{r^2}\left[\frac{\partial^2 f}{\partial k^2} - \frac{1}{k}\frac{\partial f}{\partial k}\right]G_2\,dr + k_0^2k^2\int_0^\infty [R'_{\mu\mu} + R'_{\mu\epsilon}]G_1\frac{1}{rk}\frac{\partial f}{\partial k}\,dr - k_0^2\int_0^\infty [R'_{\mu\mu} + R'_{\mu\epsilon}]\frac{1}{r^2}\left[\frac{\partial^2 f}{\partial k^2} - \frac{1}{k}\frac{\partial f}{\partial k}\right]\left[G'_1 - \frac{1}{r}G_2\right]dr - k^2\int_0^\infty R''_{\mu\mu}\frac{1}{rk}\frac{\partial f}{\partial k}\left[G'_1 - \frac{1}{r}G_2\right]dr. \quad (6.4)$$

In writing (6.3) and (6.4), we have substituted (99)–(101) into (103) and (104) of Ref. 1.

The integrals in (6.3) and (6.4) are of the same type as those we encountered in Sec. 4 for $M_{\alpha\beta\gamma}$ and $N_{\alpha\beta\gamma}$. To evaluate them it is convenient to write (6.3) and (6.4) in the forms

$$D(k) = k_0^2[I_{\mu\mu}^{(3)} + 2I_{\mu\epsilon}^{(3)} + I_{\epsilon\epsilon}^{(3)}] - k_0^2[I_{\mu\mu}^{(1)} + I_{\mu\epsilon}^{(1)}] - [I_{\mu\mu}^{(4)} + I_{\mu\epsilon}^{(4)}] + I_{\mu\mu}^{(5)}, \quad (6.5)$$

$$M(k) = -k_0^2[I_{\mu\mu}^{(2)} + 2I_{\mu\epsilon}^{(2)} + I_{\epsilon\epsilon}^{(2)}] + k_0^2[I_{\mu\mu}^{(1)} + I_{\mu\epsilon}^{(1)}] + [I_{\mu\mu}^{(6)} + I_{\mu\epsilon}^{(6)}] - I_{\mu\mu}^{(5)}. \quad (6.6)$$

The integrals $I^{(i)}$ are defined in Appendix I and evaluated there asymptotically for k and k_0 large, under the assumption that $R'(0) = 0$.

When the first few terms in the asymptotic expansions of the $I^{(i)}$ for k and k_0 large are used in (6.5) and (6.6), asymptotic expressions for D and M are obtained. By using the expression for D in (6.1), the dispersion equation for transverse waves becomes for k and k_0 large

$$k^2/k_0^2 = 1 + \eta^2 \times \Bigg[R_{\mu\epsilon}(0) + \{R_{\mu\mu}(0) + 2R_{\mu\epsilon}(0) + R_{\epsilon\epsilon}(0)\}\frac{5k_0^2 - k^2}{4(k^2 - k_0^2)} + \{R_{\mu\mu}''(0) + 2R_{\mu\epsilon}''(0) + R_{\epsilon\epsilon}''(0)\}\frac{k^4 - 3k^2k_0^2 - 2k_0^4}{(k^2 - k_0^2)^3} - \{R_{\mu\mu}''(0) + R_{\mu\epsilon}''(0)\}\frac{5k^4 - 13k^2k_0^2 + 8k_0^4}{3k_0^2(k^2 - k_0^2)^2} + R_{\mu\mu}''(0)\frac{k^2(4k_0^2 - k^2)}{3k_0^4(k^2 - k_0^2)}\Bigg] + O(k^{-4}). \quad (6.7)$$

Similarly by using the expressions for D and M in (6.2), the dispersion equation for longitudinal waves becomes for k and k_0 large,

$$1 = \eta^2\Big[\tfrac{1}{3}\{R_{\mu\mu}(0) + R_{\epsilon\epsilon}(0)\} + (2/3k_0^2)\{R_{\mu\mu}''(0) + R_{\mu\epsilon}''(0)\} + [2/(k^2 - k_0^2)]\{R_{\mu\epsilon}''(0) + R_{\epsilon\epsilon}''(0)\}\Big] + O(k^{-4}). \quad (6.8)$$

Before solving these equations, we shall derive the corresponding equations for k and k_0 small. To this end we must evaluate the integrals $I^{(i)}$ for k and k_0 small. This can be done in a straightforward manner by first expanding the integrands in powers of k and k_0. Then term-by-term integration yields the expansion of the integrals. When these expansions are used in (6.5) and (6.6) they lead to expansions of D and M in powers of k and k_0. Upon inserting the expansion for D into (6.1) we obtain the following dispersion equation for transverse waves for k and k_0 small:

$$k^2/k_0^2 = 1 + \eta^2 \times \Bigg[R_{\mu\epsilon}(0) - \frac{1}{3}\{3R_{\mu\mu}(0) + 4R_{\mu\epsilon}(0) + R_{\epsilon\epsilon}(0)\} + \frac{k^2}{3k_0^2}\{2R_{\mu\mu}(0) + R_{\mu\epsilon}(0)\} - \frac{2}{3k_0^2}\{R_{\mu\mu}''(0) + R_{\mu\epsilon}''(0)\} - \frac{1}{3}\frac{k^2}{k_0^4}R_{\mu\mu}''(0) + \frac{k^2(-4k^2 + 15k_0^2)}{15k_0^2}\int_0^\infty rR_{\mu\mu}(r)\,dr + \frac{(-k^4 + k^2k_0^2 + 10k_0^4)}{15k_0^2}\int_0^\infty rR_{\mu\epsilon}(r)\,dr + \frac{(k^2 + 10k_0^2)}{15}\int_0^\infty rR_{\epsilon\epsilon}(r)\,dr\Bigg] + O(k^4). \quad (6.9)$$

Next, by using the expansions of D and M in (6.2), we obtain the dispersion equation for longitudinal waves when k and k_0 are small, in the form

$$k_0^2 = -\eta^2k_0^2\Bigg[R_{\mu\epsilon}(0) - \tfrac{1}{3}\{3R_{\mu\mu}(0) + 4R_{\mu\epsilon}(0) + R_{\epsilon\epsilon}(0)\} - (2/3k_0^2)\{R_{\mu\mu}''(0) + R_{\mu\epsilon}''(0)\} - \tfrac{2}{15}(k^2 - 5k_0^2) \times \Bigg\{\int_0^\infty rR_{\mu\epsilon}(r)\,dr + \int_0^\infty rR_{\epsilon\epsilon}(r)\,dr\Bigg\}\Bigg] + O(k^4). \quad (6.10)$$

Now we shall solve each of the equations (6.7)–(6.10) for k as a series in appropriate powers of η. To solve (6.7) we write $k = k_0 + k_1\eta^{\frac{1}{2}} + k_2\eta + \cdots$, insert this expansion into (6.7) and equate coefficients of powers of η to determine k_1 and k_2. In this way we find for high-frequency transverse waves

$$k = k_0[1 + \eta^{\frac{1}{2}}(2k_0)^{-\frac{1}{2}}\{-R_{\mu\mu}''(0) - 2R_{\mu\epsilon}''(0) - R_{\epsilon\epsilon}''(0)\}^{\frac{1}{2}} - (3\eta/16k_0)\{-R_{\mu\mu}''(0) - 2R_{\mu\epsilon}''(0) - R_{\epsilon\epsilon}''(0)\}^{\frac{1}{2}}] + \cdots. \quad (6.11)$$

There are four solutions represented by (6.11) corresponding to the four fourth roots in the second term on the right. The square root in the third term is the square of the fourth root in the second term. We see that the difference between k and k_0 is proportional to $\eta^{\frac{1}{2}}$ which is of larger order of magnitude than the random inhomogeneities in ϵ', μ, and σ. The difference to the order shown in (6.11) depends only on the second derivatives of the correlation functions at zero separation, which is not unreasonable for short waves. We note that $R_{\mu\mu}''(0) \leq 0$ and the real parts of the other $R''(0)$ are also nonpositive. If the positive fourth root is chosen in (6.11), then the real part of k exceeds that of k_0 and the propagation speed is reduced. But then when $\sigma = 0$, k is real and there is no attenuation to the order shown. If the pure imaginary fourth root is taken, then there is attenuation of order $\eta^{\frac{1}{2}}$

when $\sigma = 0$ and a reduction in propagation speed of order η. The attenuation and change in speed are both due to scattering. The solutions corresponding to increased propagation speed or to growing waves must be discarded as being spurious.

To solve (6.9) we write $k = k_0 + k_1\eta^2 + k_2\eta^4 + \cdots$, insert into (6.9), equate coefficients of powers of η and determine k_1 and k_2. Thus we find for low-frequency transverse waves

$$k = k_0 - \frac{k_0\eta^2}{6}\left[\frac{3}{k_0^2}R''_{\mu\mu}(0) + \frac{2}{k_0^2}R''_{\mu\epsilon}(0) + R_{\mu\mu}(0) + R_{\epsilon\epsilon}(0) - \frac{k_0^2}{5}\int_0^\infty (11R_{\mu\mu} + 10R_{\mu\epsilon} + 11R_{\epsilon\epsilon})r\,dr\right] + k_0\eta^4\left[-\frac{k_1^2}{2k_0^2} + \frac{k_1}{3k_0}\left\{2R_{\mu\mu}(0) + 2R_{\mu\epsilon}(0) - \frac{1}{k_0^2}R''_{\mu\mu}(0)\right\} + \frac{k_0k_1}{15}\int_0^\infty (7R_{\mu\mu} - R_{\mu\epsilon} + R_{\epsilon\epsilon})r\,dr\right] + \cdots . \quad (6.12)$$

In (6.12) k_1 denotes the coefficient of η^2. From (6.12) we see that $k - k_0$ is of order η^2 which is of smaller order of magnitude than the random inhomogeneities in the medium. We also see that when $\sigma = 0$, k is real to the order shown in (6.12) so the attenuation due to scattering does not appear to this order. The phase speed is reduced by the scattering since Re $k >$ Re k_0.

For longitudinal high-frequency waves, we solve (6.8) by the method used for (6.9) and obtain

$$k = k_0[1 + \eta^2k_0^{-2}\{R''_{\mu\epsilon}(0) + R''_{\epsilon\epsilon}(0)\} + (\tfrac{1}{2}\eta^4k_0^{-2})\{R_{\mu\mu}(0) + R_{\epsilon\epsilon}(0) + (1/3k_0^2) \times [4R''_{\mu\mu}(0) + R''_{\mu\epsilon}(0) - 3R''_{\epsilon\epsilon}(0)]\} \times \{R''_{\mu\epsilon}(0) + R''_{\epsilon\epsilon}(0)\}] + \cdots . \quad (6.13)$$

From (6.13) we see that k is real when $\sigma = 0$ so there is no attenuation due to scattering to the order shown. However Re $k <$ Re k_0 so the phase speed is greater for this solution than for the case $\eta = 0$. Therefore this solution is spurious. For longitudinal low-frequency waves, the solution of (6.10) for k is of order η^{-2} which is large rather than small. Therefore it is spurious, since (6.10) was derived on the assumption that k was small. Thus we have found no satisfactory solution of the dispersion equation for longitudinal waves.

APPENDIX I: ASYMPTOTIC EVALUATION OF $M_{\alpha\beta\gamma}$ AND $N_{\alpha\beta\gamma}$ FOR LARGE k_0 AND k.

The asymptotic evaluation of $M_{\alpha\beta\gamma}$ and $N_{\alpha\beta\gamma}$ for large k_0 and k can be carried out by first defining the integrals

$$I^{(1)} = k^2\int_0^\infty R'G_1\frac{1}{rk}\frac{\partial f}{\partial k}\,dr, \quad (A1)$$

$$I^{(2)} = k_0^2\int_0^\infty RG_2\frac{1}{r^2}\left(\frac{\partial^2 f}{\partial k^2} - \frac{1}{k}\frac{\partial f}{\partial k}\right)dr, \quad (A2)$$

$$I^{(3)} = k_0^2\int_0^\infty R\left(G_1 f - G_2\frac{1}{r^2k}\frac{\partial f}{\partial k}\right)dr. \quad (A3)$$

The double subscripts, which are to be attached to R and $I^{(j)}$, have been omitted for convenience. In terms of these integrals, the expressions (3.10) and (3.11) for M and N are

$$M_{\alpha\beta\gamma} = I^{(3)}_{\alpha\gamma} + I^{(3)}_{\alpha\beta} - I^{(1)}_{\alpha\beta}, \quad (A4)$$

$$N_{\alpha\beta\gamma} = I^{(1)}_{\alpha\beta} - I^{(2)}_{\alpha\gamma} - I^{(2)}_{\alpha\beta}. \quad (A5)$$

Thus the evaluation of M and N is reduced to the calculation of the three integrals $I^{(j)}$.

Substitution for G_1, G_2, and f into (A1)–(A3) yields

$$I^{(1)} = +\frac{1}{kk_0^2}\int_0^\infty R'\frac{e^{ik_0r}}{r^3}(\sin kr - kr\cos kr)\,dr - \frac{i}{kk_0}\int_0^\infty R'\frac{e^{ik_0r}}{r^2}(\sin kr - kr\cos kr)\,dr - \frac{1}{k}\int_0^\infty R'\frac{e^{ik_0r}}{r}(\sin kr - kr\cos kr)\,dr, \quad (A6)$$

$$I^{(2)} = \frac{3}{k^3}\int_0^\infty R\frac{e^{ik_0r}}{r^4}\{3(\sin kr - kr\cos kr) - k^2r^2\sin kr\}\,dr - \frac{3ik_0}{k^3}\int_0^\infty R\frac{e^{ik_0r}}{r^3}\{3(\sin kr - kr\cos kr) - k^2r^2\sin kr\}\,dr - \frac{k_0^2}{k^3}\int_0^\infty R\frac{e^{ik_0r}}{r^2}\{3(\sin kr - kr\cos kr) - k^2r^2\sin kr\}\,dr, \quad (A7)$$

$$I^{(3)} = \frac{1}{k^3}\int_0^\infty R\frac{e^{ik_0r}}{r^4}\{3(\sin kr - kr\cos kr) - k^2r^2\sin kr\}\,dr - \frac{ik_0}{k^3}\int_0^\infty R\frac{e^{ik_0r}}{r^3}\{3(\sin kr - kr\cos kr) - k^2r^2\sin kr\}\,dr + \frac{k_0^2}{k}\int_0^\infty Re^{ik_0r}\sin kr\,dr - \frac{k_0^2}{k^3}\int_0^\infty R\frac{e^{ik_0r}}{r^2}(\sin kr - kr\cos kr)\,dr - \frac{R(0)}{3}. \quad (A8)$$

In (A6)–(A8) six basic integrals occur. They are

$$J_1 = \int_0^\infty R\, e^{ik_0 r} \cos kr\, dr, \tag{A9}$$

$$J_2 = \int_0^\infty R\, e^{ik_0 r} \sin kr\, dr, \tag{A10}$$

$$J_3 = \int_0^\infty R\, e^{ik_0 r} \frac{\sin kr}{r}\, dr, \tag{A11}$$

$$J_4 = \int_0^\infty R\, e^{ik_0 r} \frac{1}{r}\left(\frac{\sin kr}{kr} - \cos kr\right) dr, \tag{A12}$$

$$J_5 = \int_0^\infty R\, e^{ik_0 r} \frac{1}{r^2}\left(\frac{\sin kr}{kr} - \cos kr\right) dr, \tag{A13}$$

$$J_6 = \int_0^\infty R\, e^{ik_0 r} \frac{1}{r^3}\left\{3\left(\frac{\sin kr}{kr} - \cos kr\right) - kr \sin kr\right\} dr. \tag{A14}$$

These integrals can be evaluated asymptotically for large k and k_0 provided $R(r)$ has a power series expansion about the origin.

To illustrate the procedure, let us consider J_4 and assume that

$$R(r) = \sum_{n=0}^{\infty} \frac{r^n}{n!} R^{(n)}(0). \tag{A15}$$

From (A9) and (A15) we have

$$\begin{aligned} J_4 = {} & \int_0^\infty \{R(r) - R(0) - rR'(0)\}\, e^{ik_0 r} \\ & \times \frac{1}{r}\left(\frac{\sin kr}{kr} - \cos kr\right) dr \\ & + R(0) \int_0^\infty e^{ik_0 r} \frac{1}{r}\left(\frac{\sin kr}{kr} - \cos kr\right) dr \\ & + R'(0) \int_0^\infty e^{ik_0 r}\left(\frac{\sin kr}{kr} - \cos kr\right) dr. \end{aligned} \tag{A16}$$

By replacing the trigonometrical terms in (16) by their exponential representations and evaluating some of the resulting integrals, we obtain

$$\begin{aligned} J_4 = {} & -\frac{1}{2k} \int_0^\infty \{R(r) - R(0) - rR'(0)\} \\ & \times \frac{1}{r^2} \{(i + kr)\, e^{i(k_0+k)r} - (i - kr)\, e^{i(k_0-k)r}\}\, dr \\ & + R(0)\left\{1 + \frac{ik_0}{k} \cot^{-1} \frac{k_0}{ik}\right\} \\ & + R'(0)\left\{\frac{1}{k} \cot^{-1} \frac{k_0}{ik} + \frac{ik_0}{k^2 - k_0^2}\right\}. \end{aligned} \tag{A17}$$

Now successive integration by parts yields the following asymptotic expansion of J_4 for large k and k_0:

$$\begin{aligned} J_4 \approx {} & R(0)\left\{1 + \frac{ik_0}{k} \cot^{-1} \frac{k_0}{ik}\right\} \\ & + R'(0)\left\{\frac{1}{k} \cot^{-1} \frac{k_0}{ik} + \frac{ik_0}{k^2 - k_0^2}\right\} + \frac{k^2 R''(0)}{(k^2 - k_0^2)^2}. \end{aligned} \tag{A18}$$

By applying the same method to the remaining integrals we obtain the following asymptotic expressions for them for large k and k_0:

$$\begin{aligned} J_1 \approx {} & -\frac{ik_0 R(0)}{(k^2 - k_0^2)} - \frac{(k_0^2 + k^2)R'(0)}{(k^2 - k_0^2)^2} \\ & + i\frac{k_0(k_0^2 + 3k^2)R''(0)}{(k^2 - k_0^2)^3}, \end{aligned} \tag{A19}$$

$$J_2 \approx \frac{kR(0)}{(k^2 - k_0^2)} - \frac{i2kk_0 R'(0)}{(k^2 - k_0^2)^2} - \frac{k(k^2 - 3k_0^2)R''(0)}{(k^2 - k_0^2)^3}, \tag{A20}$$

$$J_3 \approx R(0) \cot^{-1} \frac{k_0}{ik} + \frac{kR'(0)}{(k^2 - k_0^2)} - \frac{ik_0 kR''(0)}{(k^2 - k_0^2)^2}, \tag{A21}$$

$$\begin{aligned} J_5 \approx {} & \frac{kR(0)}{2}\left[\frac{ik_0}{k} + \left(1 - \frac{k_0^2}{k^2}\right) \cot^{-1} \frac{k_0}{ik}\right] \\ & + R'(0)\left[1 + \frac{ik_0}{k} \cot^{-1} \frac{k_0}{ik}\right] \\ & + \frac{R''(0)}{2k}\left[\cot^{-1} \frac{k_0}{ik} + \frac{ik_0 k}{k^2 - k_0^2}\right], \end{aligned} \tag{A22}$$

$$\begin{aligned} J_6 \approx {} & \frac{k^2 R(0)}{2}\left[\frac{1}{6} - \frac{k_0^2}{k^2} + \frac{ik_0}{k}\left(1 - \frac{k_0^2}{k^2}\right) \cot^{-1} \frac{k_0}{ik}\right] \\ & + \frac{kR'(0)}{2}\left[3\frac{ik_0}{k} + \left(1 - \frac{3k_0^2}{k^2}\right) \cot^{-1} \frac{k_0}{ik}\right] \\ & + \frac{R''(0)}{2}\left[3 - \frac{k^2}{k^2 - k_0^2} + \frac{3ik_0}{k} \cot^{-1} \frac{k_0}{ik}\right]. \end{aligned} \tag{A23}$$

We now use the above results for the J_i in (A6)–(A8) to obtain the following asymptotic expressions for $I^{(i)}$ valid for k and k_0 large:

$$\begin{aligned} I^{(1)} \approx {} & \frac{R'(0)}{2k_0}\left[-\frac{i(k^2 + k_0^2)}{(k^2 - k_0^2)} + \frac{k}{k_0}\left(1 - \frac{k_0^2}{k^2}\right) \cot^{-1} \frac{k_0}{ik}\right] \\ & + \frac{R''(0)}{k_0^2}\left[\frac{k^2(k^2 - 3k_0^2)}{(k^2 - k_0^2)^2}\right], \end{aligned} \tag{A24}$$

$$\begin{aligned} I^{(2)} \approx {} & R(0)\left[\frac{k^2 + 3k_0^2}{4(k^2 - k_0^2)}\right] \\ & + \frac{R'(0)}{2k_0}\left[-\frac{ik_0^2(3k^4 - 2k^2k_0^2 + 3k_0^4)}{k^2(k^2 - k_0^2)^2} \right. \\ & \left. + 3\frac{k_0}{k}\left(1 + \frac{k_0^2}{k^2}\right) \cot^{-1} \frac{k_0}{ik}\right] \\ & + \frac{R''(0)}{k_0^2}\left[\frac{k_0^2 k^2(3k^2 - 7k_0^2)}{(k^2 - k_0^2)^3}\right], \end{aligned} \tag{A25}$$

$$I^{(3)} \approx R(0)\left[\frac{5k_0^2 - k^2}{4(k^2 - k_0^2)}\right] + \frac{R'(0)}{2k_0}\left[-\frac{ik_0^2(k^2 + k_0^2)^2}{k^2(k^2 - k_0^2)} + \frac{k_0}{k}\left(1 + \frac{k_0^2}{k^2}\right)\cot^{-1}\frac{k_0}{ik}\right] + \frac{R''(0)}{k_0^2}\left[\frac{k_0^2(k^4 - 3k^2k_0^2 - 2k_0^4)}{(k^2 - k_0^2)^3}\right]. \quad \text{(A26)}$$

When the results (A24)–(A26) are used in (A4) and (A5), the asymptotic expressions (4.1) and (4.2) for $M_{\alpha\beta\gamma}$ and $N_{\alpha\beta\gamma}$ are obtained.

Integrals similar to $I^{(j)}$ occur in the dispersion equation for the propagation constant derived in our previous paper.[1] They are

$$I^{(4)} = k_0^2 \int_0^\infty R'\left(f + \frac{1}{r^2k}\frac{\partial f}{\partial k}\right)\left(G_1' - \frac{1}{r}G_2\right)dr, \quad \text{(A27)}$$

$$I^{(5)} = k^2 \int_0^\infty R''\frac{1}{rk}\frac{\partial f}{\partial k}\left(G_1' - \frac{1}{r}G_2\right)dr, \quad \text{(A28)}$$

$$I^{(6)} = k_0^2 \int_0^\infty R'\frac{1}{r^2}\left(\frac{\partial^2 f}{\partial k^2} - \frac{1}{k}\frac{\partial f}{\partial k}\right)\left(G_1' - \frac{1}{r}G_2\right)dr. \quad \text{(A29)}$$

If $R(r)$ has a power series expansion about the origin and if, in addition $R'(0) = 0$, these integrals can also be evaluated asymptotically by the procedure just described. The results are

$$I^{(4)} \approx \left[\frac{2(k^4 - 2k^2k_0^2 + 4k_0^4)}{3(k^2 - k_0^2)^2}\right]R''(0) + ik_0^3\left[\frac{1}{2k^4}\left(\frac{k^2}{k^2 - k_0^2}\cot^{-1}\frac{k_0}{ik}\right) - \frac{(k^2 + 3k_0^2)}{(k^2 - k_0^2)^3}\right]R'''(0), \quad \text{(A30)}$$

$$I^{(5)} \approx \left[\frac{k^2(4k_0^2 - k^2)}{3k_0^2(k^2 - k_0^2)}\right]R''(0) - \frac{ik_0}{k^2}\left[\frac{k^2(k^2 + k_0^2)}{(k^2 - k_0^2)^2} + \frac{ik}{k_0}\cot^{-1}\frac{k_0}{ik}\right]R'''(0), \quad \text{(A31)}$$

$$I^{(6)} \approx -\left[\frac{2k^2k_0^2}{(k^2 - k_0^2)^2}\right]R''(0) + \frac{3ik_0^3}{2k^4}\left[\frac{k^2(k^2 + 3k_0^2)(3k^2 - k_0^2)}{3(k^2 - k_0^2)^3} + \frac{ik}{k_0}\cot^{-1}\frac{k_0}{ik}\right]R'''(0). \quad \text{(A32)}$$

These results are used in Sec. 6, where the solutions of the dispersion equations are considered.

APPENDIX II

The following corrections should be made in Ref. 1:

Eq. (37) $\delta(\mathbf{r})$ should be $\delta(r)/4\pi r^2$.

In the sentence after Eq. (75), (4.32) should be (63).

Eqs. (76)–(79) $-\epsilon^2\langle\rho_1^2\rangle/\rho_0^2$ should be added to the right side of each of these equations.

Eq. (91) $-\mathbf{I}\delta(\mathbf{x} - \mathbf{x}')/3k_0^2$ should be added to the right side.

Eq. (93) $-\delta(r)/12\pi k_0^2 r^2$ should be added to the right side.

Eq. (103) $\partial F/\partial k$ should be $\partial f/\partial k$.

Eq. (117) ω' should be ω^{-1}.

Eq. (118) $G_1(r)^{-1}kr$ should be $G_1(r)k^{-1}\mathbf{r}$.

Eqs. (121) and (122) The $\frac{2}{3}$ should be omitted from the right side of each of these equations.

Eq. (123) $\frac{1}{2}\eta\langle(\epsilon_1')^2\rangle^{\frac{1}{2}}$ should be $\frac{1}{2}\eta\langle(\epsilon_1')^2\rangle^{\frac{1}{2}}[1 + i\sigma_0/\omega\epsilon_0']^{-1}$.

Eq. (124) The $\frac{2}{3}$ should be 1.

In the first sentence of Appendix I, the word "is" should follow "use". In the next to last equation of Appendix II, the term $-(\alpha/k)\cot^{-1}(\beta/k)$ should be $-(\alpha/k)\cot^{-1}(\alpha/k)$.

Talmi Transformation for Unequal-Mass Particles and Related Formulas

KAILASH KUMAR
Research School of Physical Sciences, The Australian National University, Canberra, Australia
(Received 11 October 1965)

Three-dimensional polynomials which occur as coefficients of the exponential in the wavefunctions of the harmonic oscillator are used in nuclear physics and kinetic theory of gases. A generating function for these polynomials is used to simplify the calculation of several integrals. These include the integrals involving products of two and three polynomials and the coefficients of the Talmi transformation. Explicit formula in terms of recoupling coefficients of angular momentum theory are obtained.

IN the course of an investigation into the method of solving the Boltzmann equation by means of polynomial expansion of the distribution function we had occasion to derive the formulas referred to in the title. Our derivations are simpler than the ones published so far and do not involve the use of group theory. The results also have a simple structure and would perhaps be more suited for the formal study of the quantities involved. Because of its applications in nuclear theory and in kinetic theory of gases, the following may be of interest to mathematical physicists in general and is offered with little reference to any particular physical situation.

I. PRELIMINARIES

We are concerned with the orthogonal polynomials constructed from the components of three-dimensional vectors denoted by the usual bold-face symbols, $\mathbf{a}$, $\mathbf{b}$, $\mathbf{r}$, $\mathbf{r}_1$, $\cdots$, etc. The polynomials are fully specified by a set of three indices n, l, m. The last two indices indicate the irreducible tensor character of the polynomial. For the algebra of irreducible tensors we follow the notation and phase conventions given in the book by Fano and Racah.[1] According to this book an irreducible tensor can be standard or contrastandard depending upon the way it transforms under rotations of the coordinate system. The standard tensors are characterized by a superscript in round brackets and the contrastandard ones by a superscript in square brackets. The prototypes of these tensors are the spherical harmonics which are defined in terms of the rotation matrix $\mathfrak{D}$ as follows

$$\mathcal{Y}_m^{[l]}(\theta, \varphi) = i^l(2l + 1/4\pi)^{\frac{1}{2}}\mathfrak{D}_{0m}^{(l)}(\theta, \varphi) \tag{1.1}$$

This differs from the more common definition according to the convention of Condon and Shortley.[2] In the usual notation[3] the relationship is

$$\mathcal{Y}_m^{[l]}(\theta, \varphi) = i^l \mathrm{Y}_{lm}(\theta, \varphi). \tag{1.2}$$

We have

$$\mathcal{Y}_m^{[l]*} = \mathcal{Y}_m^{(l)} = (-)^{l-m}\mathcal{Y}_{-m}^{[l]}. \tag{1.3}$$

The coupling rule for spherical harmonics consequently becomes (e.g., Ref. 3)

$$\mathcal{Y}_{m_1}^{[l_1]}(\theta, \varphi)\mathcal{Y}_{m_2}^{[l_2]}(\theta, \varphi) = \sum_l \sigma(l_1 l_2 l)(l_1 m_1 l_2 m_2 \mid l\ m_1 + m_2)\mathcal{Y}_{m_1+m_2}^{[l]}(\theta, \varphi) \tag{1.4}$$

where

$$\sigma(l_1 l_2 l) = i^{l_1+l_2-l}\left[\frac{(2l_1 + 1)(2l_2 + 1)}{4\pi(2l + 1)}\right]^{\frac{1}{2}}(l_1 0 l_2 0 \mid l0). \tag{1.5}$$

The Clebsch–Gordan or Wigner coefficients denoted here by $(l_1 m_1 l_2 m_2 \mid lm)$ or $(lm \mid l_1 m_1 l_2 m_2)$ are the same as those of Condon and Shortley[2] and usually employed in angular momentum theory.[3]

The addition theorem of spherical harmonics for

$$\cos\theta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2)$$

has the form

$$P_l(\cos\theta) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l}\mathcal{Y}_m^{[l]}(\theta_1, \varphi_1)\mathcal{Y}_m^{(l)}(\theta_2, \varphi_2). \tag{1.6}$$

The following forms of the usual plane-wave expansion will be needed:

$$e^{2\mathbf{a}\cdot\mathbf{b}} = \sum_{l,m} 4\pi i^l j_l(-2iab)\mathcal{Y}_m^{[l]}(\hat{\mathbf{a}})\mathcal{Y}_m^{(l)}(\hat{\mathbf{b}})$$

$$= \sum \frac{2\pi^{\frac{3}{2}}}{\Gamma(n+1)\Gamma(n+l+\frac{3}{2})}(ab)^{2n+l}\mathcal{Y}_m^{[l]}(\hat{\mathbf{a}})\mathcal{Y}_m^{(l)}(\hat{\mathbf{b}}). \tag{1.7}$$

[1] U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press Inc., New York, 1959).

[2] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1953).

[3] M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957).

By $\hat{\mathbf{a}}$ we denote the angular variables associated with the vector $\mathbf{a}$. Differentiation with respect to a vector variable $\mathbf{a}$ will be written as $\partial/\partial\mathbf{a}$ or ∇_a. The polynomials constructed from the vector $\mathbf{r}$ will be denoted, e.g., by $\psi_m^{[nl]}(\mathbf{r})$ or $\psi_m^{(nl)}(\mathbf{r})$ depending upon their tensor character. For the sake of brevity, we sometimes write $\mathbf{n}$ for the set of indices n, l, m in which case, e.g.,

$$\psi_m^{[nl]} \equiv \psi^{[n]}. \tag{1.8}$$

No confusion can arise since the positions in which the indices $\mathbf{n}$ occur are quite different from those in which the vectors $\mathbf{a}$, $\mathbf{r}$, $\cdots$, etc., occur.

We shall sometimes use the abbreviation

$$(2l+1)^{\frac{1}{2}} = \hat{l}. \tag{1.9}$$

The Talmi transformation[4-16] arises when one expresses the functions of the position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ of two particles in terms of their center of mass and relative coordinates $\mathbf{R}$ and $\mathbf{r}$. For unequal masses the relations between the vectors are

$$\Gamma^2\mathbf{R} = \alpha_1^2\mathbf{r}_1 + \alpha_2^2\mathbf{r}_2, \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2; \tag{1.10a}$$

$$\mathbf{r}_1 = \mathbf{R} + (\alpha_2/\Gamma)^2\mathbf{r}, \qquad \mathbf{r}_2 = \mathbf{R} - (\alpha_1/\Gamma)^2\mathbf{r}; \tag{1.10b}$$

$$\Gamma^2 = \alpha_1^2 + \alpha_2^2, \qquad \gamma^{-2} = \alpha_1^{-2} + \alpha_2^{-2}. \tag{1.10c}$$

The quantities α_1^2 and α_2^2 are proportional to the masses of the particles, Γ^2 is proportional to the total mass, and γ^2 to the reduced mass. These relations hold also in kinetic theory work but the transformation is taken to apply to the velocities rather than to the positions.

II. GENERATING FUNCTION FOR THREE-DIMENSIONAL POLYNOMIALS

Consider the polynomials $\xi_m^{[nl]}(\mathbf{r})$ defined through the generating function

$$G(\mathbf{a},\mathbf{r}) \equiv e^{-a^2+2\mathbf{a}\cdot\mathbf{r}} = \sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{(-)^n}{n!}a^{2n+l}\mathcal{Y}_m^{(l)}(\hat{\mathbf{a}})\xi_m^{[nl]}(\mathbf{r}). \tag{2.1}$$

Since the generating function is a scalar, $\xi_m^{[nl]}$ must transform like a spherical harmonic. The parity property, $\xi_m^{[nl]}(-\mathbf{r}) = (-)^l\xi_m^{[nl]}(\mathbf{r})$, is appropriately reflected in the relation

$$G(\mathbf{a},-\mathbf{r}) = G(-\mathbf{a},\mathbf{r}). \tag{2.2}$$

Using the identity

$$\begin{aligned} a(\partial/\partial a)G(\mathbf{a},\mathbf{r}) &\equiv \mathbf{a}\cdot(\partial/\partial\mathbf{a})G(\mathbf{a},\mathbf{r}) \\ &= -2\mathbf{a}\cdot(\mathbf{a}-\mathbf{r})G(\mathbf{a},\mathbf{r}), \end{aligned} \tag{2.3}$$

one can show that

$$\nabla_r^2\{G(\mathbf{a},\mathbf{r})e^{-\frac{1}{2}r^2}\} = \left(r^2 - 2a\frac{\partial}{\partial a} - 3\right)G(\mathbf{a},r)e^{-\frac{1}{2}r^2}, \tag{2.4}$$

from which, on using (2.1), it follows that

$$(-\nabla^2 + r^2)(e^{-\frac{1}{2}r^2}\xi_m^{[nl]}) = [2(2n+l)+3]e^{-\frac{1}{2}r^2}\xi_m^{[nl]}. \tag{2.5}$$

This shows that, apart from the normalization, $\exp(-\frac{1}{2}r^2)\xi_m^{[nl]}$ are the wavefunctions of the 3-dimensional harmonic oscillator. We shall write

$$\begin{aligned} \psi_m^{[nl]}(\alpha\mathbf{r}) &= N_{nl}^{-1}\left(\frac{\alpha^2}{\pi}\right)^{\frac{3}{4}}e^{-\frac{1}{2}\alpha^2r^2}\xi_m^{[nl]}(\alpha\mathbf{r}) \\ &\equiv \mathcal{R}_{nl}(\alpha r)\mathcal{Y}_m^{[l]}(\theta,\varphi). \end{aligned} \tag{2.6}$$

The function $\mathcal{R}_{nl}(\alpha r)$ then agrees with the usual definition of the radial function if the constant N_{nl} is chosen such that

$$\int \psi_m^{(nl)}(\alpha\mathbf{r})\psi_{m'}^{[n'l']}(\alpha\mathbf{r})\,d\mathbf{r} = \delta_{nn'}\,\delta_{ll'}\,\delta_{mm'}. \tag{2.7}$$

The explicit form of ξ is obtained by using on the left-hand side of (2.1), Eq. (1.7) and the relation (Ref. 17, p. 189)

$$e^{-a^2}j_{l+\frac{1}{2}}(-2iar) = (-)^{l+\frac{1}{2}}(iar)^{l+\frac{1}{2}}\sum_{n=0}^{\infty}\frac{(-a^2)^n}{\Gamma(n+l+\frac{3}{2})}L_n^{l+\frac{1}{2}}(r^2). \tag{2.8}$$

Accordingly,

$$\xi_m^{[nl]}(\mathbf{r}) = \frac{2\pi^{\frac{1}{4}}\Gamma(n+1)}{\Gamma(n+l+\frac{3}{2})}L_n^{l+\frac{1}{2}}(r^2)r^l\mathcal{Y}_m^{[l]}(\hat{\mathbf{r}}). \tag{2.9}$$

The Laguerre polynomials L_n^{α} occurring here have been defined in Ref. 17, p. 188. This definition is the same as that of the Sonine polynomials $S_\alpha^{(n)}$

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[17] A. Erdélyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II.

used in kinetic theory work, e.g., in the book of Chapman and Cowling.[18] The use of this function provides the link between the two subjects.

If $A(\mathbf{r})$ is any function of $\mathbf{r}$, possibly containing differential operators, then the integral

$$\int e^{-r^2}\xi_m^{(nl)}(\mathbf{r})A(\mathbf{r})\xi_{m'}^{[n'l']}(\mathbf{r})\,d\mathbf{r} \tag{2.10}$$

can be obtained by evaluating the coefficient of $\chi_m^{[nl]}(\mathbf{a})\chi_{m'}^{(n'l')}(\mathbf{b})$ in the integral

$$\int e^{-r^2}G(\mathbf{a},\mathbf{r})A(\mathbf{r})G(\mathbf{b},\mathbf{r})\,d\mathbf{r}, \tag{2.11}$$

where

$$\chi_m^{(nl)}(\mathbf{a}) = \frac{(-)^n}{n!}a^{2n+l}\mathcal{Y}_m^{(l)}(\hat{\mathbf{a}}). \tag{2.12}$$

The integral (2.10) is related to the matrix element of the operator $A(\mathbf{r})$ with respect to harmonic oscillator wavefunctions. It is often more convenient to evaluate the integral (2.11).

When $A \equiv 1$, (2.11) becomes

$$\pi^{\frac{3}{2}}\exp(2\mathbf{a}\cdot\mathbf{b}), \tag{2.13}$$

from which, on using (1.7), it follows that

$$\int e^{-r^2}\xi_m^{(nl)}(\mathbf{r})\xi_{m'}^{[n'l']}(\mathbf{r})\,d\mathbf{r}$$

$$= \frac{2\pi^3\Gamma(n+1)}{\Gamma(n+l+\frac{3}{2})}\delta_{nn'}\,\delta_{ll'}\,\delta_{mm'}. \tag{2.14}$$

Hence in (2.6)

$$N_{nl}^2 = \frac{2\pi^{\frac{3}{2}}\Gamma(n+1)}{\Gamma(n+l+\frac{3}{2})}. \tag{2.15}$$

The main advantage of the generating function arises from the separability of its arguments, because of which many integrals can be evaluated in the form (2.11). We list these properties

$$G(\mathbf{a},\mathbf{r})G(\mathbf{b},\mathbf{r}) = G(\mathbf{a}+\mathbf{b},\mathbf{r})e^{2\mathbf{a}\cdot\mathbf{b}}, \tag{2.16a}$$

$$G(\mathbf{a},\mathbf{r})G(\mathbf{b},\mathbf{r})G(\mathbf{c},\mathbf{r})$$

$$= G(\mathbf{a}+\mathbf{b}+\mathbf{c},\mathbf{r})e^{2(\mathbf{a}\cdot\mathbf{b}+\mathbf{b}\cdot\mathbf{c}+\mathbf{c}\cdot\mathbf{a})}. \tag{2.16b}$$

From (1.10),

$$G(\mathbf{a},\Gamma\mathbf{R}) = G\left(\frac{\alpha_1}{\Gamma}\mathbf{a},\alpha_1\mathbf{r}_1\right)G\left(\frac{\alpha_2}{\Gamma}\mathbf{a},\alpha_2\mathbf{r}_2\right), \tag{2.17}$$

$$G(\mathbf{a},\gamma\mathbf{r}) = G\left(\frac{\alpha_2}{\Gamma}\mathbf{a},\alpha_1\mathbf{r}_1\right)G\left(\frac{\alpha_1}{\Gamma}\mathbf{a},-\alpha_2\mathbf{r}_2\right), \tag{2.18}$$

$$G(\mathbf{a},\alpha_1\mathbf{r}_1) = G\left(\frac{\alpha_1}{\Gamma}\mathbf{a},\Gamma\mathbf{R}\right)G\left(\frac{\alpha_2}{\Gamma}\mathbf{a},\gamma\mathbf{r}\right), \tag{2.19}$$

$$G(\mathbf{a},\alpha_2\mathbf{r}_2) = G\left(\frac{\alpha_2}{\Gamma}\mathbf{a},\Gamma\mathbf{R}\right)G\left(\frac{\alpha_1}{\Gamma}\mathbf{a},-\gamma\mathbf{r}\right), \tag{2.20}$$

$$\int e^{-r^2}G(\mathbf{a},\mathbf{r})\,d\mathbf{r} = \int e^{-(\mathbf{a}-\mathbf{r})^2}\,d\mathbf{r} = \pi^{\frac{3}{2}}. \tag{2.21}$$

It is convenient to introduce the weight function

$$w(\alpha,r) = (\alpha^2/\pi)^{\frac{3}{4}}\exp(-\alpha^2r^2);\quad w(r) \equiv w(1,r) \tag{2.22}$$

with the aid of which an arbitrary function of $\mathbf{r}$ may be expanded as

$$f(\mathbf{r}) = w(\alpha,r)\sum_n f^{(n)}(\alpha)\xi^{[n]}(\alpha\mathbf{r}), \tag{2.23a}$$

$$f^{(n)}(\alpha) = N_{nl}^{-2}\int d\mathbf{r}\,f(\mathbf{r})\xi^{(n)}(\alpha\mathbf{r}). \tag{2.23b}$$

The quantities $f^{(n)}(\alpha)$ are linear combinations of a finite number of moments of the function $f(\mathbf{r})$ and occur in kinetic theory of gases when functions of velocity are expanded near the local equilibrium. This expansion is quite different from the expansion in terms of harmonic oscillator wavefunctions which may be used in shell model theory,

$$f(\mathbf{r}) = \sum f_{\text{ho}}^{(n)}(\alpha)\psi^{[n]}(\alpha\mathbf{r}), \tag{2.24a}$$

$$f_{\text{ho}}^{(n)}(\alpha) = \int d\mathbf{r}\,f(\mathbf{r})\psi^{(n)}(\alpha\mathbf{r}). \tag{2.24b}$$

There is a third possibility, also utilized in shell theory[4]:

$$f(\mathbf{r}) = \sum_n f_t^{(n)}\xi^{[n]}(\mathbf{r}), \tag{2.25a}$$

$$f_t^{(n)} = N_{nl}^{-2}\int w(r)f(\mathbf{r})\xi^{(n)}(\mathbf{r})\,d\mathbf{r}. \tag{2.25b}$$

For the special case $f(\mathbf{r}) \equiv f(r)\mathcal{Y}_{m'}^{[l']}(\hat{\mathbf{r}})$, we have

$$f_t^{(n)} = \delta_{ll'}\,\delta_{mm'}\int w(r)f(r)r^lL_n^{l+\frac{1}{2}}(r^2)r^2\,dr \tag{2.26}$$

which may be further expressed in terms of the Talmi integrals[4] $I_p(f)$ by using the power series for $L_n^{l+\frac{1}{2}}(r^2)$,

$$f_t^{(n)} = \delta_{ll'}\,\delta_{mm'}\sum_{p=\frac{1}{2}l}^{2n+\frac{1}{2}l}A(nl,p)I_p(f), \tag{2.27}$$

$$I_p(f) = 2[\Gamma(p+\tfrac{3}{2})]^{-1}\int_0^\infty r^{2p}e^{-r^2}f(r)r^2\,dr, \tag{2.28}$$

$$A(nl;p) = \frac{(-)^{p-l/2}}{2\pi^{\frac{3}{4}}}\binom{n+l+\frac{1}{2}}{n-p+\frac{1}{2}l}\frac{\Gamma(p+\frac{3}{2})}{\Gamma(p+1-\frac{1}{2}l)}, \tag{2.29}$$

$$\binom{n+\alpha}{n} = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}. \tag{2.30}$$

[18] S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-uniform Gases* (Cambridge University Press, Cambridge, England, 1939), also 2nd ed. (1952).

III. INTEGRALS INVOLVING TRIPLE PRODUCTS OF ξ's

In view of (2.25), the evaluation of (2.10) often involves an integration of products of three ξ's. From the Wigner–Eckart theorem or Eq. (1.4) we can write

$$\int w(r)\xi_{m_3}^{(n_3 l_3)}(\mathbf{r})\xi_{m_2}^{[n_2 l_2]}(\mathbf{r})\xi_{m_1}^{[n_1 l_1]}(\mathbf{r})\,d\mathbf{r}$$

$$\equiv K(\mathbf{n}_3;\mathbf{n}_2\mathbf{n}_1) = (l_1 m,\ l_2 m_2 \mid l_3 m_3)K(n_3 l_3; n_2 l_2 n_1 l_1). \tag{3.1}$$

This may be considered a definition of the symbols K, to evaluate which we have to pick out the coefficient of $\chi^{[n_3]}(\mathbf{c})\chi^{(n_2)}(\mathbf{b})\chi^{(n_1)}(\mathbf{a})$ in the integral [Eqs. (2.16b) and (2.21)]

$$\int w(r)G(\mathbf{c},\mathbf{r})G(\mathbf{b},\mathbf{r})G(\mathbf{a},\mathbf{r})\,d\mathbf{r}$$

$$= \exp\,[2(\mathbf{a}\cdot\mathbf{b} + \mathbf{b}\cdot\mathbf{c} + \mathbf{c}\cdot\mathbf{a})]. \tag{3.2}$$

In expanding the right-hand side according to (1.7), the angular parts can be reexpressed by means of the following formula:

$$\sum_{m_1',m_2',m_3'} (-)^{l_3'-m_3'}\mathcal{Y}_{m_1'}^{[l_1']}(\hat{\mathbf{c}})\mathcal{Y}_{m_2'}^{[l_2']}(\hat{\mathbf{c}})\mathcal{Y}_{-m_3'}^{(l_3')}(\hat{\mathbf{b}})$$
$$\times \mathcal{Y}_{m_1'}^{(l_1')}(\hat{\mathbf{b}})\mathcal{Y}_{m_2'}^{(l_2')}(\hat{\mathbf{a}})\mathcal{Y}_{m_3'}^{(l_3')}(\hat{\mathbf{a}})$$
$$= \sum_{l_1,l_2,l_3}\sum_{m_1,m_2,m_3}(l_1 m_1\ l_2 m_2 \mid l_3 m_3)\bar{W}\begin{pmatrix} l_1 & l_2 & l_3 \\ l_1' & l_2' & l_3' \end{pmatrix}$$
$$\times \hat{l}_1\hat{l}_2\sigma(l_1'\ l_2'\ l_3)\sigma(l_2'\ l_3'\ l_1)\sigma(l_3'\ l_1'\ l_2)$$
$$\times \mathcal{Y}_{m_3}^{[l_3]}(\hat{\mathbf{c}})\mathcal{Y}_{m_2}^{(l_2)}(\hat{\mathbf{b}})\mathcal{Y}_{m_1}^{(l_1)}(\hat{\mathbf{a}}). \tag{3.3}$$

Both sides are evidently scalar and the formula represents the effect of a recoupling as evidenced by the appearance of the coefficient $\bar{W}$ which is the same as Wigner's 6-j symbol [Fano and Racah,[1] Eq. (11.7)].

Finally,

$$K(n_3 l_3; n_2 l_2 n_1 l_1) = (-)^{n_1+n_2+n_3} n_1!\, n_2!\, n_3!\ \hat{l}_1\hat{l}_2$$
$$\times \sum \sigma(l_1'\ l_2'\ l_3)\sigma(l_2'\ l_3'\ l_1)\sigma(l_3'\ l_1'\ l_2)$$
$$\times \bar{W}\begin{pmatrix} l_1 & l_2 & l_3 \\ l_1' & l_2' & l_3' \end{pmatrix}\left[\frac{N_{n_1' l_1'}N_{n_2' l_2'}N_{n_3' l_3'}}{n_1'!\, n_2'!\, n_3'!}\right]^2. \tag{3.4}$$

The summation variables are l_1', l_2', and l_3' whose values are restricted by the functions occurring in the sum. The values of n_i' are given by the three relations obtained by equating the powers of a, b, and c,

$$2n_1 + l_1 = 2n_2' + l_2' + 2n_3' + l_3',$$
$$2n_2 + l_2 = 2n_3' + l_3' + 2n_1' + l_1',$$
$$2n_3 + l_3 = 2n_1' + l_1' + 2n_2' + l_2'.$$

It follows that for given n_i, l_i, the sum $2n_i' + l_i' = p_i'$ has a fixed value which depends only on the former numbers,

$$2p_i' = p_j + p_k - p_i, \qquad p_i = 2n_i + l_i, \tag{3.5}$$

(i, j, k) cyclic permutation of 1, 2, and 3.

Thus, the quantities in the square brackets in (3.4) actually are

$$[N_{n_1' l_1'}(n_1'!)^{-1}]^2 = 2\pi^{\frac{1}{2}}\{\Gamma[\tfrac{1}{2}(p_1' - l_1' + 2)]$$
$$\times \Gamma[\tfrac{1}{2}(p_1' + l_1' + 3)]\}^{-1}. \tag{3.6}$$

The restrictions above establish also a relation between the p_i (hence n_i) values. Since $p_1 + p_2 = p_3 + 2p_3'$ and $p_3' \geq 0$, it follows that the integral vanishes unless

$$p_i + p_j \geq p_k, \quad (i, j, k) \text{ cyclic permutation of 1, 2, and 3.} \tag{3.7}$$

This is a symmetric relation between the free indices of independent polynomials on the left-hand side of (3.1). This may be called a scalar triangular relation corresponding to the fact that the sum of two sides of a triangle is always greater than the third. This is to be contrasted with the *vector* triangular relations which hold between the numbers l_i in virtue of the Wigner coefficient.

IV. RELATIONS INVOLVING MOSHINSKY'S COEFFICIENT $B(nl,n'l',p)$

This coefficient is defined by means of the formula[7,12,14]

$$\int_0^\infty \mathcal{R}_{nl}(r)V(r)\mathcal{R}_{n'l'}(r)r^2\,dr = \sum_p B(nl, n'l', p)I_p(V). \tag{4.1}$$

The explicit form of B has been obtained using the explicit power series for $\mathcal{R}$ functions. This coefficient occurs in calculations of nuclear shell theory and has been well tabulated.[12–14] It is related to the triple product integral of the last section—a relation which also shows the role of the $\bar{W}$-coefficient in this coefficient.

Let the Talmi integral of the function $N_{nl}r^l L_n^{l+\frac{1}{2}}(r^2)$ be denoted by $I_p(nl)$. By (2.28)

$$I_p(nl) = 2[\Gamma(p + \tfrac{3}{2})]^{-1}N_{nl}\int_0^\infty r^{2p}\,e^{-r^2}r^l L_n^{l+\frac{1}{2}}(r^2)r^2\,dr. \tag{4.2}$$

Performing the angular integrals in (3.1) and converting the radial parts to the form (4.1) by using (2.6) we obtain the relations

$$K(n_3 l_3; n_2 l_2\ n_1 l_1) = N_{n_1 l_1}N_{n_2 l_2}N_{n_3 l_3}\sigma(l_1\ l_2\ l_3)$$
$$\times \sum B(n_2 l_2, n_3 l_3, p)I_p(n_1 l_1). \tag{4.3}$$

Also

$$\sum_p B(n_2l_2, n_3l_3, p)I_p(n_1l_1) = \sum_p B(n_3l_3, n_1l_1, p)I_p(n_2l_2) = \sum_p B(n_1l_1, n_2l_2, p)I_p(n_3l_3). \quad (4.4)$$

These relations may be used to calculate the coefficients K, since B's have already been tabulated[12-14] and $I_p(nl)$ can be calculated easily.

On the other hand, the coefficient B may also be expressed in terms of K's. The integral

$$\int w(r)\xi^{(n_3)}f(\mathbf{r})\xi^{[n_1]}\,d\mathbf{r}$$

may be evaluated in two ways for the special case when $f(\mathbf{r}) \equiv f(r)\mathcal{Y}_{m_3}^{[l_3]}$. Using (2.25), (2.27), and (3.1) one gets

$$(l_1m_1\ l_2m_2 \mid l_3m_3) \sum_{n_2,p} K(n_3l_3; n_2l_2\ n_1l_1)A(n_2l_2, p)I_p(f).$$

Performing the angular integrals first and then using (4.1) on the radial part, one gets for the same quantity

$$(l_1m_1\ l_2m_2 \mid l_3m_3)\sigma(l_1\ l_2\ l_3)N_{n_1l_1}N_{n_3l_3} \times \sum_p B(n_1l_1\ n_3l_3, p)I_p(f);$$

hence the relation

$$B(n_1l_1, n_3l_3, p) = [N_{n_1l_1}N_{n_3l_3}\sigma(l_1\ l_2\ l_3)]^{-1} \times \sum_{n_2} K(n_3l_3; n_2l_2\ n_1l_1)A(n_2l_2; p). \quad (4.5)$$

With (3.4) it shows the role of the $\bar{W}$-coefficient in the formation of B. Of course, l_2 must satisfy the triangular restrictions, $l_1 + l_3 < l_2 < |l_1 - l_3|$, if this relation is to hold. The sum over n_2 is restricted among other things by l_2 and p. It serves eventually to eliminate l_2 on the right-hand side. A symmetric expression in l_1 and l_3 is obtained by setting $l_2 = l_1 + l_3$.

V. TALMI COEFFICIENTS FOR UNEQUAL MASSES

In nuclear physics where the harmonic oscillator functions can be applied, the particles in general have the same mass. Hence that is the case most often studied. However, Smirnov[16] has drawn attention to the problem of separating the center-of-mass motion of several nucleons in which harmonic oscillator functions of different masses may be used. In kinetic theory the case of unequal masses arises in the study of transport properties of gas mixtures.

Talmi coefficients[4-16] are defined by the following relation:

$$\psi_{m_1}^{[n_1l_1]}(\alpha_1\mathbf{r}_1)\psi_{m_2}^{[n_2l_2]}(\alpha_2\mathbf{r}_2) = \sum_{NLM,nlm} T\begin{bmatrix}(\Gamma)NLM & (\alpha_1)n_1l_1m_1\\ (\gamma)nlm & (\alpha_2)n_2l_2m_2\end{bmatrix} \times \psi_M^{[NL]}(\Gamma\mathbf{R})\psi_m^{[nl]}(\gamma\mathbf{r}). \quad (5.1)$$

Various notations have been used for this quantity. We use the one which is most descriptive. We shall also use the abbreviated form $T(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2)$. Sometimes the scale parameters on one or both sides will also be dropped,

$$T(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2) = \int \psi^{(N)}(\Gamma\mathbf{R})\psi^{(n)}(\gamma\mathbf{r})\psi^{[n_1]}(\alpha_1\mathbf{r}_1)\psi^{[n_2]}(\alpha_2\mathbf{r}_2)\,d\mathbf{R}\,d\mathbf{r}. \quad (5.2)$$

Using (2.6) and (1.10) we may write

$$T(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2) = \frac{\bar{T}(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2)}{N_{NL}N_{ni}N_{n_1l_1}N_{n_2l_2}}, \quad (5.3)$$

$$\bar{T}(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2) = \int w(\Gamma, R)w(\gamma, r)\xi^{(N)}(\Gamma\mathbf{R})\xi^{(n)}(\gamma\mathbf{r}) \times \xi^{[n_1]}(\alpha_1\mathbf{r}_1)\xi^{[n_2]}(\alpha_2\mathbf{r}_2)\,d\mathbf{R}\,d\mathbf{r}. \quad (5.4)$$

It follows that

$$\xi^{[n_1]}(\alpha_1\mathbf{r}_1)\xi^{[n_2]}(\alpha_2\mathbf{r}_2) = \sum_{NLM,nlm} \bar{T}(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2)\xi^{[N]}(\Gamma\mathbf{R})\xi^{[n]}(\gamma\mathbf{r}). \quad (5.5)$$

The dependence on the numbers m can be separated in two Wigner coefficients and the T-coefficient can then be expressed in terms of the transformation brackets of Moshinsky,[7,8,11-14] which has been often investigated for the equal-mass case and for which tables have been prepared.

$$T(\mathbf{N}\,\mathbf{n} \mid \mathbf{n}_1\mathbf{n}_2) = \sum_\lambda (lm\ LM \mid \lambda\mu)(\lambda\mu \mid l_1m_1\ l_2m_2) \times i^{l_1+l_2-l-L}\langle nl, NL, \lambda \mid n_1l_1, n_2l_2, \lambda\rangle. \quad (5.6)$$

To obtain explicit formulas for $\bar{T}$ note that from (2.19) and (2.20)

$$G(\mathbf{a}_1, \alpha_1\mathbf{r}_1)G(\mathbf{a}_2, \alpha_2\mathbf{r}_2) = G\left(\frac{\alpha_1}{\Gamma}\mathbf{a}_1, \Gamma\mathbf{R}\right)G\left(\frac{\alpha_2}{\Gamma}\mathbf{a}_1, \gamma\mathbf{r}\right) \times G\left(\frac{\alpha_2}{\Gamma}\mathbf{a}_2, \Gamma\mathbf{R}\right)G\left(\frac{\alpha_1}{\Gamma}\mathbf{a}_2, -\gamma\mathbf{r}\right). \quad (5.7)$$

Then from (2.16b), (2.22), and (3.2)

$$\int w(\Gamma, R)w(\gamma, r)G(\mathbf{a}_1, \alpha_1\mathbf{r}_1)G(\mathbf{a}_2, \alpha_2\mathbf{r}_2) \times G(\mathbf{A}, \Gamma\mathbf{R})G(\mathbf{a}, \gamma\mathbf{r})\, d\mathbf{R}\, d\mathbf{r} \equiv \exp\left[\frac{2}{\Gamma}(\alpha_1\mathbf{a}_1\cdot\mathbf{A} + \alpha_2\mathbf{a}_2\cdot\mathbf{A} + \alpha_2\mathbf{a}_1\cdot\mathbf{a} - \alpha_1\mathbf{a}_2\cdot\mathbf{a})\right]. \tag{5.8}$$

In virtue of (5.4), then, $\bar{T}$ is obtained by picking the coefficient of $\chi^{(n_1)}(\mathbf{a}_1)\chi^{(n_2)}(\mathbf{a}_2)\chi^{[N]}(\mathbf{A})\chi^{[n]}(\mathbf{a})$ in the right-hand side. This procedure is similar to the one described for the case of triple product integrals. The right-hand sides of (5.8) and (3.8) are thus the generating functions for $\bar{T}$ and K coefficients. Multiplying by appropriate spherical harmonics and integrating over all angles, one obtains, because of (1.4), a product over four Wigner coefficients which is to be summed over the m numbers of four l's. This gives rise to an X-coefficient

$$\sum_{m', m'', M' M''} (l'm'\ L'M' \mid l_1m_1)(l''m''\ L''M'' \mid l_2m_2) \times (l'm'\ l''m'' \mid lm)(L'M'\ L''M'' \mid LM) = \hat{l}_1\hat{l}_2\hat{l}\hat{L} \times \sum_{\lambda} (lm\ LM \mid \lambda\mu)(\lambda\mu \mid l_1m_1\ l_2m_2)X\begin{bmatrix} l' & l'' & l \\ L' & L'' & L \\ l_1 & l_2 & \lambda \end{bmatrix}. \tag{5.9}$$

From (1.7) and (2.15) the nonangular factors are

$$\left[\frac{N_{N'L'}\, N_{N''L''}\, N_{n'l'}\, N_{n''l''}}{N'!\quad N''!\quad n'!\quad n''!}\right]^2 \times (\alpha_1a_1A)^{P'}(\alpha_2a_2A)^{P''}(\alpha_2a_1a)^{p'}(-\alpha_1a_2a)^{p''}$$

where $P = 2N + L$, etc.

Comparing the powers of a_1, a_2, A, and a, respectively we have

$$P' + p' = p_1, \qquad P'' + p'' = p_2; \qquad P' + P'' = P, \qquad p' + p'' = p, \tag{5.10}$$

so that $P + p = p_1 + p_2$ or

$$2n_1 + l_1 + 2n_2 + l_2 = 2N + L + 2n + l. \tag{5.11}$$

This is referred to as the equation for conservation of energy in nuclear theory literature and also follows from (5.1) by using the differential equation (2.5).

Collecting all the terms we get finally

$$\bar{T}\left[\begin{matrix}(\Gamma)NLM \\ (\gamma)nlm\end{matrix}\middle|\begin{matrix}(\alpha_1)n_1l_1m_1 \\ (\alpha_2)n_2l_2m_2\end{matrix}\right] = (-)^{n_1+n_2+N+n} n_1!\, n_2!\, N!\, n!\, \hat{l}_1\hat{l}_2\hat{L}\hat{l} \times \sum (-)^{l'''}(\alpha_1/\Gamma)^{2N'+L'+2n'''+l'''}(\alpha_2/\Gamma)^{2N'''+L'''+2n'+l'} \times \left[\frac{N_{N'L'}\, N_{N''L''}\, N_{n'l'}\, N_{n''l''}}{N'!\quad N''!\quad n'!\quad n''!}\right]^2 \times \sigma(l'L'l_1)\, \sigma(l''L''l_2)\, \sigma(l'l''l)\, \sigma(L'L''L) \times X\begin{bmatrix} l' & l'' & l \\ L' & L'' & L \\ l_1 & l_2 & \lambda \end{bmatrix}(lm\,LM \mid \lambda\mu)(\lambda\mu \mid l_1m_1\, l_2m_2). \tag{5.12}$$

The sum is over all the primed variables and λ. The restrictions on the sum are those arising from the functions occurring in the expression and the conditions (5.10) and (5.11). Because of the latter, (5.10) fixes only three out of the four variables N', N'', n', n'' for a given set of l-values. A sum over all allowable values of the one independent one must be performed. This expression is fully symmetric under the indices of $\bar{T}$-coefficient and involves only standard functions. The derivation given here and the formula (5.12) may be compared with those given previously in the literature,[4-16] even those for the equal-mass case. Many of the results of previous workers have been expressed in terms of the transformation bracket defined in (5.6). An expression for it is obtained by comparing (5.6) and (5.12).

Other less symmetric formulas can be derived for the $\bar{T}$-coefficient. In one form $\bar{T}$ is expressed as a sum over to K-functions and one X-function.

The following special case is useful when it is required to transform the functions of one vector variable:

$$\bar{T}\left[\begin{matrix}\Gamma\ \mathbf{N} \\ \gamma\ \mathbf{n}\end{matrix}\middle|\begin{matrix}\alpha_1\ \mathbf{n}_1 \\ \alpha_2\ \mathbf{0}\end{matrix}\right] = (4\pi)^{\frac{1}{2}}(-)^{N+n+n_1}\frac{n_1!\, N_{NL}^2 N_{nl}^2}{N!\, n!} \times \left(\frac{\alpha_1}{\Gamma}\right)^{2N+L}\left(\frac{\alpha_2}{\Gamma}\right)^{2n+l}\sigma(l\,L\,l_1)(lm\,LM \mid l_1m_1). \tag{5.13}$$

This is most easily derived by considering the generating function integral (5.8) without the term depending on $\mathbf{r}_2$, i.e., put $\mathbf{a}_2 = 0$. Of course, it follows also from (5.12). For the case $\alpha_1 = \alpha_2 = 1$, Moshinsky has given a formula [Ref. 7, Eq. (60)] for the quantity $\langle nl, NL, \lambda \mid 0l_1, 0l_2, \lambda\rangle$ which may also be derived from (5.6) and (5.12). Since all the numbers n and l are either positive or zero; the requirement $|L' - l'| \leq l_1 \leq L' + l'$ together with Eq. (5.10) and $n_1 = 0$ gives $N' = n' = 0$ and $l_1 = L' + l'$. Similarly for $n_2 = 0$, $N'' = n'' = 0$, and $l_2 = L'' + l''$. The rest is straightforward.

VI. SYMMETRY RELATIONS, SUM RULES, AND RECURSION FORMULAS

By putting $\mathbf{a}_1 = 0$ in (5.8) instead of $\mathbf{a}_2$ and using (5.13) one finds

$$\bar{T}(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{0}) = (-)^l(\alpha_1/\alpha_2)^{2N+L-2n-l}\bar{T}(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{0}, \alpha_2\mathbf{n}_2) = (\alpha_1/\alpha_2)^{2N+L-2n-l}\bar{T}(\Gamma\mathbf{n}, \gamma\mathbf{N} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{0}). \quad (6.1)$$

Similarly,

$$T(\Gamma\mathbf{N}, \gamma\mathbf{0} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2) = (-)^{l_2}(\alpha_1/\alpha_2)^{2n_1+l_1-2n_2-l_2}T(\Gamma\mathbf{0}, \gamma\mathbf{N} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2). \quad (6.2)$$

There does not seem to be any such simple relation when all indices are nonvanishing.

From the integral (5.4) it is seen that the change of scale $(\alpha_1, \alpha_2) \rightarrow (\beta\alpha_1, \beta\alpha_2)$ can be compensated by a corresponding change $(\mathbf{r}_1, \mathbf{r}_2) \rightarrow (\beta^{-1}\mathbf{r}_1, \beta^{-1}\mathbf{r}_2)$; since the integral remains unaltered by the latter we have

$$T(\Gamma\mathbf{N}\ \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1\ \alpha_2\mathbf{n}_2) = T((\beta\Gamma)\mathbf{N}, (\beta\gamma)\mathbf{n} \mid (\beta\alpha_1)\mathbf{n}_1, (\beta\alpha_2)\mathbf{n}_2). \quad (6.3)$$

In particular for the equal-mass transformation, $\alpha_1 = \alpha_2 = \alpha$,

$$T((2^{\frac{1}{2}}\alpha)\mathbf{N}, (2^{-\frac{1}{2}}\alpha)\mathbf{n} \mid \alpha\mathbf{n}_1, \alpha\mathbf{n}_2) = T((2^{\frac{1}{2}})\mathbf{N}, (2^{-\frac{1}{2}})\mathbf{n} \mid 1\mathbf{n}_1, 1\mathbf{n}_2). \quad (6.4)$$

The right-hand side is the standard form in which equal-mass transformation is calculated. To establish a relation between the equal-mass and unequal-mass case we note that from the identity

$$G(\mathbf{a}, \alpha\mathbf{r}) = \exp[(\alpha^2 - 1)a^2]G(\alpha\mathbf{a}, \mathbf{r}) \quad (6.5)$$

it follows that

$$\xi_m^{[nl]}(\alpha\mathbf{r}) = \sum_{n'=0}^{n} \epsilon(\alpha, n'nl)\xi_m^{[n'l]}(\mathbf{r}), \quad (6.6)$$

$$\epsilon(\alpha, n'nl) = \binom{n}{n'}(1 - \alpha^2)^{n-n'}\alpha^{2n'+l}. \quad (6.7)$$

Then from (5.5)

$$\sum_{N=N'}^{\infty}\sum_{n=n'}^{\infty} \epsilon(2^{-\frac{1}{2}}\Gamma, N'NL)\ \epsilon(2^{\frac{1}{2}}\gamma, n'nl) \times \bar{T}(\Gamma\mathbf{N}, \gamma\mathbf{n} \mid \alpha_1\mathbf{n}_1, \alpha_2\mathbf{n}_2) = \sum_{n_1'=0}^{n_1}\sum_{n_2'=0}^{\infty} \epsilon(\alpha_1, n_1'n_1l_1)\ \epsilon(\alpha_2, n_2'n_2l_2) \times \bar{T}(2^{\frac{1}{2}}N'LM, 2^{-\frac{1}{2}}n'lm \mid 1n_1'l_1m_1, 1n_2l_2m_2). \quad (6.8)$$

The simplest form of sum rules are, of course, the orthogonality relations in which a product of two T-coefficients is summed over common indices $(\mathbf{N}, \mathbf{n})$ or $(\mathbf{n}_1\mathbf{n}_2)$. These follow from the completeness of the $\psi^{(n)}$ functions. A variety of other relations may be obtained by the use of the generating functions. For example, in Eq. (5.8) one may set $\mathbf{A} = \mathbf{a} = \mathbf{a}_1 = \mathbf{a}_2$; then the right-hand side becomes a scalar. By comparing the coefficients of a power of A on the two sides one has the result that product of a $\bar{T}$-coefficient with $\bar{W}$-coefficient and two Wigner coefficients and summed over an appropriate number of indices is equal to a constant. It is now clear that other sum rules result by setting a different set of vectors equal in expression (5.8). Similar sum rules for the K-coefficients can be obtained.

In numerical evaluation of these complicated expressions, especially for constructing tables of values, it is often more convenient to work with recursion relations. For Talmi coefficients such recursion relations have been derived using the corresponding ones for Laguerre polynomials and spherical harmonics.[11,13,14] Since we now have generating function for composite polynomials the recursion relations for ξ or ψ may be obtained more directly. The normalization of ξ-function is especially useful for this purpose as it avoids many square rooted coefficients in such formulas. We give some brief examples. Let the contrastandard components of a vector $\mathbf{a}$ be denoted by

$$a_{\pm1}^{[1]} = (\mp ia_x + a_y)/\sqrt{2}, \qquad a_0^{[1]} = ia_z. \quad (6.9)$$

Then taking account of the phase conventions and using (1.4) we have

$$a_\nu^{[1]}\chi_m^{(nl)}(\mathbf{a}) = -(n+1) \times \left(\frac{l}{2l+1}\right)^{\frac{1}{2}}(l\ 1\ m-\nu\ 1\nu \mid lm)\chi_{m-\nu}^{(n+1,l-1)}(\mathbf{a}) + \left(\frac{l+1}{2l+1}\right)^{\frac{1}{2}}(l\ 1\ m-\nu\ 1\nu \mid lm)\chi_{m-\nu}^{(n,l+1)}(\mathbf{a}), \quad (6.10)$$

and using the gradient formula (e.g., Ref. 3, p. 124 with appropriate phase changes),

$$\nabla_a^{[1]}{}_\nu\chi_m^{(nl)}(\mathbf{a}) = (2n+2l+1) \times \left(\frac{l}{2l+1}\right)^{\frac{1}{2}}(l\ 1\ m+\nu\ 1\nu \mid lm)\chi_{m-\nu}^{(n,l-1)}(\mathbf{a}) - 2\left(\frac{l+1}{2l+1}\right)^{\frac{1}{2}}(l\ 1\ m-\nu\ 1\nu \mid lm)\chi_{m-\nu}^{(n-1,l+1)}(\mathbf{a}). \quad (6.11)$$

The generating function yields

$$\nabla_a^{[1]}{}_\nu G(\mathbf{a}, \mathbf{r}) = (2r_\nu^{[1]} - 2a_\nu^{[1]})G(\mathbf{a}, \mathbf{r}), \quad (6.12)$$

$$\nabla_r^{[1]}{}_\nu G(\mathbf{a}, \mathbf{r}) = 2a_\nu^{[1]}G(\mathbf{a}, \mathbf{r}). \quad (6.13)$$

Hence comparing the coefficients with the help of (6.10) and (6.11) we immediately get

$$\nabla_\nu^{[1]}\xi_m^{[nl]} = 2\left(\frac{l}{2l-1}\right)^{\frac{1}{2}}(lm\ 1\nu \mid l-1\ m+\nu)\xi_{m+\nu}^{[n,l-1]} - 2n\left(\frac{l+1}{2l+3}\right)^{\frac{1}{2}}(lm\ 1\nu \mid l+1\ m+\nu)\xi_{m+\nu}^{[n-1,l+1]}, \quad (6.14)$$

$$r_\nu^{[1]}\xi_m^{[nl]} = \left(\frac{l}{2l-1}\right)^{\frac{1}{2}}(lm\ 1\nu \mid l-1\ m+\nu) \times [\xi_{m+\nu}^{[n,l-1]} - \xi_{m+\nu}^{[n+1,l-1]}] + \left(\frac{l+1}{2l+3}\right)^{\frac{1}{2}}(lm\ 1\nu \mid l+1\ m+\nu) \times [-n\xi_{m+\nu}^{[n-1,l+1]} + (n+l+\tfrac{3}{2})\xi_{m+\nu}^{[n,l+1]}]. \quad (6.15)$$

Of course, these expressions can be calculated by using the definition (2.9) and corresponding formulas for L_n^α, etc., but the calculations would be rather long. The calculation of relations involving scalar operators such as $r\partial/\partial r$ or r^2 are even shorter as will be seen from the following:

$$4r^2G(\mathbf{a},\mathbf{r}) = \left(2\mathbf{a}+\frac{\partial}{\partial \mathbf{a}}\right)\cdot\left(2\mathbf{a}+\frac{\partial}{\partial \mathbf{a}}\right)G(\mathbf{a},\mathbf{r}) = \left(4a^2 + 4a\frac{\partial}{\partial a} + 6 + \nabla_a^2\right)G(a,r); \quad (6.16)$$

$$r\frac{\partial}{\partial r}G \equiv \mathbf{r}\cdot\frac{\partial}{\partial r}G = \mathbf{a}\cdot\left(2\mathbf{a}+\frac{\partial}{\partial \mathbf{a}}\right)G = \left(2a^2 + a\frac{\partial}{\partial a}\right)G; \quad (6.17)$$

$$a^2\chi_m^{(nl)} = -(n+1)\chi_m^{(n+1,l)}; \quad (6.18)$$

$$a\frac{\partial}{\partial a}\chi_m^{(nl)} = (2n+l)\chi_m^{(nl)}; \quad (6.19)$$

$$\nabla_a^2\chi_m^{(nl)} = -\frac{1}{n}[(2n+l)(2n+l+1) - l(l+1)] \times \chi_m^{(n-1,l)}. \quad (6.20)$$

The generating function (2.1) may also be expanded in Cartesian coordinates in which case it generates products of three Hermite polynomials in x, y, and z (e.g., Ref. 17, p. 194). Such a product can be expressed as a linear combination of $\xi_m^{[nl]}(r, \theta, \varphi)$. The coefficients of this expansion are related to the transformation brackets $(n_x n_y n_z \mid nlm)$ which have been discussed in connection with the nuclear shell model.[19,20] The use of generating function may be expected to simplify these calculations also.

[19] Z. Pluhař and J. Tolar, Czech. J. Phys. **B14**, 287 (1964).
[20] E. Chacón and M. de Llano, Rev. Mex. Fis. **12**, 57 (1963).

Analyticity Properties of the Scattering Amplitude

A. MINGUZZI
Istituto di Fisica della Universita' di Bologna, Istituto Nazionale di Fisica Nucleare - Sezione di Bologna, Bologna, Italy
(Received 1 June 1965)

Analyticity properties in three variables, energy, momentum transfer, and "squared mass" are deduced from single-variable dispersion relations.

ANALYTICITY properties of the scattering amplitude in more than one variable are proved as a consequence of the PT invariance, the microcausality condition, and the stability of the elementary particles. The scattering of equal-mass, uncharged particles is discussed; the extension to arbitrary stable particles presents no difficulty. The tools of the proof are:

(1) For every physical value of the momentum transfer t, there exists a function $T_t(s)$, holomorphic in the center-of-mass energy s in a strip $\text{Im } s > 0$ near the physical axis, so that

$$\lim_{\epsilon \to 0^+} T_t(s + i\epsilon)$$

is the scattering amplitude.[1]

(2) For every physical value of s, there exists a function $T_s(t)$, holomorphic in t in an ellipse ("small Lehmann ellipse"), so that

$$\lim_{\eta \to 0} T_s(t + i\eta)$$

is the scattering amplitude.[2]

Mandelstam has postulated a representation of the scattering amplitude, the double dispersion relations, and has proved analyticity properties in two variables in the set

$$|st(s + t - 4\mu^2)| < 288\mu^6.$$

From (1) and (2), by straightforward application of a theorem, conjectured by Wightman[3] and proved by Zerner,[4] we prove the existence and uniqueness of a function $T(s, t)$ holomorphic in s, t in an open set of C^2 of which $T_s(t)$ and $T_t(s)$ are restrictions.

[1] A. Minguzzi, Nuovo Cimento **32**, 198 (1964).
[2] H. Lehmann, Nuovo Cimento Suppl. **13**, 57 (1959).
[3] A. S. Wightman, "Axiomatic Field Theory" in *Theoretical Physics* (International Atomic Energy Agency, Vienna, 1963), note on p. 38.
[4] M. Zerner, "Quelques résultats sur le prolongement analytique des fonctions de variables complexes" (Seminar in Mathematical Physics, Université d'Aix-Marseille).

Proof: The proof of Zerner has been carried out when the analyticity domains in (1) and (2) are replaced by the half planes $\text{Re } s > 0$, $\text{Re } t > 0$, respectively. We now do his proof with the modification necessary to cope with (1) and (2). Let us take the compact in R^2,

$$F = [s, t : 4\mu^2 \leq s \leq S; 0 \leq -t \leq s - 4\mu^2],$$

where μ is the mass of the particles and S an arbitrary real constant. Every $(s, t) \in F$ belongs to the physical range of the elastic scattering process of which s and t are the center-of-mass energy and the momentum transfer. Let us also consider the sets in $C^1 \times R^1$:

$$A_s = [s : |\text{Re } s - s_0| < \epsilon_1; 0 \leq \text{Im } s < \epsilon_2] \times [t : \text{Im } t = 0; |\text{Re } t - t_0| < \epsilon_3],$$

$$A_t = [t : |\text{Re } t - t_0| < \epsilon_3; 0 \leq \text{Im } t < \epsilon_4] \times [s : \text{Im } s = 0; |\text{Re } s - s_0| < \epsilon_1],$$

$$(s_0, t_0) \in \text{Int } (F),$$

and the sets A_s', A_t' in which strict inequalities only occur. By a proper choice of the ϵ_i, $(\text{Re } s, \text{Re } t) \in \text{Int } (F)$ and $[s: |\text{Re } s - s_0| < \epsilon_1; 0 < \text{Im } s < \epsilon_2]$ is contained in the strip of holomorphy of $T_t(s)$, for each $|\text{Re } t - t_0| < \epsilon_3$; $[t: |\text{Re } t - t_0| < \epsilon_3; 0 < \text{Im } t < \epsilon_4]$ is contained in the smallest Lehmann ellipse when $|\text{Re } s - s_0| < \epsilon_1$. (The reason we restrict ourselves to a compact set is due to the shrinking to zero of the Lehmann ellipse when $s \to \infty$.) Let us call $f(s, t)$ the function defined in $A = A_s U A_t$ by

$$f(s, t) = T_t(s), \qquad (s, t) \in A_s,$$

$$f(s, t) = T_s(t), \qquad (s, t) \in A_t,$$

and suppose that it is continuous in A. Let us do the change of variables,

$$s = s_0 + i[w^2 + 2w + \tau], \qquad w = w_r + iw_i,$$
$$t = t_0 + i[w^2 - 2w + \tau], \qquad \tau = \tau_r + i\tau_i. \tag{1}$$

The points (w_r, w_i), images of $\mathrm{Im}\, t = 0$ ($\mathrm{Im}\, s = 0$), are lying on the two branches of the hyperbola $w_r = 1 \pm (1 + w_i^2 - \tau_r)^{\frac{1}{2}}$; $[w_r = -1 \pm (1 + w_i^2 - \tau_r)^{\frac{1}{2}}]$. For every value of (τ_r, τ_i), when $0 \leq \tau_r < 1$, the points of the w-plane

$$[w_r, w_i : w_r = 1 - (1 + w_i^2 - \tau_r)^{\frac{1}{2}};\ -(\tau_r)^{\frac{1}{2}} \leq w_i \leq (\tau_r)^{\frac{1}{2}}]$$
$$\cup\ [w_r, w_i : w_r = -1 + (1 + w_i^2 - \tau_r)^{\frac{1}{2}};\ -(\tau_r)^{\frac{1}{2}} \leq w_i \leq (\tau_r)^{\frac{1}{2}}]$$

are lying on a Jordan curve Γ_τ. Γ_τ shrinks to zero when $\tau_R = 0$. τ will be allowed to move only in the set Δ for which $\Gamma_\tau \subset A$. Let us call $g_\tau(w)$ the restriction of $f(s, t)$ to Γ_τ. For each value of τ,

$$G_\tau(w) = \int_{\Gamma_\tau} \frac{g_\tau(\xi)}{\xi - w}\, d\xi \tag{2}$$

is an analytic function of w in R_τ, Γ_τ being the boundary of $\bar{R}_\tau$. We now prove also that $G_\tau(w)$ on Γ_τ is equal to $g_\tau(w)$. This is true if and only if, for every $h(w)$ holomorphic in an open set containing $\bar{R}_\tau$, we have

$$L(\tau) = \int_{\Gamma_\tau} h(w) g_\tau(w)\, dw = 0, \quad \text{for} \quad \tau \in \Delta.$$

Now: (a) $L(\tau) = 0$ when $\tau_R = 0$; (b) $L(\tau)$ is continuous in Δ; (c) $L(\tau)$ is holomorphic in the Int (Δ). The last statement will be proved later and it will be seen to follow from the holomorphy in A_s' and A_t'. From (a), (b), and (c) it follows that $L(\tau)$ vanishes in Δ. We conclude that $G_\tau(w)$ for each $\tau \in \Delta$ is an analytic function of $w \in R_\tau$ and $G_\tau(w)\,|_{w \in \Gamma_\tau} = g_\tau(w)$. $G_\tau(w)$ is uniquely determined from $g_\tau(w)$. Let us prove also that $G_\tau(w)$ for each value of w is holomorphic in τ. If $w = \bar{w}$, $\tau_r(\bar{w})$ is the real part of that τ value, so that $\bar{w} \in \Gamma_{\tau(\bar{w})}$. When $\tau_r > \tau_r(\bar{w})$ the denominator in (2) can never vanish; $G_\tau(\bar{w})$ is also continuous in τ. $G_\tau(\bar{w})$ will be holomorphic in τ when $\tau_r > \tau_r(\bar{w})$ if it is true that

$$\oint G_\tau(\bar{w})\, d\tau = 0$$

for each Jordan curve. The proof of the last step is the same as the proof of the point (c), with the choice

$$h(\bar{w}) = (\xi - \bar{w})^{-1}.$$

By means of the Hartog theorem, $G_\tau(w)$ is an analytic function in an open set of C^2 in (w, τ). Since from (1) w and τ are polynomials in s, t, it follows that

$$T(s, t) = G_{\tau(s,t)}[w(s, t)],$$

is analytic in the image $u(s_0, t_0)$ of the open set in C^2 in which $G_\tau(w)$ is holomorphic. $T_s(t)$, $T_t(s)$ are its restrictions. Provided that $0 < \epsilon_i' < \epsilon_i$, it is easy to see that

$$[s : |\mathrm{Re}\, s - s_0| < \epsilon_1';\ 0 < \mathrm{Im}\, s < \epsilon_2'] \times [t : |\mathrm{Re}\, t - t_0| < \epsilon_3';\ 0 < \mathrm{Im}\, t < \epsilon_4']$$

is contained in $u(s_0, t_0)$. By repeated application of this procedure to each of the open sets covering F, the proof is concluded.

We can also establish a more general result: in Ref. 1 it was proved also that the scattering amplitude is an analytic function of the "squared external mass" ρ in a strip $0 < \mathrm{Im}\, \rho < |\delta|$, $\mathrm{Re}\, \rho < 4\mu^2$ (stability condition) for each physical pair s, t. Since the theorem of Zerner holds for an arbitrary number of variables, it follows that there exists a function

$$T(s, t, \rho),$$

holomorphic in some open sets of C^3, whose value on the boundary

$$\lim_{\substack{\epsilon, \epsilon' \to 0^+ \\ \eta \to 0}} T(\mathrm{Re}\, s + i\epsilon, \mathrm{Re}\, t + i\eta, \mathrm{Re}\, \rho + i\epsilon')$$

is the scattering amplitude.

Proof of (c): From the continuity of $L(\tau)$, the holomorphy of $L(\tau)$ follows if

$$\oint L(\tau)\, d\tau = 0$$

holds for any rectangle in the τ-plane with its sides parallel to the axis. Let us choose an infinitesimal rectangle whose center is $\tau_r^{(0)}$, $\tau_i^{(0)}$. We have

$$\oint L(\tau)\, d\tau = -2\, d\tau_r [f(\tau_r^{(0)}, \tau_i^{(0)} + d\tau_i) - f(\tau_r^{(0)}, \tau_i^{(0)} - d\tau_i)] + 2i\, d\tau_i [f(\tau_r^{(0)} + d\tau_r, \tau_i^{(0)}) - f(\tau_r^{(0)} - d\tau_r, \tau_i^{(0)})], \tag{3}$$

where $f(\tau_r, \tau_i)$ is conveniently written

$$f(\tau_r, \tau_i) = \int_{-\tau_i - 2(\tau_r)^{\frac{1}{2}}}^{-\tau_i + 2(\tau_r)^{\frac{1}{2}}} dx_2 \frac{dw}{dx_2} h[w_r(x_2, \tau), w_i(x_2, \tau)] \times g[x_1(x_2, \tau), y_1(x_2, \tau); x_2, y_2 = 0] + \int_{-\tau_i - 2(\tau_r)^{\frac{1}{2}}}^{-\tau_i + 2(\tau_r)^{\frac{1}{2}}} dx_1 \frac{dw}{dx_1} h[w_r(x_1, \tau), w_i(x_1, \tau)] \times g[x_1, y_1 = 0; x_2(x_1, \tau), y_2(x_1, \tau)], \tag{4}$$

where

$$g[x_1(x_2, \tau), y_1(x_2, \tau); x_2, y_2 = 0] \equiv T_{t'}(s'),$$

$$g[x_1, y_1 = 0; x_2(x_1, \tau); y_2(x_1, \tau)] \equiv T_{s'}(t').$$

An elementary proof of the vanishing of (3) is the following. The limits of integrations in (4) and the arguments of $dw/dx_{1,2}$, h, g depend on τ_r, τ_i. (3) vanishes due to the continuity of the integral function when the limits of integrations are varied. The contribution to (3) coming from $(\partial/\partial\tau_{i,r})(\partial w/\partial x_{1,2})$ can be proved to vanish on account of

$$\frac{\partial^2 w_r}{\partial\tau_r\,\partial x_{1,2}} = -\frac{\partial^2 w_i}{\partial\tau_i\,\partial x_{1,2}}, \text{ and } \frac{\partial^2 w_r}{\partial\tau_i\,\partial x_{1,2}} = \frac{\partial^2 w_i}{\partial\tau_r\,\partial x_{1,2}}.$$

Finally, the contributions to (3) coming from the variation of the arguments of h and g are proportional, respectively, to

$$\frac{\partial h}{\partial w_r} + i\frac{\partial h}{\partial w_i}; \qquad \frac{\partial g}{\partial x_{1,2}} + i\frac{\partial g}{\partial y_{1,2}}.$$

The first vanishes on Γ_τ and the second vanishes almost everywhere on Γ_τ, on account of the analyticity properties of h and g.

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Continuity of Bound and Unbound States in a Fermi Gas: A Soluble Example*

CHANCHAL K. MAJUMDAR
Carnegie Institute of Technology, Pittsburgh, Pennsylvania
(Received 20 August 1965)

Considering a gas of independent fermions in the presence of an attractive localized potential, one can show that the properties of the system as a whole are smooth (analytic) functions of the strength parameter of the potential, even at those values where new single-particle bound states appear. Thus for the system as a whole, the transition from "unbound" to "bound" states is continuous and the concept of a bound state cannot be made precise. This is illustrated here for a simple mathematically soluble model—noninteracting spinless fermions moving in the presence of a delta-function potential in one dimension. Some related physical ideas are also presented.

IN an article on electrons in transition metals, Mott discussed the question of the existence of bound states in a potential embedded inside a Fermi gas and reached the conclusion[1]: "In terms of a many electron wave function, the question whether a bound state exists does not admit of a precise answer." A mathematical discussion of this problem does indeed lead to the concept of the continuity of bound and unbound states in a Fermi gas as demonstrated recently.[2] The proof given for short-range potentials (in three dimensions) is necessarily abstract. The purpose of this article is to present a simple example—one-dimensional spinless fermions moving in the presence of a single delta-function potential. It is well-known that the attractive delta-function potential in one dimension has always a bound state, and the lowest single-particle level will show a nonanalytic behavior as the strength parameter of the potential λ becomes attractive. One has here a particularly fortunate opportunity to study the detailed analytic behavior of the properties of the Fermi gas while the potential is present, since the delta function is mathematically so simple.

We shall first formulate the problem in fairly general terms for a general class of potentials. We shall then restrict ourselves to the delta-function case, and show the following: Although the lowest single-particle level shows a nonanalytic behavior at $\lambda = 0$ as the size of the system goes to infinity, the ground-state energy and the single-particle density matrix of the Fermi gas remain analytic functions of λ in a finite strip containing the entire real axis.

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[1] N. F. Mott, Advan. Phys. 13, 325 (1964), p. 360.
[2] W. Kohn and C. Majumdar, Phys. Rev. 138, A1617 (1965).

1. FORMULATION OF THE PROBLEM

The formulation of the problem for one dimension is slightly different from that for three dimensions.[2] We consider a system of N noninteracting fermions in the presence of an external potential $\lambda V(x)$, λ being the strength parameter of the potential. The complete description of the system is given by the quantum mechanical density matrix of N particles;

$$\langle x_1, x_2, \cdots x_N| \rho_N |x_1', x_2', \cdots x_N'\rangle = \Psi^*(x_1', x_2', \cdots x_N')\Psi(x_1, x_2, \cdots x_N). \quad (1.1)$$

$\Psi(x_1, x_2, \cdots x_N)$ is the wavefunction of the N-particle system. For noninteracting fermions in an external potential, this is just the ordinary Slater determinant made up of single-particle eigenfunctions of the potential. The density matrix ρ_N can then be completely written out in terms of the one-particle density matrix ρ_1:

$$\langle x_1, x_2, \cdots x_N| \rho_N |x_1', x_2', \cdots x_N'\rangle = \frac{1}{N!}\begin{vmatrix} \langle x_1|\rho_1|x_1'\rangle & \langle x_1|\rho_1|x_2'\rangle & \cdots & \langle x_1|\rho_1|x_N'\rangle \\ \langle x_2|\rho_1|x_1'\rangle & \langle x_2|\rho_1|x_2'\rangle & \cdots & \langle x_2|\rho_1|x_N'\rangle \\ \vdots & \vdots & & \vdots \\ \langle x_N|\rho_1|x_1'\rangle & \langle x_N|\rho_1|x_2'\rangle & \cdots & \langle x_N|\rho_1|x_N'\rangle \end{vmatrix}, \quad (1.2)$$

where, in our case of real boundary conditions,

$$\langle x|\rho_1|x'\rangle = \sum_{i=1}^{N} \phi_i(x')\phi_i(x). \quad (1.3)$$

The sum over i goes over the N single-particle orthonormal real eigenfunctions ϕ_i occupied and therefore occurring in the Slater determinant. The eigenfunctions in the absence of the potential are solutions of the equation ($\hbar = 1$, $m = \frac{1}{2}$)

$$(d^2\psi/dx^2) + E\psi(x) = 0, \quad (1.4)$$

with the boundary conditions that the wavefunctions be zero at the walls of the one-dimensional box, $x = \pm\frac{1}{2}L$. In the presence of the potential, the eigenfunctions satisfy

$$(d^2\psi/dx^2) + E\psi(x) - \lambda V(x)\psi(x) = 0, \qquad (1.5)$$

while the boundary conditions remain unchanged. We assume $V(x)$ to be short-ranged and sufficiently well-behaved (for instance, Lebesgue-integrable). Now we construct functions which are solutions of (1.5), $\psi(x; E, \lambda)$, satisfying the boundary conditions

$$\psi(\tfrac{1}{2}L; E, \lambda) = 0, \qquad \psi'(\tfrac{1}{2}L; E, \lambda) = 1. \qquad (1.6)$$

Since the boundary conditions are independent of λ, it follows from a theorem of Poincaré[3] that for fixed E and x, $\psi(x; E, \lambda)$ is an integral function of λ. We can now obtain eigenfunctions $\psi_i(x; E, \lambda)$ of our problem from this family of functions ψ by satisfying the other boundary condition

$$\psi(-\tfrac{1}{2}L; E, \lambda) = 0. \qquad (1.7)$$

Equation (1.7) is actually an eigenvalue equation, and will give a set of eigenvalues $E_i(\lambda)$ with a set of eigenfunctions $\psi_i[x; E_i(\lambda), \lambda]$ which, however, are not normalized. Since this is a Sturm–Liouville problem, the eigenvalues will be in general non-degenerate.[4] $\psi_i[x; E_i(\lambda), \lambda]$ need not be integral functions of λ, for $E_i(\lambda)$ is not fixed, but is a function of λ. We define also the normalization

$$N[E_i(\lambda), \lambda] = \int_{-\frac{1}{2}L}^{\frac{1}{2}L} \psi_i^2[x; E_i(\lambda), \lambda]\, dx. \qquad (1.8)$$

By normalization we obtain the real orthonormal eigenfunctions ϕ_i used in (1.3).

To determine the analytic behavior of ρ_1 as a function of λ, we now write $\langle x|\ \rho_1\ |x'\rangle$ as a contour integral:

$$\begin{aligned}\langle x|\ \rho_1\ |x'\rangle &= \sum_{i=1}^{N} \phi_i(x')\phi_i(x) \\ &= \sum_{i=1}^{N} \frac{\psi_i[x; E_i(\lambda), \lambda]\psi_i[x'; E_i(\lambda), \lambda]}{N[E_i(\lambda), \lambda]} \\ &= \frac{1}{2\pi i}\int_C \sum_i \frac{\psi(x; E, \lambda)\psi(x'; E, \lambda)}{N(E, \lambda)[E - E_i(\lambda)]}\, dE.\end{aligned} \qquad (1.9)$$

The contour C encloses only the first N eigenvalues on the real E-axis for a certain real λ; the singularities coming from the zeros of the normalization $N(E, \lambda)$, as shown below, lie off the real axis and are not included inside C. The contour C crosses the real E-axis at the chemical potential μ, which is fixed, and is closed on the left (Fig. 1). Of course we will ultimately take the limit $N \to \infty$, $L \to \infty$, keeping N/L constant. It may be noted that we have used two "unstarred" functions, $\psi(x; E, \lambda)$. The advantage is as follows. When we make λ or E complex, the functions $\psi(x; E, \lambda)$ are integral functions by Poincaré's theorem, but the complex conjugated or "starred" functions are not. For real λ, the expression (1.9) reduces to the correct expression for the density matrix, because we have taken real boundary conditions and the eigenfunctions are real.

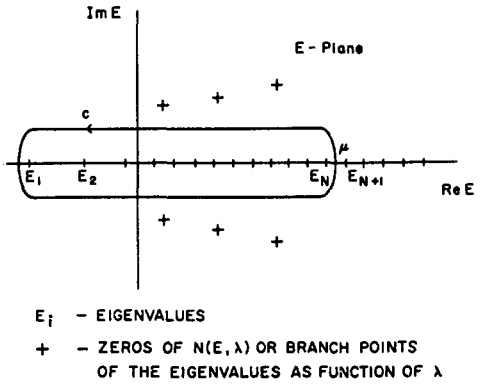


FIG. 1. Contour C for $\langle x|\ \rho_1\ |x'\rangle$ in Eq. (1.9). μ is the fixed chemical potential of the electron system.

We now go back to the normalization

$$N(E, \lambda) = \int_{-\frac{1}{2}L}^{\frac{1}{2}L} \psi^2(x; E, \lambda)\, dx. \qquad (1.10)$$

For fixed λ, this is an integral function of E. The singularities of (1.9) in the E-plane, besides the poles $E_i(\lambda)$, are the zeros of $N(E, \lambda)$. It is easy to find these zeros. Consider two eigenfunctions ψ_1 and ψ_2, fulfilling the boundary conditions as above, which satisfy

$$\begin{aligned}&(d^2\psi_1/dx^2) + E\psi_1(x) - \lambda V\psi_1(x) = 0, \\ &(d^2\psi_2/dx^2) + (E + \delta E)\psi_2(x) \\ &\qquad - (\lambda + \delta\lambda)V\psi_2(x) = 0.\end{aligned} \qquad (1.11)$$

Then we have

$$\begin{aligned}\delta E \int_{-\frac{1}{2}L}^{\frac{1}{2}L} \psi_1\psi_2\, dx - \delta\lambda \int_{-\frac{1}{2}L}^{\frac{1}{2}L} V\psi_1\psi_2\, dx \\ = [\psi_2\psi_1' - \psi_1\psi_2']_{-\frac{1}{2}L}^{\frac{1}{2}L}.\end{aligned} \qquad (1.12)$$

[3] H. Poincaré, Acta Math. 4, 215 (1884); R. Jost, and A. Pais, Phys. Rev. 82, 840 (1951).

[4] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1953), Vol. I, p. 293.

Since by the boundary conditions, the right-hand side vanishes, we have

$$\frac{d\lambda}{dE} = \int_{-\frac{1}{2}L}^{\frac{1}{2}L} \psi_1^2\, dx \Big/ \int_{-\frac{1}{2}L}^{\frac{1}{2}L} V\psi_1^2\, dx, \\ = N(E, \lambda) \Big/ \int_{-\frac{1}{2}L}^{\frac{1}{2}L} V(x)\psi_1^2(x)\, dx. \tag{1.13}$$

Thus the zeros of $N(E, \lambda)$ correspond to $d\lambda/dE = 0$ (cf. Ref. 2). In orther words they occur at the branch points of the eigenvalues $E_i(\lambda)$ regarded as a function of λ. For real λ and real E, the normalization is never zero; this ties in with the fact that the eigenvalues of the Sturm–Liouville problem are simple. This fact was used in writing (1.9) as a contour integral by keeping λ real.

Now we make λ complex. By Poincaré's theorem, the eigenfunctions $\psi(x; E, \lambda)$ are integral functions of E for any definite (x, λ). But the eigenvalues $E_i(\lambda)$ wander off into the complex plane. It is known from some considerations of Hadamard[5] that $\langle x|\ \rho_1(\lambda)\ |x'\rangle$ will have a singularity in the λ-plane when two poles of the integrand in (1.9) in the E-plane, one from inside the contour C and another from outside it, tend to coalesce at some value of λ and the contour becomes "pinched" between these singularities. We have to consider two possibilities: (1) Two poles $E_i(\lambda)$ may coalesce or (2) a pole $E_i(\lambda)$ from inside may approach a zero of $N(E, \lambda)$ which was outside. Since the zeros of $N(E, \lambda)$ are coincident with the branch points of $E_i(\lambda)$ we do not get any additional singularities from the second case, and will simply investigate the coalescence of two poles $E_i(\lambda)$ from two sides of the contour. This, therefore, requires the knowledge of the movement of the eigenvalues E_i as a function of λ. For almost any potential this would be difficult; only in the case of the delta function have we carried out the investigation completely.

So far as the ground-state energy is concerned, we have a formula similar to (1.9):

$$E_0(\lambda) = \frac{1}{2\pi i}\int_C E\ \mathrm{Tr}\frac{1}{E - H}\, dE \\ = \frac{1}{2\pi i}\int_C E \sum_i \frac{dE}{E - E_i(\lambda)}, \tag{1.14}$$

where the contour C is the same as before. By using the eigenfunctions themselves in evaluating the trace, one can avoid explicit appearance of the functions ψ in the numerator. The problem of determining $E_i(\lambda)$ remains the same as before.

[5] J. Hadamard, Acta Math. 22, 191 (1898); J. Tarski, J. Math. Phys. 1, 154 (1960).

2. ONE-DIMENSIONAL FERMION SYSTEM WITH A δ-FUNCTION POTENTIAL

Consider now a system of spinless fermions of mass $\frac{1}{2}$, enclosed in a one-dimensional box of length L, $-\frac{1}{2}L \leq x \leq \frac{1}{2}L$. The eigenfunctions with rigid wall boundary conditions are sine waves:

$$\phi_n = (2/L)^{\frac{1}{2}} \sin(2\pi n x/L); \tag{2.1}$$

$$p = (2\pi n/L), \qquad n = 1, 2, 3, \cdots. \tag{2.2}$$

We have chosen the odd solutions; a completely analogous discussion can be given for the even solutions. The energy of the N-particle system is obtained by simply putting in the particles in accordance with the Pauli enclusion principle up to the Fermi energy. The Fermi momentum is defined by

$$k_F = 2\pi N/L. \tag{2.3}$$

It is supposed that N $\to \infty$, L $\to \infty$, *keeping the ratio* N/L *constant.* The ground-state energy of the N-particle system can be calculated in this way to be

$$E_0 = \frac{L}{2\pi}\int_0^{k_F} p^2\, dp = \tfrac{1}{3}Nk_F^2, \tag{2.4}$$

so that the energy per particle is $\frac{1}{3}k_F^2$. Now we imagine that we have at the origin a short-range potential, in fact a delta-function potential of strength parameter λ. It is known that this potential has always a bound state and the lowest single-particle level cannot be an analytic function of λ, and has actually a singularity $\lambda = 0$. However, we consider again the N-particle system and compute the ground-state energy $E_0(\lambda)$ as above. We propose to show that $E_0(\lambda)$ has in fact a region of analyticity in the λ-plane, namely, a strip of finite width containing the entire real λ-axis.

The Hamiltonian for the system is

$$H = \sum_p \epsilon_p C_p^+ C_p + \lambda \sum_{p,q} V_q C_{p+q}^+ C_p. \tag{2.5}$$

λ will be a complex number in general. The fermion operators satisfy the usual anticommutation rules

$$\{C_p, C_{p'}^+\} = \delta_{p,p'}. \tag{2.6}$$

The equation of motion is

$$[C_p^+, H] = -\epsilon_p C_p^+ - \lambda \sum_q V_q C_{p+q}^+. \tag{2.7}$$

Let $|\Psi_0\rangle$ be the exact state of energy E_0, and $|\Psi\rangle$ that of energy E. Then

$$\langle\Psi|\ C_p^+ H - HC_p^+\ |\Psi_0\rangle \\ = -\epsilon_p\langle\Psi|\ C_p^+\ |\Psi_0\rangle - \lambda \sum_q V_{p-q}\langle\Psi|\ C_q^+\ |\Psi_0\rangle,$$

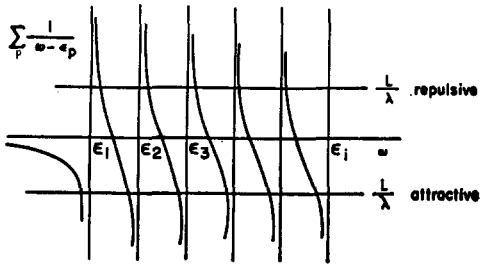


FIG. 2. Solution of Eq. (2.13) for the eigenvalues.

or

$$(\omega - \epsilon_p)\langle\Psi|\, C_p^+\, |\Psi_0\rangle = \lambda \sum_q V_{p-q}\langle\Psi|\, C_q^+\, |\Psi_0\rangle, \quad (2.8)$$

where

$$\omega = E - E_0. \quad (2.9)$$

Putting

$$\langle\Psi|\, C_p^+\, |\Psi_0\rangle = f_p, \quad (2.10)$$

we get

$$(\omega - \epsilon_p) f_p = \lambda \sum_q V_{p-q} f_q. \quad (2.11)$$

Since we take the potential to be a delta-function, we put

$$V_{p-q} \equiv 1/L. \quad (2.12)$$

Hence

$$(\omega - \epsilon_p) f_p = \frac{\lambda}{L} \sum_q f_q,$$

and the eigenvalue equation becomes

$$\frac{L}{\lambda} = \sum_p \frac{1}{\omega - \epsilon_p}. \quad (2.13)$$

Schematically the solution of (2.13) is shown in Fig. 2. For repulsive potential nothing particular happens—all the energy levels are pushed up a little. For negative real λ, i.e., attractive potential, there is always one solution below the unperturbed eigenvalues. The behavior of the eigenvalues ω as a function of real λ is shown in Fig. 3. In the limit $L \to \infty$, for the attractive case, there is a bound state for any λ with energy proportional to λ^2, while for repulsive potential there is no such splitting off of a state from the continuum. These are well-known facts.

The unperturbed energies $\epsilon_p = p^2$, and using (2.2) we get

$$\frac{L}{\lambda} = \sum_{n=1}^{\infty} \frac{1}{\omega - (2\pi n/L)^2} = \frac{L^2}{8} \frac{\frac{1}{2}L\omega^{\frac{1}{2}} \cot(\frac{1}{2}L\omega^{\frac{1}{2}}) - 1}{(\frac{1}{2}L\omega^{\frac{1}{2}})^2}, \quad (2.14)$$

or

$$\frac{\lambda L}{8} = \frac{(\frac{1}{2}L\omega^{\frac{1}{2}})^2}{\frac{1}{2}L\omega^{\frac{1}{2}} \cot(\frac{1}{2}L\omega^{\frac{1}{2}}) - 1} \equiv f(\omega). \quad (2.15)$$

In (2.14) we make use of the well-known partial fraction decomposition of the cotangent[6] and $\omega^{\frac{1}{2}}$ is defined to be the positive square root.

Equation (2.15) gives the strength parameter λ as a function of ω, the energy variable. The problem now is to obtain the inverse relation ω as a function of λ, $\omega = f^{-1}(\lambda) \equiv F(\lambda)$. Clearly ω is a multivalued function of λ; for real λ, the eigenvalues of physical interest are obtained (Fig. 3).

To ascertain the presence of algebraic singularity, we want the roots of

$$d\lambda/d\omega \equiv df(\omega)/d\omega = 0. \quad (2.16)$$

If we assume these zeros of $f(\omega)$ to be simple, the values of λ obtained from (2.15) from these zeros represent branch points of order one. At such a branch point, two sheets of the Riemann surface of the function $\omega = F(\lambda)$ are connected. A general argument that the zeros will be simple can be supplied[2] and we verify explicitly that they are simple in Fig. 8 where only double points appear. Now

$$f'(\omega) = \tfrac{1}{8}L^2/\{\tfrac{1}{2}L\omega^{\frac{1}{2}} \cot(\tfrac{1}{2}L\omega^{\frac{1}{2}}) - 1\}^2 \times (\tfrac{1}{4}L^2\omega \operatorname{cosec}^2 \tfrac{1}{2}L\omega^{\frac{1}{2}} - 2 + \tfrac{1}{2}L\omega^{\frac{1}{2}} \cot \tfrac{1}{2}L\omega^{\frac{1}{2}}). \quad (2.17)$$

Put $\omega = k^2$, the upper-half k-plane is, by definition, the physical sheet. Setting $\frac{1}{2}Lk = Z$, we have to solve

$$f'(\omega) \equiv \frac{L^2}{8} \frac{Z^2 \csc^2 Z - 2 + Z \cot Z}{(Z \cot Z - 1)^2} = 0. \quad (2.18)$$

The numerator and the denominator diverge together, so the infinities of the denominator are excluded. In the numerator, $Z = 0$ is obviously a solution, but at that point the denominator also vanishes. Besides $Z = 0$, which is not a true solution, all the other solutions are obtained from the zeros

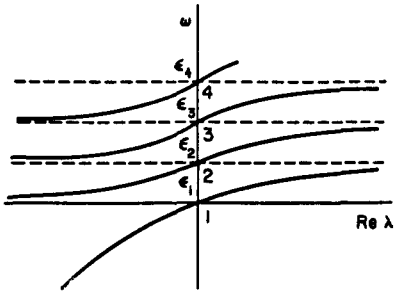


FIG. 3. The eigenvalues plotted as a function of Re λ. These define the different sheets of the Riemann surface of the function $\omega = \omega(\lambda)$.

[6] E. C. Titchmarsh, *The Theory of Functions* (Oxford University Press, London, 1939), p. 113.

of the numerator:

$$u(Z) = Z^2 - 2 + Z^2 \cot^2 Z + Z \cot Z = 0. \quad (2.19)$$

Obviously

$$u(-Z) = u(Z). \quad (2.20)$$

Also u is a real analytic function[7] so that

$$u(Z^*) = u^*(Z). \quad (2.21)$$

This means that all the zeros of (2.19), if they exist, must come in groups of four, that is, $\pm Z_i$ and $\pm Z_i^*$ are simultaneously roots of (2.19). We are interested in the roots of the upper-half plane only, which corresponds to the physical sheet. Clearly, it is enough to investigate the roots in the first quadrant.

Except $Z = 0$, there are no other zeros of $u(Z)$ on the real or the imaginary axis, so all other zeros must be complex. For real $Z \equiv x$, $u(x)$ shows a series of minima between infinities at $n\pi$ but remains positive. By the usual argument of function theory,[8] one expects that the function will decrease at right angles to the real axis at these minima and the zeros may be expected to straddle the real axis in the complex Z-plane. Also the minima are successively larger in height as one proceeds along the real axis (Fig. 4), hence the zeros will be probably moving away from the real axis.

For any fixed value of x, there cannot be any solution to (2.19) for sufficiently large values of $\operatorname{Im} Z \equiv y$; for,

$$\cot Z = i \frac{e^{i(x+iy)} + e^{-i(x+iy)}}{e^{i(x+iy)} - e^{-i(x+iy)}} \underset{y\to\infty}{\to} -i,$$

and

$$-2 + i^2 Z^2 \neq 0.$$

Thus, sufficiently far from the real axis, there are no zeros.

The location of complex zeros is always a complicated problem. In our case, the existence of the complex zeros as solutions of Eq. (2.19) is assured by Picard's theorem.[9] We note that $u(Z)$ is a meromorphic function of Z, and therefore by Hadamard's theorem,[10] can be written as the quotient of two integral transcendental functions of Z. The zeros of the integral function in the numerator are the zeros of the meromorphic function. We know that this integral function has a zero at $Z = 0$. Now Picard's theorem states that an integral function that is not a polynomial will take every value, with at most one exception, an infinity of times. Clearly 0 is not an exceptional value[11] and thus $u(Z)$ has an infinite number of zeros.[12]

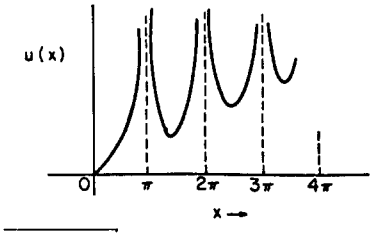


FIG. 4. The function $u(x)$ has no other zeros except the one at the origin.

We can find out the distribution of zeros for large $|Z|$ as follows. Write (2.19) as

$$Z \cot Z + Z^2 \csc^2 Z = 2,$$

or

$$Z \csc^2 Z + \cot Z = 2/Z \approx 0. \quad (2.22)$$

for large $|Z|$. (Notice that, by definition, Z is proportional to L and we will make $L \to \infty$.) Thus the roots are approximately given by

$$Z \csc Z + \cos Z = 0,$$

or

$$Z = -\sin Z \cos Z;$$

putting $W = 2Z$, we get

$$\sin W = -W. \quad (2.23)$$

Decomposing into real and imaginary parts, $W = x' + iy'$,

$$\sin x' \cosh y' = -x', \quad (2.24)$$

$$\cos x' \sinh y' = -y'. \quad (2.25)$$

We have to solve the two transcendental equations simultaneously. The solutions are the intersections of the two curves

$$\begin{aligned} &\text{(i)} \quad x' = \cos^{-1}(-y'/\sinh y'), \\ &\text{(ii)} \quad y' = \cosh^{-1}(-x'/\sin x'), \end{aligned} \quad (2.26)$$

and are given qualitatively in Fig. 5.

[7] Reference 6, p. 155.
[8] Reference 6, p. 167.
[9] Reference 6, p. 277.
[10] Reference 6, p. 284g.
[11] Reference 6, p. 278.
[12] Actually what we have proved is this: *If* there are zeros as solutions of (2.18), they are obtained from (2.19). But we have not shown the existence of complex zeros of (2.18) as yet. The function (2.18) is itself a meromorphic function. An extension of Picard's theorem states that a meromorphic function takes every value, with at most two exceptions, an infinity of times [see R. Nevanlinna, *Le Théorème de Picard–Borel*, (Gauthier-Villars, Paris, 1929)]. We have not shown that the zeros of (2.19) are not canceled by some zeros of the denominator, that is, zero may still be an exceptional value of (2.18). In order to settle this point, if not for the sake of completeness, we have to draw the Riemann surfaces of Figs. 8 and 9 to convince ourselves that double points indeed appear at the expected solutions of (2.19).

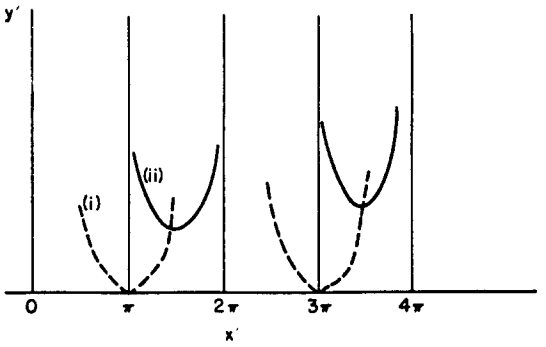


FIG. 5. Schematic solution of (2.26).

The branch points occur for

$$x' \approx (4n - 1)\tfrac{1}{2}\pi \quad \text{or} \quad x \approx n\pi - \tfrac{1}{4}\pi. \tag{2.27}$$

Using the definition of z, this gives

$$L \operatorname{Re} k \simeq 2n\pi - \tfrac{1}{2}\pi. \tag{2.28}$$

Writing the first of Eqs. (2.25) for large y',

$$\tfrac{1}{2}e^{y'} \sin x' \simeq -x'. \tag{2.29}$$

Hence, when x' is sufficiently large, the solution of (2.29) gives

$$y' \simeq \ln x' \quad \text{or} \quad y \simeq \tfrac{1}{2} \ln x. \tag{2.30}$$

This gives the asymptotic relation between x and y for those values of Z which are solutions of (2.19). To determine the branch points in the λ-plane, we go back to Eq. (2.15) written in terms of Z: For large y, $\cot Z \simeq -i$, and

$$\tfrac{1}{8}\lambda L = Z^2/Z \cot Z - 1 \simeq Z^2/-iZ - 1 \simeq iZ = ix - y. \tag{2.31}$$

Hence

$$\tfrac{1}{8}L \operatorname{Im} \lambda \simeq x = \tfrac{1}{2}L \operatorname{Re} k \quad \text{or} \quad \operatorname{Im} \lambda \simeq 4 \operatorname{Re} k. \tag{2.32}$$

Also

$$\operatorname{Re} \lambda \simeq -8y/L \simeq -8 \ln x/L \simeq -O(\ln L/L). \tag{2.33}$$

Similarly from the values $(-x + iy)$ in the Z-plane we get the complex conjugate branch points in the λ-plane:

$$\operatorname{Re} \lambda = -O(\ln L/L), \quad \operatorname{Im}\lambda = -4 \operatorname{Re} k. \tag{2.34}$$

The interesting result is that, asymptotically, the imaginary part of λ is independent of L, the length of the box. The distribution of the double points in the Z-plane and the branch points in the λ-plane are schematically shown in Figs. 6 and 7.

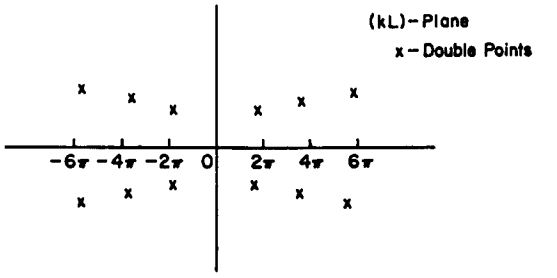


FIG. 6. Structure of the (kL)-plane showing double points.

3. STRUCTURE OF THE REIMANN SURFACE[13]

The next problem is to construct the complete Riemann surface $\omega = F(\lambda)$ and to establish the connectivity of the different sheets. We have found no other way than to plot out a portion of the Riemann surface explicitly and examine it. For this purpose we write (2.15) as

$$\lambda' = Z^2/(Z \cot Z - 1). \tag{3.1}$$

Putting $Z = x + iy$, and separating real and imaginary parts of λ', we have

$$\begin{aligned} \operatorname{Re} \lambda' &= r \cos \theta = (AC + BD)/(C^2 + D^2), \\ \operatorname{Im} \lambda' &= r \sin \theta = (BC - AD)/(C^2 + D^2), \end{aligned} \tag{3.2}$$

where

$$\begin{aligned} A &= (x^2 - y^2) \sin x \cosh y - 2xy \cos x \sinh y, \\ B &= 2xy \sin x \cosh y + (x^2 - y^2) \cos x \sinh y, \\ C &= x \cos x \cosh y + y \sin x \sinh y - \sin x \cosh y, \\ D &= y \cos x \cosh y - x \sin x \sinh y - \cos x \sinh y. \end{aligned} \tag{3.3}$$

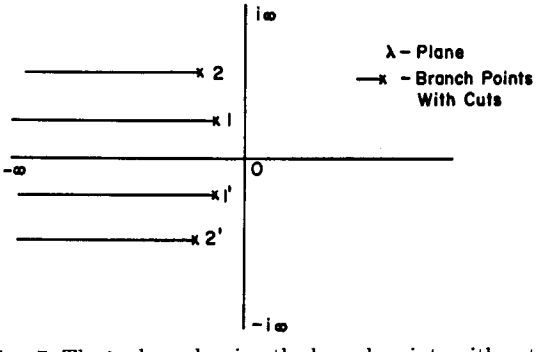
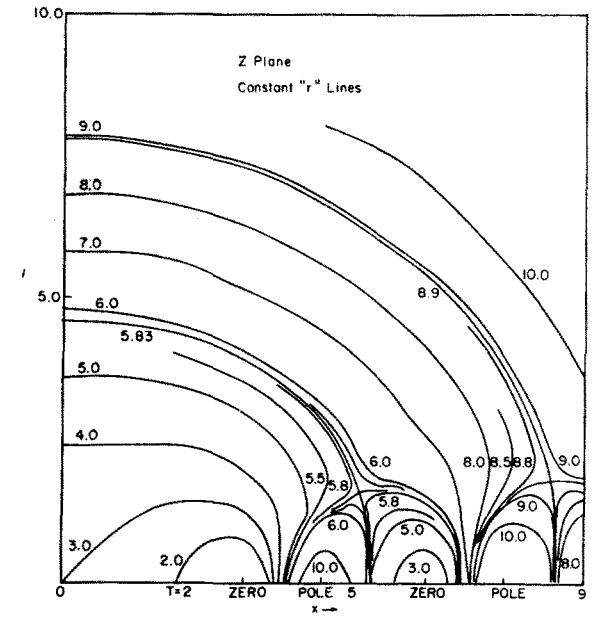
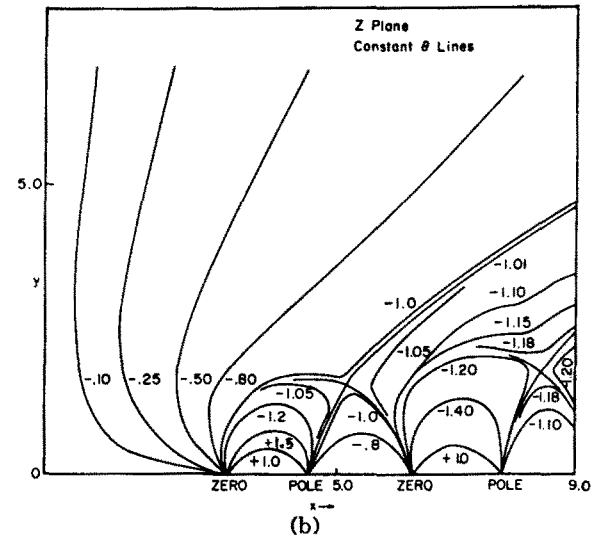


FIG. 7. The λ-plane showing the branch points with cuts.

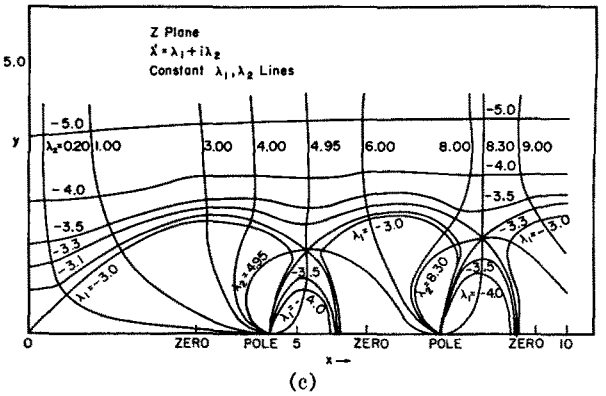
[13] H. Weyl, *Die Idee der Riemannschen Fläche* (Teubner, Stuttgart, Germany, 1923). F. Klein, *On Riemann's Theory of Algebraic Functions and Their Integrals* (Dover Publications, Inc., New York, 1963).



(a)



(b)

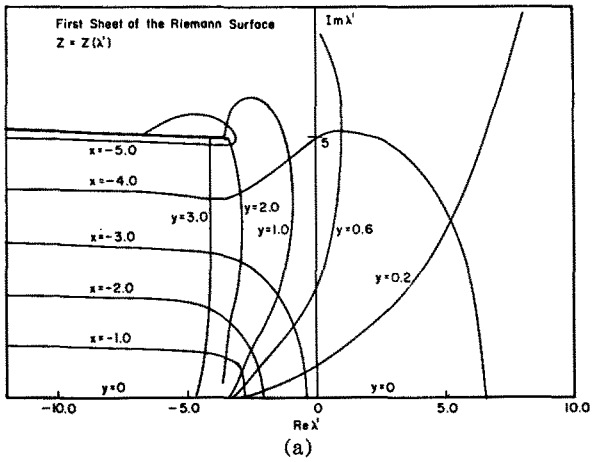


(c)

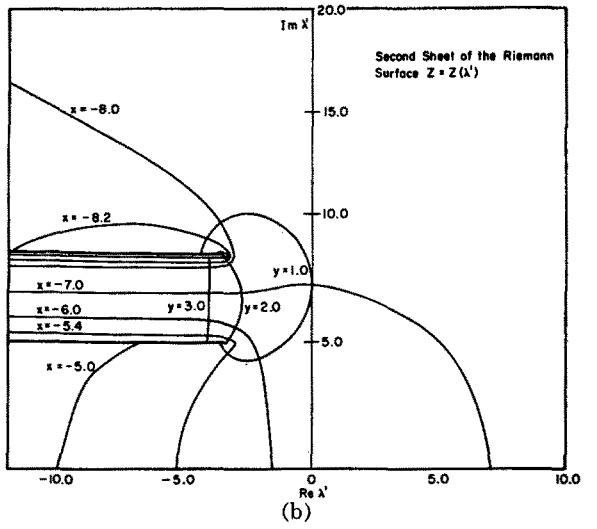
FIG. 8. (a) The Z-plane with constant r-lines. Notice the two double points. (b) The Z-plane with constant θ-lines. These are orthogonal to the constant r-lines. (c) The Z-plane with contours for real and imaginary parts of the function $\lambda' = \lambda'(Z)$.

First we plot out the r = constant and θ = constant contours, and obtain the double points [Figs. 8(a)–(c)]. Incidentally the plot demonstrates that the assumption of simple zeros [Eq. (2.16)] is valid. One also notices that the periodic structure of the double points is of great help in constructing the Riemann surface. Finally, in Figs. 9(a) and 9(b) we have plotted parts of the first and second sheets of the Riemann surface $Z(\lambda')$. This is enough to find the behavior of the function $\omega = F(\lambda)$. The x = constant lines in Fig. 9 clearly show the linking of the sheets across the cuts.

Obviously for real λ, we can arrange the sheets in a definite order (Fig. 3) as there is no crossover. We number them as 1, 2, $\cdots$, starting with the lowest unperturbed eigenvalue. We also number the branch points in the order of their increasing imag-



(a)



(b)

FIG. 9. (a) The first sheet of the Riemann surface, $Z = Z(\lambda')$. Note the single cut. The scales along Re λ' and Im λ' are not the same. (b) The second sheet of the Riemann surface $Z = Z(\lambda')$. Note the two cuts. The lower one is the same cut as in (a). All the higher sheets have similar appearance.

inary parts in the upper-half λ-plane as 1, 2, $\cdots$. The associated complex conjugate branch points are 1′, 2′, $\cdots$, respectively.

At the pair (1, 1′) the first sheet containing the eigenvalue ϵ_1 is connected to the sheet that contains ϵ_2. Clearly the pair (N, N') connects the branch containing the eigenvalue ϵ_N to that containing ϵ_{N+1}. Also every sheet, except the first one, has two pairs of branch points, one conjugate pair connecting it to the next lower one and the other conjugate pair to the next higher one.

Starting from $\lambda = 0$, $\omega = \epsilon_1$, if we go around the branch point 1 (or 1′) and come back to $\lambda = 0$, we reach $\omega = \epsilon_2$. Any other path not containing these branch points brings us back to ϵ_1. Similarly, proceeding from $\omega = \epsilon_{N+1}$ and $\lambda = 0$, and going around the branch point N (or N') to $\lambda = 0$, we arrive at $\omega = \epsilon_N$. If we go around the branch point $(N + 1)$ or $(N + 1)'$, we arrive at ϵ_{N+2}. In Fig. 9 we have drawn the cuts connecting the first to the second sheet and the second to the third sheet. Starting at $\lambda = 0$, $\omega = \epsilon_2$, and going around both the branch points 2 and 1 back to $\lambda = 0$ along a positively oriented contour, that is, a path that keeps the branch points to its left, one clearly ends up at ϵ_3. A traversal of the same path in the reverse direction leads however to ϵ_1.

4. CONTINUITY OF BOUND AND UNBOUND STATE

We are now ready to examine the analyticity of the ground-state properties in the λ-plane. Consider Eq. (1.14) first. We have the first N eigenvalues inside the contour C (Fig. 1) and we want to determine the smallest value of λ for which the contour is pinched.[5] From the structure of the Riemann surface described above, we know that the only coalescence we will have to consider is that of the Nth root with the $(N + 1)$st root. It follows from (2.32) that the critical value of λ is of order k_F, as the imaginary part is $O(k_F)$. Note that the result is independent of L, the length of the box, in the limit $L \to \infty$.

The branch points responsible for the singularity are the Nth and N'th branch points of the Riemann surface, and they are away from the real axis by a distance $O(k_F)$. This leaves a strip of finite width parallel to the real axis in which one can analytically continue from the positive-λ to the negative-λ side.

Similarly we can apply the above argument to the single-particle density matrix (1.9). Combining this with our discussion in Sec. 1,[14] we conclude that the density matrix $\rho_1(\lambda)$ is analytic in a strip of finite width enclosing the real λ-axis. Obviously, there is a possibility that the density matrix has a larger region of analyticity. For instance, if the limiting singularity in the energy $E_0(\lambda)$ happens to be a zero of $N(E, \lambda)$ in (1.9), this generates a double pole for $\langle x| \rho_1 |x'\rangle$, and we can move the contour around it. This possibility has not been completely settled.

5. CONCLUSIONS

With the mathematical formalism finished, we turn to its physical interpretation, and expatiate on some examples already mentioned in Ref. 2. The existence of a continuity of state between liquid and gas is of course universally known. In a classic paper on phase transitions, Yang and Lee[15] demonstrated that this could be interpreted as analyticity of pressure and density in a finite strip in the complex plane of fugacity enclosing the entire positive real axis (the physical region). We have simply reversed the procedure to show a continuity between bound and unbound states by finding the analytic behavior of $E_0(\lambda)$ and $\rho_1(\lambda)$ in a domain in the λ-plane including the physical region.

An example of great heuristic value is the well-known phase transformation of metallic Cerium.[16] Solid face-centered-cubic Ce shows a phase transformation with a critical point.[17] Both the phases involved (α and γ) have the same structural symmetry; otherwise such a continuous transition is not possible.[18] The classical expanation of this transition, due to Pauling and Zachariasen,[19] asserts that in the γ-to-α transformation, the bound f-electron

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[14] It is convenient at this point to think of the even solutions of (1.5), in order that Eq. (1.13) may apply unchanged. For odd solutions one can derive the equation

$$EN(E, \lambda) = -\int_{-\frac{1}{2}L}^{\frac{1}{2}L} \psi'^2 \, dx.$$

For real λ and therefore real E, $N(E, \lambda)$ cannot vanish, and the zeros lie again in the complex plane. We have not been able to find their locations. Since the ground-state energy is analytic in a finite strip in the λ-plane, it seems plausible that a similar result holds for the density matrix ρ_1 even for odd solutions. Considering the peculiar nature of the delta function (an "ideal element" in the function space), we are not surprised to face such a difficulty. On the other hand, it is extremely fortunate that is does provide an example of a pathological as well as of a normal situation.

[15] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952).

[16] A. Jayaraman, Phys. Rev. **137**, A179 (1965). We are indebted to Dr. T. Geballe for drawing attention to this work.

[17] For a complete phase diagram, see K. A. Gschneidner, Jr., R. O. Elliott, and R. R. McDonald, J. Phys. Chem. Solids **23**, 555 (1962).

[18] L. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Press, Ltd., London, 1958), p. 260.

[19] L. Pauling [quoted by A. F. Schuch and J. H. Sturdivant, J. Chem. Phys. **18**, 145 (1950)]; W. Zachariasen [quoted by A. Lawson and T. Y. Tang, Phys. Rev. **76**, 301 (1949)].

becomes unbound ($4f \rightarrow 5d$ promotion). The critical point marks the end of this transition of the f-electron, when the degree of ionization $4f \rightarrow 5d$ is 50%. Here in complete analogy with the liquid–gas case, one can think of a continuity between bound and unbound states. It must be emphasized, however, that we are using this as an aid to comprehension rather than a *fait accompli*. Phase transitions are cooperative phenomena and depend critically on electron correlations—a fact not taken into account in our demonstration above. In the presence of weak electron–electron interaction, our conclusion about the analyticity of $E_0(\lambda)$ and $\rho_1(\lambda)$ will not be affected and a continuity between bound and unbound states persists.

It is easy to see that the existence of the limit $N \rightarrow \infty$, $L \rightarrow \infty$, keeping N/L constant, is crucial to the result. If we simply let $L \rightarrow \infty$ without the concomitant $N \rightarrow \infty$, we get the usual results of the potential theory. It is known that the use of a finite box and then the limit $L \rightarrow \infty$, $N \rightarrow \infty$, N/L constant, is a physicist's way of handling the nonseparable Hilbert space appearing in the many-body problem.[20] Perhaps a more sophisticated mathematical treatment would establish our result almost trivially from this basic fact.

Note added in proof. Dr. S. Vosko has kindly pointed out that a different example of the continuity of bound and unbound states may be found in D. Butler, Proc. Phys. Soc. (London) **80**, 741 (1962).

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I would like to thank Professor Walter Kohn for suggesting the problem and patient guidance throughout the course of this work. The financial support of the Office of Naval Research is gratefully acknowledged. Discussions with Dr. L. J. Sham and Dr. R. Griffiths led to clarification of ideas.

[20] R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics and All That* (W. A. Benjamin, Inc., New York, 1964). I am indebted to Professor F. J. Dyson for a discussion on this point.

Gelfand States and the Irreducible Representations of the Symmetric Group*

M. MOSHINSKY
Institudo de Física, Universidad de México, México, D.F.
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The set of Gelfand states corresponding to a given partition $[h_1 \cdots h_n]$ form a basis for an irreducible representation of the unitary group U_n. The special Gelfand states are defined as those for which $[h_1 \cdots h_n]$ is a partition of n and the weight is restricted to $(11 \cdots 1)$. We show that the special Gelfand states constitute basis for the irreducible representations of the symmetric group S_n and use this property to construct explicitly states in configuration and spin–isospin space with definite permutational symmetry.

I. INTRODUCTION

THE symmetric group plays a fundamental role in many branches of physics and particularly in atomic and nuclear shell theory. The construction of states that are bases for irreducible representations (BIR) of the symmetric group is therefore an important task on which much work has been done.[1]

The purpose of this paper is to show that recent developments in the BIR for the unitary groups, i.e., the Gelfand states[2-4] allow us to discuss the BIR for the symmetric group from a simple and fruitful angle. We shall introduce the concept of special Gelfand (SG) states and discuss their properties under permutation showing that they are BIR of the symmetric group. We will then use this concept for the explicit construction of states with permutational symmetry, illustrating our technique by the discussion of states in configuration space, as well as in the spin–isospin space of supermultiplet theory.[5]

II. GELFAND STATES

The work of Gelfand,[2] and later of others,[3,4] indicates that the BIR for the n-dimensional unitary group U_n are given by the Gelfand states

$$|h_{rs}\rangle, \qquad 1 \leq r \leq s \leq n, \tag{1}$$

in which the sth row $[h_{rs}]$ gives the irreducible representation of the subgroup U_s in the chain $U_n \supset U_{n-1} \supset \cdots U_s \supset \cdots \supset U_1$, which defines the bases.

The Gelfand states have been constructed explicitly[3,4] in terms of polynomial expressions in the creation operators $a^+_{\mu s}$ applied to a vacuum state $|0\rangle$. The $a^+_{\mu s}$ can be considered as vectors in an n-dimensional space. We shall interpret[6] $s = 1, \cdots, n$ as the component index of this vector while μ will be the index distinguishing between vectors. We introduce the annihilation operators $a^{\mu s}$ satisfying the commutation rules

$$[a^{\mu' s'}, a^+_{\mu s}] = \delta^{\mu'}_{\mu}\, \delta^{s'}_{s}, \tag{2}$$

and with their help we can write the generators of U_n as

$$C^{s'}_{s} \equiv \sum_{\mu} a^+_{\mu s} a^{\mu s'}, \qquad s, s' = 1, \cdots n. \tag{3}$$

The Gelfand states (1) are eigenstates of the operators C^s_s, $s = 1, \cdots, n$ with eigenvalues w_s given by[3,4,7]

$$w_s = \sum_{r=1}^{s} h_{rs} - \sum_{r=1}^{s-1} h_{r,s-1}. \tag{4}$$

The set of eigenvalues $(w_1 \cdots w_n)$ gives the weight of the state.

The Gelfand state for which $h_{rs} = h_{rn}$ for all $1 \leq r \leq s \leq n$ has, from (4), the weight $(h_{1n} \cdots h_{nn})$, i.e., is of highest weight.[3,4,7] This state will be denoted by $|h_{rn}\rangle$ and its explicit form is

$$|h_{rn}\rangle = \mathrm{N}(h_{rn})(\Delta^1_1)^{h_{1n}-h_{2n}}(\Delta^{12}_{12})^{h_{2n}-h_{3n}} \cdots (\Delta^{1\cdots n}_{1\cdots n})^{h_{nn}} |0\rangle \tag{5}$$

where N is the normalization constant[3,4]

$$\mathrm{N}(h_{rn}) = \left[\prod_{s=2}^{n}\prod_{r=1}^{s-1}(h_{rn} - h_{sn} + s - r)!\right]^{\frac{1}{2}} \times \left[\prod_{r=1}^{n}(h_{rn} + n - r)!\right]^{-\frac{1}{2}} \tag{6}$$

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[1] An excellent summary of many of the aspects of the work done on the symmetric group is given by M. Hamermesh, *Group Theory and its application to physical problems* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1962), Chap. VII and also Chaps. X, XI.

[2] I. M. Gelfand and M. I. Zetlin, Dokl. Akad. Nauk, SSSR 71, 825 (1950).

[3] M. Moshinsky, J. Math. Phys. 4, 1128 (1963).

[4] G. E. Baird and L. C. Biedenham, J. Math. Phys. 4, 1449 (1963).

[5] E. P. Wigner, Phys. Rev. 51, 106 (1937).

[6] We use here an interpretation of the indices μ, s opposite to that employed in Ref. 3. This proves useful when we construct states with permutational symmetry in Secs. V and VI.

[7] J. Nagel and M. Moshinsky, J. Math. Phys. 6, 682 (1965).

and Δ is the determinant

$$\Delta^{s_1 s_2 \cdots s_r}_{\mu_1 \mu_2 \cdots \mu_r} = \sum_{\mathfrak{P}} (-1)^{\mathfrak{P}} \mathfrak{P} a^+_{\mu_1 s_1} a^+_{\mu_2 s_2} \cdots a^+_{\mu_r s_r}, \qquad (7)$$

where $\mathfrak{P}$ stands for a permutation of $s_1, s_2, \cdots s_r$.

III. LOWERING OPERATORS

To obtain all the Gelfand states (1) from the highest-weight state (5), Nagel and Moshinsky[7] introduced the concept of the lowering operator. Specifically, the lowering operator L^r_s, $1 \leq r < s \leq n$ is a polynomial function of the generators $C^{r'}_r$, $r, r' = 1, \cdots, s$ of the U_s group that transforms a Gelfand state of highest weight in U_{s-1}, characterized by the partition $[h_{ps-1}]$ into a Gelfand state, again of highest weight in U_{s-1}, characterized by the partition $[h_{ps-1} - \delta_{pr}]$. The explicit form of the lowering operator is[8]

$$L^r_s = \sum_{p=0}^{s-r-1} \sum_{q_p > q_{p-1} > \cdots q_2 > q_1 = r+1}^{s-1} C^r_{q_1} C^{q_1}_{q_2} \cdots C^{q_p}_s \times \prod_{i=1}^{p} E^{-1}_{rq_i} \prod_{q=r+1}^{s-1} E_{rq}, \qquad (8)$$

where

$$E_{pq} \equiv C^p_p - C^q_q + q - p. \qquad (9)$$

The lowering operators L^r_s and the h_{rs} are only defined for $1 \leq r < s$ and $1 \leq r \leq s$, respectively. We shall introduce though, for convenience in the following discussion, the definitions

$$L^s_s \equiv 1, \qquad h_{s\,s-1} \equiv 0, \qquad s = 1, \cdots, n. \qquad (10)$$

With the help of the lowering operators, the general Gelfand state (1) is obtained from the highest-weight state (5) by the expression

$$|h_{rs}\rangle = \left\{ N(h_{rs}) (L^1_1)^{h_{11}} \prod_{r=1}^{2} (L^r_2)^{h_{r2}-h_{r1}} \cdots \times \prod_{r=1}^{s} (L^r_s)^{h_{rs}-h_{rs-1}} \cdots \prod_{r=1}^{n} (L^r_n)^{h_{rn}-h_{rn-1}} \right\} |h_{rn}\rangle, \qquad (11a)$$

where $N(h_{rs})$ is a normalization constant that, from the discussion in Ref. 7, has the form

$$N(h_{rs}) = \left\{ \prod_{m=2}^{n} \left[\prod_{q \geq p=1}^{m-1} \frac{(h_{pm-1} - h_{qm-1} + q - p)!}{(h_{pm} - h_{qm-1} + q - p)!} \times \prod_{q>p=1}^{m} \frac{(h_{pm-1} - h_{qm} + q - p - 1)!}{(h_{pm} - h_{qm} + q - p - 1)!} \right] \right\}^{\frac{1}{2}}. \qquad (11b)$$

The operators L^r_s with the same lower index s, but with different indices r, when acting on highest weight states of U_s commute, and so their order in (11) is irrelevant. The operators L^r_s with different lower indices s do not commute, and so care should be taken to apply them in the order indicated in (11a).

IV. SPECIAL GELFAND (SG) STATES AND THE BIR OF THE SYMMETRIC GROUP

Let us now define the SG states of U_n as the states (1) for which (a) the representation $[h_{pn}]$ of U_n as a partition of n; (b) the states have weight $(11 \cdots 1)$.

From (4) we see that the condition (b) implies that

$$h_{pn-1} = h_{pn} - \delta_{pr_n}, \qquad h_{pn-2} = h_{pn-1} - \delta_{pr_{n-1}}, \cdots, h_{11} = 1, \qquad (12)$$

and from (a) and the restrictions[2-4] imposed on the representations $[h_{rs}]$, we see that the set of numbers $(1r_2 \cdots r_{n-1} r_n)$ has all the properties of a Yamanouchi symbol.[9] We see that the SG states are fully characterized by $[h_p]$, (r_p) (where we drop the index n in $[h_{pn}]$) and from (11) they are given by

$$|[h_p](r_p)\rangle \equiv |[h_1 \cdots h_n](1r_2 \cdots r_n)\rangle = N([h_p](r_p))(L^1_1 L^{r_2}_2 \cdots L^{r_s}_s \cdots L^{r_n}_n) |h_p\rangle, \qquad (13)$$

where N is a normalization coefficient given by (11b) when the h_{rs} are particularized to the values (12).

The Gelfand states are BIR of U_n and therefore also bases for an, in general, reducible representation of the symmetric subgroup S_n of U_n. The SG states, which are a subset of the set of Gelfand states satisfying (a), will also be a basis for a representation of S_n as the set of operators $C^1_1, C^2_2, \cdots, C^n_n$ is only permuted by the elements of S_n. From the appearance in the SG states of both $[h_p]$ which is a partition of n and (r_p) which has all the properties of a Yamanouchi symbol, we expect the SG states to be BIR of S_n.

To prove this point we shall first determine an operator function of the generators $C^{s'}_s$, $s, s' = 1, \cdots, n$, whose effect on the SG states is the same as that of a permutation.

We start by noticing that because of (a), the SG states are given by homogeneous polynomials in the $a^+_{\mu s}$ of degree n acting on the vacuum state, while because of (b), the polynomials must be of first degree in each value $s = 1, \cdots, n$ of the index s .Therefore the SG states can always be written as

[8] Note that the appearance in (8) of the reciprocal operators $E_{rq_i}{}^{-1}$ is spurious as they are canceled by the operators E_{rq} in the next product. The notation is compact and so we shall use it in preference to stating that the last product in (8) must not contain factors E_{rq_i}.

[9] See Ref. 1, p. 221. We use notation $(1r_2 \cdots r_n)$ for the Yamanouchi symbol rather than $(r_n \cdots r_2 1)$ as it is a more natural one for expressions such as (13).

$$|[h_p](r_p)\rangle = \sum_{\mu_1 \cdots \mu_n} A^{\mu_1 \cdots \mu_n}_{[h_p](r_p)} a^+_{\mu_1 1}\, a^+_{\mu_2 2} \cdots a^+_{\mu_n n}\, |0\rangle, \quad (14)$$

where the A's are some constants.

Let us now apply to the states (14) the operator

$$(rs) \equiv C^r_s C^s_r - 1. \quad (15)$$

Taking a typical term in the summation (14), we immediately see from the definition (3) and the commutation rules (2) that the operator (rs) interchanges the indices r and s in this term. Therefore the operator (rs), when acting on SG states, behaves as a transposition. As all permutations can be expressed by products of transpositions, we see that the effect of a permutation on a SG state can be reproduced by an operator which is a polynomial function of C^s_r, $r, s = 1, \cdots, n$.

We can now ask what is the representation of the symmetric group S_n with respect to SG states. Clearly we can restrict ourselves to representations of transpositions and in fact, only to the transposition $(n-1, n)$ as the other transpositions $(n-2, n-1)$, $(n-3, n-2)$ $\cdots$ (12) are given in terms of the generators of the subgroups U_{n-1}, U_{n-2}, $\cdots$, U_2 of U_n and so are obtained when we discuss the representations of $S_{n-1}, S_{n-2}, \cdots, S_2$, respectively.

The representation of the transposition $(n-1, n)$ is given by the matrix

$$||\langle [h_p](r'_p)|\, C^{n-1}_n C^n_{n-1} - 1\, |[h_p](r_p)\rangle||. \quad (16)$$

To evaluate the matrix elements, let us first write $r_n \equiv r$, $r_{n-1} \equiv s$ so that the Yamanouchi symbols become $(1r_2 \cdots r_{n-2}sr)$ and similarly for (r'_p). Noticing[2,4,10] then that the matrix elements of C^{n-1}_n are independent of the representations of $U_{n-3} \supset \cdots \supset U_2 \supset U_1$, and diagonal in those of U_{n-2}, and that C^n_{n-1} is a raising generator[3] with the Hermitian property $C^n_{n-1} = (C^{n-1}_n)^+$, we obtain

$$\begin{aligned}
&\langle [h_1 \cdots h_n](1r'_2 \cdots r'_{n-2}s'r')| \\
&\times (C^{n-1}_n C^n_{n-1} - 1)\, |[h_1 \cdots h_n](1r_2 \cdots r_{n-2}sr)\rangle \\
&= \Bigg\{ \delta_{r'r}\, \delta_{s's} \Bigg[(1+\delta_{rs})^{-1} \left\langle \begin{array}{c} h_p \\ h_p - \delta_{pr} \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right| C^{n-1}_n \left| \begin{array}{c} h_p \\ h_p \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right\rangle \\
&\times C^{n-1}_n \left| \begin{array}{c} h_p \\ h_p \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right\rangle \Bigg]^2 - 1 \Bigg] + \delta_{r's}\, \delta_{s'r} (1+\delta_{rs})^{-1}
\end{aligned}$$

$$\begin{aligned}
&\times \left\langle \begin{array}{c} h_p \\ h_p - \delta_{pr} \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right| C^{n-1}_n \left| \begin{array}{c} h_p \\ h_p \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right\rangle \\
&\times \left\langle \begin{array}{c} h_p \\ h_p - \delta_{ps} \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right| C^{n-1}_n \left| \begin{array}{c} h_p \\ h_p \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right\rangle \Bigg\} \prod_{p=1}^{n-2} \delta_{r_p' r_p},
\end{aligned} \quad (17)$$

where the appearance of $(1+\delta_{rs})^{-1}$ is due to the factor $\frac{1}{2}$ that we have to put in the general formula (17) if it is going to remain valid for $r = s$.

From the analysis of Gelfand and Zetlin,[2,3,10] we see that the matrix element of C^{n-1}_n required in (17), is given by[11]

$$\begin{aligned}
&\left\langle \begin{array}{c} h_p \\ h_p - \delta_{pr} \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right| C^{n-1}_n \left| \begin{array}{c} h_p \\ h_p \\ h_p - \delta_{pr} - \delta_{ps} \\ \cdots \end{array} \right\rangle \\
&= \left[(h_{r,n} - 1) \prod_{p=1}^{n-2} (h_{r,p} + \delta_{pr} + \delta_{ps}) \Big/ \prod_{\substack{p=1 \\ p \neq r}}^{n-1} (h_{r,p}) \right]^{\frac{1}{2}},
\end{aligned} \quad (18)$$

where

$$h_{r,s} \equiv h_r - h_s + s - r. \quad (19)$$

Using (18) we could immediately write down the explicit expression for the matrix of the transposition $(n-1, n)$ with respect to the SG states. This matrix turns out to be identical to the coorresponding one in the irreducible representation of S_n derived by standard methods.[9] For example, when $r, s < n-1$, $r \neq s$, we get from (17) and (18)

$$\begin{aligned}
&\langle [h_p](r'_p)|\, (n-1, n)\, |[h_p](r_p)\rangle \\
&= (h_{r,s})^{-1}\, \delta_{rr'}\, \delta_{ss'} + [1 - (h_{r,s})^{-2}]^{\frac{1}{2}}\, \delta_{rs'}\, \delta_{sr'},
\end{aligned} \quad (20)$$

which coincides with the corresponding case in Eq. (7–111) of Ref. 1, p. 221.

We conclude therefore that the SG states are BIR of the S_n group.

V. CONFIGURATION-SPACE STATES WITH PERMUTATIONAL SYMMETRY

When we are dealing with systems of identical particles, all observables are invariant under permutations and so it is important to construct n-particle states with permutational symmetry,[12] i.e., states characterized by the partition $[h_p]$ of n and by the Yamanochi symbol (r_p).

[10] J. Nagel and M. Moshinsky, Rev. Mex. Fis. 14, 29 (1965).

[11] There is a misprint in a phase factor in the formula of Gelfand's paper that is corrected in Refs. 4 and 10.

[12] See Ref. 1, pp. 243–249.

In this section we shall show how to express, as special Gelfand states, the configuration-space states with permutational symmetry.

The single-particle states in configuration space will be denoted by

$$\psi_\mu(\mathbf{r}), \tag{21}$$

where $\mathbf{r}$ is the position vector of the particle and μ characterizes the state, i.e.,

$$\mu = (\nu lm), \qquad \mu = (k_x k_y k_z), \quad \text{etc.,} \tag{22a, b}$$

depending on whether we are dealing with particles in a central potential with radial quantum number ν, angular momentum l, and projection m, or free particles with $(k_x k_y k_z)$ being the components of the momentum, etc. We shall limit our discussion to problems in which the number of single-particle states is finite, say ρ and so, choosing an appropiate enumeration convention, we have $\mu = 1, 2, \cdots, \rho$.

We introduce now the correspondence[13]

$$\psi_\mu(\mathbf{r}_s) \leftrightarrow a^+_{\mu s} |0\rangle, \tag{23}$$

where s is the particle index, $a^+_{\mu s}$ are commuting creation operators of the type discussed in Sec. II, and $|0\rangle$ is the vacuum state. An n-particle wavefunction formed from products of the ψ's corresponds to the state

$$a^+_{\mu_1 s_1} a^+_{\mu_2 s_2} \cdots a^+_{\mu_n s_n} |0\rangle, \tag{24}$$

where $(s_1 s_2 \cdots s_n)$ is a permutation of $(12 \cdots n)$ while the μ's can take any of the values $\mu = 1, 2, \cdots, \rho$.

We can use well known techniques, such as those of Young symmetrizers,[12] to build up linear combinations of the states (23) that have definite permutational symmetry though, in general, the states formed in this way do not give an orthonormal basis. In this paper we will construct the states by the procedures indicated in the previous sections. We notice first that from the $a^+_{\mu s}$, $a^{\mu' s'}$ we can define the following operators

$$\mathbf{C}^{\mu' s'}_{\mu s} \equiv a^+_{\mu s} a^{\mu' s'}, \quad \mathcal{C}^{\mu'}_{\mu} = \sum_{s=1}^{n} a^+_{\mu s} a^{\mu' s}, \quad C^{s'}_{s} = \sum_{\mu=1}^{\rho} a^+_{\mu s} a^{\mu s'}. \tag{25a, b, c}$$

From (2) we obtain the commutation relations of the operators and show that they are the generators of the groups $\mathbf{U}_{\rho n}$, $\mathfrak{U}_\rho$, U_n, respectively.[14]

With respect to $\mathbf{U}_{\rho n}$, $a^+_{\mu s}$ corresponds to a single vector of dimension ρn, and so the set of all linearly independent states (24), with arbitrary μ_i, s_i, form a BIR for the completely symmetric representation of $\mathbf{U}_{\rho n}$ characterized by $[n]$. The unitary group $\mathbf{U}_{\rho n}$ admits as subgroup the direct product $\mathfrak{U}_\rho \times U_n$ whose generators are given by (25b, c), and so we can characterize further our states by the representations $[k_{\lambda\rho}]$, $1 \le \lambda \le \rho$ of $\mathfrak{U}_\rho$ and $[h_{pn}]$, $1 \le p \le n$ of U_n. It is well known[3,13] that, to be contained in the representation $[n]$ of $\mathbf{U}_{\rho n}$, both $[k_{\lambda\rho}]$ and $[h_{pn}]$ must be the same partition of n, i.e.,

$$h_{1n} = k_{1\rho}, \qquad h_{2n} = k_{2\rho}, \cdots. \tag{26}$$

We can further characterize our states by the representations $[k_{\lambda\mu}]$, $1 \le \lambda \le \mu < \rho$ of the subgroups $\mathfrak{U}_\mu$ in the chain $\mathfrak{U}_\rho \supset \mathfrak{U}_{\rho-1} \supset \cdots \mathfrak{U}_\mu \supset \cdots \mathfrak{U}_1$, and by the representations $[h_{rs}]$, $1 \le r \le s < n$ of the subgroups U_s in the chain $U_n \supset U_{n-1} \supset \cdots U_s \supset \cdots U_1$, i.e., our states become Gelfand states with respect to both the $\mathfrak{U}_\rho$ and U_n groups, and could be represented by

$$|[k_{\lambda\mu}]; [h_{rs}]\rangle. \tag{27}$$

The highest-weight state in the set (27) is obtained when

$$\begin{aligned} k_{\lambda\mu} &= k_{\lambda\rho}, \qquad 1 \le \lambda \le \mu \le \rho, \\ h_{rs} &= h_{rn}, \qquad 1 \le r \le s \le n, \end{aligned} \tag{28}$$

and its explicit expression[3,13] is given by (5). An arbitrary state (27) can be obtained from the one of highest weight by means of lowering operators both for the U_n group, i.e., L^r_s, as well as for the $\mathfrak{U}_\rho$ group, i.e., $\mathfrak{L}^\lambda_\mu$, where the latter are given by a definition identical to (8) when we replace $C^{s'}_s$ by $\mathcal{C}^{\mu'}_\mu$.

As indicated above, the states (24) correspond to n-particle states formed from the $\psi_\mu(\mathbf{r}_s)$ only if $(s_1 \cdots s_n)$ is a permutation of $(12 \cdots n)$ and so their weight is $(11 \cdots 1)$. We see therefore that when we expand the states (24) in terms of the states (27), we need only concern ourselves with those of the latter type that are SG states of U_n. Assuming, then, that we have, at most, ρ single-particle states, the most general n-particle state with permutational symmetry is given by

$$\left| \begin{matrix} k_{1\rho}\ k_{2\rho} \cdots\cdots k_{\rho\rho} & [h_1 \cdots h_n] \\ k_{1\rho-1} \cdots k_{\rho-1\rho-1}\ ; & \\ \cdots\cdots\cdots & (1r_2 \cdots r_n) \\ k_{11} & \end{matrix} \right\rangle$$

$$= \left\{ \mathfrak{N}(k_{\lambda\mu}) (\mathfrak{L}^1_1)^{k_{11}} \prod_{\lambda=1}^{2} (\mathfrak{L}^\lambda_2)^{k_{\lambda 2} - k_{\lambda 1}} \cdots \prod_{\lambda=1}^{\rho} (\mathfrak{L}^\lambda_\rho)^{k_{\lambda\rho} - k_{\lambda\rho-1}} \times N([h_p](r_p))\, L^1_1\, L^{r_2}_2 \cdots L^{r_n}_n \right\} |h_p\rangle, \tag{29}$$

where we have dropped the index n in $[h_{pn}]$, the state $|h_p\rangle$ is given by (5) and $[k_{p\rho}] = [h_p]$ as in (26).

[13] M. Moshinsky, Nucl. Phys. **31**, 384 (1962).
[14] T. A. Brody, M. Moshinsky, and I. Renero, J. Math. Phys. **6**, 1540 (1965).

The $\mathcal{L}^{\lambda}_{\mu}$, L^{r}_{s} are the lowering operators and $\mathfrak{N}(k_{\lambda\mu})$, $N([h_p](r_p)$ the normalization coefficients of the groups $\mathfrak{U}_\rho$, U_n, respectively. The operators L^{r}_{s}, $\mathcal{L}^{\lambda}_{\mu}$ commute, as from (2),

$$[C^{r}_{s},\ \mathcal{C}^{\lambda}_{\mu}] = 0. \tag{30}$$

While the states (29) form a complete set, their characterization with respect to the chain $\mathfrak{U}_\rho \supset \mathfrak{U}_{\rho-1} \supset \cdots \mathfrak{U}_1$ has no particular physical significance. We would like rather to choose a chain of subgroups of $\mathfrak{U}_\rho$ that would be related with significant physical observables. For example, if we are dealing with single-particle states in a common central potential, i.e., $\mu = (\nu lm)$ it is very convenient to characterize the states by the total arbital angular momentum of the n-particle system and by its projection.

It can be easily shown[13,15] that the operator of angular momentum $\mathfrak{L}_q$, $q = 1, 0, -1$ can be given in terms of the generators of $\mathfrak{U}_\rho$ by the expression

$$\mathfrak{L}_q = \sum_{\nu l} \sum_{m,m'} \{[l(l+1)]^{\frac{1}{2}} \langle l1m'q\ |lm\rangle \mathcal{C}^{\nu lm'}_{\nu lm}\}, \tag{31}$$

where $\langle|\rangle$ is a Wigner coefficient of the ordinary rotation group. The operators $\mathfrak{L}_q$ satisfy the usual commutation rules and so are the generators of a R_3 subgroup of $\mathfrak{U}_\rho$.

We would like now to find linear combinations of the states (29) with definite $[h_p](r_p)$ but variable $[k_{\lambda\mu}]$, $1 \leq \lambda \leq \mu < \rho$ that would be eigenstates of $\mathfrak{L}_0$ and

$$\mathfrak{L}^2 = \sum_{q=-1}^{1} (-1)^q \mathfrak{L}_q \mathfrak{L}_{-q}, \tag{32}$$

with eigenvalues M and $L(L+1)$, with L integer. We have no problem for $\mathfrak{L}_0$, as from (31) we see that it is expressed only in terms of the generators $\mathcal{C}^{\nu lm}_{\nu lm} = \mathcal{C}^{\mu}_{\mu}$, while from (4) we see that the Gelfand states are eigenstates of these generators. As the matrix elements of the $\mathcal{C}^{\mu'}_{\mu}$ with respect to Gelfand states have been obtained by Gelfand and Zetlin,[2,4,10] we could immediately obtain from (31) the matrix elements of $\mathfrak{L}_q$ and so finally determine the matrix

$$||\langle k''_{\lambda\mu}|\ \mathfrak{L}^2\ |k'_{\lambda\mu}\rangle|| = ||\sum_{k\lambda\mu} \sum_{q} (-1)^q \langle k''_{\lambda\mu}|\ \mathfrak{L}_q\ |k_{\lambda\mu}\rangle\langle k_{\lambda\mu}|\ \mathfrak{L}_{-q}\ |k'_{\lambda\mu}\rangle||. \tag{33}$$

The diagonalization of this matrix would provide, besides the eigenvalues $L(L+1)$, i.e., the irreducible representations L of R_3 contained in a given representation of U_ρ, the eigenvectors with whose help we could construct the linear combinations of the states (29) that are eigenstates of $\mathfrak{L}^2$ and $\mathfrak{L}_0$, i.e., the states

$$|\alpha LM;\ [h_p](r_p)\rangle, \tag{34}$$

where α is an index or set of indices that distinguishes between states with the same angular momentum L, projection M, and permutational symmetry $[h_p](r_p)$.

The index or indices α could be correlated with eigenvalues of other operators formed from the $\mathcal{C}^{\mu'}_{\mu}$ that commute with the $\mathfrak{L}_q$ and among themselves. Some of these operators can be easily found if there are chains of subgroups of U_ρ that contain R_3, but the problem of finding a complete set of operators is, in general, a difficult one.[16]

The states (34) are expressed in terms of homogeneous polynomials of degree n in the $a^{+}_{\mu_s}$ acting on $|0\rangle$, but they could be immediately translated into the usual notation in terms of the single-particle states $\psi_\mu(\mu_s)$ by means of the correspondence (23).

Example: States of permutational symmetry in the p-shell.

As an example of the previous developments, we consider the problem of the determination of n-particle states of definite permutational symmetry and orbital angular momentum when the single-particle states νlm are restricted to a particular ν and to $l = 1$. The single-particle states are then characterized by $m = 1, 0, -1$ and can be enumerated as follows:

μ	1	2	3
m	1	0	-1

. (35)

The states of permutational symmetry corresponding to (29) can then be written as

$$\left|\begin{matrix} h_1\ h_2\ h_3 \\ u_1\ u_2 \\ v_1 \end{matrix}\ ;\ [h_1\ h_2\ h_3\ 0 \cdots 0] \atop (1\ r_2\ r_3\ r_4 \cdots r_n)\right\rangle$$

$$= \left\{ \mathfrak{N} \begin{pmatrix} h_1\ h_2\ h_3 \\ u_1\ u_2 \\ v_1 \end{pmatrix} (\mathcal{L}^1_2)^{u_1-v_1} (\mathcal{L}^1_3)^{h_1-u_1} (\mathcal{L}^2_3)^{h_2-u_2} \right.$$

$$\left. \times N([h_p](r_p))\ L^1_1\ L^{r_2}_2 \cdots L^{r_n}_n \right\}$$

$$\times N(h_1\ h_2\ h_3)(\Delta^1_1)^{h_1-h_2} (\Delta^{12}_{12})^{h_2-h_3} (\Delta^{123}_{123})^{h_3}\ |0\rangle, \tag{36}$$

[15] M. Moshinsky, "Group Theory and the Many Body Problem," in *Physics of Many Particle Systems* (Gordon and Breach Science Publishers, Inc., New York, 1965).

[16] V. Bargmann and M. Moshinsky, Nucl. Phys. **23**, 177 (1961).

TABLE I. Characterization of the generators of $\mathfrak{U}_3$ by their Racah tensor prperties with respect to R_3.

$\mathfrak{K} = \mathfrak{C}_1^1 + \mathfrak{C}_2^2 + \mathfrak{C}_3^3$
$\mathfrak{L}_1 = -(\mathfrak{C}_1^2 + \mathfrak{C}_2^3),\ \mathfrak{L}_0 = (\mathfrak{C}_1^1 - \mathfrak{C}_3^3),\ \mathfrak{L}_{-1} = (\mathfrak{C}_2^1 + \mathfrak{C}_3^2)$
$\mathfrak{Q}_2 = \mathfrak{C}_1^3,\ \mathfrak{Q}_1 = \frac{1}{\sqrt{2}}(-\mathfrak{C}_1^2 + \mathfrak{C}_2^3),\ \mathfrak{Q}_0 = \frac{1}{\sqrt{6}}(\mathfrak{C}_1^1 - 2\mathfrak{C}_2^2 + \mathfrak{C}_3^3),$ $\mathfrak{Q}_{-1} = \frac{1}{\sqrt{2}}(\mathfrak{C}_2^1 - \mathfrak{C}_3^2),\ \mathfrak{Q}_{-2} = \mathfrak{C}_3^1.$

where we used (26) and the notation $k_{12} = u_1$, $k_{22} = u_2$, $k_{11} = v_1$. The $N(h_1h_2h_3)$ is given by (6) while the other normalization constants can be obtained from (11b). The lowering operators L_s^r simplify considerably[17] when they act on states in which only the first three terms in the partition are different from zero. The r_p in the Yamanouchi symbols are restricted to $r_p = 1, 2, 3$.

To obtain states equivalent to (34), we first give in Table I the linear combination of the generators $\mathfrak{C}_\mu^{\mu'}$ of $\mathfrak{U}_3$ that are Racah tensors[15] of rank 0, 1, 2, denoted, respectively, by $\mathfrak{K}$, $\mathfrak{L}_q$, $\mathfrak{Q}_\tau$.

From (31) we see that the $\mathfrak{L}_q$ are the operators of orbital angular momenta, and from the fact that

$$\Omega \equiv \sum_{q,q',\tau} (-1)^\tau \langle 11qq' \mid 2\tau\rangle\ \mathfrak{Q}_{-\tau}\ \mathfrak{L}_q\ \mathfrak{L}_{q'} \tag{37}$$

is a scalar, we conclude that

$$\mathfrak{L}_0,\ \mathfrak{L}^2,\ \Omega \tag{38}$$

are three commuting operators. These operators were shown to characterize completely the states that are BIR of $\mathfrak{U}_3$ in the $\mathfrak{U}_3 \supset R_3$ chain.[16]

The states (36) are eigenstates of $\mathfrak{L}_0$ with eigenvalue

$$M = -h_1 - h_2 - h_3 + u_1 + u_2 + v_1. \tag{39}$$

The matrix of $\mathfrak{L}^2$ with respect to the states (36) was obtained explicitly in Ref. 15, and by a similar procedure to the one followed there one could obtain the matrix of Ω. As these matrices commute, we obtain from their simultaneous diagonalization the completely defined eigenvectors with whose help we could construct the linear combinations of the states (36) that are eigenstates of Ω, $\mathfrak{L}^2$, $\mathfrak{L}_0$, i.e., the states

$$|\omega LM; [h_p](r_p)\rangle, \tag{40}$$

where we denote by ω the eigenvalue of Ω.

[17] P. Kramer and M. Moshinsky, Nucl. Phys. (in press).

One can also obtain the states (40) by directly evaluating the states in the $\mathfrak{U}_3 \supset R_3$ chain[16] that are of maximum weight in U_n and then, applying the operators L_s^r as in (36).

VI. SPIN–ISOSPIN STATES WITH PERMUTATIONAL SYMMETRY

The construction of spin–isospin states with permutational symmetry can be done along lines very similar to those discussed in the previous section. The only difference is that now the single-particle state is $\chi_{\sigma\tau}(s)$ where $\sigma = \frac{1}{2}, -\frac{1}{2}$ is the spin index, $\tau = \frac{1}{2}, -\frac{1}{2}$ is the isospin index, and s is the particle index. The single-particle states are then characterized by the indices $\sigma\tau$ and can be enumerated as follows:

μ	1	2	3	4
$(\sigma\tau)$	$(\frac{1}{2}\ \frac{1}{2})$	$(\frac{1}{2}\ -\frac{1}{2})$	$(-\frac{1}{2}\ \frac{1}{2})$	$(-\frac{1}{2}\ -\frac{1}{2})$

. (41)

We establish the correspondence

$$\chi_{\sigma\tau}(s) \leftrightarrow a_{\mu s}^+ \mid 0\rangle \tag{42}$$

and see immediately that the states with permutational symmetry are given by (29) when $\rho = 4$.

To obtain states characterized by definite spin and isospin, we first give, in Table II, the linear combinations of the generators $\mathfrak{C}_\mu^{\mu'}$ of $\mathfrak{U}_4$ that are Racah tensors of definite rank with respect to spin and isospin.

From (31) we see[15] that S_q, $q = 1, 0, -1$ are the operators of spin; $T_{\bar{q}}$, $\bar{q} = 1, 0, -1$ are those of isospin; while $R_{q\bar{q}}$ is a Racah tensor of rank 1 with respect to both spin and isospin with projections q, $\bar{q}$, respectively. The trace of the generators of $\mathfrak{U}_4$ is denoted by $\mathfrak{N}$ and is a scalar[15] with respect to both spin and isospin, as it commutes with S_q, $T_{\bar{q}}$. The operators

$$\Xi \equiv S^q R_{q\bar{q}} T^{\bar{q}}, \tag{43a}$$

$$\Theta \equiv S^q S_{q'} R_{q\bar{q}} R^{q'\bar{q}} + R_{q\bar{q}} R^{q\bar{q}'} T^{\bar{q}} T_{\bar{q}'} - \epsilon^{qq'q''} \epsilon^{\bar{q}\bar{q}'\bar{q}''} S_q R_{q'\bar{q}'} R_{q''\bar{q}''} T_{\bar{q}}, \tag{43b}$$

in which repeated indices are summed and where the $\epsilon^{qq'q''}$ are the completely antisymmetric tensors, are clearly scalar with respect to both spin and isospin and so commute with

$$S^2,\ S_0, \qquad T^2,\ T_0. \tag{44}$$

Furthermore, Ξ, Θ commute,[18] and so we could use

[18] M. Moshinsky and J. Nagel, Phys. Letters 5, 173 (1963).

TABLE II. Characterization of the generators of $\mathfrak{U}_4$ by their Racah tensor properties with respect to spin and isospin.

$\mathfrak{N} = \mathfrak{C}_1^1 + \mathfrak{C}_2^2 + \mathfrak{C}_3^3 + \mathfrak{C}_4^4$		
$S_1 = -\frac{1}{\sqrt{2}}(\mathfrak{C}_1^3 + \mathfrak{C}_2^4)$	$S_0 = \frac{1}{2}(\mathfrak{C}_1^1 + \mathfrak{C}_2^2 - \mathfrak{C}_3^3 - \mathfrak{C}_4^4)$	$S_{-1} = \frac{1}{\sqrt{2}}(\mathfrak{C}_3^1 + \mathfrak{C}_4^2)$
$T_1 = -\frac{1}{\sqrt{2}}(\mathfrak{C}_1^2 + \mathfrak{C}_3^4)$	$T_0 = \frac{1}{2}(\mathfrak{C}_1^1 - \mathfrak{C}_2^2 + \mathfrak{C}_3^3 - \mathfrak{C}_4^4)$	$T_{-1} = \frac{1}{\sqrt{2}}(\mathfrak{C}_2^1 + \mathfrak{C}_4^3)$
$R_{11} = \frac{1}{2}\mathfrak{C}_1^4$	$R_{10} = -\frac{1}{\sqrt{8}}(\mathfrak{C}_1^3 - \mathfrak{C}_2^4)$	$R_{1-1} = -\frac{1}{2}\mathfrak{C}_2^3$
$R_{01} = -\frac{1}{\sqrt{8}}(\mathfrak{C}_1^2 - \mathfrak{C}_3^4)$	$R_{00} = \frac{1}{4}(\mathfrak{C}_1^1 - \mathfrak{C}_2^2 - \mathfrak{C}_3^3 + \mathfrak{C}_4^4)$	$R_{0-1} = \frac{1}{\sqrt{8}}(\mathfrak{C}_2^1 - \mathfrak{C}_4^3)$
$R_{-11} = -\frac{1}{2}\mathfrak{C}_3^2$	$R_{-10} = \frac{1}{\sqrt{8}}(\mathfrak{C}_3^1 - \mathfrak{C}_4^2)$	$R_{-1-1} = \frac{1}{2}\mathfrak{C}_4^1$

these six commuting operators to characterize the states that are BIR of $\mathfrak{U}_4$ in the $\mathfrak{U}_4 \supset S\mathfrak{U}_2 \times S\mathfrak{U}_2$ single-chain, where the $S\mathfrak{U}_2$ refer to the spin and isospin spaces.

From the general analysis of Gelfand and Zetlin,[2,4,10] we could obtain the matrix elements of $\mathfrak{C}_\mu^{\mu'}$, $\mu, \mu' = 1, \cdots 4$ with respect to the states (29) with $\rho = 4$, and so, in principle, obtain the matrices of the operators (43), (44), with respect to these states. From the simultaneous diagonalization of these commuting matrices we obtain the eigenvectors with whose help we construct the linear combinations of the states (29) that are eigenstates of these six operators, i.e., the states

$$|\xi\theta SM_S TM_T; [h_p](r_p)\rangle, \tag{45}$$

where we denote by ξ, θ the eigenvalues of Ξ, Θ.

The determination of states of the form (40) and (45), besides being conceptually simple, seems to be highly mechanizable. Therefore we plan to have programs for electronic computers that will construct states with definite permutational symmetry.

Note added in proof. It is interesting to relate the states with definite permutational symmetry obtained in this paper with those derived by the standard projection technique,[19] i.e.,

$$\Psi^{[h_p]}_{(r_p)(r_{p'})} \equiv \frac{l_{[h_p]}}{n!} \sum_{\mathfrak{P}} D^{[h_p]}(\mathfrak{P})^*_{(r_p)(r_{p'})} \psi_1(\mathbf{r}_1) \cdots \psi_n(\mathbf{r}_n), \tag{46}$$

where $\mathfrak{P}$ stands for an arbitrary permutation of the vectors $\mathbf{r}_1, \cdots, \mathbf{r}_n$, D is the IR $[h_p]$ of dimension $l_{[h_p]}$ and with its rows characterized by the Yamanouchi symbols (r_p), (r'_p), and $\psi_s(\mathbf{r}_s)$ is a single-particle state with s being a state index. If we assume that all the single-particle states are different, the state indices can be denoted by $1 \cdots n$.

Replacing $\mathfrak{P}$ by $\mathfrak{P}^{-1}$ in (46), and making use of the unitary and real character[9] of the D's, we can also write

$$\Psi^{[h_p]}_{(r_p)(r_{p'})} = \frac{l_{[h_p]}}{n!} \sum_{\mathfrak{P}} D^{[h_p]}(\mathfrak{P})^*_{(r_{p'})(r_p)} \times \mathfrak{P}^{-1}\psi_1(\mathbf{r}_1) \cdots \psi_n(\mathbf{r}_n). \tag{47}$$

From (46) we conclude that $\Psi^{[h_p]}_{(r_p)(r_{p'})}$ is a BIR of the S_n group for the vectors $\mathbf{r}_1, \cdots \mathbf{r}_n$, characterized by $[h_p]$ and corresponding to the row (r_p). From (47) (taking into account that $\mathfrak{P}^{-1}$ acting on $\mathbf{r}_1 \cdots \mathbf{r}_n$ has the same effect that $\mathfrak{P}$ acting on the state indices $1 \cdots n$), we conclude that $\Psi^{[h_p]}_{(r_p)(r_{p'})}$ is a BIR of the S_n group for the state indices $1 \cdots n$, characterized by $[h_p]$ and corresponding to the row (r'_p).

We now note that, if in Sec. 5 $\rho = n$ and the weight in $\mathfrak{U}_n$ is also $(11 \cdots 1)$, the state (29) can be characterized by the Yamanouchi symbols (r'_p), (r_p) with respect to the groups $\mathfrak{U}_n$ and U_n respectively, i.e., we have the state

$$|[h_p](r'_p), [h_p](r_p)\rangle. \tag{48}$$

If we establish the correspondance (23) between $a^+_{\mu_s}|0\rangle$ and the wavefunction $\psi_\mu(\mathbf{r}_s)$, we see that the states (48) will be linear combinations of the wavefunctions

$$\psi_{\mu_1}(\mathbf{r}_{s_1}) \cdots \psi_{\mu_n}(\mathbf{r}_{s_n}),$$

where both $(\mu_1 \cdots \mu_n)$ and $(s_1 \cdots s_n)$ are permuta-

[19] Ref. 1, pp. 111–113 and pp. 246 and 247.

tions of $(12 \cdots n)$. Furthermore the states (48) are BIR of S_n characterized by $[h_p]$ with respect to both the particle indices and state indices, with the rows of the representation being (r_p) and (r'_p) respectively.

The states (46) and the states (48), in which we use the correspondance (23), are then clearly equivalent, and so we could construct the standard projection states by applying lowering operators in the explicit fashion indicated in (29).

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Poles of the Proper Vertex Function in the Bethe–Salpeter Formalism*

NOBORU NAKANISHI
Applied Mathematics Department, Brookhaven National Laboratory, Upton, Long Island, New York
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A formal general proof of the statement of Goebel and Sakita is presented on the basis of the Bethe–Salpeter formalism; namely, it is shown that the poles of a proper vertex function cannot appear in the corresponding scattering amplitude. Some related conjectures are also verified. An exactly solvable example is presented and discussed in this connection.

1. INTRODUCTION

ON criticizing the work of Geshkenbein and Ioffe[1] concerning an upper bound on the coupling constant, Goebel and Sakita[2] pointed out, on the basis of the nonrelativistic theory, that the poles in the a channel of the proper vertex function $\Gamma(s)$ of three particles a, b, c do not appear in the scattering amplitude of the two particles b and c. Subsequently, this statement has been verified in an extended Lee model by Drell, Finn, and Hearn,[3] and in the case in which $\Gamma(s)$ has no branch cut below the elastic threshold by Jin and MacDowell.[4] The latter[4] have proposed the conjecture that the poles of $\Gamma(s)$ will lie on a Regge trajectory of the b-c scattering amplitude.

The purpose of this paper is to present a general proof of the statement of Goebel and Sakita on the basis of the Bethe–Salpeter formalism. We also verify the proposition of Jin and MacDowell. The general proof is given in the next section, and an exactly solvable example, which exhibits the Regge behavior, is discussed in the final section.

2. GENERAL PROOF

We consider the scattering Green's function $\mathbf{G}$ of two particles b and c, in which an elementary particle a can appear as an intermediate state. On the basis of the Bethe–Salpeter formalism, $\mathbf{G}$ satisfies the integral equation

$$\mathbf{G} = K^{-1} + K^{-1}(I + A)\mathbf{G}, \tag{2.1}$$

where K^{-1} denotes the product of the propagator of b and that of c, and $I + A$ is the irreducible kernel (i.e., the sum over all Feynman graphs for $b + c \to b + c$ which contains no $b + c$ intermediate states) in the operator notation. The part A is characterized by the property that it contains at least one one-particle intermediate state of a. Hence A can be written as

$$A = \Lambda K_a^{-1} \bar{\Lambda}, \tag{2.2}$$

where Λ denotes the irreducible vertex part for $a \to b + c$, which contains neither a nor $b + c$ intermediate states, while $\bar{\Lambda}$ is related to the process $b + c \to a$, and K_a^{-1} is the "free" propagator[5] of a in the sense that it has no $b + c$ intermediate states.

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[1] B. V. Geshkenbein and B. L. Ioffe, Phys. Rev. Letters **11**, 55 (1963); Zh. Eksperim. i Teor. Fiz. **44**, 1211 (1963); *ibid.* **45**, 555 (1963) [English transls.: Soviet Phys.—JETP **17**, 820 (1963); *ibid.* **18**, 382 (1964)].

[2] C. J. Goebel and B. Sakita, Phys. Rev. Letters **11**, 293 (1963).

[3] S. D. Drell, A. C. Finn, and A. C. Hearn, Phys. Rev. **136**, B1439 (1964).

[4] Y. S. Jin and S. W. MacDowell, Phys. Rev. **137**, B688 (1965).

[5] If the particle a can be converted into other virtual states without passing through the $b + c$ state, K_a^{-1} must include such radiative corrections.

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where Λ denotes the irreducible vertex part for $a \to b + c$, which contains neither a nor $b + c$ intermediate states, while $\bar{\Lambda}$ is related to the process $b + c \to a$, and K_a^{-1} is the "free" propagator[5] of a in the sense that it has no $b + c$ intermediate states.

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[4] Y. S. Jin and S. W. MacDowell, Phys. Rev. **137**, B688 (1965).

[5] If the particle a can be converted into other virtual states without passing through the $b + c$ state, K_a^{-1} must include such radiative corrections.

We also consider the $b + c$ scattering Green's function G in the absence of the particle a. It satisfies

$$G = K^{-1} + K^{-1}IG. \tag{2.3}$$

Now, assuming the existence[6] of $(K - \lambda I)^{-1}$ and $[K - \lambda(I + A)]^{-1}$ for small λ, by analytic continuation in λ we may write

$$G = (K - I)^{-1}, \tag{2.4}$$

and

$$\begin{aligned} \mathbf{G} &= (K - I - A)^{-1} \\ &= (G^{-1} - A)^{-1} \\ &= (1 - GA)^{-1}G \\ &= H + G, \end{aligned} \tag{2.5}$$

where

$$\begin{aligned} H &\equiv GA(1 - GA)^{-1}G \\ &= G\Lambda K_a^{-1}\bar{\Lambda}(1 - G\Lambda K_a^{-1}\bar{\Lambda})^{-1}G. \end{aligned} \tag{2.6}$$

Since

$$\alpha(1 - \beta\alpha)^{-1} = (1 - \alpha\beta)^{-1}\alpha \tag{2.7}$$

for two arbitrary operators α and β, provided that $(1 - \alpha\beta)^{-1}$ and $(1 - \beta\alpha)^{-1}$ exist, (2.6) is rewritten as

$$\begin{aligned} H &= G\Lambda(1 - K_a^{-1}\bar{\Lambda}G\Lambda)^{-1}K_a^{-1}\bar{\Lambda}G \\ &= G\Lambda(K_a - \bar{\Lambda}G\Lambda)^{-1}\bar{\Lambda}G \\ &= \Gamma\Delta_a'\bar{\Gamma}. \end{aligned} \tag{2.8}$$

Here

$$\Gamma \equiv G\Lambda, \qquad \bar{\Gamma} \equiv \bar{\Lambda}G \tag{2.9}$$

are the proper vertex functions, and

$$\Delta_a' \equiv (K_a - \bar{\Lambda}G\Lambda)^{-1} \tag{2.10}$$

is the modified propagator of a. From (2.5) and (2.8), we see

$$\mathbf{G} = \Gamma\Delta_a'\bar{\Gamma} + G. \tag{2.11}$$

The graphical interpretation of (2.11) will be obvious.

Now, let s be the invariant square of the total 4-momentum, and suppose that G has a pole at $s = s_B$:

$$G = \frac{i\phi_B\bar{\phi}_B}{s - s_B} + \hat{G}. \tag{2.12}$$

Here ϕ_B denotes the Bethe–Salpeter amplitude for a bound state B of b and c in the absence of a, and $\hat{G}$ is nonsingular at $s = s_B$. Then (2.9) and (2.10) lead to

$$\begin{aligned} \Gamma &= \frac{i\phi_B(\bar{\phi}_B\Lambda)}{s - s_B} + \hat{G}\Lambda, \\ \bar{\Gamma} &= \frac{i(\bar{\Lambda}\phi_B)\bar{\phi}_B}{s - s_B} + \bar{\Lambda}\hat{G}, \end{aligned} \tag{2.13}$$

and

$$\begin{aligned} \Delta_a' &= \left[K_a - \frac{i(\bar{\Lambda}\phi_B)(\bar{\phi}_B\Lambda)}{s - s_B} - \bar{\Lambda}\hat{G}\Lambda\right]^{-1} \\ &= i(s - s_B)[(\bar{\phi}_B\Lambda)^{-1}(\bar{\Lambda}\phi_B)^{-1} + O(s - s_B)]. \end{aligned} \tag{2.14}$$

Here we have assumed that $\bar{\Lambda}\phi_B$ *and therefore* $\bar{\phi}_B\Lambda$ *are nonvanishing*. Hence

$$H = -\frac{i\phi_B\bar{\phi}_B}{s - s_B} + \hat{H}, \tag{2.15}$$

where $\hat{H}$ is nonsingular at $s = s_B$. *Thus* $\mathbf{G} = H + G$ *has no pole at* $s = s_B$. This is nothing but the statement of Goebel and Sakita,[2] but we should add some comments.

(1) The existence of a pole in Γ does not necessarily imply a pole of G, namely Λ may have a pole at $s = s_0$. Then Δ_a' has a double zero at $s = s_0$, so that both H and G are nonsingular there.

(2) In the above proof, the assumption that $\bar{\Lambda}\phi_B$ is nonzero is very essential. This assumption is equivalent to the statement that B has the same quantum numbers with a. This justifies the proposition of Jin and MacDowell.[4] For example, if one considers the case in which a, b, c are scalar, then the cancellation cannot occur for the poles of G which correspond to the bound states having angular momentum $l \neq 0$. Thus the Regge trajectories of $\mathbf{G}$ are the same with those of G. Correspondingly, the high-energy behavior of $\mathbf{G}$ in the crossed channel is governed essentially by that of G because H tends to a constant.

(3) Okubo and Feldman[7] analyzed the Bethe–Salpeter equation for bound states of a scalar nucleon and a scalar antinucleon in the ladder-chain approximation. In that case, they found that the Bethe–Salpeter amplitude is proportional to the proper vertex function. A general proof of this statement immediately follows from (2.11) because the poles of Δ_a' other than that of the particle a represent true bound states of b and c. Let s_B' be a pole of Δ_a', which will tend to s_B as $\Lambda \to 0$, and

$$Z_B \equiv -i \lim_{s \to s_B'} (s - s_B')\Delta_a'. \tag{2.16}$$

[6] If they do not exist, one should introduce a cutoff in order to make them exist. The cutoff should tend to infinity in the final stage.

[7] S. Okubo and D. Feldman, Phys. Rev. 117, 279 (1960).

Then the Bethe–Salpeter amplitude is given by $Z_B^{\frac{1}{2}}\Gamma$ with $s = s_B'$.

(4) The bound state obtained above is quite akin to an elementary particle. *It does not lie on a Regge trajectory and has a nonzero Z-factor* if (2.16) is accepted as a definition of a Z factor. Thus it provides an interesting counterexample to the usual criterion for bound states.

(5) If the particle a itself is a bound state, all the above reasoning no longer holds. In this case, it is not clear how to define the proper vertex function Γ. If a is spinless, the improper vertex function may be defined by[8]

$$\int d^4q\, G, \tag{2.17}$$

where q denotes the relative momentum of b and c in the initial state. The poles of (2.17), of course, correspond to bound states of b and c.

3. EXACTLY SOLVABLE EXAMPLE

In this section, we consider an exactly solvable example which exhibits the Regge behavior. Let b and c be two scalar particles having unit mass. They exchange massless scalar particles with scalar coupling g. Then the integral equation for $\mathbf{G}$ in the case of vanishing total 4-momentum is

$$\mathbf{G}(p, q) = \frac{1}{(1-p^2)^2}\left\{-\delta^4(p-q) + \int d^4p' \times \left[\frac{\lambda/\pi^2 i}{-(p-p')^2} + \frac{\lambda_a/\pi^2 i}{m_0^2}\right]\mathbf{G}(p', q)\right\} \tag{3.1}$$

in the ladder-chain approximation. Here, q and p are the relative momenta in the initial and in the final state, respectively; $\lambda = g^2/(4\pi)^2$, $\lambda_a = g_a^2/(4\pi)^2$, and g_a and m_0 denote the unrenormalized (abc) coupling constant and the unrenormalized mass of a, respectively. For simplicity, $-i\epsilon$ has been omitted in all denominators.

We also consider the following auxiliary integral equations:

$$G(p, q) = \frac{1}{(1-p^2)^2}\left[-\delta^4(p-q) + \frac{\lambda}{\pi^2 i} \times \int d^4p' \frac{G(p', q)}{-(p-p')^2}\right], \tag{3.2}$$

$$\psi(p) = \frac{1}{(1-p^2)^2}\left[1 + \frac{\lambda}{\pi^2 i}\int d^4p' \frac{\psi(p')}{-(p-p')^2}\right]. \tag{3.3}$$

[8] I. Sato, J. Math. Phys. 4, 24 (1963).

Then it is evident that

$$\psi(p) = -\int d^4q\, G(p, q). \tag{3.4}$$

The solution to (3.2) is known already[9,10]:

$$G(p, q) = -(1-q^2)^{-2}[\delta^4(p-q) + (\lambda/\pi^2 i) f((p-q)^2, p^2, q^2)]. \tag{3.5}$$

where

$$f((p-q)^2, p^2, q^2) \equiv 2\int_0^1 dy \frac{(1-y)\varphi(y, q^2)}{[(1-y)(1-p^2) - y(p-q)^2]^3}, \tag{3.6}$$

with

$$\varphi(y, q^2) \equiv F\{-\nu, \nu+1; 2; -[(1-y)/y(1-q^2)]\}, \tag{3.7}$$

and

$$\nu \equiv (\lambda + \tfrac{1}{4})^{\frac{1}{2}} - \tfrac{1}{2}. \tag{3.8}$$

Since $G(p, q) = G(q, p)$, (3.5) with (3.6) leads to

$$\psi(q) = -\int d^4p\, G(p, q) = (1-q^2)^{-2}\left[1 + \lambda\int_0^1 dy \frac{\varphi(y, q^2)}{1-yq^2}\right]. \tag{3.9}$$

Using p in place of q, and assuming $p^2 < 1$ for the moment, we obtain

$$\psi(p) = (1-p^2)^{-2} \times \left\{1 + \lambda\int_0^\infty dx \frac{F(-\nu, \nu+1; 2; -x)}{(1+x)[1+x(1-p^2)]}\right\}, \tag{3.10}$$

a result which is identical with a formula given by Okubo.[11] But, according to Okubo and Feldman,[7] it is convenient to employ an integral representation

$$\psi(p) = 2\int_0^\infty dx \frac{x\varphi(x)}{[1+x(1-p^2)]^3}. \tag{3.11}$$

Then it is straightforward to find[11]

$$\varphi(x) = F(-\nu, \nu+1; 2; -x) \tag{3.12}$$

from (3.3). The equivalence between (3.10) and (3.11) can be easily seen by substituting (3.11) in the right-hand side of (3.3).

We are now ready to solve (3.1). Making an ansatz

$$\mathbf{G}(p, q) = \alpha\psi(p)\psi(q) + G(p, q), \tag{3.13}$$

[9] N. Nakanishi, Nuovo Cimento **34**, 795 (1964).
[10] N. Nakanishi, Phys. Rev. **138**, B 1182 (1965).
[11] S. Okubo, Progr. Theoret. Phys. (Kyoto) **10**, 692 (1953).

and using (3.2), (3.3), and the first equality of (3.9), we obtain

$$\alpha = -i(\Sigma/m_0^2)\alpha + i\lambda_a/\pi^2 m_0^2, \tag{3.14}$$

where a quantity

$$\Sigma \equiv (\lambda_a/\pi^2)\int d^4p\ \psi(p) = i\lambda_a \int_0^\infty dx \frac{\varphi(x)}{x(1+x)} \tag{3.15}$$

is the proper self-energy of a. Substitution of the solution α of (3.14) in (3.13) yields

$$G(p, q) = \Gamma(p)\Delta_a'\bar{\Gamma}(q) + G(p, q), \tag{3.16}$$

with

$$\bar{\Gamma}(p) = \Gamma(p) \equiv [ig_a/(2\pi)^2]\psi(p), \tag{3.17}$$

and

$$\Delta_a' \equiv -i/(m_0^2 + i\Sigma). \tag{3.18}$$

Here the divergence of Σ should be removed by mass renormalization. Evidently, (3.16) corresponds to (2.11).

Though our model does not contain the variable s, we can still consider the poles of $\Gamma(p)$ in terms of ν. It was shown that $G(p, q)$ has a simple pole at $\nu = N$, where N is a positive integer. Its residue is given by[10]

$$\lim_{\nu\to N}(\nu - N)G(p, q) = i\sum_{L=0}^{N-1} \frac{(-1)^L(L+1)N(N+1)(N-L-1)!}{\pi^2(N+L+1)!} \times (p^2)^{\frac{1}{2}L}(q^2)^{\frac{1}{2}L}C_L^1(pq/(p^2q^2)^{\frac{1}{2}})f_{NL}(p^2)f_{NL}(q^2), \tag{3.19}$$

where $C_i^a(z)$ is a Gegenbauer polynomial, and $f_{NL}(p^2)$ is the radial part of the Bethe–Salpeter amplitude, which is given by[10]

$$f_{NL}(p^2) = -i\frac{(2L+2)!}{(L+1)!}\cdot\frac{1}{(1-p^2)^{L+3}} \times C_{N-L-1}^{L+\frac{3}{2}}\left(\frac{1+p^2}{1-p^2}\right). \tag{3.20}$$

The appearance of various angular-momentum states in (3.19) is due to the degeneracy at zero energy.

The integral in (3.11) can be easily carried out[12]:

$$\psi(p) = \frac{\pi\nu(\nu+1)}{\sin\pi\nu}\cdot\frac{1}{(1-p^2)^3} \cdot F[-\nu+1, \nu+2; 2; -p^2/(1-p^2)]. \tag{3.21}$$

Hence[13]

$$\lim_{\nu\to N}(\nu - N)\psi(p) = \frac{2(-1)^N}{(1-p^2)^3}C_{N-1}^{\frac{3}{2}}\left(\frac{1+p^2}{1-p^2}\right) = i(-1)^N f_{N0}(p^2). \tag{3.22}$$

This is of course equal to

$$-\int d^4q \lim_{\nu\to N}(\nu - N)G(p, q), \tag{3.23}$$

as is seen from (3.19) together with

$$\int d^4q\, f_{N0}(q) = -\pi^2(-1)^N. \tag{3.24}$$

Likewise, we may calculate the residue of Σ in the following way:

$$\lim_{\nu\to N}(\nu - N)\Sigma = (\lambda_a/\pi^2)\int d^4p \lim_{\nu\to N}(\nu - N)\psi(p) = -i\lambda_a. \tag{3.25}$$

Thus, from (3.17), (3.22), (3.18), and (3.25), we have

$$H(p, q) \equiv \Gamma(p)\Delta_a'\bar{\Gamma}(q) = -\frac{1}{\pi^2}\cdot\frac{if_{N0}(p^2)f_{N0}(q^2)}{\nu - N} + \hat{H}(p, q), \tag{3.26}$$

where $\hat{H}(p, q)$ is nonsingular at $\nu = N$. Therefore, the $L = 0$ part of the residue of $G(p, q)$ exactly cancels with that of $H(p, q)$ in $G(p, q)$ as it should.

The high-energy asymptotic expansion of $G(p, q)$ in the crossed channel was already given elsewhere.[9] The high-energy behavior of $G(p, q)$ is exactly the same with that of $G(p, q)$ apart from a constant term. Thus the poles of $\Gamma(p)$ are related to the high-energy behavior of $G(p, q)$.

Note added in proof. Dowker [Nuovo Cimento **33**, 110 (1964)] presented a consideration similar to our proof of the cancellation of a vertex pole, but in his paper the external-mass dependence of the amplitudes was not taken into account. The author appreciates his notice.

[12] A. Erdélyi *et al.*, *Tables of Integral Transforms*, (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 400. For explicit derivation, see N. Nakanishi, Phys. Rev. 137, B1352 (1965), Appendix A.

[13] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, (National Bureau of Standards, Washington, D. C., 1964), p. 779.

Analytic Continuations of Higher-Order Hypergeometric Functions*

PER O. M. OLSSON
Institutionen för Teoretisk Pysik, Stockholms Universitet, Stockholm, Sweden
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Solutions in powers of $1-x$ of the differential equation associated with the hypergeometric function ${}_pF_{p-1}$ are derived and the function is continued analytically in terms of these solutions. The analytic continuation is derived in a simple way from an expansion which is well suited for the purpose and which is valid for all values of the argument x. The usefulness of the ${}_3F_2$ function in studying certain hypergeometric functions of two variables is emphasized.

INTRODUCTION

In a previous investigation of the analytic properties of the Appell function $F_1(a, b_1, b_2, c, x, y)$[1] it was shown that all solutions of the partial differential equations associated with the F_1 function which are expressible in terms of the Appell function F_1 and Horn's function G_2 could be obtained in an elementary way by expanding known solutions in ${}_2F_1$ functions and then using transformations and analytic continuations of the latter functions. In this way, new solutions as well as connections between the various solutions were obtained and analytic continuations of the F_1 function to the whole domain of its variables were derived.

The success and simplicity of the method inspired an attempt to derive solutions of the equations associated with the Appell function $F_2(a, b_1, b_2, c_1, c_2, x, y)$ in the same way. It was then found that higher-order hypergeometric functions had to be taken into account. The lack of simple representations of the analytic continuations of these functions to the neighborhood of $x = 1$ caused considerable difficulties which difficulties gave the incitement to the present investigation.

In continuing ${}_3F_2$ functions and functions of higher order we are concerned with the neighborhood of $x = 1$ only, since the behavior near the singularity at infinity has long been known and offers in fact no difficulties.

In the first section of this paper we derive an explicit analytic continuation of the function ${}_pF_{p-1}$ in the neighborhood of $x = 1$. In deriving this result we use certain convenient expansions of hypergeometric functions in series of hypergeometric functions of lower order. These expansions have the advantage of being valid for all values of the variable x. With the aid of these expansions, a hypergeometric function can be expanded in hypergeometric functions whose properties are well known and can be taken advantage of in order to derive solutions of the differential equation associated with the function as well as connections between the various solutions and their transformations.

The intimate relations between some of the Appell functions and ${}_3F_2$ functions are revealed by the fact that the former functions, provided that they are finite, are ${}_3F_2$ functions in one variable if the other variable is equal to unity. Relations of this kind are given in the last section. They suggest strongly the usefulness of the ${}_3F_2$ function in the theory of certain hypergeometric functions of several variables frequently occurring in mathematical physics.

ANALYTIC CONTINUATIONS

A simple way of obtaining analytic continuations of the hypergeometric series

$$ {}_pF_{p-1}\left(\begin{matrix} a_1, a_2, \cdots, a_p \\ b_1, b_2, \cdots, b_{p-1} \end{matrix}; x\right) = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n \cdots (a_p)_n x^n}{(b_1)_n (b_2)_n \cdots (b_{p-1})_n n!}, \qquad |x| < 1, \tag{1} $$

is to expand it in functions of lower order and then make use of the analytic continuations of the latter functions. We carry this out in detail on ${}_3F_2$ functions only and merely outline the fairly straightforward generalization to functions of higher order at the end of this section.

There exist many expansions of ${}_3F_2$ functions in terms of ${}_2F_1$ functions but most of them are inconvenient for our purpose. There are, however, also expansions which deliver the desired result in a very direct way. We show that

$$ {}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix}; x\right) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a_1)\Gamma(b_1 + b_2 - a_1)} \sum_{n=0}^{\infty} \frac{(b_1 - a_1)_n (b_2 - a_1)_n}{(b_1 + b_2 - a_1)_n n!} \times {}_2F_1(a_2, a_3, b_1 + b_2 - a_1 + n, x), \tag{2} $$

* This work was carried out under the auspices of the Swedish Atomic Research Council.

[1] P. O. M. Olsson, J. Math. Phys. 5, 420 (1964).

and that this expansion converges absolutely if Re $a_1 > 0$ for all finite values of x except possibly $x = 1$, where the function on the left-hand side (lhs) may be infinite. Since the ${}_3F_2$ function is symmetric in the parameters a_i, an expansion of the type (2) exists as soon as the real part of any of the parameters a_i is positive.

The convergence follows easily from the estimate

$$\frac{(b_1 - a_1)_n(b_2 - a_1)_n}{(b_1 + b_2 - a_1)_n n!} = \frac{\Gamma(b_1 + b_2 - a_1)}{\Gamma(b_1 - a_1)\Gamma(b_2 - a_1)n^{1+a_1}}\left[1 + 0\left(\frac{1}{n}\right)\right],$$

and from the asymptotic behavior[2]

$${}_2F_1(a_2, a_3, b_1 + b_2 - a_1 + n, x) \sim 1 + 0(1/n).$$

The equality can be proved by expanding the right-hand side (rhs) of (2) in a McLaurin series. The derivatives of the expansion may be calculated by term-by-term differentiation

$$\frac{d^m}{dx^m}\sum_{n=0}^{\infty}\frac{(b_1 - a_1)_n(b_2 - a_1)_n}{(b_1 + b_2 - a_1)_n n!} \times {}_2F_1(a_2, a_3, b_1 + b_2 - a_1 + n, x)$$
$$= \frac{(a_2)_m(a_3)_m}{(b_1 + b_2 - a_1)_m}\sum_{n=0}^{\infty}\frac{(b_1 - a_1)_n(b_2 - a_1)_n}{(b_1 + b_2 - a_1 + m)_n n!} \times {}_2F_1(a_2 + m, a_3 + m, b_1 + b_2 - a_1 + m + n, x),$$

from which we obtain the derivatives for $x = 0$

$$\left[\frac{d^m}{dx^m}\sum_{n=0}^{\infty}\frac{(b_1 - a_1)_n(b_2 - a_1)_n}{(b_1 + b_2 - a_1)_n n!} \times {}_2F_1(a_2, a_3, b_1 + b_2 - a_1 + n, x)\right]_{x=0}$$
$$= \frac{(a_2)_m(a_3)_m}{(b_1 + b_2 - a_1)_m}\sum_{n=0}^{\infty}\frac{(b_1 - a_1)_n(b_2 - a_1)_n}{(b_1 + b_2 - a_1 + m)_n n!}$$
$$= \frac{\Gamma(b_1 + b_2 - a_1)\Gamma(a_1)}{\Gamma(b_1)\Gamma(b_2)}\cdot\frac{(a_1)_m(a_2)_m(a_3)_m}{(b_1)_m(b_2)_m},$$

since

$$\sum_{n=0}^{\infty}\frac{(b_1 - a_1)_n(b_2 - a_1)_n}{(b_1 + b_2 - a_1 + m)_n n!} = \frac{\Gamma(a_1 + m)\Gamma(b_1 + b_2 - a_1 + m)}{\Gamma(b_1 + m)\Gamma(b_2 + m)},$$

provided Re $a_1 > 0$.

From the derivatives at $x = 0$ it is easily seen that the McLaurin expansion of the rhs of (2) is identical with the hypergeometric series (1) for $p = 3$ which proves the expansion.

Since the ${}_2F_1$ functions are analytic functions in a plane cut from $x = 1$ to $x = +\infty$, the ${}_3F_2$ function is analytic in the same domain.

In order to obtain also an explicit analytic continuation in the neighborhood of $x = 1$, we replace the ${}_2F_1$ functions in (2) by their analytic continuations in this neighborhood.

We have[3]

$${}_2F_1(a_2, a_3, b_1 + b_2 - a_1 + n, x) = A_1\,{}_2F_1(a_2, a_3, a_1 + a_2 + a_3 - b_1 - b_2 - n + 1, 1 - x) + A_2\,x^{a_1 - b_1 - b_2 + 1}(1 - x)^{b_1 + b_2 - a_1 - a_2 - a_3}\left(\frac{1 - x}{x}\right)^n \times {}_2F_1(1 - a_2, 1 - a_3, b_1 + b_2 - a_1 - a_2 - a_3 + n + 1, 1 - x),$$

where

$$A_1 = \frac{\Gamma(b_1 + b_2 - a_1 + n)\Gamma(b_1 + b_2 - a_1 - a_2 - a_3 + n)}{\Gamma(b_1 + b_2 - a_1 - a_2 + n)\Gamma(b_1 + b_2 - a_1 - a_3 + n)},$$

and

$$A_2 = \frac{\Gamma(b_1 + b_2 - a_1 + n)\Gamma(a_1 + a_2 + a_3 - b_1 - b_2 - n)}{\Gamma(a_2)\Gamma(a_3)}.$$

Using

$$\Gamma(a + n) = \Gamma(a)(a)_n,$$
$$\Gamma(a - n) = \frac{(-1)^n\Gamma(a)}{(1 - a)_n},$$

[2] O. Perron, Sitzber. Heidelberg. Akad. Wiss. Math. Naturw. Kl. Abhandl. **8A**, 3 (1917).

[3] Bateman Manuscript Project, *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill Book Company, Inc., New York, 1953), Vol. I, p. 109.

we obtain

$$ {}_3F_2\left(\begin{matrix}a_1, a_2, a_3, \\ b_1, b_2\end{matrix} x\right) = F_R\left(\begin{matrix}a_1, a_2, a_3, \\ b_1, b_2\end{matrix} x\right) + \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(a_1+a_2+a_3-b_1-b_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)}\,\xi\left(\begin{matrix}a_1, a_2, a_3, \\ b_1, b_2\end{matrix} x\right), \tag{3} $$

where

$$ F_R\left(\begin{matrix}a_1, a_2, a_3, \\ b_1, b_2\end{matrix} x\right) $$

$$ = \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(b_1+b_2-a_1-a_2-a_3)}{\Gamma(a_1)\Gamma(b_1+b_2-a_1-a_2)\Gamma(b_1+b_2-a_1-a_3)} \sum_{n=0}^{\infty} \frac{(b_1-a_1)_n(b_2-a_1)_n(b_1+b_2-a_1-a_2-a_3)_n}{(b_1+b_2-a_1-a_2)_n(b_1+b_2-a_1-a_3)_n n!} $$

$$ \times {}_2F_1(a_2, a_3, a_1+a_2+a_3-b_1-b_2-n+1, 1-x), \qquad \operatorname{Re} a_1 > 0, \quad \operatorname{Re} x > \tfrac{1}{2}, \tag{4} $$

and

$$ \xi\left(\begin{matrix}a_1, a_2, a_3, \\ b_1, b_2\end{matrix} x\right) = x^{a_1-b_1-b_2+1}(1-x)^{b_1+b_2-a_1-a_2-a_3} \sum_{n=0}^{\infty} \frac{(b_1-a_1)_n(b_2-a_1)_n}{(b_1+b_2-a_1-a_2-a_3+1)_n n!}\left(\frac{x-1}{x}\right)^n $$

$$ \times {}_2F_1(1-a_2, 1-a_3, b_1+b_2-a_1-a_2-a_3+n+1, 1-x), \qquad \operatorname{Re} x > \tfrac{1}{2}. \tag{5} $$

The second series (5) converges absolutely for

$$ \left|\frac{x-1}{x}\right| < 1, \quad \text{or} \quad \operatorname{Re} x > \tfrac{1}{2}, $$

since, as we have seen,

$$ {}_2F_1(1-a_2, 1-a_3, b_1+b_2-a_1-a_2-a_3+n+1, 1-x) \sim 1 + 0(1/n), $$

and we conclude that the first series (4) also converges absolutely for $\operatorname{Re} x > \frac{1}{2}$ provided $\operatorname{Re} a_1 > 0$, since its terms are the differences between the terms of two series which converge under these conditions.

The two functions (4) and (5) are solutions of the differential equation associated with the ${}_3F_2$ function in (1). This is not difficult to prove, but follows directly from a result derived by Nørlund[4]

$$ {}_3F_2\left(\begin{matrix}a_1, a_2, a_3, \\ b_1, b_2\end{matrix} x\right) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)}\,\varphi(x) $$

$$ + \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(a_1+a_2+a_3-b_1-b_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)}\,\xi(x), $$

where $\varphi(x)$ is a regular solution at the point $x = 1$ of the differential equations associated with the ${}_3F_2$ function. For the function Nørlund gives the integral representation[4]

$$ \varphi(x) = \frac{\Gamma(a_1+a_2+a_3-b_1-b_2)}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{\xi(t)}{t-x}\,dt, \qquad 0 < c < 1, $$

where x lies on the right of the path of integration.

The function $\xi(x)$ is an irregular solution for which Nørlund gives expansions of the type

$$ \xi(x) = x^{1-b_2}(1-x)^{b_1+b_2-a_1-a_2-a_3} $$

$$ \times \sum_{n=0}^{\infty} \frac{(b_1-a_1-a_3+1)_n(b_1-a_2-a_3+1)_n}{(b_1+b_2-a_1-a_2-a_3+1)_n n!}\cdot(1-x)^n $$

$$ \times {}_3F_2\left(\begin{matrix}-n, 1-a_3, b_1-a_3, \\ b_1-a_1-a_3+1, b_1-a_2-a_3+1\end{matrix} 1\right), \qquad |1-x| < 1, $$

as well as integral representations.

Clearly the two functions (4) and (5) can be identified with the solutions $\varphi(x)$ and $\xi(x)$, respectively, and are thus solutions.

If $\operatorname{Re}(b_1+b_2-a_1-a_2-a_3) > 0$, the hypergeometric series (1) converges also for $x = 1$ and we obtain from (3), (4), and (5)

$$ {}_3F_2\left(\begin{matrix}a_1, a_2, a_3, \\ b_1, b_2\end{matrix} 1\right) $$

$$ = \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(b_1+b_2-a_1-a_2-a_3)}{\Gamma(a_1)\Gamma(b_1+b_2-a_1-a_2)\Gamma(b_1+b_2-a_1-a_3)} $$

$$ \times {}_3F_2\left(\begin{matrix}b_1-a_1, b_2-a_1, b_1+b_2-a_1-a_2-a_3, \\ b_1+b_2-a_1-a_2, b_1+b_2-a_1-a_3\end{matrix} 1\right), \qquad \operatorname{Re} a_1 > 0, $$

$$ \operatorname{Re}(b_1+b_2-a_1-a_2-a_3) > 0, \tag{6} $$

a result that was first derived by Thomae.[5] It con-

[4] N. E. Nørlund, Act. Mat. 94, 289 (1955).

[5] J. Thomae, J. für Math. 87, 26 (1879); also G. H. Hardy, Proc. Cambridge Phil. Soc. 21, 492 (1923).

tains all known two-term relations between ${}_3F_2$ functions of unit argument. Further relations can be obtained by repeated application of the formula and by permuting the parameters a_i or b_i.

Both sides of (6) are analytic functions of any one of the parameters but they are not defined in the same domain by their series expansions. We can take advantage of this fact by using (6) to obtain analytic continuations of ${}_3F_2$ functions of unit argument as functions of the parameters.

Defining the ${}_3F_2$ function of unit argument in this way it is permitted to use (6) to transform the series obtained. This can be used to simplify the expansion of the F_R function. It is first transformed by carrying out an Euler transformation on the ${}_2F_1$ functions which gives, e.g.,

$$F_R\left(\begin{matrix}a_1, a_2, a_3\\ b_1, b_2\end{matrix}, x\right)$$
$$= \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(b_1+b_2-a_1-a_2-a_3)}{\Gamma(a_1)\Gamma(b_1+b_2-a_1-a_2)\Gamma(b_1+b_2-a_1-a_3)}\, x^{-a_3} \sum_{n=0}^{\infty} \frac{(b_1-a_1)_n(b_2-a_1)_n(b_1+b_2-a_1-a_2-a_3)_n}{(b_1+b_2-a_1-a_2)_n(b_1+b_2-a_1-a_3)_n n!}$$
$$\times {}_2F_1\left(a_1+a_3-b_1-b_2-n+1,\ a_3,\ a_1+a_2+a_3-b_1-b_2-n+1,\ \frac{x-1}{x}\right).$$

The series is a uniformly convergent series of analytic functions when $\operatorname{Re} a_1 > 0$ and $\operatorname{Re} x > \frac{1}{2}$ and may thus be differentiated any number of times. Its power series expansion is then easily derived.

$$F_R\left(\begin{matrix}a_1, a_2, a_3\\ b_1, b_2\end{matrix}, x\right)$$
$$= \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(b_1+b_2-a_1-a_2-a_3)}{\Gamma(a_1)\Gamma(b_1+b_2-a_1-a_2)\Gamma(b_1+b_2-a_1-a_3)}\, x^{-a_3} \sum_{n=0}^{\infty} \frac{(a_3)_n(a_1+a_3-b_1-b_2+1)_n}{(a_1+a_2+a_3-b_1-b_2+1)_n n!} \left(\frac{x-1}{x}\right)^n$$
$$\times {}_3F_2\left(\begin{matrix}b_1-a_1, b_2-a_1, b_1+b_2-a_1-a_2-a_3-n\\ b_1+b_2-a_1-a_2, b_1+b_2-a_1-a_3-n\end{matrix}, 1\right), \qquad \operatorname{Re} x > \tfrac{1}{2}.$$

Applying now the transformation (6) on the ${}_3F_2$ functions of unit argument, the above expansion can be written in the simple form

$$F_R\left(\begin{matrix}a_1, a_2, a_3\\ b_1, b_2\end{matrix}, x\right) = x^{-a_3} \sum_{n=0}^{\infty} \frac{(a_3)_n}{n!} \left(\frac{x-1}{x}\right)^n$$
$$\times {}_3F_2\left(\begin{matrix}a_1, a_2, a_3+n\\ b_1, b_2\end{matrix}, 1\right), \qquad \operatorname{Re} x > \tfrac{1}{2}. \tag{8}$$

Here as well as in the irregular solution, we may, permute the parameters a_i or b_i arbitrarily since the ${}_3F_2$ function is symmetric in these parameters and the regular part of the function cannot be changed.

Since six distinct solutions of the equation associated with the ${}_3F_2$ function which are expressible in terms of ${}_3F_2$ functions are known, we obtain six regular solutions by taking the regular parts of the functions according to (3). Obviously any three of them must be linearly dependent.

There exists a slightly different kind of regular solutions which are obtained not by taking the regular part of a ${}_3F_2$ function, but by forming a regular combination of two solutions in terms of ${}_3F_2$ functions which is possible since there exists only one irregular solution. The expression

$$\frac{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)}{\Gamma(b_1)\Gamma(b_2)}\, {}_3F_2\left(\begin{matrix}a_1, a_2, a_3\\ b_1, b_2\end{matrix}, x\right)$$
$$- \frac{\Gamma(a_1-b_1+1)\Gamma(a_2-b_1+1)\Gamma(a_3-b_1+1)}{\Gamma(2-b_1)\Gamma(b_2-b_1+1)} \cdot x^{1-b_1}$$
$$\times {}_3F_2\left(\begin{matrix}a_1-b_1+1, a_2-b_1+1, a_3-b_1+1\\ 2-b_1, b_2-b_1+1\end{matrix}, x\right) = y_{12}(x),$$

which is the difference between two solutions, is easily seen to be such a combination.

With the aid of (8) we may write

$$y_{12}(x) = x^{-a_1} \sum_{n=0}^{\infty} \frac{(1-1/x)^n}{n!} \left[\frac{\Gamma(a_1+n)\Gamma(a_2)\Gamma(a_3)}{\Gamma(b_1)\Gamma(b_2)}\, {}_3F_2\left(\begin{matrix}a_1+n, a_2, a_3\\ b_1, b_2\end{matrix}, 1\right)\right.$$
$$\left. - \frac{\Gamma(a_1-b_1+n+1)\Gamma(a_2-b_1+1)\Gamma(a_3-b_1+1)}{\Gamma(2-b_1)\Gamma(b_2-b_1+1)}\, {}_3F_2\left(\begin{matrix}a_1-b_1+n+1, a_2-b_1+1, a_3-b_1+1\\ 2-b_1, b_2-b_1+1\end{matrix}, 1\right)\right].$$

The expression within the bracket can be replaced by[6]

$$\frac{\Gamma(a_2)\Gamma(a_3)\Gamma(a_1-b_1+n+1)\Gamma(a_2-b_1+1)\Gamma(a_3-b_1+1)}{\Gamma(b_1)\Gamma(1-b_1)\Gamma(a_2+a_3-b_1+1)\Gamma(b_2-b_1+1)}\,{}_3F_2\left(\begin{matrix}b_2-a_1-n,\ a_2-b_1+1,\ a_3-b_1+1\\ a_2+a_3-b_1+1,\ b_2-b_1+1\end{matrix};1\right)$$

which is one of the many known three-term relations between ${}_3F_2$ functions of unit argument. This gives

$$y_{12}(x)=\frac{\Gamma(a_2)\Gamma(a_3)\Gamma(a_1-b_1+1)\Gamma(a_2-b_1+1)\Gamma(a_3-b_1+1)}{\Gamma(b_1)\Gamma(1-b_1)\Gamma(a_2+a_3-b_1+1)\Gamma(b_2-b_1+1)}\,x^{-a_1}\sum_{n=0}^{\infty}\frac{(a_1-b_1+1)_n}{n!}\left(\frac{x-1}{x}\right)^n$$
$$\times\,{}_3F_2\left(\begin{matrix}b_2-a_1-n,\ a_2-b_1+1,\ a_3-b_1+1\\ a_2+a_3-b_1+1,\ b_2-b_1+1\end{matrix};1\right),\qquad \mathrm{Re}\,x>\tfrac{1}{2}. \tag{9}$$

The regular combination (9) has been derived in a different way by Nørlund and is subject to more extensive study than the regular parts F_R which we have considered here. The series (9) is slightly simpler than Nørlund's expansion but can be identified with the aid of a Thomae transformation. When Re $a_1>0$ we may expand the ${}_3F_2$ function in (9). If we sum over n in this double series we obtain an expansion in ${}_2F_1$ functions. Carrying out a suitable transformation on the ${}_2F_1$ functions we can derive

$$y_{12}(x)=Cx^{1-b_1}\sum_{n=0}^{\infty}\frac{(a_2-b_1+1)_n(a_3-b_1+1)_n}{(a_2+a_3-b_1+1)_n n!}$$
$$\times\,{}_2F_1(-n,\ a_1-b_1+1,\ b_2-b_1+1,\ x),$$
$$\mathrm{Re}\,a_1>0,\ |1-x|<1.$$

This is an expansion in hypergeometric polynomials, and can be found in the paper by Nørlund. The constant C appearing here is the same constant as appears in front of the function in (9).

An instructive example of the analytic continuation is obtained if we put $b_2=a_3$ in the result (3). All three functions are then ordinary hypergeometric functions. Interchanging a_1 and a_3 we obtain from (3)

$${}_2F_1(a_1,a_2,b_1,x)=x^{-a_1}\sum_{n=0}^{\infty}\frac{(a_1)_n}{n!}\left(\frac{x-1}{x}\right)^n$$
$$\times\,{}_2F_1(a_1+n,a_2,b_1,1)$$
$$+\frac{\Gamma(b_1)\Gamma(a_1+a_2-b_1)}{\Gamma(a_1)\Gamma(a_2)}\,x^{1-b_1}(1-x)^{b_1-a_1-a_2}$$
$$\times\,{}_2F_1(1-a_1,1-a_2,b_1-a_1-a_2+1,1-x),$$

which continues a ${}_2F_1$ function in the neighborhood of $x=1$. The ${}_2F_1$ functions of unit argument in the regular part are defined by their hypergeometric series when they converge, or by analytic continuation of n from a domain of convergence. From the Thomae transformation (6) we obtain the sum of the series which converges if Re $(b_1-a_1-a_2-n)>0$,

$${}_2F_1(a_1+n,a_2,b_1,1)$$
$$=\frac{\Gamma(b_1)\Gamma(b_1-a_1-a_2)(a_1-b_1+1)_n}{\Gamma(b_1-a_1)\Gamma(b_1-a_2)(a_1+a_2-b_1+1)_n},$$

which sum delivers the desired analytic continuation in case the series does not converge. Inserting the sum into the regular part we obtain

$$F_R\left(\begin{matrix}a_1,a_2\\ b_1\end{matrix};x\right)$$
$$=x^{-a_1}\sum_{n=0}^{\infty}\frac{(a_1)_n}{n!}\left(\frac{x-1}{x}\right)^n{}_2F_1(a_1+n,a_2,b_1,1)$$
$$=\frac{\Gamma(b_1)\Gamma(b_1-a_1-a_2)}{\Gamma(b_1-a_1)\Gamma(b_1-a_2)}\,x^{-a_1}$$
$$\times\,{}_2F_1\left(a_1,a_1-b_1+1,a_1+a_2-b_1+1,\frac{x-1}{x}\right)$$
$$=\frac{\Gamma(b_1)\Gamma(b_1-a_1-a_2)}{\Gamma(b_1-a_1)\Gamma(b_1-a_2)}$$
$$\times\,{}_2F_1(a_1,a_2,a_1+a_2-b_1+1,1-x),$$

and we have derived a well-known analytic continuation of the ${}_2F_1$ function in terms of ${}_2F_1$ functions.[3]

Clearly we can expand the regular and the irregular parts of a ${}_3F_2$ function in the corresponding parts of a ${}_2F_1$ function

$$F_R\left(\begin{matrix}a_1,a_2,a_3\\ b_1,b_2\end{matrix};x\right)=\frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a_3)\Gamma(b_1+b_2-a_3)}$$
$$\times\sum_{n=0}^{\infty}\frac{(b_1-a_3)_n(b_2-a_3)_n}{(b_1+b_2-a_3)_n n!}\,F_R\left(\begin{matrix}a_1,a_2\\ b_1+b_2-a_3+n\end{matrix};x\right), \tag{10}$$

a result that is obtained simply by replacing the hypergeometric functions in (2) by their regular parts. Introducing the notation

[6] G. H. Hardy, Proc. Cambridge Phil. Soc. 21, 492 (1923).

$$F_I\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2\end{matrix}\right) = \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(a_1+a_2+a_3-b_1-b_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)} \times \xi\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2\end{matrix}\right),$$

we obtain a corresponding expansion for the irregular part

$$F_I\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2\end{matrix}\right) = \frac{\Gamma(b_1)\Gamma(b_2)}{\Gamma(a_3)\Gamma(b_1+b_2-a_3)} \times \sum_{n=0}^{\infty} \frac{(b_1-a_3)_n(b_2-a_3)_n}{(b_1+b_2-a_3)_n n!} F_I\left(\begin{matrix}a_1, a_2, x\\ b_1+b_2-a_3+n\end{matrix}\right), \tag{11}$$

where

$$F_I\left(\begin{matrix}a_1, a_2, x\\ b_1\end{matrix}\right) = \frac{\Gamma(b_1)\Gamma(a_1+a_2-b_1)}{\Gamma(a_1)\Gamma(a_2)} \cdot x^{1-b_1}(1-x)^{b_1-a_1-a_2} \times {}_2F_1(1-a_1, 1-a_2, b_1-a_1-a_2+1, 1-x).$$

The expansions (10) and (11) are easily generalized to hypergeometric series of arbitrary order.

We have

$${}_pF_{p-1}\left(\begin{matrix}a_1, a_2, \cdots a_p, x\\ b_1, b_2, \cdots b_{p-1}\end{matrix}\right) = \frac{\Gamma(b_{p-1})\Gamma(b_{p-2})}{\Gamma(a_p)\Gamma(b_{p-1}+b_{p-2}-a_p)} \times \sum_{n=0}^{\infty} \frac{(b_{p-1}-a_p)_n(b_{p-2}-a_p)_n}{(b_{p-1}+b_{p-2}-a_p)_n n!} \times {}_{p-1}F_{p-2}\left(\begin{matrix}a_1, a_2, \cdots a_{p-1}, x\\ b_1, b_2, \cdots b_{p-3}, b_{p-1}+b_{p-2}-a_p+n\end{matrix}\right), \quad \text{Re } a_p > 0, \quad x \neq 1, \tag{12}$$

which identity can be proved exactly as the proof was carried out for $p = 3$. From this relation we obtain the regular and irregular parts of a ${}_4F_3$ function in terms of the corresponding parts of a ${}_3F_2$ function, etc.

Consider, as an example, a ${}_4F_3$ function. We have

$${}_4F_3\left(\begin{matrix}a_1, a_2, a_3, a_4, x\\ b_1, b_2, b_3\end{matrix}\right) = \frac{\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_4)\Gamma(b_2+b_3-a_4)} \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_4)_n n!} {}_3F_2\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2+b_3-a_4+n\end{matrix}\right)$$

$$= \frac{\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_4)\Gamma(b_2+b_3-a_4)} \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_4)_n n!} \times \left[F_R\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2+b_3-a_4+n\end{matrix}\right) + F_I\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2+b_3-a_4+n\end{matrix}\right)\right].$$

For the irregular part we obtain the double series

$$F_I\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2+b_3-a_4+n\end{matrix}\right) = \frac{\Gamma(b_1)\Gamma(b_2)\Gamma(b_3)\Gamma(a_1+a_2+a_3+a_4-b_1-b_2-b_3)}{\Gamma(a_1)\Gamma(a_2)\Gamma(a_3)\Gamma(a_4)} x^{a_3+a_4-b_1-b_2-b_3+1}$$

$$\times (1-x)^{b_1+b_2+b_3-a_1-a_2-a_3-a_4} \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_1+b_2+b_3-a_1-a_2-a_3-a_4+1)_n n!} \left(\frac{x-1}{x}\right)^n$$

$$\times \sum_{m=0}^{\infty} \frac{(b_1-a_3)_m(b_2+b_3-a_3-a_4+n)_m}{(b_1+b_2+b_3-a_1-a_2-a_3-a_4+n+1)_m m!} \left(\frac{x-1}{x}\right)^m$$

$$\times {}_2F_1(1-a_1, 1-a_2, b_1+b_2+b_3-a_1-a_2-a_3-a_4+m+n+1, 1-x).$$

Since the ${}_2F_1$ functions tend to unity for large values of $m+n$, the series converges as the simpler series

$$\sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_3-a_4)_n n!} \left(\frac{x-1}{x}\right)^n \sum_{m=0}^{\infty} \frac{(b_1-a_3)_m(b_2+b_3-a_3-a_4)_{m+n}}{(b_1+b_2+b_3-a_1-a_2-a_3-a_4+1)_{m+n} m!} \left(\frac{x-1}{x}\right)^m,$$

which converges absolutely if

$$\left|\frac{x-1}{x}\right| < 1, \quad \text{or} \quad \text{Re } x > \tfrac{1}{2}.$$

Then the series

$$F_I\left(\begin{matrix}a_1, a_2, a_3, a_4, x\\ b_1, b_2, b_3\end{matrix}\right) = \frac{\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_4)\Gamma(b_2+b_3-a_4)} \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_4)_n n!} F_I\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2+b_3-a_4+n\end{matrix}\right), \quad \text{Re } x > \tfrac{1}{2},$$

converges for Re $x > \frac{1}{2}$ and we conclude that the series

$$F_R\left(\begin{matrix}a_1, a_2, a_3, a_4, x\\ b_1, b_2, b_3\end{matrix}\right) = \frac{\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_4)\Gamma(b_2+b_3-a_4)} \times \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_4)_n n!} F_R\left(\begin{matrix}a_1, a_2, a_3, x\\ b_1, b_2+b_3-a_4+n\end{matrix}\right), \quad \text{Re } a_4 > 0, \quad \text{Re } x > \tfrac{1}{2},$$

converges if Re $a_4 > 0$ and Re $x > \frac{1}{2}$, since its terms are the differences between the terms of two series which converges under these conditions.

For $x = 1$ we obtain

$$F_R\left(\begin{matrix}a_1, a_2, a_3, a_4, 1\\ b_1, b_2, b_3\end{matrix}\right) = \frac{\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_4)\Gamma(b_2+b_3-a_4)} \times \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_4)_n n!} {}_3F_2\left(\begin{matrix}a_1, a_2, a_3, 1\\ b_1, b_2+b_3-a_4+n\end{matrix}\right), \quad \text{Re } a_4 > 0,$$

since, from (8),

$$F_R\left(\begin{matrix}a_1, a_2, a_3, 1\\ b_1, b_2+b_3-a_4+n\end{matrix}\right) = {}_3F_2\left(\begin{matrix}a_1, a_2, a_3, 1\\ b_1, b_2+b_3-a_4+n\end{matrix}\right).$$

If Re $(b_1 + b_2 + b_3 - a_1 - a_2 - a_3 - a_4) > 0$, the hypergeometric series of the ${}_4F_3$ function converges for $x = 1$, and we obtain the value of the function for $x = 1$,

$$ {}_4F_3\left(\begin{matrix}a_1, a_2, a_3, a_4, 1\\ b_1, b_2, b_3\end{matrix}\right) = \frac{\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_4)\Gamma(b_2+b_3-a_4)} \times \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_4)_n n!} {}_3F_2\left(\begin{matrix}a_1, a_2, a_3, 1\\ b_1, b_2+b_3-a_4+n\end{matrix}\right), \quad \text{Re } a_4 > 0, \tag{13}$$

$$\text{Re } (b_1 + b_2 + b_3 - a_1 - a_2 - a_3 - a_4) > 0.$$

The rhs converges for Re $a_4 > 0$, the lhs for Re $(b_1 + b_2 + b_3 - a_1 - a_2 - a_3 - a_4) > 0$. Since the ${}_4F_3$ function is symmetric in the parameters a_i or b_i the parameters a_i or b_i may be permuted arbitrarily.

From (8) we obtain

$$F_R\left(\begin{matrix}a_1, a_2, a_3, a_4, x\\ b_1, b_2, b_3\end{matrix}\right) = \frac{\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_4)\Gamma(b_2+b_3-a_4)} x^{-a_1} \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_4)_n n!} \times \sum_{m=0}^{\infty} \frac{(a_1)_m}{m!}\left(\frac{x-1}{x}\right)^m {}_3F_2\left(\begin{matrix}a_1+m, a_2, a_3, 1\\ b_1, b_2+b_3-a_4+n\end{matrix}\right)$$

$$= x^{-a_1} \sum_{m=0}^{\infty} \frac{(a_1)_m}{m!}\left(\frac{x-1}{x}\right)^m \frac{\Gamma(b_2)\Gamma(b_3)}{\Gamma(a_4)\Gamma(b_2+b_3-a_4)} \times \sum_{n=0}^{\infty} \frac{(b_2-a_4)_n(b_3-a_4)_n}{(b_2+b_3-a_4)_n n!} {}_3F_2\left(\begin{matrix}a_1+m, a_2, a_3, 1\\ b_1, b_2+b_3-a_4+n\end{matrix}\right),$$

where the change of the order of summation is allowed since the series is absolutely convergent. The rhs of (13) is an analytic function of, e.g., a_1 when Re $a_4 > 0$. It is defined also for large values of Re a_1 when the condition Re $(b_1 + b_2 + b_3 - a_1 - a_2 - a_3 - a_4) > 0$ is not valid and continues analytically the lhs, which, so far, is defined by its hypergeometric series only. In this sense we can replace the sum over n, above, by a ${}_4F_3$ function of unit argument.

Then

$$F_R\left(\begin{matrix}a_1, a_2, a_3, a_4, x\\ b_1, b_2, b_3\end{matrix}\right) = x^{-a_1} \sum_{n=0}^{\infty} \frac{(a_1)_n}{n!}\left(\frac{x-1}{x}\right)^n \times {}_4F_3\left(\begin{matrix}a_1+n, a_2, a_3, a_4, 1\\ b_1, b_2, b_3\end{matrix}\right). \tag{14}$$

CONNECTIONS WITH APPELL FUNCTIONS

Appell introduced the hypergeometric functions[7]

$$F_2(a, b_1, b_2, c_1, c_2, x_1, x_2) = \sum_{m,n=0}^{\infty} \frac{(a)_{m+n}(b_1)_m(b_2)_n x_1^m x_2^n}{(c_1)_m(c_2)_n m!\, n!}, \quad |x_1| + |x_2| < 1,$$

$$F_3(a_1, a_2, b_1, b_2, c, x_1, x_2) = \sum_{m,n=0}^{\infty} \frac{(a_1)_m(a_2)_n(b_1)_m(b_2)_n x_1^m x_2^n}{(c)_{m+n} m!\, n!}, \quad |x_1| < 1, \ |x_2| < 1, \tag{15}$$

as well as two other series denoted by F_1 and F_4, but we are concerned here with F_2 and F_3 only, since they are the only functions that contain the same number of parameters as the ${}_3F_2$ functions. Later Horn made a classification of hypergeometric series of two variables.[8] In Horn's classification there is, in addition to the F_2 and F_3 functions, only one more function with five parameters. This function is defined by the series

$$H_2(a, b, c, d, e, x_1, x_2) = \sum_{m,n=0}^{\infty} \frac{(a)_{m-n}(b)_m(c)_n(d)_n x_1^m x_2^n}{(e)_m m!\, n!}. \tag{16}$$

The functions F_2, F_3, and H_2 satisfy certain systems of partial differential equations which, however, can be transformed into one another. The solutions of one system satisfy, then, the other systems after suitable transformations. Appell has given four independent solutions of the equations associated with the F_2 function in terms of F_2 func-

[7] P. Appell and J. Kampé de Fériet, *Fonctions hypergéometriques et hypersphériques* (Gauthier-Villars, Paris, 1926).

[8] J. Horn, Math. Ann. 105, 381 (1931); also Ref. 3, p. 224.

tions, but there are also solutions in terms of F_3 and H_2 functions, which solutions are connected with ${}_3F_2$ functions in the sense that they are ${}_3F_2$ functions in one variable if the other variable is equal to unity.

The connections between ${}_3F_2$ functions and F_3 functions are easily established from the formulas we have derived here. By summing over m in (15) we obtain

$$F_3(a_1, a_2, b_1, b_2, c, x_1, x_2) = \sum_{n=0}^{\infty} \frac{(a_2)_n (b_2)_n x_2^n}{(c)_n n!} {}_2F_1(a_1, b_1, c+n, x_1).$$

This series converges, as we have seen, for $x_2 = 1$ provided Re $(c - a_2 - b_2) > 0$ and we obtain, using (2) and the symmetry of the F_3 function,

$$F_3(a_1, a_2, b_1, b_2, c, x, 1) = F_3(a_2, a_1, b_2, b_1, c, 1, x) = \frac{\Gamma(c)\Gamma(c-a_2-b_2)}{\Gamma(c-a_2)\Gamma(c-b_2)} {}_3F_2\left(\begin{matrix} a_1, b_1, c-a_2-b_2 \\ c-a_2, c-b_2 \end{matrix}, x\right),$$

$$\text{Re}\,(c - a_2 - b_2) > 0. \qquad (17)$$

If also Re $(c - a_1 - b_1) > 0$, the hypergeometric series of the ${}_3F_2$ function converges for $x = 1$ and we have

$$F_3(a_1, a_2, b_1, b_2, c, 1, 1) = \frac{\Gamma(c)\Gamma(c-a_2-b_2)}{\Gamma(c-a_2)\Gamma(c-b_2)} {}_3F_2\left(\begin{matrix} a_1, b_1, c-a_2-b_2 \\ c-a_2, c-b_2 \end{matrix}, 1\right),$$

$$\text{Re}\,(c-a_1-b_1)>0, \quad \text{Re}\,(c-a_2-b_2)>0. \qquad (18)$$

Here the lhs is invariant for interchange of indices 1 and 2 as well as for interchange of all the a's and b's, which gives us the Thomae transformations obtained in connection with the analytic continuation.

In order to establish the connections between H_2 functions and ${}_3F_2$ functions we use an analytic continuation of the F_3 function[9]

$$F_3(a_1, a_2, b_1, b_2, c, x_1, x_2) = \frac{\Gamma(c)\Gamma(b_1-a_1)}{\Gamma(b_1)\Gamma(c-a_1)} (-x_1)^{-a_1} \times H_2(a_1-c+1, a_1, a_2, b_2, a_1-b_1+1, 1/x_1, -x_2)$$
$$+ \frac{\Gamma(c)\Gamma(a_1-b_1)}{\Gamma(a_1)\Gamma(c-b_1)} (-x_1)^{-b_1} \times H_2(b_1-c+1, b_1, a_2, b_2, b_1-a_1+1, 1/x_1, -x_2).$$

In the expansion (16) of the H_2 function we may sum over m,

$$(-x_1)^{-a_1} H_2(a_1-c+1, a_1, a_2, b_2, a_1-b_1+1, 1/x_1, -x_2) = (-x_1)^{-a_1} \sum_{m=0}^{\infty} \frac{(a_1-c+1)_m (a_1)_m (1/x_1)^m}{(a_1-b_1+1)_m m!} \times {}_2F_1(a_2, b_2, c-a_1-m, x_2). \qquad (19)$$

The series converges for Re $x_2 < \frac{1}{2}$ and for $|x_1| \geq 1$ provided Re $(c - a_1 - b_1) > 0$, since, for Re $x_2 < \frac{1}{2}$ we have[10]

$${}_2F_1(a_2, b_2, c-a_1-m, x_2) \sim 1 + O(1/m).$$

We next put $x_1 = 1$. The functions on the rhs are, however, many-valued due to the factors $(-x_1)^{-a_1}$ and $(-x_1)^{-b_1}$, and, by letting $x_1 \to 1$ from above or below the cut from $x_1 = 0$ to $x_1 = \infty$, two different expressions will be obtained for the F_3 function. We can then argue that one of the H_2 functions can be eliminated and that there must exist an expansion of the type (19) for the ${}_3F_2$ function. We have, indeed, after a suitable change of the parameters

$${}_3F_2\left(\begin{matrix} a_1, a_2, a_3 \\ b_1, b_2 \end{matrix}, x\right) = C \sum_{n=0}^{\infty} \frac{(b_2-a_1)_n (1-b_1)_n}{(b_2-b_1+1)_n n!} {}_2F_1(a_2, a_3, b_1-n, x),$$

$$\text{Re}\, a_1 > 0, \qquad \text{Re}\, x < \tfrac{1}{2}. \qquad (20)$$

The result is easily proved in the same way as the result (2) by expanding the rhs in a McLaurin series. This determines the constant

$$C = \frac{\Gamma(a_1-b_1+1)\Gamma(b_2)}{\Gamma(b_2-b_1+1)\Gamma(a_1)}.$$

From (19) and (20) we obtain for an H_2 function

$$H_2(a, b, c, d, e, 1, -x_2) = \frac{\Gamma(e)\Gamma(e-a-b)}{\Gamma(e-a)\Gamma(e-b)} {}_3F_2\left(\begin{matrix} e-a-b, c, d \\ 1-a, e-a \end{matrix}, x_2\right),$$

$$\text{Re}\,(e - a - b) > 0. \qquad (21)$$

Provided that the ${}_3F_2$ series converges for $x_2 = 1$, which is the case when Re $(b - a - c - d + 1) > 0$, we have

$$H_2(a, b, c, d, e, 1, -1) = \frac{\Gamma(e)\Gamma(e-a-b)}{\Gamma(e-a)\Gamma(e-b)} {}_3F_2\left(\begin{matrix} e-a-b, c, d \\ 1-a, e-a \end{matrix}, 1\right),$$

$$\text{Re}\,(e-a-b)>0,$$

$$\text{Re}\,(b-a-c-d+1)>0.$$

[9] A. Erdélyi, Proc. Roy. Soc. (Edinburgh) **A62**, 378 (1949).

[10] O. Perron, Ref. 2, p. 11.

This result, as well as (18), holds in fact independent of how the two variables x_1 and x_2 approach unity.

The case of an F_2 function of unit arguments is more complicated due to the fact that we are no longer dealing with unique limits.

There are also connections between Appell functions and other solutions of the equations associated with the ${}_3F_2$ function. One immediate example is the function $\xi(x)$ in (5). Expanding the ${}_2F_1$ function we obtain the double series defining the Appell function F_3, and we may write

$$\xi\left(\begin{matrix} a_1, a_2, a_3, x \\ b_1, b_2 \end{matrix}\right) = x^{a_1-b_1-b_2+1}(1-x)^{b_1+b_2-a_1-a_2-a_3} \times F_3(b_1-a_1, 1-a_2, b_2-a_1, 1-a_3, b_1+b_2-a_1-a_2-a_3+1, 1-1/x, 1-x). \quad (22)$$

There are numerous similar examples relating not only the functions F_2, F_3, and H_2 to solutions of the equations associated with the ${}_3F_2$ function, but also higher-order hypergeometric functions which are solutions of the equations associated with the Appell functions. Certain higher-order hypergeometric series have been investigated by Appell.[6] However, the fact that the equation associated with the ${}_3F_2$ function does not permit solutions in powers of $1 - x$, which are hypergeometric series in the sense that the expansion coefficients are quotients of Γ functions as in (1), indicates that the equations associated with the Appell functions considered here have no solutions in terms of double hypergeometric series in powers of $1 - x_1$ and $1 - x_2$, whatever is the order.

A classification of the hypergeometric functions, based on the equations they satisfy, is in many respects more natural than a classification based on properties of expansion coefficients, but requires an introduction of associated Appell functions which do not seem to be hypergeometric in the sense of the functions in Horn's list.

Permutation-Algebraic Formulation of Spin-Free Transition Density Matrices*

R. D. POSHUSTA AND F. A. MATSEN
Molecular Physics Group, The University of Texas, Austin, Texas
(Received 25 August 1965)

Spin-free transition density matrices are derived from spin-free kets which are symmetry-adapted to the symmetric group and its algebra. The Dirac identity establishes that these spin-free density matrices are identical to those obtained by integrating the spin from the full-spin density martices. Derivations are first given for arbitrary primitive kets which may be geminals of higher polymals, after which we consider products of orbitals, either orthonormal or nonorthonormal.

Correlation in the spin-free space is discussed and we show the influence of permutational symmetry on the probability of coincidence of pairs. A special case of this correlation is the well-known Fermi hole.

INTRODUCTION

REDUCED density matrices[1,2] introduce considerable economy in the description of systems of identical particles. First- and second-order density matrices contain enough information to compute all observable properties of such systems. This represents an enormous saving over the full eigenkets when the number of particles is much larger than 2. Additional saving results if the observables do not involve spin; for then one may use the spin-free[1] density matrices. Computer programs can advantageously use density matrix formulations in calculating matrix elements of observables. Besides their economy of description, density matrices have interest because of the possibility[3,4] that they can be obtained directly from the Hamiltonian, thereby circumventing the determination of the full eigenkets.

In this paper we formulate the spin-free transition density matrices in the language of permutation group algebra.[5] This enables us to exploit the permutational symmetry without introducing an explicit form for the spin-free kets. That is, our kets might be products of orbitals, geminals or higher polymals. Before beginning the derivation of spin-free density matrices, we present a brief review of notation and the mathematical tools to be used.

A.

Kets and bras of an N-particle system are denoted by $|U\rangle$ and $\langle V|$ and can be expanded in orthonormal basis kets and bras:

$$|U\rangle = \sum_{i(N)} |i(N)\rangle\langle i(N) \mid U\rangle \tag{1.1a}$$

and

$$\langle U| = \sum_{i(N)} \langle U \mid i(N)\rangle\langle i(N)|, \tag{1.1b}$$

where

$$\langle i(N) \mid U\rangle = \langle U \mid i(N)\rangle^*. \tag{1.2}$$

Here $|i(N)\rangle$ and $\langle i(N)|$ stand for the N-fold tensor product[6] of single-particle kets and bras:

$$|i(N)\rangle \equiv |i_1\rangle\,|i_2\rangle \cdots |i_N\rangle, \tag{1.3a}$$

$$\langle i(N)| \equiv \langle i_N| \cdots \langle i_2|\,\langle i_1|. \tag{1.3b}$$

Bra-kets between these basis bras and kets are chosen to be

$$\langle i(N) \mid j(N)\rangle = \begin{cases} 1 & \text{if } i_r = j_r \text{ for each } r, \\ 0 & \text{otherwise.} \end{cases} \tag{1.4}$$

Particle numbers and coordinates never appear in this notation. The order of single-particle kets takes the place of particle numbers. The first ket in $|i(N)\rangle$ represents the state of particle one, the second represents that of particle two, and so forth. In the dual bra, the order is reversed as required for the "adjoint of a product."

B.

Density matrices are tensor products between kets and bras and are denoted by either $|U\rangle\langle V|$, $|U\rangle \otimes \langle V|$, or $\langle V| \otimes |U\rangle$. Such a "tensor" is called

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[1] R. McWeeny, Rev. Mod. Phys. **32**, 335 (1960).
[2] P.-O. Löwdin, Phys. Rev. **97**, 1474 (1955).
[3] A. J. Coleman, Rev. Mod. Phys. **35**, 668 (1963).
[4] C. Garrod and J. K. Percus, J. Math. Phys. **5**, 1756 (1964).
[5] F. A. Matsen and R. D. Poshusta, *Theorie des Groupes en Physique Classique et Quantique*, edited by T. Kahan (Dunod Cie., Paris, to be published), Vol. 3. (Available as a technical report from Molecular Physics Group, the University of Texas, Austin.)
[6] The elementary properties of tensor products and their use in many-particle quantum mechanics are discussed by W. Band in *The Mathematics of Physics and Chemistry* edited by H. Magenau and G. M. Murphy (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1964), Vol. II, Chap. 8.

a ket-bra and acts as a linear transformation on both kets and bras; it sends the ket $|W\rangle$ into $|U\rangle\langle V|W\rangle$ and the bra $\langle W|$ into $\langle W|U\rangle\langle V|$. One may interpret $|U\rangle\langle V|$ as a transformation which annihilates all of $|W\rangle$ except the $|V\rangle$ component which it projects onto $|U\rangle$. By means of (1.1a) and (1.1b) such a ket-bra has an expansion in basis ket-bras:

$$|U\rangle\langle V| = \sum_{i(N),j(N)} |i(N)\rangle\langle i(N) \mid U\rangle\langle V \mid j(N)\rangle\langle j(N)|. \quad (1.5)$$

Successive application of transition density matrices $|U\rangle\langle V|$ and $|W\rangle\langle X|$ to bras and kets indicates that transition density matrices form a linear associative algebra:

$$(|U\rangle\langle V|)\ |W\rangle\langle X| = |U\rangle\langle V \mid W\rangle\langle X|.$$

For example, the density matrix of a normalized ket $|U\rangle$ is idempotent:

$$(|U\rangle\langle U|)\ |U\rangle\langle U| = |U\rangle\langle U \mid U\rangle\langle U| = |U\rangle\langle U|.$$

In fact, the homomorphism algebra[7] of all linear mappings of the N-particle ket space into itself is spanned by a collection of such ket-bras.

Partial traces are linear operators on N-particle ket-bras which we define by means of basis ket-bras:

$$\mathrm{Tr}^m\ |i(N)\rangle\langle j(N)| \equiv |i(n)\rangle\langle j(n)|\ \langle j(m) \mid i(m)\rangle \quad (1.6)$$

where

$$|i(n)\rangle \equiv |i_1\rangle\ |i_2\rangle \cdots |i_n\rangle, \qquad |i(m)\rangle \equiv |i_{n+1}\rangle \cdots |i_N\rangle. \quad (1.7)$$

We adopt the convention that $i(n)$ stands for the first n indices from $i(N)$, and $i(m)$ stands for the last m indices where $n + m = N$. Thus $\mathrm{Tr}^m|U\rangle\langle V|$ is a transformation on n-particle kets and bras where $|U\rangle\langle V|$ was a transformation on N-particle kets and bras. One also speaks of Tr^m as a contraction on the last m indices or the last m particles of $|U\rangle\langle V|$. If $m = N$, the contraction sends $|U\rangle\langle V|$ into a complex number and we call Tr^N the full trace or simply the trace operator:

$$\mathrm{Tr}^N\ |U\rangle\langle V| = \langle V \mid U\rangle. \quad (1.8)$$

[7] A discussion of abstract vector spaces, tensor spaces, contractions, homomorphism algebras, and related mathematical concepts is to be found in the freshman text by G. D. Mastow, J. H. Sampson, and J. Meyer, *Fundamental Structure of Algebra* (McGraw–Hill Book Company, Inc., New York, 1963).

C.

S_N denotes the symmetric group[8] of all $N!$ permutations of the N particles in any N-particle ket or bra. The effect of an element P of S_N on an arbitrary ket is expressed in terms of the basis bras and kets:

$$P \equiv \begin{pmatrix} p_1 & p_2 & \cdots & p_N \\ 1 & 2 & \cdots & N \end{pmatrix}, \quad (1.9)$$

$$P\ |i(N)\rangle \equiv |i_{p_1}\rangle\ |i_{p_2}\rangle \cdots |i_{p_N}\rangle, \quad (1.10a)$$

$$\langle i(N)|\ P^{-1} \equiv \langle i_{p_N}| \cdots \langle i_{p_2} \mid \langle i_{p_1}|. \quad (10.1b)$$

It follows from the definition that

$$\langle U|\ P\ |V\rangle = \langle V|\ P^{-1}\ |U\rangle^*. \quad (1.11)$$

D.

A_N denotes the Frobenius algebra[5,9] of S_N and consists of all linear combinations of permutations with complex coefficients. A matric basis of A_N is denoted by $\{e^\alpha_{rs}; \alpha = 1, 2, \cdots, M; r, s = 1, 2, \cdots f^\alpha\}$. Partitions[8] of N, $\alpha = \{1^{\alpha_1}, 2^{\alpha_2}, \cdots, H^{\alpha_H}\}$, are used to label the matric basis and $\alpha = 1, 2, \cdots, M$ means that α ranges over all M partitions of N. Matric basis elements have the following properties:

$$e^\alpha_{rs}e^\beta_{tu} = \delta^{\alpha\beta}\delta_{st}e^\alpha_{ru}. \quad (1.12)$$

This is the matric basis multiplication rule in which $\delta^{\alpha\beta}$ and δ_{st} are Kronecker deltas.

The invertable relation between the matric basis and the so-called regular basis of the algebra is

$$e^\alpha_{rs} = \frac{f^\alpha}{N!} \sum_P [P^{-1}]^\alpha_{sr} P, \quad (1.13)$$

$$P = \sum_{\alpha=1}^{M} \sum_{r,s=1}^{f^\alpha} [P]^\alpha_{rs} e^\alpha_{rs}. \quad (1.14)$$

Here the expansion coefficient, $[P]^\alpha_{rs}$, is the r, s element of the $f^\alpha \times f^\alpha$ matrix of P in the αth irreducible representation of S_N.

A unitary matric basis can always be found for which the adjoint of e^α_{rs}, defined to be

$$e^{\alpha\dagger}_{rs} \equiv \frac{f^\alpha}{N!} \sum_P [P^{-1}]^{\alpha *}_{sr} P^{-1} \quad (1.15)$$

is given by

$$e^{\alpha\dagger}_{rs} = e^\alpha_{sr}. \quad (1.16)$$

[8] D. E. Littlewood, *The Theory of Group Characters and Matrix Representations of Groups* (Oxford University Press, New York, 1958).

[9] H. Boerner, *Representations of Groups* (North–Holland Publishing Company, Amsterdam, 1963).

Hence there is also a unitary irreducible representation:

$$[P]^{\alpha *}_{rs} = [P^{-1}]^{\alpha}_{sr}. \tag{1.17}$$

E.

A quantum mechanical system of N indistinguishable particles must undergo no observable change if the particles are permuted (equivalent to relabeling the particles). It follows that observables correspond to linear operators which commute with all the elements of A_N. Consequently,[5,10] A_N induces the following structure on the eigenkets of any observable operator, H.

(i) The matrix of H is factored:

$$\begin{aligned}\langle V; \beta ut| H |U; \alpha rs\rangle &\equiv \langle V| e^{\beta\dagger}_{ut} H e^{\alpha}_{rs} |U\rangle \\ &= \langle V| He^{\beta}_{tu} e^{\alpha}_{rs} |U\rangle \\ &= \delta^{\alpha\beta}\delta_{ur}\langle V| e^{\alpha\dagger}_{vt} H e^{\alpha}_{vs} |U\rangle \\ &= \delta^{\alpha\beta}\delta_{ur}\langle V; \alpha vt| H |U; \alpha vs\rangle. \end{aligned} \tag{1.18}$$

In words, H has zero intersection between matric basis projections of arbitrary kets $|U\rangle$ and $|V\rangle$ unless the symmetries α, β match and the first indices u, r are equal. Further, the matrix element is independent of the first index $u = r$.

(ii) Symmetry-adapted kets are defined to be those of the form

$$|U; \sigma\alpha r\rangle \equiv \sum_{s} (\sigma)_{s} e^{\alpha}_{rs} |U\rangle. \tag{1.19}$$

Because of the factorization of (i), the eigenkets of H assume this form. The partition, α, is called the permutation quantum number of the state $|U; \sigma\alpha r\rangle$. The collection of all kets with permutation quantum number α is called a permutation state. The zeros $\delta^{\alpha\beta}$ forbid mixing between different permutation states. A permutation P transforms a symmetry-adapted ket according to an irreducible representation of S_N:

$$P |U; \sigma\alpha r\rangle = \sum_{r'} [P]^{\alpha}_{r'r} |U; \sigma\alpha r'\rangle \tag{1.20}$$

and similarly for the bras:

$$\langle U; \sigma\alpha r| P^{-1} = \sum_{r'} \langle U; \sigma\alpha r'| [P^{-1}]^{\alpha}_{rr'}. \tag{1.21}$$

Matrix elements of H over these symmetry-adapted kets are easily expressed in the following form:

$$\begin{aligned}&\langle V; \tau\alpha r| H |U; \sigma\alpha r\rangle \\ &\quad = \sum_{s'} \sum_{s} (\tau)^{*}_{s'} \langle V; \alpha rs'| H |U; \alpha rs\rangle (\sigma)_{s} \\ &\quad = \tau^{\dagger} \mathbf{H} \sigma. \end{aligned} \tag{1.22}$$

Here σ and τ denote the column matrices of coefficients $(\sigma)_s$ and $(\tau)_s$, while $\mathbf{H}$ is the $f^{\alpha} \times f^{\alpha}$ matrix of Eq. (1.18). For example, the normalization of $|U; \sigma\alpha r\rangle$ depends on the matrix element

$$\langle U; \sigma\alpha r | U; \sigma\alpha r\rangle = \sigma^{\dagger} \mathbf{\Delta} \sigma, \tag{1.23}$$

where $\mathbf{\Delta}$ is the matrix of the identity.

We treat a system of N electrons whose Hamiltonian contains no spin interactions.[5,10] The Pauli principle for spin-free eigenkets is: α has the form $\{2^p, 1^{N-2p}\}$ for electrons; no more than two electrons may occupy the same orbital.

Permutational symmetry is connected with spin through the Dirac identity. Briefly, the spin quantum number, S, of electronic systems is related to the permutation quantum number $\alpha = \{2^p, 1^{N-2p}\}$ by the equation[5]

$$S = \tfrac{1}{2}N - p. \tag{1.24}$$

A spin-free N-electron ket with permutation quantum number α, gives the same matrix elements of spin-free observables as does its corresponding spin-eigenket with spin quantum number S.

SPIN-FREE DENSITY MATRICES

Consider an n-particle operator on a system of N identical particles. We denote such an operator by G^n and define it by the equation

$$G^n \equiv \sum_{i_1=1}^{(N-n+1)} \sum_{i_2>i_1} \cdots \sum_{i_n>i_{n-1}}^{N} g_{i_1 i_2 \cdots i_n}, \tag{2.1}$$

where $g_{1,2,\cdots,n}$ is a transformation on the kets representing particles 1, 2, $\cdots$ n. Further $g_{12\cdots n}$ is assumed to be symmetric in the indices 1, 2, $\cdots$ n, so that, e.g., $g_{213\cdots n} = g_{123\cdots n}$, etc. The remaining terms of G^n are defined by means of the transpositions

$$(i,r) \equiv \begin{pmatrix} i, & r \\ r, & i \end{pmatrix}:$$

$$\begin{aligned} g_{i_1 i_2 \cdots i_n} &\equiv (i_n n) \cdots (i_2 2)(i_1 1) \\ &\quad \times g_{12\cdots n}(i_1 1)(i_2 2) \cdots (i_n n). \end{aligned}$$

When the abbreviation $P_{i(n)} \equiv (i_1 1)(i_2 2) \cdots (i_n n)$ is used, this definition becomes

$$g_{i_1 i_2 \cdots i_n} \equiv P^{-1}_{i(n)} g_{12\cdots n} P_{i(n)}. \tag{2.2}$$

It follows from (2.1) that G^n commutes with every

[10] F. A. Matsen, *Advances in Quantum Chemistry* (Academic Press Inc., New York, 1964), Vol. I.

permutation from S_N. The observables on our system are linear combinations of operators of this kind. For example, the Hamiltonian is $H = H^1 + H^2$, where H^1 represents the sum of one-particle energies (kinetic and potential) and H^2 represents the sum of interparticle interaction energies.

nth-order reduced spin-free transition density matrices are suggested by the matrix elements of G^n between symmetry-adapted kets. First, from Eq. (1.18), one may conclude that matrix elements are independent of the index r in symmetry-adapted kets (1.19) and therefore may be averaged. Second, one forms the completely random average:

$$\langle V;\, \tau\alpha r|\, G^n\, |U;\, \sigma\alpha r\rangle = \frac{1}{f^\alpha} \sum_t \langle V;\, \tau\alpha t|\, G^n\, |U;\, \sigma\alpha t\rangle. \tag{2.3}$$

We next substitute (2.1), (2.2), (1.20), and (1.21) into (2.3) to obtain

$$\langle V;\, \tau\alpha r|\, G^n\, |U;\, \sigma\alpha r\rangle = \frac{1}{f^\alpha} \sum_{i_1(i_2\cdots(i_n} \sum_{s,s'} \Big(\sum_t [P_{i(n)}]^\alpha_{st} \times [P^{-1}_{i(n)}]^\alpha_{ts'}\Big)\langle V;\, \tau\alpha s'|\, g_{12\ldots n}\, |U;\, \sigma\alpha s\rangle. \tag{2.4}$$

The sum on t in parenthesis gives $\delta_{ss'}$ regardless of the summation indices $i_1, i_2, \cdots, i_n$ so that we find

$$\langle V;\, \tau\alpha r|\, G^n\, |U;\, \sigma\alpha r\rangle = \binom{N}{n} \frac{1}{f^\alpha} \sum_s \langle V;\, \tau\alpha s|\, g_{12\ldots n}\, |U;\, \sigma\alpha s\rangle. \tag{2.5}$$

In words, this equation states that G^n may be replaced by the single operator $g_{12\ldots n}$ (on the first n particles) if a random average is made on the index r and the result multiplied by $\binom{N}{n}$. The bra-ket of (2.5) is the trace of a ket-bra:

$$\begin{aligned}\langle V;\, \tau\alpha r|\, G^n\, |U;\, \sigma\alpha r\rangle &= \mathrm{Tr}^N\,(G^n\, |U;\, \sigma\alpha r\rangle\langle V;\, \tau\alpha r|) \\ &= \mathrm{Tr}^n\left(g_{12\ldots n}\binom{N}{n}\frac{1}{f^\alpha}\sum_s \mathrm{Tr}^m\, |U;\, \sigma\alpha s\rangle\langle V;\, \tau\alpha s|\right) \\ &= \mathrm{Tr}^n\,(g_{12\ldots n} nP^n[U;\, \sigma\alpha r \mid V;\, \tau\alpha r]).\end{aligned} \tag{2.6}$$

Here we have introduced the definition of the nth-order reduced spin-free transition density matrix:

$$P^n[U;\, \sigma\alpha r \mid V;\, \tau\alpha r] \equiv \binom{N}{n}\frac{1}{f^\alpha}\sum_s \mathrm{Tr}^m\,(|U;\, \sigma\alpha s\rangle\langle V;\, \tau\alpha s|). \tag{2.7}$$

We use the convention of Eq. (1.6), that $n + m = N$.

In the notation of McWeeny[1] (which is similar to that of Lowdin[2]), the reduced density matrix between states $\psi_{U;\sigma\alpha r}(1, \cdots, N)$ and $\psi_{V;\tau\alpha r}(1, \cdots N)$ is defined

$$\begin{aligned}&\rho^n_{U;\sigma\alpha r|V;\tau\alpha r}(1, \cdots, n;\, 1', \cdots, n') \\ &\equiv \binom{N}{n}\int\cdots\int \psi_{U;\sigma\alpha r}(1, \cdots, N) \\ &\quad\times \psi^*_{V;\tau\alpha r}(1', \cdots, n', n+1, \cdots, N)\, d\tau_{n+1}\cdots d\tau_N,\end{aligned}$$

where 1, 2, $\cdots$ stand for ordinary and spin coordinates of particles 1, 2, $\cdots$. The spin-free reduced density matix is

$$\begin{aligned}P^n_{U;\sigma\alpha r|V;\tau\alpha r}(1, \cdots n;\, 1', \cdots n') &= \iint [\rho^n_{U;\sigma\alpha r|V;\tau\alpha r} \\ &\quad\times (1, \cdots, n;\, 1', \cdots, n')]_{\omega_r'\to\omega_r}\, d\omega_1 \cdots d\omega_n,\end{aligned}$$

where $\omega_r' \to \omega_r$ means that the primes are removed from the spin coordinates before integration. In spin-free density matrices, 1, 2, $\cdots$ stand for ordinary space coordinates only.

One can interpret the sum on s in (2.7) as a random statistical average of the pure-state density matrices

$$\binom{N}{n}\mathrm{Tr}^m\, |U;\, \sigma\alpha s\rangle\langle V;\, \tau\alpha s|.$$

It should be emphasized that Eq. (2.7) is an nth-order spin-free transition density matrix derived from a spin-free ket. No change would result if one began from a antisymmetric space and spin ket and contracted on spin indices after finding the usual nth-order density matrix. Equation (1.24) gives the connection between spin quantum numbers and permutation quantum numbers.

It follows from (2.7) that the various orders of reduced density matrices are related by the recursion formula

$$(N - n)P^n[U;\, \sigma\alpha r \mid V;\, \tau\alpha r] = \mathrm{Tr}^1\, P^{n+1}[U;\, \sigma\alpha r \mid V;\, \tau\alpha r]. \tag{2.8}$$

Density matrices for *arbitrary* kets can be obtained from Eq. (2.7), the density matrix of symmetry-adapted kets. Such symmetry-adapted kets receive the most attention in the following sections because they represent pure states (either of permutational symmetry or spin eigenvalue). But the density matrices between arbitrary kets can be derived in a similar manner. Briefly, the resolution of the identity into matric basis elements [Eq. (1.14)] resolves $|U\rangle$ into its symmetry-adapted components. The matrix elements of G^n then become

$$\langle V|\, G^n\, |U\rangle = \sum_{\alpha,\alpha'}\sum_{r,r'}\langle V;\, \alpha' r' r'|\, G^n\, |U;\, \alpha r r\rangle$$

and by Eq. (1.18):

$$\langle V|\, G^n\, |U\rangle = \sum_\alpha \sum_r \langle V; \alpha rr|\, G^n\, |U; \alpha rr\rangle. \qquad (2.9)$$

Since the components $|U; \alpha rr\rangle$ are symmetry-adapted (with $\mathfrak{d}$ = a unit column vector with a single one in row r), the definition (2.7) may be used to introduce the nth-order density matrix:

$$\langle V|\, G^n\, |U\rangle = \sum_\alpha \sum_r \mathrm{Tr}^n\, g_{12\ldots n} P^n[U; \alpha sr \mid V; \alpha sr]. \qquad (2.10)$$

Thus, the nth-order reduced spin-free transition density matrix between arbitrary kets is defined to be

$$P^n[U \mid V] \equiv \sum_\alpha \sum_r P^n[U; \alpha sr \mid V; \alpha sr]. \qquad (2.11)$$

[Notice (2.11) is independent of s.] The sum on α in (2.11) resolves $P^n[U|V]$ into symmetry components. The density matrix between arbitrary kets has components of each permutation quantum number. If $|U\rangle$ and $|V\rangle$ are replaced by symmetry-adapted kets, (2.11) reduces to

$$P^n[U; \sigma\alpha r \mid V; \tau\beta u] = \delta^{\alpha\beta}\delta_{ru} P^n[U; \sigma\alpha r \mid V; \tau\alpha r]. \qquad (2.12)$$

EVALUATION OF SPIN-FREE DENSITY MATRICES

The properties of A_N permit us to express the spin-free density matrices of Eq. (2.7) in more elementary form.

The permutational symmetry of the adapted kets $|U; \sigma\alpha r\rangle$ and $|V; \tau\alpha r\rangle$ is used by substituting (1.19) and (1.13) into (2.7):

$$P^n[U; \sigma\alpha r \mid V; \tau\alpha r] = \left(\frac{f^\alpha}{N!\, n!}\right) \sum_P \sum_{P'} \frac{1}{m!} \times \Big(\sum_\iota \sum_{\iota'} (\tau)^*_{\iota'} \sum_s [P']^\alpha_{\iota' s} [P]^\alpha_{s\iota} (\sigma)_\iota\Big) \times \mathrm{Tr}^m\, (P \mid U\rangle\langle V \mid P'). \qquad (3.1)$$

The triple sum enclosed in parenthesis in (3.1) is recognized as the matrix product $\tau^\dagger[\mathbf{P}'\mathbf{P}]^\alpha \mathfrak{d}$, where $[\mathbf{P}]^\alpha$ is the matrix of P in the αth-irreducible representation of S_N and $\mathfrak{d}$, τ are the column vectors of coefficients from (1.19). We define the following expansion density matrices in terms of $|U\rangle$ and $|V\rangle$:

$$p^n_{UV}[P \mid P'] \equiv \mathrm{Tr}^m\, (P \mid U\rangle\langle V \mid P'). \qquad (3.2)$$

When these are introduced in (3.1), the transition density matrix between $|U; \sigma\alpha r\rangle$ and $|V; \tau\alpha r\rangle$ becomes

$$P^n[U; \sigma\alpha r \mid V; \tau\alpha r] = \frac{f^\alpha}{N!\, n!} \sum_P^{N!} \sum_{P'}^{N!} \frac{1}{m!}\, \tau^\dagger[\mathbf{P}'\mathbf{P}]^\alpha \mathfrak{d} p^n_{UV}[P \mid P']. \qquad (3.3)$$

Expansion density matrices consist of contractions on particles $n+1$ through N; consequently, they have the property

$$p^n_{UV}[P \mid P'] = p^n_{UV}[\pi P \mid P'\pi^{-1}], \qquad (3.4)$$

where π is any permutation from $S_m \subset S_N$, the group of all $m!$ permutations on the last m particles. To make use of this property, we decompose S_N in left cosets relative to S_m:

$$S_N = \sum_f^{N!/m!} P_f S_m, \qquad (3.5)$$

where P_f is a left coset representative and $P_f S_m$ is the left coset generated by P_f. In view of (3.5), we are able to express a sum over the whole group S_N as a double sum over S_m and the generators of distinct left cosets of S_m. Thus, we write $P' = P_f\pi$ and (3.3) becomes

$$P^n[U; \sigma\alpha r \mid V; \tau\alpha r] = (f^\alpha/N!\, n!) \times \sum_P^{N!} \sum_f^{N!/m!} \sum_\pi^{m!} \frac{1}{m!}\, \tau^\dagger[\mathbf{P}_f\pi\mathbf{P}]^\alpha \mathfrak{d} p^n_{UV}[P \mid P_f\pi]. \qquad (3.6)$$

By the property of (3.4), this becomes

$$P^n[U; \sigma\alpha r \mid V; \tau\alpha r] = (f^\alpha/N!\, n!) \times \sum_P \sum_f \sum_\pi \frac{1}{m!}\, \tau^\dagger[\mathbf{P}_f\pi\mathbf{P}]^\alpha \mathfrak{d} p^n_{UV}[\pi P \mid P_f]. \qquad (3.7)$$

As π varies over S_m and P varies over S_N, the product πP varies over S_N a total of $m!$ times; therefore,

$$P^n[U; \sigma\alpha r \mid V; \tau\alpha r] = \frac{f^\alpha}{N!\, n!} \sum_P \sum_f \tau^\dagger[\mathbf{P}_f\mathbf{P}]^\alpha \mathfrak{d} p^n_{UV}[P \mid P_f]. \qquad (3.8)$$

This expression represents the simplest form of the nth-order reduced spin-free transition density matrix for arbitrary $|U\rangle$ and $|V\rangle$. For electronic systems, (3.8) gives the spin-free density matrices identical to those of pure spin states with spin quantum numbers given by (1.24).

ORBITAL PRODUCT DENSITY MATRICES

In this section we enploy kets $|U\rangle$ and $|V\rangle$ with the special form

$$|U\rangle \equiv |u(N)\rangle, \qquad (4.1a)$$

$$|V\rangle \equiv |v(N)\rangle, \qquad (4.1b)$$

where $|u_r\rangle$ is a single-particle ket or orbital (not necessarily orthonormal). The partial traces of ket-bras between products of non-orthonormal kets are given by the same expression (1.6) as for orthonormal kets. This is seen by substituting the expansion of

$|u_r\rangle$ and $|v_s\rangle$ in orthonormal orbitals,

$$|u_r\rangle = \sum_i |i\rangle\langle i \mid u_r\rangle,$$

into the partial trace expression and using the linear property of Tr^m:

$$\begin{aligned}\mathrm{Tr}^m & |u(N)\rangle\langle v(N)| \\ &= \mathrm{Tr}^m \sum_{i(N)} \sum_{j(N)} |i(N)\rangle\langle i(N) \mid u(N)\rangle\langle v(N) \mid j(N)\rangle\langle j(N)| \\ &= \sum_{i(n)} \sum_{j(n)} |i(n)\rangle\langle i(n) \mid u(n)\rangle\langle v(n) \mid j(n)\rangle\langle j(n)| \\ &\qquad \times \sum_{i(m)} \langle i(m) \mid u(m)\rangle\langle v(m) \mid i(m)\rangle \\ &= |u(n)\rangle\langle v(n)| \langle v(m) \mid u(m)\rangle.\end{aligned}$$

Equation (1.6), the definition of partial trace, thus applies to nonorthonormal orbitals as well as orthonormal orbitals.

Expansion density matrices between orbital product primitive kets become, from Eqs. (3.2) and (3.8),

$$\begin{aligned}p^n_{UV}[P \mid P_f] &= \mathrm{Tr}^m (P(u)P_f^{-1}(v) \; |u_1\rangle\langle v_1| \otimes |u_2\rangle \\ &\qquad \times \langle v_2| \otimes \cdots \otimes |u_N\rangle\langle v_N|). \qquad (4.2)\end{aligned}$$

Here $P(u)$ is a permutation on the ordered u-orbitals and $P_f^{-1}(v)$ is a permutation on the v-orbitals. The effect of Tr^m is to send the last m of the single particle ket-bras $|u_r\rangle\langle v_r|$ into the complex numbers $\rangle v_r|u_r\rangle$. Permutations $P(u)$ and $P_f^{-1}(v)$ on $\mathrm{Tr}^m(|u(N)\rangle\langle v(N)|)$ give the same reduced density matrix as results from applying the permutations before the partial trace. Hence, (4.2) can be written

$$\begin{aligned}p^n_{UV}[P \mid P_f] &= P(u)P_f^{-1}(v) \; \mathrm{Tr}^m \, (|u(N)\rangle\langle v(N)|) \\ &= P(u)P_f^{-1}(v) \; |u(n)\rangle\langle v(n)| \, \langle v(m) \mid u(m)\rangle \\ &= P(u)P_f^{-1}(v) \; |u_1\rangle\langle v_1| \otimes |u_2\rangle\langle v_2| \otimes \cdots \\ &\qquad \otimes |u_n\rangle\langle v_n| \, \langle v_{n+1} \mid u_{n+1}\rangle \cdots \langle v_N \mid u_N\rangle. \qquad (4.3)\end{aligned}$$

and the nth-order reduced spin-free transition density matrix (3.8) becomes

$$\begin{aligned}P^n[U; \sigma\alpha r \mid V; \tau\alpha r] &= \frac{f^\alpha}{N!\, n!} \sum_P \sum_f \tau^\dagger[\mathbf{P}_f\mathbf{P}] \\ &\times \mathfrak{d}P(u)P_f^{-1}(v) \; |u(n)\rangle\langle v(n)| \, \langle v(m) \mid u(m)\rangle. \qquad (4.4)\end{aligned}$$

As P ranges over S_N, the first orbital of $|u(N)\rangle$ ranges from $|u_1\rangle$ through $|u_N\rangle$ and similarly for the second, third, etc., orbitals. Hence, the sums on P and P_f may be replaced by multiple sums on orbitals:

$$\begin{aligned}P^n[U; \sigma\alpha r \mid V; \tau\alpha r] &= \sum_{i(n)}{}' \sum_{j(n)}{}' \gamma^n_{UV}(i(n) \mid j(n)) \; |u_{i(n)}\rangle\langle v_{j(n)}|, \qquad (4.5)\end{aligned}$$

where each summation index i_r ranges from 1 through N and the prime indicates that no two indices are equal. By $|u_{i(n)}\rangle$ is meant $|u_{i_1}\rangle|u_{i_2}\rangle \cdots |u_{i_n}\rangle$ and the coefficient $\gamma^n_{UV}(i(n)|j(n))$ is the sum of all coefficients of $|u_{i(n)}\rangle\langle v_{j(n)}|$ in 4.4. In Appendix A we show that

$$\begin{aligned}&\gamma^n_{UV}(i(n) \mid j(n)) \\ &= \frac{f^\alpha}{N!\, n!} \sum_{i(m)}{}'' \tau^\dagger\left[\begin{pmatrix} \mathrm{i(n)\,i(m)} \\ \mathrm{j(n)\,j(m)} \end{pmatrix}\right]^\alpha \mathfrak{d}\langle v_{j(m)} \mid u_{i(m)}\rangle, \qquad (4.6)\end{aligned}$$

where the double prime indicates that no two indices of $i(m)$ are equal and none is equal to an index of $i(n)$. $j(m)$ is any arrangement of the integers which remain from (N) after $j(n)$ is specified.

If the single-particle kets and bras are orthonormal, the expansion density matrices $|u_{i(n)}\rangle\langle v_{j(n)}|$ form a matric basis of the homomorphism algebra of all linear transformations on n-particle kets and bras:

$$\begin{aligned}(|u_{i(n)}\rangle\langle v_{j(n)}|) \; |u_{k(n)}\rangle\langle v_{l(n)}| \\ = \begin{cases} |u_{i(n)}\rangle\langle v_{l(n)}| & \text{if} \quad j(n) = k(n) \\ 0 \quad \text{otherwise.} \end{cases}\end{aligned}$$

In this case, the coefficients $\gamma^n_{UV}(i(n)|j(n))$ may be interpreted, as is done by Löwdin[2] and others, as representations of transition density matrices on the homomorphism algebra. The coefficient $\gamma^n_{UU}(i(n)|i(n))$ of the density matrix is interpreted as $\binom{N}{n}$ times the probability of finding n particles occupying the space-orbitals $|u_{i_1}\rangle, |u_{i_2}\rangle, \cdots, |u_{i_n}\rangle$. The off-diagonal elements in the representation of the first-order density matrix, $\gamma^1_{UU}(i|j)$, are the bond orders, and the diagonal elements, $\gamma^1_{UU}(i|i)$, are the occupation numbers of the space-orbitals. The unitary transformation which diagonalizes $\gamma^1_{UU}(i|j)$ will transform the orbitals into a set of natural spin-free orbitals in analogy with Löwdin's natural spin orbitals.

Equation (4.6) can be simplified when the orbitals are orthonormal. The $\mathbf{\Delta}$ matrix of (1.23) becomes the scalar matrix $(f^\alpha/N!)\,\mathbf{1}$, and $|U; \sigma\alpha r\rangle$ is normalized if $\mathfrak{d}^\dagger\mathfrak{d} = N!/f^\alpha$. The density matrix coefficients $\gamma^n_{UV}(i(n)|j(n))$ vanish unless $i(n)$ is a permutation of $j(n)$: the sum on $i(m)$ in (4.6) is replaced by the single term

$$\gamma^n_{UV}(i(n) \mid j(n)) = \begin{cases} (f^\alpha/N!\, n!) \; \tau^\dagger[\binom{\mathrm{i(n)}}{\mathrm{j(n)}}]^\alpha \mathfrak{d} \\ 0 \quad \text{otherwise} \end{cases}$$

if $i(n)$ is a permutation of $j(n)$. For example, let $|U\rangle$ be the N-fold product of orthonormal orbitals; then the first and second order density matrices over $|U; \sigma\alpha r\rangle$ are given by

$$P^1[U; \sigma\alpha r \mid U; \sigma\alpha r] = \sum_{i=1}^N |u_i\rangle\langle u_i| \qquad (4.9)$$

and

$$P^2[U;\sigma\alpha r \mid U;\sigma\alpha_r] = \tfrac{1}{2}\sum_{i,j}' |u_i\rangle\langle u_i| \otimes |u_j\rangle\langle u_j| + f^\alpha/2(N!)\sum_{i,j}' \mathfrak{d}^\dagger\left[\begin{pmatrix} i & j \\ j & i \end{pmatrix}\right]^\alpha \mathfrak{d}\, |u_i\rangle\langle u_i| \otimes |u_j\rangle\langle u_i|. \tag{4.10}$$

Appendix B provides a simple example of Eqs. (4.9) and (4.10) for the case of three particles in permutation state $\alpha = \{2, 1\}$.

SINGLE-DETERMINANT DENSITY MATRICES

Symmetry-adapted kets for the permutation state $\alpha = \{1^N\}$ have the form

$$|U; \{1^N\}\rangle = \frac{1}{N!}\sum_P \epsilon(P)P\,|U\rangle, \tag{5.1}$$

where $\epsilon(p)$ is the parity of P and σ and r have been suppressed because $f^{\{1^N\}} = 1$. Alternately, Eq. (5.1) may be written

$$|U; \{1^N\}\rangle = \mathfrak{A}\,|U\rangle, \tag{5.2}$$

where $\mathfrak{A}$ is the antisymmetrizer. If $|U\rangle$ is spin-free, then (5.2) represents a state with spin quantum number $S = \frac{1}{2}N$. When $|U\rangle$ is any orbital product (spin-free or not) ket $|u(N)\rangle$, (5.2) becomes

$$|U; \{1^N\}\rangle = \mathfrak{A}\,|u(N)\rangle = \det\{u(N)\}. \tag{5.3}$$

The nth-order spin-free transition density matrix between two such kets is given by

$$P^n[U; \{1^N\} \mid V; \{1^N\}] = \sum_{i(n)}'\sum_{j(n)}' \gamma^n_{UV}(i(n) \mid j(n))\, |u_{i(n)}\rangle\langle v_{j(n)}|,$$

where

$$\gamma^n_{UV}(i(n) \mid j(n)) = \frac{1}{N!\,n!}\sum_{i(m)}'' \epsilon\begin{pmatrix} i(n)i(m) \\ j(n)j(m) \end{pmatrix}\langle v_{i(m)} \mid u_{i(m)}\rangle = \frac{1}{N!\,n!}\sum_{i(m)}'' \epsilon\begin{pmatrix} i(n)i(m) \\ j(n)j(m) \end{pmatrix}\prod_{r=n+1}^{N}\langle v_{i_r} \mid u_{i_r}\rangle \tag{5.4}$$

and $\langle v_i|u_i\rangle$ is called an "overlap integral." The $N \times N$ matrix with these overlap integrals as elements:

$$\mathbf{D}_{UV} \equiv \{d_{UV}(j \mid i)\}, \tag{5.5}$$

where

$$d_{UV}(j \mid i) \equiv \langle v_i \mid u_i\rangle$$

is labeled by v_i on rows and u_i on columns. Now the coefficient $\gamma^n_{UV}(i(n)|j(n))$ is recognized as the cofactor which results when the rows labeled $v_{j(m)}$ and columns labeled $u_{i(m)}$ are struck from the determinant of $\mathbf{D}_{UV}$. This is the useful result first given by Löwdin[2] for spin orbital wavefunctions.

Equation (5.4) applies to spin kets as well as spin-free kets. Simply consider the orbital $|u_i\rangle$ to be a spin-orbital, e.g., electron spin orbitals have the form $|u^+\rangle \equiv |u\rangle|\alpha\rangle$ and $|u^-\rangle \equiv |u\rangle|\beta\rangle$. Then $|U; \{1^N\}\rangle$ is a Slater determinant. Such a determinant is not an eigenket of S^2 unless the space orbitals are doubly occupied. That is, $|U; \{1^N\}\rangle$ (with spin-orbitals) is an eigenket of S^2 only if $|u(N)\rangle$ has the form $|u^+_1\rangle|u^-_1\rangle|u^+_2\rangle|u^-_2\rangle\cdots$. Regardless of this shortcoming, single Slater determinants are often used as approximate representations of eigenkets. Equation (5.4) may be used without change for the density matrices between Slater determinants, but the spin-free density matrices are found by contracting on the spin in (5.4).

Permutational symmetry-adapted spin-free kets may be coupled to similarly adapted pure-spin kets (analogous to Clebsh–Gordon series for rotational symmetry) with the result[5,10] that

$$\mathfrak{A}\,|U\rangle\,|\theta\rangle = \sum_\alpha \frac{1}{f^\alpha}\sum_{r,s} |U; \alpha rs\rangle\,|\theta; \hat{\alpha}rs\rangle, \tag{5.6}$$

where $|U\rangle$ is the spin-free ket, $|\theta\rangle$ the pure-spin ket (e.g., $|\theta\rangle = \alpha\beta\alpha\beta\cdots$) and $\hat{\alpha}$ is related to α by $[P]^{\hat{\alpha}} \equiv [P]^\alpha\epsilon(P)$. The nth-order reduced spin-free transition density matrix between such kets now may be expressed:

$$P^n[U\theta \mid V\theta] = \sum_{\alpha,\alpha'}\frac{1}{f^\alpha f^{\alpha'}}\sum_{r,r'}\sum_{s,s'} P^n[U; \alpha rs \mid V; \alpha' r's'] \times \langle\theta; \hat{\alpha}rs \mid \theta; \hat{\alpha}'r's'\rangle$$

$$= \sum_\alpha \frac{1}{f^\alpha}\sum_{s,s'}\langle\theta \mid \theta; \hat{\alpha}ss'\rangle\frac{1}{f^\alpha} \times \sum_r P^n[U; \alpha rs \mid V; \alpha rs'].$$

Since $P^n[U; \alpha rs \mid V; \alpha rs']$ already contains an average on the first index r, this becomes

$$P^n[U\theta \mid V\theta] = \sum_\alpha \frac{1}{f^\alpha}\sum_{s,s'}\langle\theta \mid \theta; \hat{\alpha}ss'\rangle \times P^n[U; \alpha rs \mid V; \alpha rs']. \tag{5.7}$$

Equation (5.7) expresses the resolution of $P^n[U\theta|V\theta]$ into pure permutation-state components. The weights given each component depend on the spin bra-kets:

$$\langle\theta \mid \theta; \hat{\alpha}ss'\rangle = \frac{f^\alpha}{N!}\sum_P [P]^{\hat{\alpha}}_{s's}\langle\theta|\,P\,|\theta\rangle.$$

Density matrices between Slater determinants result from (5.7) when

$$|U\rangle = |u(N)\rangle$$

and

$|\theta\rangle$ = a product of orthonormal spin kets (such as $|\alpha\rangle|\beta\rangle|\alpha\rangle \cdots$ for electrons).

In this case, $\langle\theta|\ P\ |\theta\rangle$ vanishes unless

$$P\ |\theta\rangle = |\theta\rangle$$

and we find that

$$\langle\theta\ |\ \theta; \hat{\alpha}ss'\rangle = \frac{f^{\alpha}}{N!\, n^{\theta}}\,[E^{\theta}]^{\hat{\alpha}}_{ss'},$$

where E^{θ} is the idempotent

$$E^{\theta} = \frac{1}{n^{\theta}} \sum_{P^{\theta}} P^{\theta},$$

where P^{θ} is a permutation which leaves $|\theta\rangle$ invariant and n^{θ} is the number of such permutations.

$$P^{n}[U\theta\ |\ V\theta] = \frac{n^{\theta}}{N!} \sum_{\alpha} \sum_{s,s'} [E^{\theta}]^{\hat{\alpha}}_{ss'} \times P^{n}[U; \alpha rs\ |\ V; \alpha rs']. \qquad (5.8)$$

One may choose a representation in which $[E^{\theta}]^{\hat{\alpha}}$ is diagonal with ones at the upper left. This choice gives for the nth-order spin-free transition density matrix between two Slater determinants [cf. Eq. (2.11)]

$$P^{n}[U\theta\ |\ V\theta] = \frac{n^{\theta}}{N!} \sum_{\alpha} \sum_{s=1}^{f^{\hat{\alpha}\theta}} P^{n}[U; \alpha rs\ |\ V; \alpha rs]. \qquad (5.9)$$

Here $f^{\hat{\alpha}\theta}$ is the number of ones in the diagonal of $[E^{\theta}]^{\hat{\alpha}}$.

When $|\theta\rangle$ is the spin factor of an electron Slater determinant, $f^{\hat{\alpha}\theta} = 0$ if $\hat{\alpha} < \{n_{\alpha}, n_{\beta}\}$ (or $\alpha > \{2^{p}, 1^{N-2p}\}$) where n_{α} and n_{β} are the number of $|\alpha\rangle$ and $|\beta\rangle$ kets, respectively. Equation (5.9) then contains every permutation quantum number except those forbidden by the Pauli principle. By Eq. (1.24), this is equivalent to a mixture of spin states $S = \frac{1}{2}N, \frac{1}{2}(N-1), \frac{1}{2}(N-2), \cdots (\frac{1}{2})$ or 0. If $|U\rangle$ is given the special form $|u_1\rangle\ |u_1\rangle\ |u_2\rangle\ |u_2\rangle \cdots$, one finds $|U; \alpha rs\rangle = 0$ if $\alpha < \{2^{\frac{1}{2}N}\}$ or $\{2^{\frac{1}{2}(N-1)}, 1\}$. This is the only single Slater determinant whose spin-free density matrix can have pure permutational symmetry.

CORRELATION

Probability densities of particles relative to some fixed center and relative to one another are among the quantities which can be computed from first- and second-order spin-free density matrices. Correlation of particles is often discussed[1] by comparing the probability densities of pairs with the product of two single-particle densities. We will find it sufficient to compute the pair densities alone and compare the pair density of one permutation state with that of another. As is usual, we confine our attention to probability of coincident pairs, but we do not find it necessary to resolve the probabilities into factors for parallel spin ($\alpha\alpha$ and $\beta\beta$) and for antiparallel spin ($\alpha\beta$). We find that the probability for coincidence depends on permutational symmetry; as α varies from $\{1^N\}$ to $\{N\}$ the probability of coincidence increases from zero to a certain maximum. This effect may be called permutation correlation and the general lowering of density of particles relative to one another which results from permutational symmetry may be called the permutation hole. Such correlation provides a spin-free explanation of the Hund rule.

Let ρ denote the operator which represents an observation of any pair of coincident particles at any position. Then ρ is a two-particle operator given by

$$\rho = \sum_{i,j} \rho_{ij}, \qquad (6.1)$$

where ρ_{ij} is the operator[11] for coincidence of particles i and j. For simplicity we consider correlation in kets constructed from orthonormal orbitals. Equation (4.10) then gives the second-order density matrix of a symmetry-adapted ket and hence the expectation value of ρ is

$$\begin{aligned} D_2^{\sigma\alpha} &\equiv \mathrm{Tr}^2\,(\rho_{12} P^2[U; \sigma\alpha r\ |\ U; \sigma\alpha r]) \\ &= \tfrac{1}{2} \sum{}' \langle u_i|\,\langle u_i|\ \rho_{12}\ |u_i\rangle\ |u_i\rangle \\ &\quad + \frac{f^{\alpha}}{2(N!)} \sum_{i,j}{}' \mathfrak{d}^{\dagger}\left[\begin{pmatrix} \mathrm{i} & \mathrm{j} \\ \mathrm{j} & \mathrm{i} \end{pmatrix}\right]^{\alpha} \mathfrak{d}\langle u_i|\,\langle u_i|\ \rho_{12}\ |u_i\rangle\ |u_j\rangle. \end{aligned} \qquad (6.2)$$

[If one were to ignore the uncertainty principle, particles would be distinguishable (in principle) except when they occupied the same position. In this case, one could find the probability that a specific pair of particles be coincident. For example, we might find the probability that particles one and two be coincident in a state represented by $|U; \alpha sr\rangle$. Now if the representation of the transposition (12) is diagonal one has either (12) $|U; \alpha sr\rangle = |U; \alpha sr\rangle$ or (12) $|U; \alpha sr\rangle = -|U; \alpha sr\rangle$(These two cases require electron spin functions which are antisymmetric and symmetric, respectively.) The probability of

[11] In the Schrödinger representation ρ_{ij} is the Dirac delta function $\delta(r_{ij})$.

coincidence of particles one and two is $\langle U;\ \alpha sr|\ \rho_{12}\ |U;\ \alpha sr\rangle$. Since particles 1 and 2 are indistinguishable when coincident, one may interchange them in either the bra or ket, and if $|U;\ \alpha sr\rangle$ is antisymmetric ("parallel" spins) under the interchange, the probability vanishes. This restricted example of correlation produced by permutational symmetry is called the Fermi hole. On this basis, the quantity $D_2^{\sigma\alpha}$ may be considered to be an average Fermi hole for the permutation state $|U;\ \sigma\alpha r\rangle$].

The operator ρ_{12} represents an observation of particles one and two at the same position—hence, they may be interchanged and we find

$$\langle u_i|\ \langle u_j|\ \rho_{12}\ |u_i\rangle\ |u_j\rangle = \langle u_j|\ \langle u_i|\ \rho_{12}\ |u_i\rangle\ |u_j\rangle \equiv R_{ij}. \tag{6.3}$$

Equation (6.2) may now be written

$$D_2^{\sigma\alpha} = \tfrac{1}{2}\sum_{i,j}{}' \left(1 + \frac{f^\alpha}{N!}\,\mathfrak{d}^\dagger\left[\binom{\mathrm{i}\ \mathrm{j}}{\mathrm{j}\ \mathrm{i}}\right]^\alpha \mathfrak{d}\right) R_{ij}, \tag{6.4}$$

or since $\binom{\mathrm{i}\ \mathrm{j}}{\mathrm{j}\ \mathrm{i}} = \binom{\mathrm{j}\ \mathrm{i}}{\mathrm{i}\ \mathrm{j}}$ and $R_{ij} = R_{ji}$, it may also be written

$$D_2^{\sigma\alpha} = \sum_{i,j} \left(1 + \frac{f^\alpha}{N!}\,\mathfrak{d}^\dagger\left[\binom{\mathrm{i}\ \mathrm{j}}{\mathrm{j}\ \mathrm{i}}\right]^\alpha \mathfrak{d}\right) R_{ij}. \tag{6.5}$$

The probability of coincidence of any pair of particles depends on the values of R_{ij}, on the permutation quantum number α, and on the vector $\mathfrak{d}$. There are f^α independent vectors $\mathfrak{d}$, each showing its own value of $D_2^{\sigma\alpha}$. Representative vectors $\mathfrak{d}$ are those with only one nonzero component:

$$\mathfrak{d}_1 = \left(\frac{N!}{f^\alpha}\right)^{\frac{1}{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \qquad \mathfrak{d}_2 = \left(\frac{N!}{f^\alpha}\right)^{\frac{1}{2}} \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix}, \quad \text{etc.} \tag{6.6}$$

The average pair density for these f^α independent states is invariant under similarity transformations of $[\binom{\mathrm{i}\ \mathrm{j}}{\mathrm{j}\ \mathrm{i}}]^\alpha$ since it involves only the characters

$$\bar{D}_2^\alpha \equiv \frac{1}{f^\alpha}\sum_\sigma D_2^{\sigma,\alpha} \tag{6.7}$$

$$= \binom{N}{2}(1 + \chi_2^\alpha/f^\alpha)\bar{R}. \tag{6.8}$$

Here $\bar{R}$ is the average of the expressions R_{ij}:

$$\bar{R} \equiv \binom{N}{2}^{-1}\sum_{i,j} R_{ij}. \tag{6.9}$$

Equation (6.8) gives the average probability of coincidence of pairs of particles in permutation states α. Yamanouchi[12] has given an expression for χ_2^α/f^α in terms of the partition $\alpha = \{\alpha^1, \alpha^2, \cdots\}$. In case $\alpha = \{2^p,\ 1^{N-2p}\}$ as for electrons one finds

$$\chi_2^\alpha/f^\alpha = \binom{N}{2}^{-1}\left[p^2 - p(N+1) + \frac{N(N-1)}{2}\right]. \tag{6.10}$$

From Yamansuchi's formula, we find for $\alpha = \{1^N\}$ and $\alpha = \{N\}$ that $\chi_2^\alpha/f^\alpha = -1$ and $+1$, respectively, so that

$$\bar{D}_2^{\{1^N\}} = 0 \quad \text{and} \quad \bar{D}_2^{\{N\}} = 2\binom{N}{2}\bar{R}.$$

There is zero probability of coincidence of pairs in permutation states $\alpha = \{1^N\}$ and $\bar{R}$ for each pair in states $\alpha = \{N\}$. Between these extreme cases, $\bar{D}_2^\alpha$ has intermediate values.

In as much as $\bar{D}_2^\alpha$ indicates the degree of avoidance of pairs of particles, it also indicates a rough measure of the order of energy levels among permutation states. If the particles strongly repel each other (as electrons do) then the state $\alpha = \{1^N\}$ tends to have the lowest energy and $\alpha = \{N\}$ the highest. If the particles attract each other (as nucleons apparently do) the order is reversed. This ordering of energy levels by χ_2^α/f^α is the Hund rule for permutational symmetry (or multiplicity for electronic systems).

APPENDIX A:
DERIVATION OF EQUATION (4.6)

A left coset of S_N relative to S_m is denoted by $P_f S_m$ and consists of permutations

$$P_f S_m = \left\{\binom{(n)\ \ (m)}{j(n)\ j(m)}\binom{(n)\ \ (m)'}{(n)\ \ (m)} = \binom{(n)\ \ (m)'}{j(n)\ j(m)}\right\},$$

where $(m)'$ ranges over all $m!$ permutations of the last integers (m). Aside from order, there are $\binom{N}{n}$ choices for the n integers $j(n)$ and each choice of $j(n)$ determines $j(m)$ aside from order. The coset is generated as $(m)'$ or equivalently $j(m)$, is permuted. A permutation of $j(n)$ produces another coset; hence, there are $\binom{N}{n}\, n! = N!/m!$ cosets and

$$S_N = \sum_{j(n)}{}' \binom{(n)\ \ (m)}{j(n)\ j(m)} S_m,$$

where the order of integers in $j(m)$ is arbitrary but the integers themselves are determined by $j(n)$. Hence, in Eq. (4.4), the sum on P may be replaced by a sum on $i(N)$:

$$P = \binom{i(N)}{(N)},$$

and the sum of P_f may be replaced by a sum on $j(n)$:

$$P_f^{-1} = \binom{j(n)\ j(m)}{(n)\ \ (m)}.$$

[12] T. Yamanouchi, Phys. Math. Soc. (Japan) **19**, 436 (1937).

TABLE I. Matric basis coefficients $[P]^{\alpha}_{rs}$ for $\alpha = \{2, 1\}$.

P	$\mathcal{E}$	(12)	(13)	(23)	(123)	(132)
$[P]^{\alpha}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{bmatrix}$	$\begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{bmatrix}$	$\begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$	$\begin{bmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix}$

Thus (4.4) becomes

$$P^{m}[U;\sigma\alpha r \mid V;\tau\alpha r] = \frac{f^{\alpha}}{N!\,n!}\sum_{i(N)}{}'\sum_{j(n)}{}'\tau^{\dagger}\left[\binom{(n)\ (m)}{j(n)\ j(m)}\binom{i(n)\ i(m)}{(n)\ (m)}\right]^{\alpha}\mathfrak{d} \times\left\{\binom{i(N)}{(N)}\right\}^{u}\left\{\binom{j(n)\ j(m)}{(n)\ (m)}\right\}^{*}|u(n)\rangle\langle v(m)|\,\langle v(m)\mid u(m)\rangle$$

[here $\{P\}^{u}$ is used in place of $P(u)$ to denote a permutation on u-orbitals] and when terms are collected,

$$P^{m}[U;\sigma\alpha r \mid V;\tau\alpha r] = \sum_{i(n)}{}'\sum_{j(n)}{}'\gamma^{m}_{UV}(i(n)\mid j(n)\,|u_{i(n)}\rangle\langle v_{j(n)}|,$$

where

$$\gamma^{m}_{UV}(i(n)\mid j(n)) = \frac{f^{\alpha}}{N!\,n!}\sum_{i(m)}{}''\tau^{\dagger}\left[\binom{i(n)\ i(m)}{j(n)\ j(m)}\right]^{\alpha}\mathfrak{d}\langle v_{j(m)}\mid u_{i(m)}\rangle$$

as in (4.6).

APPENDIX B: EXAMPLES

In this Appendix we apply the methods of the text to the evaluation of spin-free density matrices for $N = 3$ and $\alpha = \{2, 1\}$ (doublet state of three-electron systems). We find the first- and second-order spin-free density matrices for a spin-free eigenket of orthonormal orbitals by application of Eqs. (4.9) and (4.10). Let $|U\rangle$ be the orbital product

$$|U\rangle \equiv |u(3)\rangle = |u_1\rangle\,|u_2\rangle\,|u_3\rangle.$$

The symmetry-adapted ket $|U;\sigma\alpha r\rangle$ is given by

$$|U;\sigma\alpha r\rangle = (\sigma)_1 e^{\alpha}_{r1}\,|U\rangle + (\sigma)_2 e^{\alpha}_{r2}\,|U\rangle,$$

where e^{α}_{r1} and e^{α}_{r2} are found from Eq. (1.9) and the matric basis coefficients of Table I.

Normalization of $|U;\sigma\alpha r\rangle$ is provided by Eq. (1.23) and in our case, the elements of Δ are given by

$$\begin{aligned}\Delta_{st} &= \langle U|\, e^{\alpha\dagger}_{sr}\, e^{\alpha}_{rt}\,|U\rangle \\ &= \langle u(3)|\, e^{\alpha}_{st}\,|u(3)\rangle \\ &= \frac{f^{\alpha}}{N!}\sum_{P}[P]^{\alpha}_{st}\langle u(3)|\,P\,|u(3)\rangle \\ &= \tfrac{2}{6}\delta_{st}.\end{aligned}$$

Hence, $|U;\sigma\alpha r\rangle$ is normalized by dividing by the square root of

$$\langle U;\sigma\alpha r \mid U;\sigma\alpha r\rangle = \mathfrak{d}\Delta\mathfrak{d} = \tfrac{1}{2}(\sigma^{*}_1\sigma_1 + \sigma^{*}_2\sigma_2).$$

To normalize $|U;\sigma\alpha r\rangle$, we require $\mathfrak{d}$ to have magnitude 2, and procede to evaluate the density matrices of $|U;\sigma\alpha r\rangle$. From (4.9) and (4.10) we find

$$P^{1}[U;\sigma\alpha r \mid U;\sigma\alpha r] = \tfrac{1}{3}[|u_1\rangle\langle u_1| + |u_2\rangle\langle u_2| + |u_3\rangle\langle u_3|]$$

and

$$\begin{aligned}P^{2}[U;\sigma\alpha r \mid U;\sigma\alpha r] &= \tfrac{1}{2}[|u_1\rangle\,|u_2\rangle\langle u_2|\,\langle u_1| + |u_1\rangle\,|u_3\rangle\langle u_3|\,\langle u_1| \\ &+ |u_2\rangle\,|u_1\rangle\langle u_1|\,\langle u_2| + |u_2\rangle\,|u_3\rangle\langle u_3|\,\langle u_2| \\ &+ |u_3\rangle\,|u_1\rangle\,|u_1\rangle\langle u_3| + |u_3\rangle\,|u_2\rangle\langle u_2|\,\langle u_3|] \\ &+ \tfrac{1}{6}(\sigma^{*}_1\sigma_1 - \sigma^{*}_2\sigma_2)[|u_1\rangle\,|u_2\rangle\langle u_1|\,\langle u_2| \\ &+ |u_2\rangle\,|u_1\rangle\langle u_2|\,\langle u_1|] + \tfrac{1}{12}(-\sigma^{*}_1\sigma_1 - \sqrt{3}\,\sigma^{*}_2\sigma_1 \\ &- \sqrt{3}\,\sigma^{*}_1\sigma_2 + \sigma^{*}_2\sigma_2)[|u_1\rangle\,|u_3\rangle\langle u_1|\,\langle u_3| \\ &+ |u_3\rangle\,|u_1\rangle\langle u_3|\,\langle u_1|] + \tfrac{1}{12}(-\sigma^{*}_1\sigma_1 \\ &+ \sqrt{3}\,\sigma^{*}_2\sigma_1 + \sqrt{3}\,\sigma^{*}_1\sigma_2 + \sigma^{*}_2\sigma_2)[|u_2\rangle\,|u_3\rangle \\ &\times\langle u_2|\,\langle u_3| + |u_3\rangle\,|u_2\rangle\langle u_3|\,\langle u_2|].\end{aligned}$$

Solution of Schrödinger Equation Involving Time*

TATUYA SASAKAWA†
Wayman Crow Laboratory of Physics, Washington University, St. Louis, Missouri
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The general solution of the Schrödinger equation involving the time-dependent perturbation is presented in a compact and manageable form both for periodic and aperiodic perturbations. The method includes as a special case the solution of the Schrödinger equation involving the time-independent perturbation. Formulas ready for practical uses are explicitly described. The essential part of the procedure is the determinantal method in the Laplace-transformed space. The solution is applicable to strong perturbations as well as weak perturbations.

I. INTRODUCTION

THE time-dependent perturbation theory is the basis of calculating the probabilities for various processes including the interaction of electromagnetic field with matter.

Up to the present time, the most satisfactory time-dependent perturbation theory was the method of variation of constants (MVC) developed by Dirac.[1] This method is basically the simple power expansion in terms of the strength of the applied perturbation just as the Rayleigh–Schrödinger perturbation theory[2] (RS) in the case of the time-independent perturbation. As in RS, MVC is useful only when the perturbation is weak. If the perturbation is strong, we must perform the calculations up to very higher-order terms. However, in practice, this is almost impossible and the result may diverge. The number of terms in each order will increase very rapidly even in RS. In all cases, the number of terms appearing in MVC is much larger than in RS. Also in MVC, we must perform the time integration in each order. In short, if we apply MVC the calculation will be very laborious with the result which may diverge.

Here the author would call the reader's attention to the previous papers by the author,[3,4] in which a method for solving the time-independent Schrödinger equation was given. The method yields satisfactory convergence for the strong perturbation as well as for the weak perturbation. It is hoped, then, that we can establish the time-dependent perturbation theory which is also applicable to the strong perturbation with a good convergence, because the time independent perturbation theory should be included, as a special case, in the more general time-dependent perturbation theory. Bearing this situation in mind, the author will present a new time-dependent perturbation theory as the generalization of the previous papers.[3,4]

Here we shall explain the basic idea in the present paper. In the case of the periodic perturbation, we construct a set of the coupled equations for the function $\exp(-il\omega t)\Psi(\mathbf{x}, t)$ (ω, the characteristic frequency l, positive and negative integers). In the case of the aperiodic perturbations, we construct a set of coupled equations for $t^s\Psi(\mathbf{x}, t)$ (s, positive integers). To this set of coupled equations, we apply the Laplace transform and obtain the coupled equation in the Laplace-transformed space. Then by making the inner product of this set of coupled equations and the wavefunctions of the unperturbed stationary states, we have the set of coupled equations, all of whose elements are constants. We solve the secular equation obtained from this set of coupled equations employing the method described in Ref. 3. Once we find the eigenvalues of the secular equation in the Laplace-transformed space, we can obtain the Laplace-transformed wave function from which we get the wave function of the perturbed system by simply applying the Laplace inverse transform.

The important aspect of this method is that we are solving the set of coupled equations which does not contain any operator. All the time, we need only to do with numbers. Thus the calculations are very easily performed. Besides, we need not perform the tedious time integrations in each order, which was needed in MVC. The equivalent to the time integration is the Laplace inverse transform in the last stage. This is very easily done, once we know poles (the eigenvalues of the secular determinantal equation).

* This work was supported by the National Science Foundation.
† On leave of absence from Kyoto University. Present address: Department of Physics, Tohoku University, Sendai, Japan.
[1] P. A. M. Dirac, Proc. Roy Soc. (London) **A112**, 661 (1926); **A114**, 243 (1927).
[2] E. Schrödinger, Ann. Physik **80**, 437 (1926).
[3] T. Sasakawa, J. Math. Phys. **4**, 970 (1963).
[4] T. Sasakawa, J. Math. Phys. **5**, 379 (1964).

In the course of expanding the secular determinantal equation, we employ the Fredholm expansion, whose convergence is guaranteed by the Hadamard's theorem. The method of obtaining the eigenvalues from the secular equation is described in Ref. 3. The methods yield the results which converge very rapidly. On this account, see also the Appendix of the present paper.

The wave function thus obtained is most generally expressed as

$$\Psi(\mathbf{x}, t) = \sum_{n} |n) \sum_{l''} \sum_{n''} e^{-iE_{l''n''}t/\hbar} \chi_{n,l'n',l''n''} f^0_{n'},$$

where f^0_n denotes the inner product of the initial state and the unperturbed stationary state $|n)$. $E_{l''n''}$ is the eigenvalue of the secular determinantal equation. (The states assigned by these eigenvalues are not orthogonal in the configuration space.) $E_{l''n''}$ is real for the periodic perturbation of real frequencies and complex for the aperiodic perturbation. Therefore, the spectra are sharp lines for the periodic perturbations (Fig. 1), but not for the aperiodic perturbations. The explicit form of $\chi_{n,l'n',l''n''}$ is given by Eq. (2.19) or Eq. (6.19). This function is independent of time. In conclusion, the above form is the exact and the general solution of the time-dependent Schrödinger equation. If we know the wave functions of the unperturbed stationary states, and accordingly the matrix elements appearing in $E_{l''n''}$ and $\chi_{n,l'n',l''n''}$, the general solution is ready for use in practical problems. The result from MVC is the power expansion of this general solution in terms of the strength of the added perturbation.

The readers who are interested only in knowing the idea of the present method may read Sec. II for periodic potentials and Sec. VI for aperiodic potentials. From Sec. II to Sec. V, the method for the periodic potentials is described. Section II describes the procedure leading to the general solution. In Sec. III, as a simple example, the time-independent perturbation is discussed from the view point of the present approach. In Sec. IV, the detailed formulas for actual calculations for periodic potentials are described. In Sec. V, the comparison with MVC is made. Here we see that the result from MVC is nothing but the power expansion of the general solution in terms of the strength of the perturbation.

In Sec. VI, the method for the aperiodic potentials is described. The general solution is expressed in the same form as for the periodic potentials. One difference from the case of the periodic potential is that now the eigenvalues are degenerate up to the first order. To remove this degeneracy, the secular determinantal equation is transformed into the dispersion equation described in Sec. VII. If we pick up the terms directly concerning the state of interest [Eq. (6.14)] from the dispersion equation, we can remove the degeneracy with respect to the state of interest, by employing the method described in Ref. 3.

Using the value thus obtained as the starting value of iteration, we use the iteration formula (6.15) to find the eigenvalue. Once we obtain the eigenvalues, the wave function is calculated by the same method as described in Sec. II. In the actual calculation of the wavefunction, the formulas given in Sec. IV for periodic potentials is used also for the aperiodic potentials with slight reinterpretation of the matrix elements.

In Sec. VIII, we treat the time-dependent perturbation which is the product of periodic and aperiodic potentials. In this case, the solution of the Schrödinger equation is expressed as (8.9). Obviously, this form can be absorbed into Eq. (2.18) or Eq. (6.18) if we change the meaning of the sub-indices. The extension to a more general class of perturbations, the sum of products of periodic and aperiodic potentials, is very easily done. The general solution should again be expressed in the form of (2.18) if we change the meaning of the sub-indices. Finally, in Sec. IX, we conclude this paper.

In the Appendix, the rapidity of convergence of the weak coupling and the strong coupling methods described in Ref. 3 is discussed.

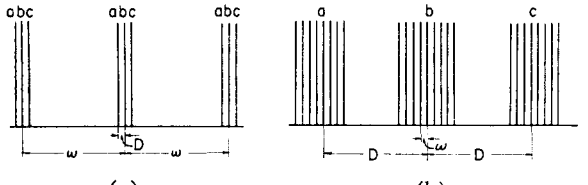

FIG. 1. The energy spectrum in the case of three unperturbed states a, b, and c. (a) $\omega \gg D$, (b) $\omega \ll D$. Here D is the distance between the perturbed energies defined by Eq. (4.18).

II. METHOD AND GENERAL SOLUTION FOR PERIODIC POTENTIALS

We let H_0 denote the unperturbed Hamiltonian of the system and $V(\mathbf{x}, t)$ the perturbation which acts after the time $t = 0$.

By the canonical transformation

$$\Psi(\mathbf{x}, t) = \exp(-iH_0 t/\hbar)\psi(\mathbf{x}, t), \qquad (2.1)$$

the original Schrödinger equation

$$i\hbar \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} = [H_0 + V(\mathbf{x}, t)]\Psi(\mathbf{x}, t) \qquad (2.2)$$

is transformed into

$$i\hbar \frac{\partial \psi(\mathbf{x}, t)}{\partial t}$$

$$= \exp(iH_0 t/\hbar) V(\mathbf{x}, t) \exp(-iH_0 t/\hbar) \psi(\mathbf{x}, t). \quad (2.3)$$

The solution of this equation is formally expressed as

$$\psi(\mathbf{x}, t) = \psi(\mathbf{x}, 0) + \frac{1}{i\hbar} \int_0^t \exp(iH_0 t'/\hbar) \times V(\mathbf{x}, t') \exp(-iH_0 t'/\hbar) \psi(\mathbf{x}, t')\, dt', \quad (2.4)$$

The simple iteration of this equation taking $\psi(\mathbf{x}, 0)$ as the starting function is MVC. We do not apply this iteration method.

In this section and Secs. III–V, we assume that the interaction $V(\mathbf{x}, t)$ is periodic.

$$V(\mathbf{x}, t) = \sum_{l=-\infty}^{\infty} V_l(\mathbf{x}) \exp(-il\omega t/\hbar). \quad (2.5)$$

Correspondingly, we express Eq. (2.4) as

$$\exp[-i(H_0 + l\omega)t/\hbar]\psi(\mathbf{x}, t)$$

$$= \exp[-i(H_0 + l\omega)(t/\hbar)]\psi(x, 0)$$

$$+ \frac{1}{i\hbar} \sum_{l'} \int_0^t \exp[-i(H_0 + l\omega)(t - t')/\hbar] V_{l'}(\mathbf{x})$$

$$\times \exp\{-i[H_0 + (l + l')\omega]t'/\hbar\}\psi(\mathbf{x}, t')\, dt'. \quad (2.6)$$

We define the Laplace transform [multiplied by $(i\hbar)^{-1}$] $f_l(\mathbf{x}, p)$ by

$$f_l(\mathbf{x}, p) = \frac{1}{i\hbar} \int_0^\infty e^{-pt} \times \exp[-i(H_0 + l\omega)t/\hbar]\psi(\mathbf{x}, t)\, dt. \quad (2.7)$$

If we use the Parceval–Borel addition theorem of the Laplace transform that

$$\int_0^\infty e^{-pt}\, dt \left[\int_0^t u(t - t')v(t')\, dt'\right] = \int_0^\infty e^{-pt} u(t)\, dt \cdot \int_0^\infty e^{-pt} v(t)\, dt, \quad (2.8)$$

the Laplace transform of Eq. (2.6) becomes

$$(i\hbar p - H_0 - l\omega) f_l(\mathbf{x}, p) = \psi(\mathbf{x}, 0) + \sum_{l'} V_{l'}(\mathbf{x}) f_{l+l'}(\mathbf{x}, p). \quad (2.9)$$

In this equation the time integration no longer appears. However, the operator is still included, namely, H_0. Therefore, we further decompose $f_l(\mathbf{x}, p)$ by the complete orthonormal set of the eigenfunctions $|n)$ of the unperturbed Hamiltonian H_0,

$$H_0 |n) = \epsilon_n |n). \quad (2.10)$$

We multiply $|n)$ from the left and integrate over the coordinate $\mathbf{x}$. (As usual, these processes will simply be expressed as $(n|.)$ As the result, we have the set of coupled equations

$$(i\hbar p - \epsilon_n - l\omega) f_{l,n} = f_n^0 + \sum_{l'} \sum_{n'} V_{l',nn'} f_{l+l',n'}, \quad (2.11)$$

where

$$f_{l,n} = (n|\, f_l(\mathbf{x}, p)),$$

$$f_n^0 = (n|\, \psi(\mathbf{x}, 0)),$$

and

$$V_{l,nn'} = (n|\, V_l(\mathbf{x})\, |n'). \quad (2.12)$$

The coupled equations (2.11) does not involve any operator: All elements are numbers. Therefore we can solve it by the elementary method of coupled equations. The number of equations is actually infinite. However, provisionally, we cut it at an arbitrary finite number $l = L$. Later, we let $L \to \infty$. In the present paper, we assume that the number of concerning unperturbed states is finite, say, N. (However, this can be easily generalized to the case of infinite number of unperturbed states.) We let ω_n denote the first-order energy

$$\omega_n = \epsilon_n + V_{0,nn}. \quad (2.13)$$

If we write out Eq. (2.11) explicitly, it assumes the form of Eq. (2.14) (shown at the top of the following page). Therefore, if we express the determinant on the left-hand side by $D(i\hbar p)$, the solution $f_{0,n}$ of Eq. (2.11) or Eq. (2.14) is expressed as

$$f_{0,n} = \frac{\sum_{l'n'} f_{n'}^0 D_{l'n',0n}(i\hbar p)}{D(i\hbar p)}, \quad (2.15)$$

where $D_{l'n',0n}$ is the cofactor of the element such that in the column to which this element belongs also belongs the element $i\hbar p - \omega_n$, and in the row to which this element belongs also does the element $i\hbar p - \omega_{n'} - l'\omega$. The expression for D and $D_{l'n',0n}$ are given in the form of the Fredholm expansion (see, Sec. IV), whose convergence is guaranteed by Hadamard's theorem.

The determinant $D(i\hbar p)$ is factorized into the

$$\begin{vmatrix} i\hbar p-\omega_a+L\omega & & & & -V_{2L,aN} \\ & \ddots & & & \\ & & i\hbar p-\omega_a+\omega & -V_{0,aN} & -V_{1,aa} & -V_{1,aN} \\ & & -V_{0,Na} & i\hbar p-\omega_N+\omega & -V_{1,Na} & -V_{1,NN} \\ & & -V_{-1,aa} & -V_{-1,aN} & i\hbar p-\omega_a & -V_{0,aN} \\ & & -V_{-1,Na} & -V_{-1,NN} & -V_{0,Na} & i\hbar p-\omega_N \\ & \ddots & & & & \\ -V_{-2L,Na} & & & & & i\hbar p-\omega_N-L\omega \end{vmatrix} \begin{vmatrix} f_{-La} \\ \vdots \\ f_{-1a} \\ f_{-1,N} \\ f_{0,a} \\ f_{0N} \\ \vdots \\ f_{L,N} \end{vmatrix} = \begin{vmatrix} f_1^0 \\ \vdots \\ f_N^0 \\ f_1^0 \\ f_N^0 \\ f_1^0 \\ f_N^0 \\ \vdots \\ f_N^0 \end{vmatrix}. \tag{2.14}$$

product

$$D(i\hbar p)=\prod_{l=-L}^{L}\prod_{n=a}^{N}(i\hbar p-E_{ln}). \tag{2.16}$$

The eigenvalues E_{ln} of the determinantal equation $D(i\hbar p)=0$ can be calculated by the method of the previous paper. (See, Sec. III of Ref. 3 and the Appendix of the present paper.)

The wave function is now given by the sum of the Laplace inverse transforms of $f_{0,n}$ multiplied by $i\hbar\,|n)$:

$$\Psi(\mathbf{x},t)=i\hbar\sum_n\frac{|n)}{2\pi i}\int_{-i\infty+\epsilon}^{i\infty+\epsilon}dp\,e^{pt}f_{0n}. \tag{2.17}$$

The path of integration is taken along the imaginary axis shifted by an arbitrarily small positive quantity ϵ (the Bromwitch integral), and the semicircle of infinite radius on the left half of the complex p-plane. If we use the expressions (2.15) and (2.16), the result is

$$\Psi(\mathbf{x},t)=\sum_{l'l''}\sum_{nn'n''}|n)e^{-iE_{l''n''}t/\hbar}f_{n'}^0\chi_{n,l'n',l''n''}, \tag{2.18}$$

where

$$\chi_{n,l'n',l''n''}=\frac{D_{l'n',0n}(E_{l''n''})}{\prod'_{l'''n'''\neq l''n''}(E_{l''n''}-E_{l'''n'''})}. \tag{2.19}$$

Equation (2.18) is the general solution which we wanted to have. The explicit expressions for E_{ln} and $D_{l'n',0n}(E_{l''n''})$ will be found in Sec. IV. In Eq. (2.18), we need no longer perform the time integration.

A similar method is applicable to the more general class of periodic potentials

$$V(\mathbf{x},t)=\sum_l\sum_m V_{lm}(\mathbf{x})\exp(-il\omega_m t/\hbar). \tag{2.20}$$

In Secs. VI and X, it will be seen that the solution of the Schrödinger equation takes the form (2.18), not only for the periodic potentials but for all kinds of time-dependent potentials.

When we compare the wavefunction (2.18) with MVC, we may use the canonical-transformed wave function

$$\psi(\mathbf{x}, t) = \exp [i\epsilon_a t/\hbar]\, \Psi(\mathbf{x}, t) \tag{2.21}$$

(a is the initial unperturbed state). The phase factor $\exp [i\epsilon_a t/\hbar]$ is not important, however, since what we actually need is the probability.

III. TIME-INDEPENDENT INTERACTION

Let us compare the solution (2.18) with the solution of the Schrödinger equation whose perturbation does not include time

$$i\hbar \frac{\partial \Psi^0(x, t)}{\partial t} = [H_0 + V(\mathbf{x})]\Psi^0(\mathbf{x}, t). \tag{3.1}$$

This is the special case that only the term with $l = 0$ appears in Eq. (2.5). Consequently, all terms in Eq. (2.18) vanish except for the terms with $l = l' = l'' = 0$. If we omit unnecessary suffixes, Eq. (2.18) is now

$$\Psi^0(\mathbf{x}, t) = \sum_{nn'n''} |n)$$

$$\times \exp (-iE_{n''}t/\hbar) \frac{f^0_{n'} D_{n'n}(E_{n''})}{\prod'_{n'''\neq n''} (E_{n''} - E_{n'''})}. \tag{3.2}$$

This result must, of course, be the same as the result derived by the usual method. We expand $\Psi^0(\mathbf{x}, t)$ by the eigenfunctions of the perturbed state, which are the solutions of the Schrödinger equation

$$(H_0 + V(\mathbf{x}))\psi_{n''}(\mathbf{x}) = E_{n''}\psi_{n''}(\mathbf{x}) \tag{3.3}$$

as

$$\Psi^0(\mathbf{x}, t) = \sum_{n''} \exp (-iE_{n''}t/\hbar)$$

$$\times \psi_{n''}(\mathbf{x}) \cdot [\psi_{n''}(\mathbf{x})\Psi^0(\mathbf{x}, 0)]. \tag{3.4}$$

The perturbed eigenfunction is expanded by the unperturbed eigenfunctions $|n)$ as

$$\psi_{n''}(\mathbf{x}) = \sum_n |n) a_{nn''}, \tag{3.5}$$

where

$$a_{nn''} = (n|\, \psi_{n''}(\mathbf{x})). \tag{3.6}$$

We put (3.5) into Eq. (3.4). The result is

$$\Psi^0(\mathbf{x}, t) = \sum_{nn'n''} \exp (-iE_{n''}t/\hbar)\, |n) \cdot a_{nn''} a^*_{n'''n'} f^0_{n'}. \tag{3.7}$$

Equations (15) and (18) in Ref. 4 show that

$$a_{nn''} a^*_{n'''n'} = \frac{D_{n'n}(E_{n''})}{\prod'_{n'''\neq n'} (E_{n''} - E_{n'''})}. \tag{3.8}$$

The equivalence of (3.2) and (3.3) is thus established, so we have now checked that our wavefunction (2.18) includes the wavefunction of the time-independent interaction.

The problem of the time-independent interaction switched on for a finite time interval is found in many text books of quantum mechanics where this problem is solved up to the first order. If the number of states involved is only two, a and b, and if the state was in the state a at the time $t = 0$, the first-order term of the usual method yields the transition probability from state a to state b

$$P_{ab} = \frac{4\,|V_{ab}|^2}{(\epsilon_a - \epsilon_b)^2} \sin^2 (\epsilon_a - \epsilon_b)t/\hbar. \tag{3.9}$$

On the other hand, if we use Eq. (3.2), it gives

$$P_{ab} = \frac{4\,|V_{ab}|^2}{(E_a - E_b)^2} \sin^2 (E_+ - E_-)t/\hbar, \tag{3.10}$$

where

$$E_\pm = \tfrac{1}{2}\{(\omega_a + \omega_b) \pm [(\omega_a - \omega_b)^2 + 4\,|V_{ab}|^2]^{\frac{1}{2}}\}. \tag{3.11}$$

Comparison of Eqs. (3.9) and (3.10) shows that Eq. (3.9) is valid only when the perturbation is small.

IV. FORMULAS OF E_{ln}, $D_{0n,\,0n}(i\hbar p)$ AND $D_{l'n',\,0n}(i\hbar p)$ FOR PERIODIC POTENTIALS

In this section, the general formulas for E, D_{aa}, and D_{ba} given in Refs. 3 and 4 are applied to obtain the explicit formulas for E_{ln}, $D_{0n,0n}(i\hbar p)$, and $D_{l'n',0n}(i\hbar p)$.

For convenience, we recall the basic idea of the treatments in these references, which was the Fredholm expansion of the determinant

$$D = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ \cdots & \cdots & \cdots & \cdots \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{vmatrix}. \tag{4.1}$$

We expand this determinant in the following way. First, we pick up all the diagonal terms and get the product $\prod_{n=1}^{N} a_{nn}$. Next, if we limit the product of diagonal terms to $\prod''_{n\neq 1,2} a_{nn}$, it must be multiplied

by the determinant $\begin{vmatrix} 0 & a_{12} \\ a_{21} & 0 \end{vmatrix}$. For the "second-order" terms, we must sum up all such possibilities;

$$\sum_{n=1}^{N}\sum_{p>n}^{N}\begin{vmatrix} 0 & a_{np} \\ a_{pn} & 0 \end{vmatrix}\prod_{n'\neq np}'' a_{n'n'}.$$

This consideration is generalized to obtain

$$D=\prod_{n=1}^{N} a_{nn}+\sum_{n=1}^{N}\sum_{p>n}^{N}\begin{vmatrix} 0 & a_{np} \\ a_{pn} & 0 \end{vmatrix}\prod_{n'\neq np}'' a_{n'n'} \tag{4.2}$$

$$+\sum_{n=1}^{N}\sum_{p>n}^{N}\sum_{q>p}^{N}\begin{vmatrix} 0 & a_{np} & a_{nq} \\ a_{pn} & 0 & a_{pq} \\ a_{qn} & a_{qp} & 0 \end{vmatrix}\prod_{n'\neq npq}''' a_{n'n'}+\cdots.$$

Therefore, if we let ϵ_n denote the energy of the unperturbed state and ω_n the first-order energy

$$\omega_n=\epsilon_n+V_{nn}, \tag{4.3}$$

the secular determinantal equation

$$D(E)=\det(E-H)=0 \tag{4.4}$$

is transformed into

$$\prod_{n=1}^{N}(E-\omega_n)$$

$$+\sum_{n=1}^{N}\sum_{p>n}^{N}\begin{vmatrix} 0 & -V_{np} \\ -V_{pn} & 0 \end{vmatrix}\prod_{n'\neq np}''(E-\omega_{n'})$$

$$+\sum_{n=1}^{N}\sum_{p>n}^{N}\sum_{q>p}^{N}\begin{vmatrix} 0 & -V_{np} & -V_{nq} \\ -V_{pn} & 0 & -V_{pq} \\ -V_{qn} & -V_{qp} & 0 \end{vmatrix}\prod_{n'\neq npq}'''(E-\omega_{n'})$$

$$+\cdots. \tag{4.5}$$

If there is no degeneracy with respect to ω_n, Eq. (4.5) is brought into the dispersion formula

$$\sum_n \frac{C_n}{E-\omega_n}=1 \tag{4.6}$$

by applying the partial fraction method. In Ref. 3, the method for solving (4.6) was given.

In the transformation coefficient of the wavefunction, the determinant $D_{aa}(E)$ is needed. This is the cofactor of the (a, a) element in $D(E)$ and is equal to the determinant $D(E)$, whose a row and a column are missing.

Next, we shall explain the method of expanding the determinant D_{ab}, the cofactor of the (a, b) element in D. This is the determinant D, whose a row and b column are missing, multiplied by the factor $(-)^{a+b}$;

$$D_{ab}=(-)^{a+b}\begin{vmatrix} a_{11} & \cdots & \phi_{1b} & \cdots & a_{1N} \\ \vdots & & \vdots & & \vdots \\ \phi_{a1} & \phi_{a2} & \cdots\ \phi_{ab} & \cdots & \phi_{aN} \\ \vdots & & \vdots & & \vdots \\ a_{N1} & \cdots & \phi_{Nb} & \cdots & a_{NN} \end{vmatrix}. \tag{4.7}$$

Now let us consider the element a_{ba} which is at the mirror image of the element a_{ab} with respect to the diagonal elements. We rearrange the determinant D_{ab} in the form that the element a_{ba} comes on the left corner in the first row. The result is

$$D_{ab}=(-)^{a+b-1}(-)^{a+b}$$

$$\times\begin{vmatrix} a_{ba} & a_{b1} & a_{b2} & \cdots & a_{ba-1} & a_{ba+1} & \cdots & a_{bN} \\ a_{1a} & a_{11} & a_{12} & \cdots & a_{1a-1} & a_{1a+1} & \cdots & a_{1N} \\ a_{2a} & a_{21} & a_{22} & \cdots & a_{2a-1} & a_{2a+1} & \cdots & a_{2N} \\ \vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{b-1a} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{b+1a} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \vdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{Na} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & a_{NN} \end{vmatrix}. \tag{4.8}$$

By this rearrangement, the determinant always changes its sign from the original arrangement. By the same consideration as used in deriving (4.2), we can expand (4.8) as

$$D_{ab}=-\prod_{n\neq ab}'' a_{nn}\left[a_{ba}+\sum_{p\neq ab}''\begin{vmatrix} a_{ba} & a_{bp} \\ a_{pa} & 0 \end{vmatrix}\frac{1}{a_{pp}}\right.$$

$$\left.+\sum_{p\neq ab}''\sum_{q>p}\begin{vmatrix} a_{ba} & a_{bp} & a_{bq} \\ a_{pa} & 0 & a_{pq} \\ a_{qa} & a_{qp} & 0 \end{vmatrix}\frac{1}{a_{pp}a_{qq}}+\cdots\right]. \tag{4.9}$$

$D_{ab}(E)$ is also needed in the transformation coefficient of the wavefunction. Further details were described in Refs. 3 and 4.

Now we apply the above general relations to our special problem. Complication comes from the fact that now the quantities have two suffixes l and n. The derivation of the formula is made by watching Eq. (2.14). In what follows we write out the results.

A. Eigenvalues

Similarly to Ref. 4, we shall define $g_{l',nn'}$, $g_{l'l'',nn'n''}$ etc. by

$$g_{l',nn'} = -\begin{vmatrix} 0 & V_{l',nn'} \\ V_{-l',n'n} & 0 \end{vmatrix},$$

$$g_{l'l'',nn'n''} = \begin{vmatrix} 0 & V_{l',nn'} & V_{l'',nn''} \\ V_{-l',n'n} & 0 & V_{(l''-l'),n'n''} \\ V_{-l'',n''n} & V_{-(l''-l'),n''n'} & 0 \end{vmatrix},$$

$$g_{l'l''l''',nn'n''n'''} = -\begin{vmatrix} 0 & V_{l',nn'} & V_{l'',nn''} & V_{l''',nn'''} \\ V_{-l',n'n} & 0 & V_{(l''-l'),n'n''} & V_{(l'''-l'),n'n'''} \\ V_{-l'',n''n} & V_{-(l''-l')n''n'} & 0 & V_{(l'''-l''),n''n'''} \\ V_{-l''',n'''n} & V_{-(l'''-l'),n'''n'} & V_{-(l'''-l''),n'''n''} & 0 \end{vmatrix}, \tag{4.10}$$

etc.

If we use these quantities, the Fredholm expansion of the determinant $D(i\hbar p)$ is

$$\begin{aligned} D(i\hbar p) = {} & \prod_{l=-L}^{L} \prod_{n=a}^{N} (i\hbar p - \omega_n - l\omega) \\ & - \sum_{l=-L}^{L} \sum_{l'=0}^{-l+N} \sum_{n=a}^{N} \sum_{\substack{n'=a \\ (n'>n,\ \text{if } l'=0)}}^{N} g_{l',nn'} \prod_{(l''n'')\neq(l,n)(l+l',n')}'' (i\hbar p - \omega_{n''} - l''\omega) \\ & - \sum_{l=-L}^{L} \sum_{l'=0}^{-l+L} \sum_{l''\geq l'}^{-l+L} \sum_{n=a}^{N} \sum_{\substack{n'=a \\ (n'>n,\ \text{if } l'=0)}}^{N} \sum_{\substack{n''=a \\ (n''>n',\ \text{if } l''=l')}}^{N} g_{l'l'',nn'n''} \\ & \times \prod_{(l''',n''')\neq(l,n),(l+l',n')(l+l'',n'')}''' (i\hbar p - \omega_{n'''} - l'''\omega) \\ & - \sum_{l=-L}^{L} \sum_{l'=0}^{-l+L} \sum_{l''\geq l'}^{-l+L} \sum_{l'''\geq l''}^{-l+L} \sum_{n=a}^{N} \sum_{\substack{n'=a \\ (n'>n,\ \text{if } l'=0)}}^{N} \sum_{\substack{n''=a \\ (n''>n',\ \text{if } l''=l')}}^{N} \sum_{\substack{n'''=a \\ (n'''>n'',\ \text{if } l'''=l'')}}^{N} g_{l'l''l''',nn'n''n'''} \\ & \times \prod_{(l'''',n'''')\neq(l,n),(l+l',n')(l+l'',n'')(l+l''',n''')}'''' (i\hbar p - \omega_{n''''} - l''''\omega) + \cdots . \end{aligned} \tag{4.11}$$

Therefore, the secular equation

$$D(i\hbar p) = 0 \tag{4.12}$$

is transformed into the dispersion equation

$$\sum_{l=-L}^{L} \sum_{n=a}^{N} \frac{C_{ln}}{(i\hbar p - \omega_n - l\omega)} = 1, \tag{4.13}$$

where

$$\begin{aligned} C_{ln} = {} & \sum_{l'=-l-L}^{-l+L} \sum_{\substack{n'=a \\ (n'\neq n,\ \text{if } l'=0)}}^{N} \frac{g_{l',nn'}}{\omega_n - \omega_{n'} - l'\omega} \\ & + \sum_{l'=-l-L}^{-l+L} \sum_{l''\geq l'}^{-l+L} \sum_{\substack{n'=a \\ (n'\neq n,\ \text{if } l'=0)}}^{N} \sum_{\substack{n''=a \\ (n''>n',\ \text{if } l''=l')}}^{N} \frac{G_{l'l'',nn'n''}}{(\omega_n - \omega_{n'} - l'\omega)(\omega_n - \omega_{n''} - l''\omega)} \\ & + \sum_{l'=-l-L}^{-l+L} \sum_{l''\geq l'}^{-l+L} \sum_{l'''\geq l''}^{-l+L} \sum_{\substack{n'=a \\ (n'\neq n,\ \text{if } l'=0)}}^{N} \sum_{\substack{n''=a \\ (n''>n',\ \text{if } l''=l')}}^{N} \sum_{\substack{n'''=a \\ (n'''>n'',\ \text{if } l'''=l'')}}^{N} \\ & \times \frac{g_{l'l''l''',nn'n''n'''}}{(\omega_n - \omega_{n'} - l'\omega)(\omega_n - \omega_{n''} - l''\omega)(\omega_n - \omega_{n'''} - l'''\omega)} + \cdots . \end{aligned} \tag{4.14}$$

Equation (4.14) shows that the l dependence of the coefficients C_{ln} comes from the upper limit of summations. However, actually, L should be infinite, so C_{ln} does not depend on l. Thus the dispersion equation (4.13) must be

$$\sum_{l=-\infty}^{\infty} \sum_{n=a}^{N} \frac{C_n}{i\hbar p - \omega_n - l\omega} = 1 \tag{4.15}$$

with the coefficient

$$C_n = \sum_{l'=-\infty}^{\infty} \sum_{\substack{n'=a \\ (n' \neq n, \text{ if } l'=0)}}^{N} \frac{g_{l',nn'}}{\omega_n - \omega_{n'} - l'\omega} + \sum_{l'=-\infty}^{\infty} \sum_{l''\geq l'}^{\infty} \sum_{\substack{n'=a \\ (n' \neq n, \text{ if } l'=0)}}^{N} \sum_{\substack{n''=a \\ (n''>n', \text{ if } l''=l')}}^{N} \frac{G_{l'l'',nn'n''}}{(\omega_n - \omega_{n'} - l'\omega)(\omega_n - \omega_{n''} - l''\omega)} + \cdots . \tag{4.16}$$

From Eq. (4.15) we see that the eigenvalues E for a fixed state n is distributed with equal distance,

$$E_{l,n} = E_{l-1,n} + \omega. \tag{4.17}$$

When the eigenvalues E_{0n} are distributed with equal distance D,

$$D = E_{0,n} - E_{0,n+1}, \tag{4.18}$$

the energy spectrum will be as shown in Fig. 1a for $\omega \gg D$ and as shown in Fig. 1b for $\omega \ll D$.

To obtain the eigenvalues from Eq. (4.15), we may apply the methods discussed in Ref. 3; the weak-coupling method, the strong-coupling method, or the nearest-neighbor-states method. These methods give very good convergence. See examples given in Ref. 3 and discussions developed in the Appendix of the present paper.

B. Formula for $D_{0n,\,0n}(i\hbar p)$

In this section we shall calculate $D_{0n,0n}(i\hbar p)$ for $n = \rho$.

The determinant $D_{0\rho,0\rho}(i\hbar p)$ is equal to the determinant $D(i\hbar p)$, but without the row and column to which the diagonal element $(i\hbar p - \omega_\rho)$ belongs. Keeping this in mind, we can write out $D_{0\rho,0\rho}(i\hbar p)$ as

$$\begin{aligned}
D_{0\rho,0\rho}(i\hbar p) = {} & \prod_{\substack{l=-L \\ (ln)\neq(0\rho)}}^{L} \prod_{n=a}^{N} (i\hbar p - \omega_n - l\omega) \\
& - \underbrace{\sum_{l=-L}^{L} \sum_{l'=0}^{-l+L} \sum_{n=a}^{N} \sum_{\substack{n'=a \\ (n'>n, \text{ if } l'=0)}}^{N}}_{\left(\substack{n\neq\rho, \text{ if } l=0 \\ n'\neq\rho, \text{ if } l'=-l(l\leq 0)}\right)} g_{l',nn'} \prod_{(l'',n'')\neq(l,n)(l+l',n')}'' (i\hbar p - \omega_{n''} - l''\omega) \\
& - \underbrace{\sum_{l=-L}^{L} \sum_{l''=0}^{-l+L} \sum_{l''\geq l'}^{-l+L} \sum_{n=a}^{N} \sum_{\substack{n'=a \\ (n'>n, \text{ if } l'=0)}}^{N} \sum_{\substack{n''=a \\ (n''>n', \text{ if } l''=l')}}^{N}}_{\left[\substack{n\neq\rho, \text{ if } l=0 \\ n'\neq\rho, \text{ if } l'=-l(l\leq 0) \\ n''\neq\rho, \text{ if } l''=-l(l\leq 0)}\right]} g_{l'l'',nn'n''} \\
& \prod_{(l''',n''')\neq(l,n)(l+l',n')(l+l'',n'')}''' (i\hbar p - \omega_{n'''} - l'''\omega) \\
& - \underbrace{\sum_{l=-L}^{L} \sum_{l'=0}^{-l+L} \sum_{l''\geq l'}^{-l+L} \sum_{l'''\geq l''}^{-l+L} \sum_{n=a}^{N} \sum_{\substack{n'=a \\ (n'>n, \text{ if } l'=0)}}^{N} \sum_{\substack{n''=a \\ (n''>n', \text{ if } l''=l')}}^{N} \sum_{\substack{n'''=a \\ (n'''>n'', \text{ if } l'''=l'')}}^{N}}_{\left(\substack{n\neq\rho, \text{ if } l=0 \\ n'\neq\rho, \text{ if } l'=-l(l\leq 0) \\ n''\neq\rho, \text{ if } l''=-l(l\leq 0) \\ n'''\neq\rho, \text{ if } l'''=-l(l\leq 0)}\right)} \\
& \times g_{l'l''l''',nn'n''n'''} \prod_{(l'''',n'''')\neq(l,n)(l+l',n')(l+l'',n'')(l+l''',n''')}'''' (i\hbar p - \omega_{n''''} - l''''\omega) + \cdots .
\end{aligned} \tag{4.19}$$

Or alternatively, this determinant is expressed as

$$
\begin{aligned}
D_{0\rho,0\rho}(i\hbar p) = {} & \prod_{\substack{l=-L \\ (l,n)\neq(0,\rho)}}^{L} \prod_{n=a}^{N} (i\hbar p - \omega_n - l\omega) \\
& \times \Bigg\{ 1 - \underbrace{\sum_{l'=-L}^{L} \sum_{l''=-l'-L}^{-l'+L} \sum_{n'=a}^{N} \sum_{\substack{n''=a \\ (n''\neq n',\ \text{if } l''=0)}}^{N}}_{\binom{n'\neq\rho,\ \text{if } l'=0}{n''\neq\rho,\ \text{if } l''=-l'}} \frac{g_{l'',n'n''}}{i\hbar p - \omega_{n'} - l'\omega} \frac{1}{\omega_{n'} - \omega_{n''} - l''\omega} \\
& - \underbrace{\sum_{l'=-L}^{L} \sum_{l''=-l'-L}^{-l'+L} \sum_{l'''\geq l''}^{-l'+L} \sum_{n'=a}^{N} \sum_{\substack{n''=a \\ (n''\neq n',\ \text{if } l''=0)}}^{N} \sum_{\substack{n'''=a \\ (n'''>n'',\ \text{if } l'''=l'')}}^{N}}_{\begin{pmatrix} n'\neq\rho,\ \text{if}\ \ l'=0 \\ n''\neq\rho,\ \text{if}\ \ l''=-l' \\ n'''\neq\rho,\ \text{if } l'''=-l' \end{pmatrix}} g_{l''l''',n'n''n'''} \\
& \times [(i\hbar p - \omega_{n'} - l'\omega)(\omega_{n'} - \omega_{n''} - l''\omega)(\omega_{n'} - \omega_{n'''} - l'''\omega)]^{-1} \\
& - \underbrace{\sum_{l'=-L}^{L} \sum_{l''=-l'-L}^{-l'+L} \sum_{l'''\geq l''}^{-l'+L} \sum_{l^{\mathrm{iv}}\geq l'''}^{-l'+L} \sum_{n'=a}^{N} \sum_{n''=a}^{N} \sum_{n'''=a}^{N}}_{\left(\begin{smallmatrix} n'\neq\rho,\ \text{if}\ \ l'=0 \\ n''\neq\rho,\ \text{if}\ \ l''=-l' \\ n'''\neq\rho,\ \text{if}\ \ l'''=-l' \\ n^{\mathrm{iv}}\neq\rho,\ \text{if}\ \ l^{\mathrm{iv}}=-l' \end{smallmatrix}\right)\left[\begin{smallmatrix} n''\neq n',\ \text{if}\ \ l''=0 \\ n'''>n'',\ \text{if } l'''=-l'' \\ n^{\mathrm{iv}}>n''',\ \text{if}\ \ l^{\mathrm{iv}}=-l''' \end{smallmatrix}\right]} \sum_{n^{\mathrm{iv}}=a}^{N} g_{l''l'''l^{\mathrm{iv}},n'n''n'''n^{\mathrm{iv}}} \\
& \times [(i\hbar p - \omega_{n'} - l'\omega)(\omega_{n'} - \omega_{n''} - l''\omega)(\omega_{n'} - \omega_{n'''} - l'''\omega)(\omega_{n'} - \omega_{n^{\mathrm{iv}}} - l^{\mathrm{iv}}\omega)]^{-1} - \cdots \Bigg\}. \qquad (4.20)
\end{aligned}
$$

As in C_{ln}, L should be set as infinite in the final result.

C. Formula for $D_{l'n',\,0n}(i\hbar p)$

The formula (25) in Ref. 4 is applied to obtain the explicit form of $D_{l'n',0n}(i\hbar p)$. First, we define $h_{l'l'',nn'n''}$, $h_{l'l''l''',nn'n''n'''}$, etc., by

$$
\begin{aligned}
h_{l'l'',nn'n''} &= -\begin{vmatrix} V_{l',nn'} & V_{(l'-l''),nn''} \\ V_{l'',n''n'} & 0 \end{vmatrix}, \\
h_{l'l''l''',nn'n''n'''} &= \begin{vmatrix} V_{l',nn'} & V_{(l'-l''),nn''} & V_{(l'-l'''),nn'''} \\ V_{l'',n''n'} & 0 & V_{(l''-l'''),n''n'''} \\ V_{l''',n'''n'} & V_{(l'''-l''),n'''n''} & 0 \end{vmatrix}, \\
h_{l'l''l'''l^{\mathrm{iv}},nn'n''n'''n^{\mathrm{iv}}} &= -\begin{vmatrix} V_{l',nn'} & V_{(l'-l''),nn''} & V_{(l'-l'''),nn'''} & V_{(l'-l^{\mathrm{iv}}),nn^{\mathrm{iv}}} \\ V_{l'',n''n'} & 0 & V_{(l''-l'''),n''n'''} & V_{(l''-l^{\mathrm{iv}}),n''n^{\mathrm{iv}}} \\ V_{l''',n'''n'} & V_{(l'''-l''),n'''n''} & 0 & V_{(l'''-l^{\mathrm{iv}}),n'''n^{\mathrm{iv}}} \\ V_{l^{\mathrm{iv}},n^{\mathrm{iv}}n'} & V_{(l^{\mathrm{iv}}-l''),n^{\mathrm{iv}}n''} & V_{(l^{\mathrm{iv}}-l'''),n^{\mathrm{iv}}n'''} & 0 \end{vmatrix}, \\
&\text{etc.} \qquad (4.21)
\end{aligned}
$$

Then we can express $D_{ln',0n}(i\hbar p)$ as

$$
\begin{aligned}
D_{l'n',0n}(i\hbar p) = {} & \prod_{(\bar{l},\bar{n})\neq(0,n),(l',n')}' (i\hbar p - \omega_{\bar{n}} - \bar{l}\omega) \\
& \times \Bigg\{ V_{l',nn'} + \sum_{l''=l'-L}^{l'+L} \sum_{\substack{n''=a \\ \binom{n''\neq n\ \text{for } l''=l'}{n''\neq n'\ \text{for } l''=0}}}^{N} h_{l'l'',nn'n''} \times \frac{1}{i\hbar p - \omega_{n''} - (l' - l'')\omega} \\
& + \sum_{l''=l'-L}^{l'+L} \sum_{l'''\geq l''}^{l'+L} \sum_{\substack{n''=a \\ \binom{n''\neq n\ \text{for } l''=l'}{n''\neq n'\ \text{for } l''=0}}}^{N} \sum_{\substack{n'''=a \\ \left[\begin{smallmatrix} n'''<n''\ \text{for } l'''=l'' \\ n'''\neq n\ \text{for } l'''=l' \\ n'''\neq n'\ \text{for } l'''=0 \end{smallmatrix}\right]}}^{N} h_{l'l''l''',nn'n''n'''}
\end{aligned}
$$

$$\times [(i\hbar p - \omega_{n''} - (l' - l'')\omega)]^{-1}[(i\hbar p - \omega_{n'''} - (l' - l''')\omega)]^{-1}$$
$$+ \sum_{l''=l'-L}^{l'+L} \sum_{l'''\geq l''}^{l'+L} \sum_{l^{iv}\geq l'''}^{l'+L} \sum_{\substack{n''=a \\ (n''\neq n \text{ for } l''=l') \\ (n''\neq n' \text{ for } l''=0)}}^{N} \sum_{\substack{n'''=a \\ n'''<n'' \text{ for } l'''=l'' \\ n'''\neq n \text{ for } l'''=l \\ n'''\neq n' \text{ for } l'''=0}}^{N} \sum_{\substack{n^{iv}=a \\ n^{iv}<n''' \text{ for } l^{iv}=l''' \\ n^{iv}\neq n \text{ for } l^{iv}=l \\ n^{iv}=0 \text{ for } l^{iv}=0}}^{N}$$
$$\times h_{l'l''l'''l^{iv},nn'n''n'''n^{iv}}[(i\hbar p - \omega_{n''} - (l' - l'')\omega)(i\hbar p - \omega_{n'''} - (l' - l''')\omega)]^{-1}$$
$$\times [(i\hbar p - \omega_{n^{iv}} - (l' - l^{iv})\omega)]^{-1} + \cdots \Big\}. \tag{4.22}$$

Or alternatively, this determinant is expressed as

$$D_{l'n',0n} = \prod_{(\bar{l},\bar{n})\neq(0,n),(l',n')}' (i\hbar p - \omega_{\bar{n}} - \bar{l}\omega)$$
$$\times \Bigg[V_{l',nn'} + \sum_{l''=l'-L}^{l'+L} \sum_{\substack{n''=a \\ (n''\neq n \text{ for } l''=l') \\ (n''\neq n' \text{ for } l''=0)}}^{N} h_{l'l'',nn'n''} \frac{1}{(i\hbar p - \omega_{n''} - (l' - l'')\omega)}$$
$$+ \underbrace{\sum_{l''=l'-L}^{l'+L} \sum_{l'''=l'-L}^{l'+L} \sum_{n''=a}^{N} \sum_{n'''=a}^{N}}_{\substack{(n''\neq n \text{ for } l''=l') \\ (n''\neq n' \text{ for } l''=0)}} \underbrace{\begin{pmatrix} n'''\neq n'' \text{ for } l'''=l'' \\ n'''\neq n \text{ for } l'''=l' \\ n'''\neq n' \text{ for } l'''=0 \end{pmatrix}}$$
$$\frac{h_{l'l''l''',nn'n''n'''}}{(i\hbar p - \omega_{n''} - (l' - l'')\omega)(\omega_{n''} - \omega_{n'''} - (l'' - l''')\omega)}$$
$$+ \underbrace{\sum_{l''=l'-L}^{l'+L} \sum_{l'''=l'-L}^{l'+L} \sum_{l^{iv}\geq l'''}^{l'+L} \sum_{n''=a}^{N} \sum_{n'''=a}^{N} \sum_{n^{iv}=a}^{N}}_{\substack{(n''\neq n \text{ for } l''=l') \\ (n''\neq n' \text{ for } l''=0) \\ (n'''\neq n \text{ for } l'''=l') \\ (n'''\neq n' \text{ for } l'''=0)}} \underbrace{\begin{pmatrix} n^{iv}\neq n \text{ for } l^{iv}=l' \\ n^{iv}\neq n' \text{ for } l^{iv}=0 \end{pmatrix} \begin{pmatrix} n''\neq n''' \text{ for } l''=l''' \\ n''\neq n^{iv} \text{ for } l''=l^{iv} \\ n'''\neq n^{iv} \text{ for } l'''=l^{iv} \end{pmatrix}}$$
$$\times \frac{h_{l'l''l'''l^{iv},nn'n''n'''n^{iv}}}{(i\hbar p - \omega_{n''} - (l' - l'')\omega)(\omega_{n''} - \omega_{n'''} - (l'' - l''')\omega)(\omega_{n''} - \omega_{niv} - (l'' - l^{iv})\omega)} + \cdots \Bigg]. \tag{4.23}$$

Again L should be taken as infinite in the final result.

V. PERTURBATION EXPANSION (PERIODIC PONTENTIAL)

The general solution (2.18) with the explicit formulas given in Sec. IV is all that we need. However, it may be interesting to compare the general solution with the perturbative result derived from MVC. In this section, we shall make this comparison up to the second-order terms.

A. General Formulas

Since the original secular determinantal equation $D(i\hbar p) = 0$ can be transformed into Eq. (4.13), the determinant $D(i\hbar p)$ must be factorized as

$$D(i\hbar p) = \prod_{\bar{l}n} (i\hbar p - \omega_{\bar{n}} - \bar{l}\omega)$$
$$\times \left(1 - \sum_{l=-L}^{L} \sum_{n=a}^{N} \frac{C_{ln}}{i\hbar p - \omega_n - l\omega}\right). \tag{5.1}$$

On the other hand, according to the weak-coupling approximation given in Ref. 3 (see also the Appendix of the present paper),

$$E_{l'n'} = \omega_{n'} + l'\omega + \frac{C_{l'n'}}{1 - \sum_{l''n''\neq l'n'} (C_{l''n''}/E_{l'n'} - \omega_{n''} - l''\omega)}. \tag{5.2}$$

Therefore, up to the second-order terms,

$$\lim_{i\hbar p\to E_{l'n'}} \frac{D(i\hbar p)}{i\hbar p - E_{l'n'}} = \prod_{\bar{l}n\neq\bar{l}'n'} (E_{l'n'} - \omega_{\bar{n}} - \bar{l}\omega)$$
$$\times \left(1 - \sum_{\substack{l=-L \\ (l,n)\neq(l',n')}}^{L} \sum_{n=a}^{N} \frac{C_{ln}}{E_{l'n'} - \omega_n - l\omega}\right), \tag{5.3}$$

where

$$C_{ln} = \sum_{l''=-l-L}^{-l+L} \sum_{\substack{n''=a \\ (n''\neq n, \text{ if } l''=0)}}^{N} \frac{V_{l'',nn''}V_{-l'',n''n}}{\omega_n - \omega_{n''} - l''\omega}. \tag{5.4}$$

From (4.20), we have

$$D_{0\rho,0\rho}(E_{0\rho}) = \prod_{(\bar{l},\bar{n})=(0,\rho)} (E_{0\rho} - \omega_{\bar{n}} - \bar{l}\omega) \times \left\{1 - \sum_{\substack{l=-L \\ (l,n)\neq(0,\rho)}}^{L} \sum_{n=a}^{L} \frac{C_{ln}(0,\rho)}{E_{0\rho} - \omega_n - l\omega}\right\}, \quad (5.5)$$

where

$$C_{ln}(0,\rho) = \sum_{\substack{l''=-l-L \\ (n''\neq n, \text{ if } l''=0) \\ (n''\neq\rho, \text{ if } l=0 \\ n''\neq\rho, \text{ if } l''=-l)}}^{-l+L} \sum_{n''=a}^{N} \frac{V_{l'',nn''}V_{-l'',n''n}}{\omega_n - \omega_{n''} - l''\omega}. \quad (5.6)$$

Then, since

$$C_{ln} - C_{ln}(0,\rho) = \frac{V_{-l,n\rho}V_{l,\rho n}}{\omega_n - \omega_\rho + l\omega}, \quad (5.7)$$

we obtain

$$\lim_{i\hbar p\to E_{0\rho}} (i\hbar p - E_{0\rho}) \frac{D_{0\rho,0\rho}(i\hbar p)}{D(i\hbar p)} = 1 + \sum_{\substack{l=-L \\ (l,n)\neq(0,\rho)}}^{L} \sum_{n=a}^{N} \frac{1}{E_{0\rho} - (\omega_n + l\omega)} \cdot \frac{V_{-l,n\rho}V_{l,\rho n}}{(\omega_n + l\omega) - \omega_\rho}. \quad (5.8)$$

For $(l', n') \neq (0, \rho)$,

$$D_{0\rho,0\rho}(E_{l'n'}) = \prod_{(\bar{l},\bar{n})\neq(0,\rho)} (E_{l'n'} - \omega_{\bar{n}} - \bar{l}\omega) \times \left\{1 - \sum_{\substack{l=-L \\ (l,n)\neq(0,\rho)}}^{L} \sum_{n=a}^{N} \frac{C_{ln}(0\rho)}{E_{l'n'} - \omega_n - l\omega}\right\}$$

$$= \prod_{(\bar{l},\bar{n})\neq(0,\rho)(l',n')} (E_{l'n'} - \omega_{\bar{n}} - \bar{l}\omega)(E_{l'n'} - \omega_{n'} - l'\omega) \times \left\{1 - \sum_{\substack{l=-L \\ (l,n)\neq(0,\rho)(l',n')}}^{L} \sum_{n=a}^{N} \frac{C_{ln}(0\rho)}{E_{l'n'} - \omega_n - l\omega} - \frac{C_{l'n'}(0\rho)}{E_{l'n'} - \omega_{n'} - l'\omega}\right\}.$$

Therefore, up to the second-order terms,

$$D_{0\rho,0\rho}(E_{l'n'}) = \prod_{(\bar{l},\bar{n})\neq(0,\rho)(l',n')} (E_{l'n'} - \omega_{\bar{n}} - \bar{l}\omega) \times \{C_{l'n'} - C_{l'n'}(0\rho)\}.$$

Thus, for $(l', n') \neq (0, \rho)$,

$$\lim_{i\hbar p\to E_{l'n'}} (i\hbar p - E_{l'n'}) \frac{D_{0\rho,0\rho}(i\hbar p)}{D(i\hbar p)} = \frac{1}{E_{l'n'} - \omega_\rho} [C_{l'n'} - C_{l'n'}(0\rho)].$$

If we use (5.7), we get

$$\lim_{i\hbar p\to E_{l'n'}} (i\hbar p - E_{l'n'}) \frac{D_{0\rho,0\rho}(i\hbar p)}{D(i\hbar p)} = \frac{1}{E_{l'n'} - \omega\rho} \frac{V_{-l',n'\rho}V_{l',\rho n'}}{\omega_{n'} - \omega_\rho + l'\omega} \quad (5.9)$$

for $(l', n') \neq (0, \rho)$.

Next, from the second-order approximation of Eq. (4.23), we have

$$D_{l\sigma,0\rho}(E_{l'n'}) = \prod_{(\bar{l},\bar{n})\neq(0,\rho)(l,\sigma)} (E_{l'n'} - \omega_{\bar{n}} - \bar{l}\omega) \times \left[V_{l,\rho\sigma} + \sum_{\substack{l''=l-L \\ (l'',n'')\neq(l,\rho)(0,\sigma)}}^{l+L} \sum_{n=a}^{N} \frac{V_{l'',n''\sigma}V_{(l-l''),\rho n''}}{(E_{l'n'} - \omega_{n''} - (l-l'')\omega)}\right].$$

Therefore,

$$\lim_{i\hbar p\to E_{0\rho}} (i\hbar p - E_{0\rho}) \frac{D_{l\sigma,0\rho}(i\hbar p)}{D(i\hbar p)} = \frac{1}{E_{0\rho} - \omega_\sigma - l\omega} \times \left[V_{l,\rho\sigma} + \sum_{\substack{l'=l-L \\ (l',n')\neq(l,\rho),(0,\sigma)}}^{l+L} \sum_{n'=a}^{N} \frac{V_{l',n'\sigma}V_{(l-l'),\rho n'}}{E_{0\rho} - \omega_{n'} - (l-l')\omega}\right]$$

$$= \frac{1}{E_{0\rho} - \omega_\sigma - l\omega} V_{l,\rho\sigma} + \sum_{\substack{l'=l-L \\ (l',n')\neq(l,\rho)(0,\sigma)}}^{l+L} \sum_{n'=a}^{N} V_{l',n'\sigma}V_{(l-l'),\rho n'} \times \{[E_{0\rho} - \omega_\sigma - l\omega]^{-1}[\omega_\sigma - \omega_{n'} + l'\omega]^{-1} + [E_{0\rho} - \omega_{n'} - (l - l')\omega]^{-1}[\omega_{n'} - \omega_\sigma - l'\omega]^{-1}\}. \quad (5.10)$$

Similarly,

$$\lim_{i\hbar p\to E_{l\sigma}} (i\hbar p - E_{l\sigma}) \frac{D_{l\sigma,0\rho}(i\hbar p)}{D(i\hbar p)} = \frac{1}{E_{l\sigma} - \omega_\rho} \times \left[V_{l,\rho\sigma} + \sum_{\substack{l'=l-L \\ (l',n')\neq(l,\rho),(0,\sigma)}}^{l+L} \sum_{n'=a}^{N} \frac{V_{l',n'\sigma}V_{(l-l'),\rho n'}}{E_{l\sigma} - \omega_{n'} - (l - l')\omega}\right]. \quad (5.11)$$

Finally, for $(l', n') \neq (l, \sigma), (0, \rho)$,

$$\lim_{i\hbar p\to E_{l'n'}} (i\hbar p - E_{l'n'}) \frac{D_{l\sigma,0\rho}(i\hbar p)}{D(i\hbar p)} = \frac{1}{(E_{l'n'} - \omega_\rho)(E_{l'n'} - \omega_\sigma - l\omega)} V_{(l-l'),n'\sigma}V_{l',\rho n'}. \quad (5.12)$$

B. Example

As the simplest example, we shall discuss the case of two unperturbed states a and b, presuming that before the time $t = 0$ the system was at a state a;

$$f^0_{n'} = \delta_{n'a} \quad (5.13)$$

in (2.18). Also, we assume that the perturbation (2.5) has only two components $l = \pm 1$, and that $V_1(x) = V_{-1}(x) \equiv V(x)$. Therefore, $\omega_a = \epsilon_a$ and $\omega_a = \epsilon_b$. The wavefunction (2.18) of the system is now

$$\Psi(x, t) = \sum_{ll'} \sum_{nn'} |n) \times \lim_{E \to E_{l'n'}} (E - E_{l'n'}) \frac{e^{-iEt/\hbar} D_{la,0n}(E)}{D(E)}. \tag{5.14}$$

From (5.8), we have

$$\lim_{E \to E_{0a}} (E - E_{0a}) \frac{D_{0a,0a}(E)}{D(E)} e^{-iEt/\hbar} = \left[1 - \frac{2|V_{aa}|^2}{\omega^2} + |V_{ab}|^2 \left\{ \frac{1}{\epsilon_a - \epsilon_b - \omega} \frac{1}{\epsilon_b + \omega - \epsilon_a} + \frac{1}{\epsilon_a - \epsilon_b + \omega} \frac{1}{\epsilon_b - \omega - \epsilon_a} \right\} \right] e^{-iE_{0a}t/\hbar}.$$

All other terms of the form

$$\lim_{E \to E_{0a}} (E - E_{0a}) \frac{D_{la,0a}(E)}{D(E)} \exp(-iEt/\hbar)$$

vanish. Therefore, the coefficient of the term $|a)$ $\times \exp(-iE_{0a}t/\hbar)$ in (5.14) is equal to

$$1 - \frac{|V_{aa}|^2}{\omega^2} + |V_{ab}|^2 \times \left[\left\{ \frac{-1}{(\epsilon_b - \epsilon_a + \omega)(2\omega)} + \frac{-1}{(\epsilon_b - \epsilon_a - \omega)(-2\omega)} \right\} - \frac{(-1)}{\epsilon_a - \epsilon_b + \omega} \left\{ \frac{1}{\epsilon_b - \epsilon_a + \omega} + \frac{1}{\epsilon_b - \epsilon_a - \omega} \right\} - \frac{(-1)}{\epsilon_a - \epsilon_b - \omega} \left\{ \frac{1}{\epsilon_b - \epsilon_a + \omega} + \frac{1}{\epsilon_b - \epsilon_a - \omega} \right\} \right]. \tag{5.15}$$

Next, from Eq. (5.9),

$$\lim_{E \to E_{\pm 1a}} (E - E_{\pm 1a}) \frac{D_{0a,0a}(E)}{D(E)} e^{-iEt/\hbar} = \frac{|V_{aa}|^2}{\omega^2} \exp(-iE_{\pm 1a}t/\hbar), \tag{5.16}$$

and

$$\lim_{E \to E_{\pm 1b}} (E - E_{\pm 1b}) \frac{D_{0a,0a}(E)}{D(E)} e^{-iEt/\hbar} = \frac{|V_{ab}|^2}{(\epsilon_b - \epsilon_a \pm \omega)^2} \exp(-iE_{\pm 1b}t/\hbar).$$

All other terms of the form

$$\lim_{E \to E_{ln}} (E - E_{ln}) \frac{D_{0a,0a}(E)}{D(E)} e^{-iEt/\hbar}, \quad (l, n) \neq (0, a),$$

vanish.

From Eq. (5.11), we have

$$\lim_{E \to E_{\pm 1a}} (E - E_{\pm 1a}) \frac{D_{1a,0a}(E)}{D(E)} e^{-iEt/\hbar} = \frac{1}{\pm\omega} V_{aa} \exp(-iE_{\pm 1a}t/\hbar), \tag{5.18}$$

and

$$\lim_{E \to E_{\pm 2a}} (E - E_{\pm 2a}) \frac{D_{\pm 2a,0a}(E)}{D(E)} e^{-iEt/\hbar} = \frac{1}{(\pm 2\omega)} \left(\frac{|V_{aa}|^2}{(\pm\omega)} + \frac{|V_{ab}|^2}{\epsilon_a - \epsilon_b \pm \omega} \right) \exp(-iE_{\pm 2a}t/\hbar). \tag{5.19}$$

All other terms of the form

$$\lim_{E \to E_{la}} (E - E_{la}) \frac{D_{la,0a}(E)}{D(E)} e^{-iEt/\hbar}$$

vanish.

From Eq. (5.12), we have

$$\lim_{E \to E_{\pm 1a}} (E - E_{\pm 1a}) \frac{D_{\pm 2a,0a}(E)}{D(E)} e^{-iEt/\hbar} = -\frac{|V_{aa}|^2}{\omega^2} \exp(-iE_{\pm 1a}t/\hbar), \tag{5.20}$$

which, however, cancels out with (5.16). Also, we have

$$\lim_{E \to E_{\pm 1b}} (E - E_{\pm 1b}) \frac{D_{\pm 2a,0a}(E)}{D(E)} e^{-iEt/\hbar} = \frac{|V_{ab}|^2 \exp(-iE_{\pm 1b}t/\hbar)}{(\epsilon_b - \epsilon_a \pm \omega)(\epsilon_b - \epsilon_a \mp \omega)}. \tag{5.21}$$

All other terms of the form

$$\lim_{E \to E_{l'n}} (E - E_{l'n}) \frac{D_{la,0a}(E)}{D(E)}, \quad (l', n) \neq (l, a),$$

vanish.

Collecting all of these results, we obtain the coefficient of the wavefunction $|a)$ in (5.14) as

$$e^{-i\epsilon_a t/\hbar} \left\{ 1 - \frac{V_{aa}}{\omega} (e^{i\omega t/\hbar} - e^{-i\omega t/\hbar}) + \frac{|V_{aa}|^2}{2\omega^2} (e^{2i\omega t/\hbar} - 2 + e^{-2i\omega t/\hbar}) - \frac{|V_{ab}|^2}{i\hbar} \left(\frac{1}{\epsilon_b - \epsilon_a + \omega} + \frac{1}{\epsilon_b - \epsilon_a - \omega} \right) t + |V_{ab}|^2 \left[\frac{e^{2i\omega t/\hbar} - 1}{(\epsilon_b - \epsilon_a + \omega)2\omega} + \frac{e^{-2i\omega t/\hbar} - 1}{(\epsilon_b - \epsilon_a - \omega)(-2\omega)} - \frac{e^{i(\epsilon_a - \epsilon_b + \omega)t/\hbar} - 1}{\epsilon_a - \epsilon_b + \omega} \left(\frac{1}{\epsilon_b - \epsilon_a + \omega} + \frac{1}{\epsilon_b - \epsilon_a - \omega} \right) - \frac{e^{i(\epsilon_a - \epsilon_b - \omega)t/\hbar} - 1}{\epsilon_a - \epsilon_b - \omega} \left(\frac{1}{\epsilon_b - \epsilon_a + \omega} + \frac{1}{\epsilon_b - \epsilon_a - \omega} \right) \right] \right\}. \tag{5.22}$$

This is just the result which we obtain by MVC. The term which is linearly proportional to the time comes from the expansion of exp $(-E_{0a}t/\hbar)$. This shows that MVC can be applicable only to the weak perturbation.

Next, we shall calculate the coefficient of the wave-function |b) in (5.14). From (5.10), we have

$$\lim_{E\to E_{0b}} (E - E_{0b}) \frac{D_{\pm 1a,0b}(E)}{D(E)} e^{-iEt/\hbar} = \frac{1}{\epsilon_b - \epsilon_a \mp \omega} V_{ba} e^{-iE_{0b}t/\hbar}, \tag{5.23}$$

$$\begin{aligned}\lim_{E\to E_{0b}} (E - E_{0b}) \frac{D_{0a,0b}(E)}{D(E)} e^{-iEt/\hbar} &= \left\{ V_{ba}V_{aa}\left[\left(\frac{1}{\epsilon_b - \epsilon_a}\cdot\frac{1}{\omega} + \frac{1}{\epsilon_b - \epsilon_a + \omega}\cdot\frac{1}{-\omega}\right)\right.\right. \\ &\quad \left. + \left(\frac{1}{\epsilon_b - \epsilon_a}\cdot\frac{1}{-\omega} + \frac{1}{\epsilon_b - \epsilon_a - \omega}\cdot\frac{1}{\omega}\right)\right] \\ &\quad + V_{bb}V_{ba}\left[\left(\frac{1}{\epsilon_b - \epsilon_a}\cdot\frac{1}{\epsilon_a - \epsilon_b + \omega} + \frac{1}{\omega}\cdot\frac{1}{\epsilon_b - \epsilon_a - \omega}\right)\right. \\ &\quad + \left(\frac{1}{\epsilon_b - \epsilon_a}\cdot\frac{1}{\epsilon_a - \epsilon_b - \omega}\right. \\ &\quad \left.\left.\left. + \frac{1}{-\omega}\cdot\frac{1}{\epsilon_b - \epsilon_a + \omega}\right)\right]\right\} e^{-iE_{0b}t/\hbar},\end{aligned} \tag{5.24}$$

and

$$\begin{aligned}\lim_{E\to E_{0b}} (E - E_{0b}) \frac{D_{\pm 2a,0b}(E)}{D(E)} e^{-iEt/\hbar} &= \left[V_{ba}V_{aa}\left(\frac{1}{\epsilon_b - \epsilon_a \mp 2\omega}\cdot\frac{1}{\pm\omega} + \frac{1}{\epsilon_b - \epsilon_a \mp \omega}\cdot\frac{1}{\mp\omega}\right)\right. \\ &\quad + V_{bb}V_{ba}\left(\frac{1}{\epsilon_b - \epsilon_a \mp 2\omega}\cdot\frac{1}{\epsilon_a - \epsilon_b \pm \omega}\right. \\ &\quad \left.\left. + \frac{1}{\mp\omega}\cdot\frac{1}{\epsilon_b - \epsilon_a \mp \omega}\right)\right] e^{-iE_{0b}t/\hbar}.\end{aligned} \tag{5.25}$$

From (5.11), we have

$$\begin{aligned}\lim_{E\to E_{0a}} (E - E_{0a}) \frac{D_{0a,0b}(E)}{D(E)} e^{-iEt/\hbar} &= \left[V_{ba}V_{aa}\left(\frac{1}{\epsilon_a - \epsilon_b}\cdot\frac{1}{\omega} + \frac{1}{\omega_a - \epsilon_b}\cdot\frac{1}{-\omega}\right)\right. \\ &\quad + V_{bb}V_{ba}\left(\frac{1}{\epsilon_a - \epsilon_b}\frac{1}{\epsilon_a - \epsilon_b + \omega}\right. \\ &\quad \left.\left. + \frac{1}{\epsilon_a - \epsilon_b}\frac{1}{\epsilon_a - \epsilon_b - \omega}\right)\right] e^{-iE_{0a}t/\hbar},\end{aligned} \tag{5.26}$$

$$\begin{aligned}\lim_{E\to E_{\pm 2a}} (E - E_{\pm 2a}) \frac{D_{\pm 2a,0b}(E)}{D(E)} &= \left[\frac{V_{ba}V_{aa}}{(\epsilon_a - \epsilon_b \pm 2\omega)(\pm\omega)}\right. \\ &\quad \left. + \frac{V_{bb}V_{ba}}{(\epsilon_a - \epsilon_b \pm 2\omega)(\epsilon_a - \epsilon_b \pm \omega)}\right] e^{-iE_{\pm 2a}t/\hbar}.\end{aligned} \tag{5.27}$$

Finally, from (5.12) we have

$$\lim_{E\to E_{\pm 1a}} (E - E_{\pm 1a}) \frac{D_{0a,0b}(E)}{D(E)} e^{-iEt/\hbar} = \frac{V_{ba}V_{aa}}{(\epsilon_a - \epsilon_b \pm \omega)(\pm\omega)} e^{-iE_{\pm 1a}t/\hbar}, \tag{5.28}$$

$$\lim_{E\to E_{\pm 1a}} (E - E_{\pm 1a}) \frac{D_{\pm 2a,0b}(E)}{D(E)} e^{-iEt/\hbar} = \frac{V_{ba}V_{aa}}{(\epsilon_a - \epsilon_b \pm \omega)(\mp\omega)} e^{-iE_{\pm 1a}t/\hbar}, \tag{5.29}$$

$$\lim_{E\to E_{\pm 1b}} (E - E_{\pm 1b}) \frac{D_{0a,0b}(E)}{D(E)} e^{-iEt/\hbar} = \frac{V_{ba}V_{bb}}{(\pm\omega)(\epsilon_b - \epsilon_a \pm \omega)} e^{-iE_{\pm 1b}t/\hbar}, \tag{5.30}$$

$$\lim_{E\to E_{\pm 1b}} (E - E_{\pm 1b}) \frac{D_{\pm 2a,0b}(E)}{D(E)} e^{-iEt/\hbar} = \frac{V_{bb}V_{ba}}{(\pm\omega)(\epsilon_b - \epsilon_a \pm \omega)} e^{-iE_{\pm 1b}t/\hbar}, \tag{5.31}$$

Up to second-order terms, all terms which are not listed vanish. Collecting equations from (5.23) to (5.31), we obtain as the coefficient of the unperturbed wave function |b),

$$\begin{aligned} e^{-i\epsilon_b t/\hbar}\Bigg\{ &- V_{ba}\left[\frac{e^{i(\epsilon_b - \epsilon_a + \omega)t/\hbar} - 1}{\epsilon_b - \epsilon_a + \omega}\right. \\ &\left. + \frac{e^{i(\epsilon_b - \epsilon_a - \omega)t/\hbar} - 1}{\epsilon_b - \epsilon_a - \omega}\right] \\ &+ \frac{V_{ba}V_{aa}}{\omega}\left[-\frac{e^{i(\epsilon_b - \epsilon_a - 2\omega)t/\hbar} - 1}{\epsilon_b - \epsilon_a - 2\omega}\right. \\ &\left. + \frac{e^{i(\epsilon_b - \epsilon_a + 2\omega)t/\hbar} - 1}{\epsilon_b - \epsilon_a + 2\omega}\right] \\ &+ \frac{V_{bb}V_{ba}}{\epsilon_b - \epsilon_a - \omega}\left[\frac{e^{i(\epsilon_b - \epsilon_a - 2\omega)t/\hbar} - 1}{\epsilon_b - \epsilon_a - 2\omega} + \frac{e^{-i\omega t/\hbar} - 1}{\omega}\right. \\ &\left. + \frac{e^{i(\epsilon_b - \epsilon_a)t/\hbar} - 1}{\epsilon_b - \epsilon_a} - \frac{e^{i\omega t/\hbar} - 1}{\omega}\right] \\ &+ \frac{V_{bb}V_{ba}}{\epsilon_b - \epsilon_a + \omega}\left[\frac{e^{i(\epsilon_b - \epsilon_a)t/\hbar} - 1}{\epsilon_b - \epsilon_a} + \frac{e^{-i\omega t/\hbar} - 1}{\omega}\right. \\ &\left.\left. + \frac{e^{i(\epsilon_b - \epsilon_a + 2\omega)t/\hbar} - 1}{\epsilon_b - \epsilon_a + 2\omega} - \frac{e^{i\omega t/\hbar} - 1}{\omega}\right]\right\}. \end{aligned} \tag{5.32}$$

This is the result which we obtain also from MVC.

VI. METHOD AND GENERAL SOLUTION FOR APERIODIC POTENTIALS

In this section, we demonstrate the method of treating potentials which are not periodic in time. The basic idea in this section is almost the same as in Sec. II. The general solution assumes formally the same form as that given in Sec. II.

We assume that the potential is not singular in time. Then, the potential may be expressed by

$$V(\mathbf{x}, t) = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{t}{i\hbar}\right)^k V^{(k)}(\mathbf{x}), \tag{6.1}$$

where

$$V^{(k)}(\mathbf{x}) = (i\hbar)^k \left(\frac{\partial^k V(\mathbf{x}t)}{\partial t^k}\right)_{t=0}. \tag{6.2}$$

The solution of the Schrödinger equation (2.2) is expressed then as

$$\psi(\mathbf{x}, t) = \psi(\mathbf{x}, 0) + \sum_{k'=0}^{\infty} \frac{1}{k'!} \left(\frac{1}{i\hbar}\right) \times \int_0^t e^{iH_0 t'/\hbar} \left(\frac{t'}{i\hbar}\right)^{k'} V^{(k')}(\mathbf{x}) e^{-iH_0 t'/\hbar} \psi(\mathbf{x}, t)\, dt'. \tag{6.3}$$

Defining the Laplace transform

$$g_k(\mathbf{x}, p) = \frac{1}{k!} \left(\frac{1}{i\hbar}\right) \int_0^{\infty} e^{-pt} \left(\frac{t}{i\hbar}\right)^k e^{-iH_0 t/\hbar} \psi(\mathbf{x}, t)\, dt, \tag{6.4}$$

we obtain from (6.3)

$$g_k(\mathbf{x}, p) = \frac{1}{(i\hbar p - H_0)^{k+1}} \psi(\mathbf{x}, 0) + \sum_{k'=0}^{\infty} \sum_{r=0}^{k} \frac{1}{(i\hbar p - H_0)^{k-r+1}} \times \binom{k'+r}{k'} V^{(k')}(\mathbf{x}) g_{k'+r}(\mathbf{x}, \mathrm{p}). \tag{6.5}$$

Here we have used the relation

$$\int_0^{\infty} e^{-pt} t^k\, dt \int_0^t u(t-t') t'^{k'} v(t')\, dt' = \sum_{r=0}^{k} \binom{k}{r} \int_0^{\infty} e^{-pt} t^{k-r} u(t)\, dt \cdot \int_0^{\infty} e^{-pt} t^{k'+r} v(t)\, dt, \tag{6.6}$$

and

$$\int_0^{\infty} t^n e^{-(p+iH_0/\hbar)t}\, dt = \frac{n!}{(p + iH_0/\hbar)^{n+1}}. \tag{6.7}$$

Equation (6.5) is transformed into a more tractable form

$$(i\hbar p - H_0 - V^{(0)}(\mathbf{x}))g_0 - \psi(\mathbf{x}, 0) - \sum_{k'=1}^{\infty} V^{(k')} g_{k'} = 0, \tag{6.8}$$

and

$$(i\hbar p - H_0 - V^{(0)}(\mathbf{x}))g_{k+1} - g_k - \sum_{k'=1}^{\infty} \binom{k'+k+1}{k'} V^{(k')}(\mathbf{x}) g_{k'+k+1} = 0, \quad k \geq 0.$$

Similarly to Eq. (2.10), we define the inner products of the quantities appearing in Eq. (6.8) and the unperturbed stationary state $|n)$;

$$\begin{aligned} g_{k,n} &= (n|\ g_k), \\ f_n^0 &= (n|\ \psi(\mathbf{x}, 0)), \end{aligned} \tag{6.9}$$

and

$$V_{nn'}^{(k')} = (n|\ V^{(k')}(\mathbf{x})\ |n').$$

Equation (6.8) then reads

$$(i\hbar p - \epsilon_n - V_{nn}^{(0)}) g_{0,n} - \sum_{n' \neq n} V_{nn'}^{(0)} g_{0,n'} - \sum_{k'=1}^{\infty} \sum_{n'} V_{nn'}^{(k')} g_{k',n'} = f_n^0, \tag{6.10}$$

and

$$-g_{k,n} + (i\hbar p - \epsilon_n - V_{nn}^{(0)}) g_{k+1,n} - \sum_{n' \neq n} V_{nn'}^{(0)} g_{k+1,n'} - \sum_{k'=1}^{\infty} \sum_{n'} \binom{k'+k+1}{k'} V_{nn'}^{(k')} g_{k'+k+1,n} = 0, \quad (k \geq 0).$$

Equation (6.10) forms a secular equation in which the first-order energy, $\epsilon_n + V_{nn}^{(0)}$, is degenerate with respect to n. In practice, we truncate this set of equations at k ($\equiv s - 1$) and solve the equations with s-fold degenerate energies. The choice of the number s should depend on the strength of the added perturbation and/or the time after the system comes under influence of the perturbation. Numerically, we must say that our choice of s depends on the accuracy of numerical results we want to have.

We can transform the secular determinantal equation obtained from Eq. (6.10) into the dispersion equation

$$\sum_n \frac{C_n^s}{(E - \omega_n)^s} + \sum_n \frac{C_n^{(s-1)}}{(E - \omega_n)^{s-1}} + \cdots + \sum_n \frac{C_n^{(1)}}{(E - \omega_n)} = 1, \tag{6.11}$$

where we have put

$$E = i\hbar p \quad \text{and} \quad \omega_n = \epsilon_n + V^{(0)}_{nn}. \tag{6.12}$$

The method for deriving Eq. (6.11) is demonstrated in Sec. VII. To solve Eq. (6.11), we transform it as

$$\sum_{n' \neq n} \sum_{i=1}^{s} \frac{C_n^{(i)}}{(E - \omega_{n'})^i} = \frac{(E - \omega_n)^s - \sum_{i=1}^{s} C_n^{(i)} (E - \omega_n)^{s-i}}{(E - \omega_n)^s} = \frac{(E - E^{[0]}_{0,n,s})(E - E^{[0]}_{1,n,s}) \cdots (E - E^{[0]}_{s-1,n,s})}{(E - \omega_n)^s}, \tag{6.13}$$

where $E_{k,n,s}$ $(k = 0, 1, \cdots, s - 1)$ are the solutions of the equation

$$(E - \omega_n)^s - C_n^{(1)}(E - \omega_n)^{s-1} - C_n^{(2)}(E - \omega_n)^{s-2} - \cdots - C_n^{(s)} = 0. \tag{6.14}$$

Therefore the iteration formula is

$$E^{[m]}_{k,n,s} = \frac{(E^{[m-1]}_{k,n,s} - \omega_n)^s}{\prod_{j \neq k} (E^{[m-1]}_{k,n,s} - E^{[0]}_{j,n,s})} \cdot \left(\sum_{n' \neq n} \sum_{i=1}^{s} \frac{C_n^{(i)}}{(E^{[m-1]}_{k,n,s} - \omega_{n',s})^i} \right) \quad (m \geq 1). \tag{6.15}$$

Equation (6.14) may be solved in a manner described in Ref. 3, Sec. V, but without any restriction with respect to the sign of the coefficients $C_n^{(i)}$. Therefore, the eigenvalues $E_{k,n,s}$ is generally not a real number, but a complex number.

The solution $E_{k,n,s}$ thus obtained depends on s. If in $C_n^{(i)}$ all terms up to $V^{(s-1)}$ are included, we can expect the final result which is at least correct up to the terms proportional to t^{s-1}. Hereafter we omit the subindex s, with the understanding that we have chosen an s which yields sufficiently good results.

In the limit of convergence $E^{[m]}_{k,n} \to E_{k,n}$, the solution $g_{0,n}$ of Eq. (6.10) is expressed as

$$g_{0,n} = \frac{\sum_{k'} \sum_{n'} f^0_{n'} D_{k'n',0n}(i\hbar p)}{D(i\hbar p)}, \tag{6.16}$$

where

$$D(i\hbar p) = \prod_k \prod_n (i\hbar p - E_{kn}). \tag{6.17}$$

Therefore the solution of the Schrödinger equation with the aperiodic potential (6.1) is given by

$$\Psi(\mathbf{x}, t) = i\hbar \sum_n \frac{|n)}{2\pi i} \int_{-i\infty+\epsilon}^{i\infty+\epsilon} dp\, e^{pt} g_{0,n} = \sum_{k'k''} \sum_{nn'n''} |n) e^{-iE_{k''n''}t/\hbar} f^0_{n'} \chi_{n,k'n',k''n''} \tag{6.18}$$

with

$$\chi_{n,k'n',k''n''} = \frac{D_{k'n',0n}(E_{k''n''})}{\prod'_{k'''n''' \neq k''n''} (E_{k''n''} - E_{k'''n'''})}. \tag{6.19}$$

In the case of the time-independent interaction, we set $k = k' = k'' = k''' = 0$, and obtain Eq. (3.7).

Comparing the results obtained in this section with those in Sec. II, we see that the general solution of the time-dependent Schrödinger equation is expressed in the form of Eq. (2.18). The difference in the periodic and the aperiodic potential is if the potential is periodic (aperiodic) in time, the eigenvalue E_{ln} in Eq. (2.18) is a real (complex) number, so the energy spectra for the periodic perturbation should be sharp lines as shown in Fig. 1, whereas the energy spectrum for aperiodic perturbations should have the width.

Explicit expressions for $D_{k'n',0n}$ in Eq. (6.16) was given in Sec. IV. The matrix elements $V_{l,nn'}$ in Sec. IV, must, of course, be reinterpreted by comparing Eq. (2.11) with Eq. (6.10).

VII. DISPERSION EQUATION OF DEGENERATE SYSTEM

In this section, we demonstrate the method of transforming the secular equation of the s-fold degenerate system into the dispersion equation (6.11). The fundamental idea is based on the general method described in Sec. IV. Here we consider the case that the first-order energy ω_n defined by (4.3) is s-fold degenerate for each unperturbed state n. This is the case of Eq. (6.10).

We denote the element of the secular determinantal equation as $a_{\alpha n,\alpha' n'}$, where α (and α') takes on the values $0, 1, \cdots, s - 1$. Since we are considering the case that $a_{0n,0n} = a_{1n,1n} = \cdots = a_{s-1n,s-1n}$, we put

$$\omega_n \equiv a_{\alpha n,\alpha n} (\alpha = 0, 1, \cdots, s - 1). \tag{7.1}$$

We expand the secular determinantal equation in the form (4.5): First comes the product of all diagonal elements, next the sum of the products of $(sN - 2)$ diagonal elements and two nondiagonal elements, and so forth. The result is

$$\prod_n (E-\omega_n)^s + \sum_n \sum_\alpha \sum_{\beta>\alpha} \begin{vmatrix} 0 & -a_{\alpha n,\beta n} \\ -a_{\beta n,\alpha n} & 0 \end{vmatrix} (E-\omega_n)^{s-2} \prod_{n'\neq n}{}' (E-\omega_{n'})^s$$
$$+ \sum_n \sum_{n'>n} \sum_\alpha \sum_{\alpha'} \begin{vmatrix} 0 & -a_{\alpha n,\alpha' n'} \\ -a_{\alpha' n',\alpha n} & 0 \end{vmatrix} (E-\omega_n)^{s-1}(E-\omega_{n'})^{s-1} \prod_{n''\neq nn'}{}'' (E-\omega_{n''})^s$$
$$+ \sum_n \sum_\alpha \sum_{\beta>\alpha} \sum_{\gamma>\beta} \begin{vmatrix} 0 & -a_{\alpha n,\beta n} & -a_{\alpha n,\gamma n} \\ -a_{\beta n,\alpha n} & 0 & -a_{\beta n,\gamma n} \\ -a_{\gamma n,\alpha n} & -a_{\gamma n,\beta n} & 0 \end{vmatrix} (E-\omega_n)^{s-3} \prod_{n'\neq n}{}' (E-\omega_{n'})^s$$
$$+ \sum_n \sum_{n'>n} \sum_\alpha \sum_{\beta>\alpha} \sum_{\alpha'} \begin{vmatrix} 0 & -a_{\alpha n,\beta n} & -a_{\alpha n,\alpha' n'} \\ -a_{\beta n,\alpha n} & 0 & -a_{\beta n,\alpha' n'} \\ -a_{\alpha' n',\alpha n} & -a_{\alpha n',\beta n} & 0 \end{vmatrix} (E-\omega_n)^{s-2}(E-\omega_{n'})^{s-1} \prod_{n''\neq nn'}{}'' (E-\omega_{n''})^s$$
$$+ \sum_n \sum_{n'>n} \sum_\alpha \sum_{\alpha'} \sum_{\beta'>\alpha'} \begin{vmatrix} 0 & -a_{\alpha n,\alpha' n'} & -a_{\alpha n,\beta' n'} \\ -a_{\alpha' n',\alpha n} & 0 & -a_{\alpha' n',\beta' n'} \\ -a_{\beta' n',\alpha n} & -a_{\beta' n',\alpha' n'} & 0 \end{vmatrix} (E-\omega_n)^{s-1}(E-\omega_{n'})^{s-2} \prod_{n''\neq nn'}{}'' (E-\omega_{n''})^s$$
$$+ \sum_n \sum_{n'>n} \sum_{n''>n'} \sum_\alpha \sum_{\alpha'} \sum_{\alpha''} \begin{vmatrix} 0 & -a_{\alpha n,\alpha' n'} & -a_{\alpha n,\alpha'' n''} \\ -a_{\alpha' n',\alpha n} & 0 & -a_{\alpha' n',\alpha'' n''} \\ -a_{\alpha'' n'',\alpha n} & -a_{\alpha'' n'',\alpha' n'} & 0 \end{vmatrix}$$
$$\times (E-\omega_n)^{s-1}(E-\omega_{n'})^{s-1}(E-\omega_{n''})^{s-1} \prod_{n'''\neq nn'n''}{}''' (E-\omega_{n'''})^s + \cdots = 0. \tag{7.2}$$

The power of $(E-\omega_n)$, $(E-\omega_{n'})$, etc., should not be negative. For example, the second, the fifth, and the sixth terms in (7.2) appear only if $s \geq 2$, the fourth term appears only if $s \geq 3$, and so forth.

Dividing each term by the first term, we obtain

$$1 + \sum_n \sum_\alpha \sum_{\beta>\alpha} \begin{vmatrix} 0 & -a_{\alpha n,\beta n} \\ -a_{\beta n,\alpha n} & 0 \end{vmatrix} (E-\omega_n)^{-2}$$
$$+ \sum_n \sum_{n'>n} \sum_\alpha \sum_{\alpha'} \begin{vmatrix} 0 & -a_{\alpha n,\alpha' n'} \\ -a_{\alpha' n',\alpha n} & 0 \end{vmatrix} [(E-\omega_n)(E-\omega_{n'})]^{-1}$$
$$+ \sum_n \sum_\alpha \sum_{\beta>\alpha} \sum_{\gamma>\beta} \begin{vmatrix} 0 & -a_{\alpha n,\beta n} & -a_{\alpha n,\gamma n} \\ -a_{\beta n,\alpha n} & 0 & -a_{\beta n,\gamma n} \\ -a_{\gamma n,\alpha n} & -a_{\gamma n,\beta n} & 0 \end{vmatrix} (E-\omega_n)^{-3}$$
$$+ \sum_n \sum_{n'>n} \sum_\alpha \sum_{\beta>\alpha} \sum_{\alpha'} \begin{vmatrix} 0 & -a_{\alpha n,\beta n} & -a_{\alpha n,\alpha' n'} \\ -a_{\beta n,\alpha n} & 0 & -a_{\beta n,\alpha' n'} \\ -a_{\alpha' n',\alpha n} & -a_{\alpha' n',\beta n} & 0 \end{vmatrix} [(E-\omega_n)^2(E-\omega_{n'})]^{-1}$$
$$+ \sum_n \sum_{n'>n} \sum_\alpha \sum_{\alpha'} \sum_{\beta'>\alpha'} \begin{vmatrix} 0 & -a_{\alpha n,\alpha' n'} & -a_{\alpha n,\beta' n'} \\ -a_{\alpha' n',\alpha n} & 0 & -a_{\alpha' n',\beta' n'} \\ -a_{\beta' n',\alpha n} & -a_{\beta' n',\alpha' n'} & 0 \end{vmatrix} [(E-\omega_n)(E-\omega_{n'})^2]^{-1}$$
$$+ \sum_n \sum_{n'>n} \sum_{n''>n'} \sum_\alpha \sum_{\alpha'} \sum_{\alpha''} \begin{vmatrix} 0 & -a_{\alpha n,\alpha' n'} & -a_{\alpha n,\alpha'' n''} \\ -a_{\alpha' n',\alpha n} & 0 & -a_{\alpha' n',\alpha'' n''} \\ -a_{\alpha'' n'',\alpha n} & -a_{\alpha'' n'',\alpha' n'} & 0 \end{vmatrix}$$
$$\times [(E-\omega_n)(E-\omega_{n'})(E-\omega_{n''})]^{-1} + \cdots = 0. \tag{7.3}$$

We decompose the left-hand side of this equation into a partial fraction and obtain the dispersion equation of the form

$$\sum_{n} \sum_{i=1}^{s} \frac{C_n^{(i)}}{(E-\omega_n)^i} = 1. \tag{6.11}$$

Up to the fourth order terms, the coefficients are given by

$$C_n^{(1)} = -\sum_{n'\neq n} \sum_{\alpha} \sum_{\alpha'} \begin{vmatrix} 0 & a_{\alpha n,\alpha' n'} \\ a_{\alpha' n',\alpha n} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-1}$$

$$- \sum_{n'\neq n} \sum_{\alpha} \sum_{\alpha'} \left\{ \sum_{\beta>\alpha} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\alpha' n'} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\alpha' n'} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-2} \right.$$

$$\left. - \sum_{\beta'>\alpha'} \begin{vmatrix} 0 & a_{\alpha n,\alpha' n'} & a_{\alpha n,\beta' n'} \\ a_{\alpha' n',\alpha n} & 0 & a_{\alpha' n',\beta' n'} \\ a_{\beta' n',\alpha n} & a_{\beta' n',\alpha' n'} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-2} \right\}$$

$$+ \sum_{n'\neq n} \sum_{n''>n'} \sum_{\alpha} \sum_{\alpha'} \sum_{\alpha''} \begin{vmatrix} 0 & a_{\alpha n,\alpha' n'} & a_{\alpha n,\alpha'' n''} \\ a_{\alpha' n',\alpha n} & 0 & a_{\alpha' n',\alpha'' n''} \\ a_{\alpha'' n'',\alpha n} & a_{\alpha'' n'',\alpha' n'} & 0 \end{vmatrix} [(\omega_n - \omega_{n'})(\omega_n - \omega_{n''})]^{-1}$$

$$- \sum_{n'\neq n} \sum_{\alpha} \sum_{\alpha'} \left\{ \sum_{\beta>\alpha} \sum_{\gamma>\beta} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\gamma n} & a_{\alpha n,\alpha' n'} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\gamma n} & a_{\beta n,\alpha' n'} \\ a_{\gamma n,\alpha n} & a_{\gamma n,\beta n} & 0 & a_{\gamma n,\alpha' n'} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & a_{\alpha' n',\gamma n} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-3} \right.$$

$$\left. + \sum_{\beta'>\alpha'} \sum_{\gamma'>\beta'} \begin{vmatrix} 0 & a_{\alpha n,\alpha' n'} & a_{\alpha n,\beta' n'} & a_{\alpha n,\gamma' n'} \\ a_{\alpha' n',\alpha n} & 0 & a_{\alpha' n',\beta' n'} & a_{\alpha' n',\gamma' n'} \\ a_{\beta' n',\alpha n} & a_{\beta' n',\alpha' n'} & 0 & a_{\beta' n',\gamma' n'} \\ a_{\gamma' n',\alpha n} & a_{\gamma' n',\alpha' n'} & a_{\gamma' n',\beta' n'} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-3} \right\}$$

$$+ \sum_{n'\neq n} \sum_{\alpha} \sum_{\beta>\alpha} \sum_{\alpha'} \sum_{\beta'>\alpha'} 2 \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\alpha' n'} & a_{\alpha n,\beta' n'} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\alpha' n'} & a_{\beta n,\beta' n'} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & 0 & a_{\alpha' n',\beta' n'} \\ a_{\beta' n',\alpha n} & a_{\beta' n',\beta n} & a_{\beta' n',\alpha' n'} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-3}$$

$$+ \sum_{n'\neq n} \sum_{n''>n'} \sum_{\alpha} \sum_{\alpha'} \sum_{\alpha''} \left[\sum_{\beta>\alpha} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\alpha' n'} & a_{\alpha n,\alpha'' n''} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\alpha' n'} & a_{\beta n,\alpha'' n''} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & 0 & a_{\alpha' n',\alpha'' n''} \\ a_{\alpha'' n'',\alpha n} & a_{\alpha'' n'',\beta n} & a_{\alpha'' n'',\alpha' n'} & 0 \end{vmatrix} \right.$$

$$\times (2\omega_n - \omega_{n'} - \omega_{n''})/(\omega_n - \omega_{n'})^2(\omega_n - \omega_{n''})^2$$

$$\left. - \sum_{\beta'>\alpha'} \begin{vmatrix} 0 & a_{\alpha n,\alpha' n'} & a_{\alpha n,\beta' n'} & a_{\alpha n,\alpha'' n''} \\ a_{\alpha' n',\alpha n} & 0 & a_{\alpha' n',\beta' n'} & a_{\alpha' n',\alpha'' n''} \\ a_{\beta' n',\alpha n} & a_{\beta' n',\alpha' n'} & 0 & a_{\beta' n',\alpha'' n''} \\ a_{\alpha'' n'',\alpha n} & a_{\alpha'' n'',\alpha' n'} & a_{\alpha'' n'',\beta' n'} & 0 \end{vmatrix} \right] [(\omega_n - \omega_{n'})^2(\omega_n - \omega_{n''})]^{-1}$$

$$- \sum_{\beta''>\alpha''} \begin{vmatrix} 0 & a_{\alpha n,\alpha' n'} & a_{\alpha n,\alpha'' n''} & a_{\alpha n,\beta'' n''} \\ a_{\alpha' n',\alpha n} & 0 & a_{\alpha' n',\alpha'' n''} & a_{\alpha' n',\beta'' n''} \\ a_{\alpha'' n'',\alpha n} & a_{\alpha'' n'',\alpha' n'} & 0 & a_{\alpha'' n'',\beta'' n''} \\ a_{\beta'' n'',\alpha n} & a_{\beta'' n'',\alpha' n'} & a_{\beta'' n'',\alpha'' n''} & 0 \end{vmatrix} [(\omega_n - \omega_{n''})^2(\omega_n - \omega_{n'})]^{-1}$$

$$- \sum_{n'\neq n} \sum_{n''>n'} \sum_{n'''>n''} \sum_{\alpha} \sum_{\alpha'} \sum_{\alpha''} \sum_{\alpha'''} \begin{vmatrix} 0 & a_{\alpha n,\alpha' n'} & a_{\alpha n,\alpha'' n''} & a_{\alpha n,\alpha''' n'''} \\ a_{\alpha' n',\alpha n} & 0 & a_{\alpha' n',\alpha'' n''} & a_{\alpha' n',\alpha''' n'''} \\ a_{\alpha'' n'',\alpha n} & a_{\alpha'' n'',\alpha' n'} & 0 & a_{\alpha'' n'',\alpha''' n'''} \\ a_{\alpha''' n''',\alpha n} & a_{\alpha''' n''',\alpha' n'} & a_{\alpha''' n''',\alpha'' n''} & 0 \end{vmatrix}$$

$$\times [(\omega_n - \omega_{n'})(\omega_n - \omega_{n''})(\omega_n - \omega_{n'''})]^{-1} + \cdots , \tag{7.4}$$

$$C_n^{(2)} = - \sum_{\alpha} \sum_{\beta>\alpha} \begin{vmatrix} 0 & a_{\alpha n,\beta n} \\ a_{\beta n,\alpha n} & 0 \end{vmatrix}$$

$$+ \sum_{n'\neq n} \sum_{\alpha} \sum_{\alpha'} \sum_{\beta>\alpha} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\alpha' n'} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\alpha' n''} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-1}$$

$$+ \sum_{n'\neq n} \sum_{\alpha} \sum_{\alpha'} \sum_{\beta>\alpha} \sum_{\gamma>\beta} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\gamma n} & a_{\alpha n,\alpha' n'} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\gamma n} & a_{\beta n,\alpha' n'} \\ a_{\gamma n,\alpha n} & a_{\gamma n,\beta n} & 0 & a_{\gamma n,\alpha' n'} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & a_{\alpha' n',\gamma n} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-2}$$

$$- \sum_{n'\neq n} \sum_{\alpha} \sum_{\beta>\alpha} \sum_{\alpha'} \sum_{\beta'>\alpha'} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\alpha' n'} & a_{\alpha n,\beta' n'} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\alpha' n'} & a_{\beta n,\beta' n'} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & 0 & a_{\alpha' n',\beta' n'} \\ a_{\beta' n',\alpha n} & a_{\beta' n',\beta n} & a_{\beta' n',\alpha' n'} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-2}$$

$$- \sum_{n'\neq n} \sum_{n''>n'} \sum_{\alpha} \sum_{\alpha'} \sum_{\alpha''} \sum_{\beta>\alpha} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\alpha' n'} & a_{\alpha n,\alpha'' n''} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\alpha' n'} & a_{\beta n,\alpha'' n''} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & 0 & a_{\alpha' n',\alpha'' n''} \\ a_{\alpha'' n'',\alpha n} & a_{\alpha'' n'',\beta n} & a_{\alpha'' n'',\alpha' n'} & 0 \end{vmatrix}$$

$$\times [(\omega_n - \omega_{n'})(\omega_n - \omega_{n''})]^{-1} + \cdots , \tag{7.5}$$

$$C_n^{(3)} = \sum_{\alpha} \sum_{\beta>\alpha} \sum_{\gamma>\beta} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\gamma n} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\gamma n} \\ a_{\gamma n,\alpha n} & a_{\gamma n,\beta n} & 0 \end{vmatrix}$$

$$- \sum_{n'\neq n} \sum_{\alpha} \sum_{\alpha'} \sum_{\beta>\alpha} \sum_{\gamma>\beta} \begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\gamma n} & a_{\alpha n,\alpha' n'} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\gamma n} & a_{\beta n,\alpha' n'} \\ a_{\gamma n,\alpha n} & a_{\gamma n,\beta n} & 0 & a_{\gamma n,\alpha' n'} \\ a_{\alpha' n',\alpha n} & a_{\alpha' n',\beta n} & a_{\alpha' n',\gamma n} & 0 \end{vmatrix} (\omega_n - \omega_{n'})^{-1} + \cdots , \tag{7.6}$$

$$C_n^{(4)} = -\sum_{\alpha}\sum_{\beta>\alpha}\sum_{\gamma>\beta}\sum_{\delta>\gamma}\begin{vmatrix} 0 & a_{\alpha n,\beta n} & a_{\alpha n,\gamma n} & a_{\alpha n,\delta n} \\ a_{\beta n,\alpha n} & 0 & a_{\beta n,\gamma n} & a_{\beta n,\delta n} \\ a_{\gamma n,\alpha n} & a_{\gamma n,\beta n} & 0 & a_{\gamma n,\delta n} \\ a_{\delta n,\alpha n} & a_{\delta n,\beta n} & a_{\delta n,\gamma n} & 0 \end{vmatrix} + \cdots . \tag{7.7}$$

Having obtained the dispersion equation (6.11), we remove the degeneracy by solving Eq. (6.14), applying the method described in Ref. 3, Sec. V. We use the iteration formula (6.15) and then we obtain the eigenvalues.

VIII. MIXED PERTURBATION OF PERIODIC AND APERIODIC PARTS

In this section, we describe the method of calculating the wavefunction for a more general case.

If the time-dependent perturbation is the product of the periodic and aperiodic perturbations, we can express it by using the notations of Secs. II and VI as

$$V(\mathbf{x}, t) = \sum_{k=0}^{\infty}\sum_{l}\left(\frac{1}{k!}\right)\left(\frac{t}{i\hbar}\right)^k e^{-il\omega t/\hbar}V^{(k)}(\mathbf{x}). \tag{8.1}$$

(The time derivatives are taken to the aperiodic part.) The formal solution of the Schrödinger equation is

$$\psi(\mathbf{x}, t) = \psi(\mathbf{x}, 0) + \sum_{k'=0}\sum_{l'}\left(\frac{1}{k'!}\right)\left(\frac{1}{i\hbar}\right)\int_0^t e^{iH_0t'/\hbar}(t'/i\hbar)^{k'} \times V^{(k')}(\mathbf{x})e^{-il'\omega t'/\hbar}e^{-iH_0t'/\hbar}\psi(\mathbf{x}t')\,dt'. \tag{8.2}$$

We define the Laplace transform of the function

$$(1/k!)(1/i\hbar)(t/i\hbar)^k e^{-i(H_0+l\omega)t/\hbar}\psi(\mathbf{x}, t)$$

by $g_{l,k}(\mathbf{x}, p)$

$$= \left(\frac{1}{k!}\right)\left(\frac{1}{i\hbar}\right)\int_0^{\infty} e^{-pt}\left(\frac{t}{i\hbar}\right)^k e^{-i(H_0+l\omega)t/\hbar}\psi(\mathbf{x}, t)\,dt.$$

By the similar method as in Secs. II and VI, we obtain from Eq. (8.2) a set of coupled equations

$$g_{l,k}(\mathbf{x}, p) = \frac{1}{[i\hbar p - (H_0 + l\omega)]^{k+1}}\psi(\mathbf{x}, 0) + \sum_{k'}\sum_{l'}\sum_{r=0}^{k}\frac{1}{\{i\hbar p - [H_0 + (l + l')\omega]\}^{k-r+1}} \times \binom{k' + r}{k'}V_{l'}^{(k')}(\mathbf{x})g_{l+l',k'+r}(\mathbf{x}, p)$$

or

$$\{i\hbar p - [H_0 + (l + l')\omega]\}^{k+1}g_{lk}(\mathbf{x}, p) = \{i\hbar p - [H_0 + (l + l')\omega]\}^{k+1} \times \frac{1}{[i\hbar p - (H_0 + l\omega)]^{k+1}}\psi(\mathbf{x}, 0) + \sum_{k'}\sum_{l'}\sum_{r=0}^{k}\{i\hbar p - [H_0 + (l + l')\omega]\}^r \times \binom{k' + r}{k'}V_{l'}^{(k')}(\mathbf{x})g_{l+l',k'+r}(\mathbf{x}, p).$$

As in Sec. II, we multiply $|n)$ from the left and integrate over the coordinate $\mathbf{x}$. Then we obtain the set of coupled equations

$$\{i\hbar p - [\epsilon_n + (l + l')\omega]\}^{k+1}g_{lk,n} = \{i\hbar p - [\epsilon_n + (l + l')\omega]\}^{k+1}\frac{1}{[i\hbar p - (\epsilon_n + l\omega)]^{k+1}}f_n^0 + \sum_{n'}\sum_{k'}\sum_{l'}\sum_{r=0}^{k}\{i\hbar p - [\epsilon_n + (l + l')\omega]\}^r \times \binom{k' + r}{k'}V_{l',nn'}^{(k')}g_{l+l',k'+r,n'}, \tag{8.5}$$

where

$$g_{lk,n} = (n|\, g_{lk}(\mathbf{x})), \qquad f_n^0 = (n|\, \psi(\mathbf{x}, 0)), \tag{8.6}$$

and

$$V_{l',nn'}^{(k')} = (n|\, V_{l'}^{(k')}(\mathbf{x})\,|n').$$

Eq. (8.5) is alternatively expressed as

$$[i\hbar p - (\epsilon_n + l\omega + V_{0,nn}^{(0)})]g_{l0,n} - \sum_{\substack{n'\\(n'k'l')\neq(n00)}}\sum_{k'}\sum_{l'}V_{l',nn'}^{(k')}g_{l+l',k'n'} = f_n^0 \tag{8.7}$$

and

$$\{i\hbar p - [\epsilon_n + (l + l')\omega + V_{0,nn}^{(0)}]\}g_{l,k+1,n} - g_{l,k,n} - \sum_{\substack{n'\\(n'k'l')\neq(n00)}}\sum_{k'}\sum_{l'}\binom{k' + k + 1}{k'}V_{l',nn'}^{(k')}g_{l+l',k'+k+1,n'}$$

$$= \left\{ \frac{i\hbar p - [\epsilon_n + (l + l')\omega]}{[i\hbar p - (\epsilon_n + l\omega)]^{k+2}} - \frac{1}{[i\hbar p - (\epsilon_n + l\omega)]^{k+1}} \right\} f^0_{ln}, \tag{8.8}$$

for $k \geq 0$.

By the method demonstrated in Secs. IV and VII, we can diagonalize the secular equation obtained from Eqs. (8.7) and (8.8).

Once we find eigenvalues, the wavefunction is obtained by the Laplace inverse transform of $g_{00,n}$

$$\Psi(\mathbf{x}, t) = i\hbar \sum_n \frac{|n)}{2\pi i} \int_{-i\infty+\epsilon}^{i\infty+\epsilon} dp\, e^{pt} g_{00,n} = \sum_{l''l''} \sum_{k'k''} \sum_{nn'n''} |n) e^{-iE_{l''k''n''}t/\hbar} f^0_{n'} \chi_{n,l'k'n',l''k''n''}, \tag{8.9}$$

with

$$\chi_{n,l'k'n',l''k''n''} = \frac{D_{l'k'n',00n}(E_{l''k''n''})}{\prod'_{l'''k'''n'''\neq l''k''n''} (E_{l''k''n''} - E_{l'''k'''n'''})}. \tag{8.10}$$

This is the generalized form of Eq. (2.18) or Eq. (6.18). However, the expressions (8.9) and (8.10) are formally absorbed in Eqs. (2.18) and (2.19) or Eqs. (6.18) and (6.19) if we change the meaning of sub-indices.

By Eq. (8.1), we have assumed that the time-dependent perturbation is the product of the periodic and the aperiodic perturbations. The extension of the treatment to more general class, which is expressed as the sum of such products is very easily done. The general solution should again be expressed in the form (8.9) with additional sub-indices.

CONCLUSION

In conclusion, the general solution of the time-dependent Schrödinger equation is always expressible in the form (2.18). We can perform calculations with the aid of the formulas described in Sec. IV and Sec. VII.

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The author would like to express his gratitude to Professor E. Feenberg for hospitality and research facilities extended to him and interest in this work.

APPENDIX: COMMENT TO THE METHOD FOR OBTAINING EIGENVALUES

As shown in Ref. 3 and in Sec. IV of the present paper, the original secular determinantal equation is transformed into the dispersion equation

$$\sum_n \frac{C_n}{E - \omega_n} = 1. \tag{A1}$$

One of the methods of solving this equation is the weak-coupling method. (See Sec. III in Ref. 3.) The iteration formula of this method is

$$E^{[m]} = \omega_n + \frac{C_n}{1 - \sum_{p\neq n} [C_p/E^{[m-1]} - \omega_p]} \quad (m \geq 1) \tag{A2}$$

with

$$E^{[0]} = \omega_n.$$

If we expand Eq. (A2) and subtract $E^{[1]}$ from $E^{[2]}$, we obtain

$$E^{[2]} = E^{[1]} - C_n \sum_{n'\neq n} \frac{C_{n'}}{(\omega_n - \omega_{n'})^2} (E^{[1]} - \omega_n) + \text{higher-order terms.} \tag{A3}$$

In general, we have

$$E^{[m]} = E^{[m-1]} - C_n \sum_{n'\neq n} \frac{C_{n'}}{(\omega_n - \omega_{n'})^2} (E^{[m-1]} - E^{[m-2]}) + \text{higher-order terms.} \tag{A4}$$

Since the lowest-order term in C_n, $C_{n'}$ and $E^{[1]} - \omega_n$ are of second order, the difference of $E^{[2]}$ and $E^{[1]}$ is the sixth- and higher-order terms. That is, the first iteration is correct up to the fifth-order terms.

In general, the mth iteration of the weak-coupling method gives the result which is correct up to the $(4m + 1)$th-order terms. In the usual perturbation methods, the mth-order iteration gives the result which is correct up to the mth-order terms (see Ref. 3). This can be modified if we let the first-order energy absorb into the energy denominator. However, even with this modification, the usual perturbation theory gives the result which is correct at most up to the $(2m + 1)$th-order terms for the mth iteration. The important improvement in the weak-coupling method results from the presumption that we calculate all coefficients C_n in the dispersion equation (A1) before making iterations.

Another method of solving the dispersion equation (A1) is the strong-coupling method. (See, also Sec. III in Ref. 3.) We discuss it taking the case of $C_n > 0$ and $C_{n+1} > 0$.

First, we solve the equation

$$\frac{C_n}{E - \omega_n} + \frac{C_{n+1}}{E - \omega_{n+1}} = 1 \tag{A5}$$

exactly. This means that we diagonalize the original secular determinantial equation with respect to the two states. The lower solution E_- of this equation lies in between ω_n and ω_{n+1}. We take E_- as the starting value of iterations, for which we make use of the formula

$$E^{[m]} = E_- + \frac{(E^{[m-1]} - \omega_n)(E^{[m-1]} - \omega_{n+1})}{E^{[m-1]} - E_+} \times \left(\sum_{n' \neq n, n+1} \frac{C_{n'}}{E^{[m-1]} - \omega_{n'}} \right), \quad m \geq 1 \qquad \text{(A6)}$$

with

$$E^{[0]} = E_-.$$

In Eq. (A6),

$$E_\pm = \tfrac{1}{2}\{(\omega_n + \omega_{n+1} + C_n + C_{n+1}) \pm [(\omega_n + \omega_{n+1} + C_n + C_{n+1})^2 - 4(\omega_n\omega_{n+1} + C_n\omega_{n+1} + C_{n+1}\omega_n)]^{\frac{1}{2}}\}. \qquad \text{(A7)}$$

In the limit of convergence, Eq. (A6) becomes the dispersion equation (A1) because

$$\frac{(E - E_-)(E - E_+)}{(E - \omega_n)(E - \omega_{n+1})} = 1 - \frac{C_n}{E - \omega_n} - \frac{C_{n+1}}{E - \omega_{n+1}}.$$

The strong-coupling method gives the result which is correct up to $(4m + 3)$th-order terms after the mth iterations, because (1) E_- is correct up to the third-order terms, (2) $(E_- - \omega_n)$ begins from the second-order terms, (3) $(E_- - \omega_{n+1})/(E_- - E_+)$ begins from the zeroth-order terms and $c_{n'}/(E_- - \omega_{n'})$ begins from the second-order terms.

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Generalizations of the Virial and Wall Theorems in Classical Statistical Mechanics*

ARNOLD J. F. SIEGERT AND EMMANUEL MEERON
Department of Physics, Northwestern University, Evanston, Illinois
(Received 11 October 1965)

A generalized virial theorem which expresses *inverse compressibility* in terms of integrals of virials and canonical distribution functions through the four-particle distribution is transformed to the grand canonical ensemble and becomes an expression for *compressibility* in terms of the same integrals formed with *grand canonical* distribution functions. The integrals are of a mixed (virial and fluctuation) type.

While the thermodynamic functions expressed by the same integrals with canonical and grand canonical distribution functions are quite different, the two formulas agree in the thermodynamic limit because of the different asymptotic behavior of canonical and grand canonical distribution functions. We also derived an alternative form of the second virial theorem which expresses compressibility in terms of integrals over virials and grand canonical distribution functions through the three-particle distribution function only. It is shown that this form and its generalizations to higher derivatives of the density, as well as the hierarchy of fluctuation theorems and the fugacity expansions of distribution and correlation functions can all be very simply derived from a set of integro-differential equations satisfied by the grand canonical distribution functions. A generalization of the wall theorem $(P/kT = \rho_{\text{wall}})$ is derived and shown to be equivalent to the generalized virial theorem (canonical form).

1. INTRODUCTION

THERE are equations of several types which express thermodynamic functions in terms of molecular distribution functions: the virial theorem, which expresses pressure in terms of the average virial of the force of interaction; the "wall-theorem," which expresses pressure in terms of the density at the surface of the container, and the fluctuation theorems, which express compressibility and its derivatives as integrals over correlation functions. There is an infinite sequence of fluctuation theorems and we became interested in the question whether the wall theorem and the virial theorem can be extended also, to express, for instance, compressibility in terms of virials and molecular distribution functions or boundary values of the latter, respectively. In the present paper, we derive several theorems of this type, and show their relations with each other, and

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with

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In Eq. (A6),

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with integral equations for the distribution functions.

In Sec. 2 we introduce the notation and general assumptions. In Sec. 3 we state a generalization of the virial theorem, which expresses inverse compressibility as an integral over virials and the distribution functions in the canonical ensemble up to the four-point distribution. We then derive the corresponding theorem for the grand canonical ensemble and obtain the thermodynamic limit of this theorem. In Sec. 4 we obtain the thermodynamic limit of the canonical form and show agreement with the thermodynamic limit of the grand canonical form. In Sec. 5 we obtain a generalization of the virial theorem, which expresses compressibility as an integral over the virial and grand canonical distribution functions up to the three-particle distribution only, and obtain its limiting form in the thermodynamic limit.

The integrals occurring in these equations are of a mixed (virial and fluctuation) type.

In Sec. 6 we show that the fluctuation theorems, and the fugacity expansions of distribution functions and correlation functions, and the theorem of Sec. 5 and its generalizations can all be derived very simply from an integro-differential equation satisfied by the molecular distribution functions of the grand canonical ensemble. In Sec. 7 we derive heuristically an asymptotic equation for the correlation of two functions of density relative to the probability distribution of the grand canonical ensemble, and derive from it an auxiliary equation needed in Sec. 3. In Sec. 8 we derive a generalization of the wall theorem, and show its equivalence to the generalization of the virial theorem (canonical form) stated in Sec. 3.

2. NOTATION AND GENERAL ASSUMPTIONS

We consider systems of N particles without internal degrees of freedom. Quantum effects are neglected. The particles are contained in a domain V, and we use the same symbol for the volume of this domain. We want to consider the case of 1, 2, and 3 dimensions together and write ν for the number of dimensions. The position vectors of the particles are $\mathbf{r}_1, \mathbf{r}_2 \cdots$, and the volume elements are $d^\nu r_1$, $d^\nu r_2 \cdots$. We write $d^{\nu n} r$ for $\Pi_1^n d^\nu r_i$, and we frequently write only the numbers of the position vectors.

We write $Z_N(V)$ for the Gibbs integral

$$Z_N(V) = \int_V \cdots \int_V e^{-\beta U_N} \, d^{\nu N} r, \tag{2.1}$$

where $\beta = 1/kT$, and

$$U_N = U_N(\mathbf{r}_1, \mathbf{r}_2 \cdots \mathbf{r}_N) \tag{2.2}$$

is the potential energy of interaction. We use the abbreviation

$$\beta P(N, V) = \partial \log Z_N(V)/\partial V. \tag{2.3}$$

Additional assumptions concerning V and its increment are made, when necessary to ensure that $P(N, V)$ represents in the thermodynamic limit the outcome of a pressure measurement (and not, for instance, the work per volume increment required to increase the size of a small cavity in a large volume of fluid). We define the molecular distribution functions in the canonical ensemble (CE) by

$$\rho_n(\mathbf{r}_1 \cdots \mathbf{r}_n; N, V) = \frac{N!}{(N-n)!} [Z_N(V)]^{-1} \int_V \cdots \int_V e^{-\beta U_N} \prod_{i=n+1}^{N} d^\nu r_i. \tag{2.4}$$

For the grand canonical ensemble (GCE) we define the partition function by

$$\mathcal{Q}_V(z) = \sum_{N=0}^{\infty} \frac{z^N}{N!} Z_N(V) \tag{2.5}$$

and we define grand canonical averages by

$$\langle F(N) \rangle_z = \mathcal{Q}_V^{-1}(z) \sum_{N=0}^{\infty} \frac{z^N}{N!} Z_N(V) F(N). \tag{2.6}$$

We made a distinction between the GC average of the canonical pressure

$$\langle P(N, V) \rangle_z \equiv \partial \log \mathcal{Q}_V(z)/\partial V, \tag{2.7}$$

and the conventional GC pressure

$$P(z, V) = (1/V) \log \mathcal{Q}_V(z), \tag{2.8}$$

and use $\rho(z, V)$ or ρ for the GC density only.

We distinguish canonical from GC distribution functions in the notation only by replacing N by z in the argument, and define

$$\rho_n(\mathbf{r}_1, \cdots, \mathbf{r}_n; z, V) = \langle \rho_n(\mathbf{r}_1, \cdots, \mathbf{r}_n; N, V) \rangle_z. \tag{2.9}$$

We denote by $\chi_n(\mathbf{r}_1, \cdots \mathbf{r}_n; N, V)$ and

$$\chi_n(\mathbf{r}_1, \cdots, \mathbf{r}_n; z, V),$$

the correlation functions formed by the Ursell development[1] from the canonical and grand canonical distribution functions. Note that $\chi_n(\mathbf{r}_1, \cdots, \mathbf{r}_n; z, V)$ is not, in general, the grand canonical average of $\chi_n(\mathbf{r}_1, \cdots \mathbf{r}_n; N, V)$.

3. SECOND VIRIAL THEOREM WITH ρ_4

We obtained a second virial theorem for the canonical ensemble, in the case of spherically symmetric

[1] B. Kahn and G. E. Uhlenbeck, Physica 5, 399 (1938), especially p. 403.

pair interaction $u_{ij} = u(|r_i - r_j|)$, by the scaling method,[2] and found that it was given implicitely by an expression for the fluctuation of the virial calculated by Brown.[3] The calculation is straightforward and one obtains

$$\frac{\partial}{\partial V}[\beta P(N, V)V]$$
$$= \frac{\beta}{2\nu^2 V}\left\{\frac{\beta}{2}\iiiint_V \mathfrak{v}_{12}\mathfrak{v}_{34}[\rho_4(1, 2, 3, 4; N, V) - \rho_2(1, 2; N, V)\rho_2(3, 4; N, V)]\, d'r_1\, d'r_2\, d'r_3\, d'r_4 + 2\beta\iiint_V \mathfrak{v}_{12}\mathfrak{v}_{13}\rho_3(1, 2, 3; N, V)\, d'r_1\, d'r_2\, d'r_3 - \iint_V \left[r_{12}\frac{d}{dr_{12}}\mathfrak{v}_{12} - \beta\mathfrak{v}_{12}^2\right] \times \rho_2(1, 2; N, V)\, d'r_1\, d'r_2\right\}, \tag{3.1}$$

where

$$\mathfrak{v}_{ij} = r_{ij}\, du_{ij}/dr_{ij}, \tag{3.1'}$$

with

$$r_{ij} = |r_i - r_j|. \tag{3.1''}$$

Equation (3.1) can also be derived from the second wall theorem (Sec. 8) through Eq. (8.15).

The thermodynamic limit of Eq. (3.1) must not be taken under the integral in the first term. We have, therefore, derived the grand canonical form of this theorem.

All terms linear in the distribution functions on the right-hand side of Eq. (3.1) can be averaged immediately. To take care of the term $\rho_2(1, 2; N, V)\cdot\rho_2(3,4; N, V)$ we add and subtract

$$\frac{\beta^2}{4\nu^2 V}\iiiint_V \mathfrak{v}_{12}\mathfrak{v}_{34}[\langle\rho_2(1, 2; N, V)\rho_2(3, 4; N, V)\rangle_z - \rho_2(1, 2; z, V)\rho_2(3, 4; z, V)] = V\left[\left\langle\left(\frac{N}{V} - \beta P(N, V)\right)^2\right\rangle_z - \left\langle\frac{N}{V} - \beta P(N, V)\right\rangle_z^2\right] \tag{3.2}$$

on both sides. The right-hand side of Eq. (3.2) is

$$\frac{1}{V}(\langle N^2\rangle_z - \langle N\rangle_z^2) - 2\beta[\langle NP(N, V)\rangle_z - \langle N\rangle_z\langle P(N, V)\rangle_z] + V[\langle(\beta P(N, V))^2\rangle_z - \langle\beta P(N, V)\rangle_z^2] = \frac{\partial}{\partial \log z}[\rho(z, V) - 2\langle\beta P(N, V)\rangle_z] + V[\langle(\beta P(N, V))^2\rangle_z - \langle\beta P(N, V)\rangle_z^2] \tag{3.3}$$

by Eq. (A1), Appendix A. From Eq. (B3) we have

$$V\left\langle\frac{\partial}{\partial V}\beta P(N, V)\right\rangle_z + V[\langle(\beta P(N, V))^2\rangle_z - \langle\beta P(N, V)\rangle_z^2] = V\frac{\partial}{\partial V}\langle\beta P(N, V)\rangle_z. \tag{3.4}$$

Using these results one obtains for the GC average of Eq. (3.1)

$$\frac{\partial}{\partial \log z}[\rho(z, V) - 2\langle\beta P(N, V)\rangle_z] + \langle\beta P(N, V)\rangle_z + V\frac{\partial}{\partial V}\langle\beta P(N, V)\rangle_z = \frac{\beta}{2\nu^2 V}\left\{\frac{\beta}{2}\iiiint_V \mathfrak{v}_{12}\mathfrak{v}_{34}[\rho_4(1, 2, 3, 4; z, V) - \rho_2(1, 2; z, V)\rho_2(3, 4; z, V)]\, d'r_1 \cdots d'r_4 + 2\beta\iiint_V \mathfrak{v}_{12}\mathfrak{v}_{13}\rho_3(1, 2, 3; z, V)\, d'r_1\, d'r_2\, d'r_3 - \iint_V \left[r_{12}\frac{d}{dr_{12}}\mathfrak{v}_{12} - \beta\mathfrak{v}_{12}^2\right]\rho_2(1, 2; z, V)\, d'r_1\, d'r_2\right\}. \tag{3.5}$$

It is generally accepted, as the basis of the use of the conventional GC pressure $P(z, V)$, that

$$\lim_{V\to\infty}\langle\beta P(N, V)\rangle_z = \lim_{V\to\infty}\beta P(z, V), \tag{3.6}$$

and it is known that the limit on the right-hand side exists.[4] Accepting Eq. (3.6) to be true on a set $\mathcal{E}$ of measure $m(\mathcal{E})$ in the z plane, we have, by Egoroff's theorem[5]

$$\lim_{V\to\infty}\frac{\partial}{\partial \log z}\langle\beta P(N, V)\rangle_z = \lim_{V\to\infty}\frac{\partial}{\partial \log z}\beta P(z, V) \tag{3.7}$$

on a subset of $\mathcal{E}$, the measure of the subset being $m(\mathcal{E}) - \delta$ with arbitrarily small δ. It is known that in one-phase regions the limit on the right-hand side

[2] H. S. Green, Proc. Roy. Soc. (London) **A189**, 103 (1947), especially p. 115.

[3] W. B. Brown, Philo. Trans. Roy. Soc. (London) **A250**, 221 (1957/8). The explicit form is obtained by substituting, into his Eq. (A4) (p. 245), his Eqs. (7.11)–(7.12) (p. 231) and Eq. (7.4) (p. 230) with Eqs. (7.18)–(7.20), p. 232. There is a factor 1/9 missing on the right-hand side of the last three equations, which is our $1/\nu^2$ for $\nu = 3$.

[4] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952).

[5] E. C. Titchmarch, *The Theory of Functions* (Oxford University Press, New York, 1939), 2nd ed., p. 339.

of Eq. (3.7) exists,[4] and that

$$\lim_{V\to\infty} \frac{\partial}{\partial \log z}\rho(z, V) = \frac{\partial}{\partial \log z}\lim_{V\to\infty}\rho(z, V). \tag{3.8}$$

We show heuristically in Sec. 7 that in one-phase regions

$$\lim_{V\to\infty} V\frac{\partial}{\partial V}\langle \beta P(N, V)\rangle_z = 0. \tag{3.9}$$

With the notation

$$\lim P(z, V) = P \tag{3.10}$$

and

$$\lim_{V\to\infty}\rho(z, V) = \rho \tag{3.11}$$

we, therefore, have—with the provisos stated above—

$$\begin{aligned}
&\frac{\partial\rho}{\partial \log z} - 2\rho + \beta P \\
&= \lim_{V\to\infty}\frac{\beta}{2\nu^2 V}\left\{\frac{\beta}{2}\iiint_V \mathfrak{v}_{12}\mathfrak{v}_{34}[\rho_4(1, 2, 3, 4; z, V)\right. \\
&\quad - \rho_2(1, 2; z, V)\rho_2(3, 4; z, V)]\, d^3r_1\cdots d^3r_4 \\
&\quad + 2\beta\iiint_V \mathfrak{v}_{12}\mathfrak{v}_{13}\rho_3(1, 2, 3; z, V)\, d^3r_1\, d^3r_2\, d^3r_3 \\
&\quad \left. - \iint_V\left[r_{12}\frac{d}{dr_{12}}\mathfrak{v}_{12} - \beta\mathfrak{v}_{12}^2\right]\rho_2(1, 2; z, V)\, d^3r_1\, d^3r_2\right\}.
\end{aligned} \tag{3.12}$$

4. THERMODYNAMIC LIMIT OF THE SECOND VIRIAL THEOREM

We mentioned above that the thermodynamic limit of Eq. (3.1) must not be taken under the integral. If this is done and the result is expanded in powers of density, one obtains equations which are obviously wrong. We also note that the thermodynamic functions expressed by the distribution functions are quite different in the canonical and grand canonical form, Eq. (3.1) and Eq. (3.5), respectively. In the former occurs $V\partial\beta P(N, V)/\partial V$ which approaches $-\rho\partial\beta P/\partial\rho$, in the latter we have $\partial\rho/\log z = \rho\partial\rho/\partial\beta P$. The corresponding phenomenon in the case of the fluctuation theorem has been discussed by several authors.[6]

There is, of course, no paradox when the limit is carried out properly, which can be done explicitly within the range of validity of results concerning the asymptotic behavior of distribution functions which were obtained by Lebowitz and Percus[7-9]. Specialized to our case, their results are that

$$\begin{aligned}
&\rho_4(1, 2, 3, 4; N, V) - \rho_2(1, 2; N, V)\rho_2(3, 4; N, V) \\
&\quad = -\frac{1}{V\rho}\frac{\partial\rho}{\partial\beta P}\left[\rho\frac{\partial}{\partial\rho}\rho_2(1, 2)\right] \\
&\qquad \times\left[\rho\frac{\partial}{\partial\rho}\rho_2(3, 4)\right] + o(V^{-1})
\end{aligned} \tag{4.1}$$

when the pair (1, 2) is far from the pair (3, 4), while there is no term of order V^{-1} in the grand canonical case. We use the notation $\rho_n(1, \cdots, n)$ for the thermodynamic limit of the distribution functions (in this section only).

Within the range of validity of these results of Lebowitz and Percus, it is then permissible to take the thermodynamic limit on the right-hand side of Eqs. (3.5) and (3.12) under the integral. Equation (3.1), however, becomes

$$\begin{aligned}
&-\rho\frac{\partial\beta P}{\partial\rho} + \beta P \\
&\quad = \frac{\beta}{2\nu^2}\left\{\frac{\beta}{2}\iiint \mathfrak{v}_{12}\mathfrak{v}_{34}[\rho_4(1, 2, 3, 4)\right. \\
&\qquad - \rho_2(1, 2)\rho_2(3, 4)]\, d^3r_2\, d^3r_3\, d^3r_4 \\
&\qquad + 2\beta\iint \mathfrak{v}_{12}\mathfrak{v}_{13}\rho_3(1, 2, 3)\, d^3r_2\, d^3r_3 \\
&\qquad \left. - \int\left[r_{12}\frac{d\mathfrak{v}_{12}}{dr_{12}} - \beta\mathfrak{v}_{12}^2\right]\rho_2(1, 2)\, d^3r_2\right\} \\
&\qquad - \rho^{-1}\frac{\partial\rho}{\partial\beta P}\left[\rho\frac{\partial}{\partial\rho}(\rho - \beta P)\right]^2,
\end{aligned} \tag{4.2}$$

where the virial theorem has been used to evaluate the correction terms. The integrals now extend over all space and the point (1) is arbitrarily fixed. With

$$\begin{aligned}
&\rho^{-1}\frac{\partial\rho}{\partial\beta P}\left[\rho\frac{\partial}{\partial\rho}(\rho - \beta P)\right]^2 \\
&\qquad = \rho^{-1}\frac{\partial\rho}{\partial\beta P}\left[\rho - \rho\frac{\partial\beta P}{\partial\rho}\right]^2 \\
&\qquad = \rho\frac{\partial\rho}{\partial\beta P} - 2\rho + \rho\frac{\partial\beta P}{\partial\rho},
\end{aligned} \tag{4.3}$$

Eq. (4.2) becomes

[6] G. E. Uhlenbeck, P. C. Hemmer, and M. Kac, J. Math Phys. 4, 229 (1963), footnote 11, p. 234, and literature quoted there.

[7] J. L. Lebowitz and J. K. Percus, Phys. Rev. 122, 1675 (1961).

[8] H. L. Frisch and J. L. Lebowitz, *The Equilibrium Theory of Classical Fluids* (W. A. Benjamin Company, Inc., New York, 1964), pp. I-19, 20.

[9] J. L. Lebowitz and J. K. Percus, J. Math. Phys. 4, 116 (1963).

$$\rho\frac{\partial\rho}{\partial\beta P}-2\rho+\beta P$$
$$=\frac{\beta}{2v^2}\Big\{\frac{\beta}{2}\iiint v_{12}v_{34}[\rho_4(1,2,3,4)-\rho_2(1,2)\rho_2(3,4)]\,d^3r_2\,d^3r_3\,d^3r_4+2\beta\iint v_{12}v_{13}\rho_3(1,2,3)\,d^3r_2\,d^3r_3-\int\Big[r_{12}\frac{dv_{12}}{dr_{12}}-\beta v_{12}^2\Big]\rho_2(1,2)\,d^3r_2\Big\} \quad (4.4)$$

in agreement with the result obtained from Eq. (3.12) by taking the limit under the integral.

5. THE SECOND VIRIAL THEOREM WITH ρ_3

In this section we derive a form of the GC second virial theorem which contains distribution functions up to ρ_3 only. One expects such a form to exist, since integration by parts applied to the compressibility theorem will yield a term with $\nabla\rho_2$, which converts to a term with ρ_3 by the use of the Yvon–Born–Green equation.[10] The derivation from the compressibility theorem can be carried through but is somewhat tedious, and we present here a much shorter derivation.

From the virial theorem and the identity

$$\int_V \rho_3(1,2,3;N,V)\,d^3r_3=(N-2)\rho_2(1,2;N,V) \quad (5.1)$$

we obtain

$$(N-2)\Big(\frac{N}{V}-\beta P(N,V)\Big)=(N-2)\frac{\beta}{2vV}\iint_V v_{12}\rho_2(1,2;N,V)\,d^3r_1\,d^3r_2=\frac{\beta}{2vV}\iiint_V v_{12}\rho_3(1,2,3;N,V)\,d^3r_1\,d^3r_2\,d^3r_3. \quad (5.2)$$

The grand canonical average of the left-hand side is by Eq. (A1) given by

$$\Big\langle(N-2)\Big(\frac{N}{V}-\beta P(N,V)\Big)\Big\rangle_z=\langle N\rangle_z\Big\langle\frac{N}{V}-\beta P(N,V)\Big\rangle_z+\frac{\partial}{\partial\log z}\Big\langle\frac{N}{V}-\beta P(N,V)\Big\rangle_z-2\Big\langle\frac{N}{V}-\beta P(N,V)\Big\rangle_z. \quad (5.3)$$

Taking the GC average of Eq. (5.2) we thus obtain, by writing the first term on the right-hand side of Eq. (5.3) in terms of distribution functions

$$\frac{\partial}{\partial\log z}[\rho(z,V)-\langle\beta P(N,V)\rangle_z]-2[\rho(z,V)-\langle\beta P(N,V)\rangle_z]=\frac{\beta}{2vV}\iiint_V v_{12}[\rho_3(1,2,3;z,V)-\rho_2(1,2;z,V)\rho_1(3;z,V]\,d^3r_1\,d^3r_2\,d^3r_3. \quad (5.4)$$

To go to the thermodynamic limit, the arguments stated at the end of Sec. 3 apply and we obtain

$$\rho\frac{\partial\rho}{\partial\beta P}-3\rho+2\beta P=\lim_{V\to\infty}\frac{\beta}{2vV}\iiint_V v_{12}[\rho_3(1,2,3;z,V)-\rho_2(1,2;z,V)\rho_1(3;z,V)]\,d^3r_1\,d^3r_2\,d^3r_3. \quad (5.5)$$

6. SYSTEMATIC APPROACH THROUGH INTEGRO-DIFFERENTIAL EQUATIONS

If one averages the normalization equation

$$(N-n)\rho_n(1,2,\cdots,n;N,V)=\int_V\rho_{n+1}(1,\cdots,n,n+1;N,V)\,d^3r_{n+1} \quad (6.1)$$

over the GCE one obtains, using Eq. (A1), the integro-differential equations

$$\Big(\frac{\partial}{\partial\log z}-n\Big)\rho_n(1,\cdots,n;z,V)=\int_V[\rho_{n+1}(1,\cdots,n,n+1;z,V)-\rho_n(1,\cdots,n;z,V)\rho_1(n+1;z,V)]\,d^3r_{n+1}. \quad (6.2)$$

If a sequence of symmetric functions ρ_n satisfies Eq. (6.2), the Ursell functions χ_n associated with them satisfy the simpler equations

$$\Big(\frac{\partial}{\partial\log z}-n\Big)\chi_n(1,\cdots,n;z,V)=\int_V\chi_{n+1}(1,\cdots,n,n+1;z,V)\,d^3r_{n+1} \quad (6.3)$$

and, conversely, Eq. (6.2) follows from Eq. (6.3).

These two sets of equations were given by Percus[11] and can serve to derive in a unified way fluctuation

[10] A. Muenster, *Statistische Thermodynamik* (Springer-Verlag, Berlin, 1956), p. 255 Eq. (VIII 81). The first term on the right-hand side of this equation should be multiplied by $\rho^{(n)}$.

[11] J. K. Percus, "The Pair Distribution Function in Classical Statistical Mechanics" in Ref. 8, p. II-52 Eqs. (4.13), (4.14).

theorems, fugacity expansions, and the second virial theorem of Sec. 5 and its generalizations.

The fluctuation theorems[12]

$$\left\{\prod_{j=1}^{n}\left(\frac{\partial}{\partial \log z}-j\right)\right\}\rho(z, V)$$
$$\equiv\left\{\prod_{j=1}^{n}\left[\rho(z, V)\frac{\partial}{\partial\beta P(z, V)}-j\right]\right\}\rho(z, V)$$
$$=\frac{1}{V}\int_{V}\cdots\int\chi_{n+1}(1, \cdots, n, n+1; z, V)\, d^{\nu}r_{n+1} \tag{6.4}$$

follow from Eq. (6.3) by successive substitution and integration.

The fugacity expansion of $\chi_n(1, \cdots, n; z, V)$[13] is obtained by writing Eq. (6.3) in the form

$$\frac{\partial}{\partial z}\hat{\chi}_n(1, \cdots, n; z, V)$$
$$=\int_{V}\hat{\chi}_{n+1}(1, \cdots, n; n+1; z, V)\, d^{\nu}r_{n+1} \tag{6.5}$$

with

$$\hat{\chi}_n = z^{-n}\chi_n. \tag{6.6}$$

From this follows by successive substitution

$$\chi_n(1, \cdots, n; z, V)$$
$$=z^{n}\Big\{\chi_n(1, \cdots, n; 0, V)+\sum_{l\geq 1}\frac{z^{l}}{l!}$$
$$\times\int_{V}\cdots\int\chi_{n+l}(1, \cdots, n+l; 0, V)\, d^{\nu}r_{n+1}\cdots, d^{\nu}r_{n+l}\Big\}, \tag{6.7}$$

where, by definition, $\chi_n(1, \cdots, n; 0, V)$ are the ordinary Ursell functions. This derivation for finite V does not require the use of the thermodynamic limit

$$N!\, Z_{n-h}/(N-h)!\, Z_N \to z^{h} \tag{6.8}$$

which is used in Ref. 13 to introduce the fugacity, and which is known to be hard to prove rigorously.[14]

With

$$\hat{\rho}_n = z^{-n}\rho_n \tag{6.9}$$

Eq. (6.2) becomes

$$\frac{\partial}{\partial z}\hat{\rho}_n(\mathbf{n}) = \int_{V}\{\hat{\rho}_{n+1}(\mathbf{n}, n+1)$$
$$-\hat{\rho}_n(\mathbf{n})\hat{\rho}_1(n+1)\}\, d^{\nu}r_{n+1}, \tag{6.10}$$

where we have omitted the variables z and V, and written $\mathbf{n}$ for the set $(\mathbf{r}_1 \cdots \mathbf{r}_n)$. By iteration of this equation one obtains the fugacity expansion of the distribution functions,[15] again without the use of Eq. (6.8).

For central symmetric pair interaction, the virial theorem and Eq. (6.2) yield

$$\left(\frac{\partial}{\partial \log z}-2\right)[\rho(z, V)-\langle\beta P(N, V)\rangle_z]$$
$$=\frac{\beta}{2\nu V}\left(\frac{\partial}{\partial \log z}-2\right)\int_{V}\mathfrak{v}_{12}\rho_2(1, 2)\, d^{\nu}r_1\, d^{\nu}r_2$$
$$=\frac{\beta}{2\nu V}\int_{V}\mathfrak{v}_{12}\{\rho_3(1, 2, 3)-\rho_2(1, 2)\rho_1(3)\}\, d^{\nu}r_1\, d^{\nu}r_2 \tag{6.11}$$

in agreement with Eq. (5.4).

One can also easily obtain a third virial theorem from Eqs. (6.2) and (6.11):

$$\left(\frac{\partial}{\partial \log z}-3\right)\left(\frac{\partial}{\partial \log z}-2\right)[\rho(z, V)-\langle\beta P(N, V)\rangle_z]$$
$$=\frac{\beta}{2\nu V}\iint_{V}\mathfrak{v}_{12}\{\rho_4(1, 2, 3, 4)-\rho_3(1, 2, 3)\rho_1(4)$$
$$-\rho_3(1, 2, 4)\rho_1(3)-\rho_2(1, 2)\rho_2(3, 4)$$
$$+2\rho_2(1, 2)\rho_1(3)\rho_1(4)\}\, d^{\nu}r_1\cdots d^{\nu}r_4 \tag{6.12}$$

and generalizations to higher order are obtained in the same way. As is already suggested by the two examples, the functions in the integrand are in the general case obtained from the distribution functions by a modified Ursell development, the modification being that the pair $(\mathbf{r}_1, \mathbf{r}_2)$ is formally treated as one position vector.[16]

7. CORRELATION OF TWO FUNCTIONS OF DENSITY

In this section we give a heuristic derivation of the correlation of two functions of N/V and V relative to the probability distribution of the GCE, through order V^{-1}. From this we derive Eq. (3.9).

Equation (A7) in Appendix A can be written in the form

[12] The fluctuation theorem for $n = 2$ is the well-known compressibility theorem; for $n = 3$ it is given explicitly in Ref. 6, Eq. (34b). The general form is implicit in the equation for $\partial^{r}\beta P/\partial z^{r}$, Ref. 10, Eq. (VIII 226) with Eq. (VIII 159).

[13] G. E. Uhlenbeck and G. W. Ford, "The Theory of Linear Graphs with Applications to the Theory of the Virial Development of Gases," *Studies in Statistical Mechanics*, edited by J. de Boer and G. E. Uhlenbeck (North-Holland Publishing Company, Amsterdam, 1962), Vol. I, p. 143, Eqs. (47)–(49).

[14] M. E. Fisher, J. Chem. Phys. **42**, 3856 (1965).

[15] J. de Boer, Repts. Progr. Phys. **12**, 305 (1949); Sec. 7, III. The term $-W(r^{h})W(r_{kl})$ should be added on the right-hand side of the third equation of Eqs. (7.11).

[16] Reference 15, p. 338, Eqs. (7.11).

$$\left\langle N^l g\left(\frac{N}{V}, V\right)\right\rangle_z = \left(\langle N\rangle_z + \frac{\partial}{\partial \log z}\right)^l \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z. \quad (7.1)$$

Suppose now that $f(N/V, V)$ is a function which permits an expansion

$$f\left(\frac{N}{V}, V\right) = \sum_{l=1}^{\infty} B_l(V)\left(\frac{N}{V}\right)^l. \quad (7.2)$$

Then the covariance $\langle f(N/V, V)g(N/V, V)\rangle_z$ is given by

$$\left\langle f\left(\frac{N}{V}, V\right)g\left(\frac{N}{V}, V\right)\right\rangle_z = \sum_{l=1}^{\infty} B_l(V)\left[\rho(z, V) + \frac{1}{V}\frac{\partial}{\partial \log z}\right]^l \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z. \quad (7.3)$$

Expanding the brackets on the right through order V^{-1} yields

$$\begin{aligned}
&\left[\rho(z, V) + \frac{1}{V}\frac{\partial}{\partial \log z}\right]^l \\
&\times \left\langle g\left(\frac{N}{V}, V\right)\right\rangle = \rho^l \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z \\
&+ \frac{1}{V}\sum_{k=0}^{l-1} \rho^{l-1-k}\frac{\partial}{\partial \log z}\left(\rho^k \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z\right) + \cdots \\
&= \rho^l \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z + \frac{1}{V}\sum_{k=0}^{l-1}\left[k\rho^{l-2}\frac{\partial \rho}{\partial \log z}\right. \\
&\times \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z + \rho^{l-1}\frac{\partial}{\partial \log z} \\
&\left.\times \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z\right] + \cdots \\
&= \rho^l \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z + \frac{1}{V}\left[\tfrac{1}{2}l(l-1)\rho^{l-2}\frac{\partial \rho}{\partial \log z}\right. \\
&\times \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z + l\rho^{l-1}\frac{\partial}{\partial \log z} \\
&\left.\times \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z\right] + \cdots, \quad (7.4)
\end{aligned}$$

where ρ stands for $\rho(z, V)$. Substituting this into Eq. (7.3) and carrying out the sum over l we obtain

$$\begin{aligned}
&\left\langle f\left(\frac{N}{V}, V\right)g\left(\frac{N}{V}, V\right)\right\rangle_z \\
&= f[\rho(z, V), V]\left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z \\
&+ \frac{1}{V}\left(\frac{1}{2}\left\{\frac{\partial \rho}{\partial \log z}\frac{\partial^2}{\partial \rho^2} f[\rho(z, V); V]\right\}\right. \\
&\times \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z + \frac{\partial}{\partial \rho(z, V)}\left\langle f\left(\frac{N}{V}, V\right)\right\rangle_z \\
&\left.\times \frac{\partial}{\partial \log z}\left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z\right) + \cdots. \quad (7.5)
\end{aligned}$$

The first term right-hand side still deviates from the product of the averages required for the correlation. We, therefore, use the same equation, with $g(N/V, V) \equiv 1$, to obtain a relation between $f[\rho(z, V), V)]$ and $\langle f(N/V, V)\rangle_z$, namely

$$\left\langle f\left(\frac{N}{V}, V\right)\right\rangle_z = f[\rho(z, V), V] + \frac{1}{2V}\frac{\partial \rho}{\partial \log z}\frac{\partial^2}{\partial \rho(z, V)^2} f[\rho(z, V), V] + \cdots. \quad (7.6)$$

Substitution in Eq. (7.5) yields the correlation with respect to the GC probability distribution through order V^{-1}:

$$\begin{aligned}
&\left\langle f\left(\frac{N}{V}, V\right)g\left(\frac{N}{V}, V\right)\right\rangle_z - \left\langle f\left(\frac{N}{V}, V\right)\right\rangle_z \left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z \\
&= V^{-1}\frac{\partial \rho(z, V)}{\partial \log z}\frac{\partial}{\partial \rho(z, V)}\left\langle f\left(\frac{N}{V}, V\right)\right\rangle_z \\
&\times \frac{\partial}{\partial \rho(z, V)}\left\langle g\left(\frac{N}{V}, V\right)\right\rangle_z + \cdots, \quad (7.7)
\end{aligned}$$

where dots indicate terms of higher order in V^{-1}.

For $f(N/V, V) \equiv N/V$, these higher terms clearly do not appear, and we obtain Eq. (A1) of Appendix A.

In a region of values of N/V, where the series in Eq. (7.2) does not converge, but

$$f\left(\frac{N}{V}, V\right) = \sum_{l=1}^{\infty} \hat{B}_l\left(\frac{N}{V} - n_0\right)^l \quad (7.8)$$

with fixed n_0 converges, the above procedure can still be applied and yields Eq. (7.7).

Specially, with $f(N/V, V)$ and $g(N/V, V)$ put equal to the canonical pressure $P(N, V)$ we have the fluctuation of the canonical pressure in the GCE through order V^{-1}:

$$\begin{aligned}
&\beta^2[\langle P^2(N, V)\rangle_z - \langle P(N, V)\rangle_z^2] \\
&= V^{-1}\rho\frac{\partial \rho}{\partial \beta P}\left[\frac{\partial}{\partial \rho}\langle \beta P(N, V)\rangle\right]^2 + \cdots \\
&= V^{-1}\rho\frac{\partial \beta P}{\partial \rho} + \cdots. \quad (7.9)
\end{aligned}$$

We have also an exact identity for this, derived in Appendix B: With $f(N, V)$ specialized to $\beta P(N, V)$ in Eq. (B3) we have

$$\begin{aligned}
&V\{\langle[\beta P(N, V)]^2\rangle_z - \langle \beta P(N, V)\rangle_z^2\} \\
&= V\frac{\partial}{\partial V}\langle \beta P(N, V)\rangle_z - \left\langle V\frac{\partial}{\partial V}\beta P(N, V)\right\rangle_z. \quad (7.10)
\end{aligned}$$

Now, in one-phase regions, where CE and GCE must give the same result for the compressibility in the thermodynamic limit, we have

$$\lim_{V\to\infty}\left\langle V\frac{\partial}{\partial V}\beta P(N,V)\right\rangle_z = -\rho\frac{\partial\beta P}{\partial\rho} \tag{7.11}$$

and, from Eq. (7.9)

$$\lim_{V\to\infty} V\{\langle[\beta P(N,V)]^2\rangle_z - \langle\beta P(N,V)\rangle_z^2\} = \rho\frac{\partial\beta P}{\partial\rho} \tag{7.12}$$

so that

$$\lim_{V\to\infty} V\frac{\partial}{\partial V}\langle\beta P(N,V)\rangle_z = 0. \tag{7.13}$$

8. WALL THEOREMS

The derivations in this section are carried through for the case of a system contained in a spherical volume of radius R. Using polar coordinates we then write

$$\begin{aligned} &Z_N(V)\rho_n(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_n;N,V)\\ &=\frac{N!}{(N-n)!}\int_V\cdots\int e^{-\beta U(\mathbf{r}_1,\cdots,\mathbf{r}_N)}\,d^\nu r_{n+1}\cdots d^\nu r_N\\ &=\frac{N!}{(N-n)!}\int_0^R r_{n+1}^{\nu-1}\,dr_{n+1}\\ &\times\int_0^R r_{n+2}^{\nu-1}\,dr_{n+2}\cdots\int_0^R r_N^{\nu-1}\,dr_N\\ &\times\int\cdots\int d\omega_{n+1}\cdots d\omega_N e^{-\beta U(\mathbf{r}_1\cdots\mathbf{r}_N)}, \end{aligned} \tag{8.1}$$

where $\int\cdots\int d\omega_{n+1}\cdots d\omega_N$ indicates the integration over angles and is to be omitted for the case $\nu = 1$. We then obtain, for $\nu \geq 2$,

$$\begin{aligned} &\frac{\partial}{\partial V}[Z_N(V)\rho_n(1,\cdots,n;N,V)]\\ &=\frac{N!}{(N-n)!}\frac{dR}{dV}(N-n)R^{\nu-1}\\ &\times\int_0^R r_{n+2}^{\nu-1}\,dr_{n+2}\cdots\int_0^R r_N^{\nu-1}\,dr_N\\ &\times\int\cdots\int d\omega_{n+1}\cdots d\omega_N\, e^{-\beta U(\mathbf{r}_1\cdots\mathbf{r}_N)}\\ &=\frac{1}{S}\int_S d^{\nu-1}r_{n+1}\frac{N!}{(N-n-1)!}\\ &\times\int_V d^\nu r_{n+2}\,d^\nu r_{n+3}\cdots d^\nu r_N\, e^{-\beta U(\mathbf{r}_1\cdots\mathbf{r}_N)}\\ &=Z_N(V)\frac{1}{S}\int_S d^{\nu-1}r_{n+1}\rho_{n+1}(1,\cdots,n,n+1;N,V), \end{aligned} \tag{8.2}$$

where S is the surface of the sphere, and $\int_S d^{\nu-1}r_{n+1}$ the surface integral over the sphere. From this we obtain

$$\begin{aligned} &\frac{\partial}{\partial V}\rho_n(1,2,\cdots,n;N,V)\\ &\quad+\beta P(N,V)\rho_n(1,2,\cdots,n;N,V)\\ &=\frac{1}{S}\int_S d^{\nu-1}r_{n+1}\rho_{n+1}(1,\cdots,n,n+1;N,V). \end{aligned} \tag{8.3}$$

For a one-dimensional model of particles in the interval $(0, R)$ the right-hand side is replaced by $\rho_{n+1}(r_1\cdots r_{n+1};N,V)|_{r_{n+1}=R}$.

To obtain the equation corresponding to Eq. (8.3) in the GCE, we use Eq. (B3) with

$$f(N,V)\equiv\rho_n(1,\cdots,n;N,V). \tag{8.4}$$

This yields

$$\begin{aligned} &\frac{\partial}{\partial V}\rho_n(1,\cdots,n;z,V)\\ &\quad+\langle\beta P(N,V)\rangle_z\rho_n(1,2\cdots n;z,V)\\ &=\frac{1}{S}\int_S d^{\nu-1}r_{n+1}\rho_{n+1}(1,\cdots,n,n+1;z,V). \end{aligned} \tag{8.5}$$

The known wall theorem[17] is a special case of Eq. (8.3): since $\rho_0 = 1$, one has

$$\begin{aligned} \beta P(N,V) &= \frac{1}{S}\int_S \rho_1(\mathbf{r};N,V)\,d^{\nu-1}r\\ &= \rho_1(\mathbf{r};N,V)_{r\subset S} \end{aligned} \tag{8.6}$$

using the spherical symmetry.

Equation (8.6) is closely related to the virial theorem: Converting the right-hand side of Eq. (8.6) to a volume integral by means of the identity

$$\begin{aligned} \int_S\varphi(\mathbf{r})\,d^{\nu-1}r &= \frac{1}{R}\int_S\frac{\mathbf{r}}{R}\cdot\mathbf{r}\varphi\,d^{\nu-1}r\\ &= \frac{1}{R}\int_V(\nu+\mathbf{r}\cdot\nabla)\varphi(\mathbf{r})\,d^\nu r \end{aligned} \tag{8.7}$$

valid for spherical volume one obtains

$$\beta P(N,V) - \frac{N}{V} = \frac{1}{\nu V}\int_V \mathbf{r}_1\cdot\nabla_1\rho_1(\mathbf{r}_1;N,V)\,d^\nu r_1. \tag{8.8}$$

For spherically symmetric pair interaction this reduces to the virial theorem by use of the definition of ρ_1 or through the Yvon–Born–Green equation.[10]

From the ordinary wall theorem [Eq. (8.6)] one derives a second wall theorem which expresses the

[17] J. L. Lebowitz, Phys. Fluids 3, 64 (1960), Eq. 12.

inverse compressibility in terms of surface integrals. Since $\mathbf{r}$ moves with the surface when the volume decreases, we have

$$d\beta P(N, V) = \frac{dV}{S}\frac{\mathbf{r}\cdot\nabla}{R}\rho_1(\mathbf{r}; N, V) + \left[\frac{\partial\rho_1(\mathbf{r}, V)}{\partial V}\right]_{\mathbf{r}\text{ fixed}} dV. \quad (8.9)$$

Using Eq. (8.3) we then obtain

$$\frac{\partial\beta P(N, V)}{\partial V} = \left\{\frac{1}{\nu V}\mathbf{r}\cdot\nabla\rho_1(\mathbf{r}; N, V) - \beta P(N, V)\rho_1(\mathbf{r}; N, V) + \frac{1}{S}\int_S \rho_2(\mathbf{r}, \mathbf{r}_2; N, V)\, d^{\nu-1}r_2\right\}_{r\subset S}, \quad (8.10)$$

Using Eq. 8.6 and the spherical symmetry we then obtain

$$V\frac{\partial\beta P(N, V)}{\partial V} = \frac{1}{\nu S}\int_S \mathbf{r}\cdot\nabla\rho_1(\mathbf{r}; N, V)\, d^{\nu-1}r + \frac{V}{S^2}\iint_S \chi_2(\mathbf{r}_1, \mathbf{r}_2; N, V)\, d^{\nu-1}r_1\, d^{\nu-1}r_2 \quad (8.11)$$

with

$$\chi_2(\mathbf{r}_1, \mathbf{r}_2; N, V) = \rho_2(\mathbf{r}_1, \mathbf{r}_2; N, V) - \rho_1(\mathbf{r}_1; N, V)\rho_1(\mathbf{r}_2, N, V). \quad (8.12)$$

The second wall theorem is closely related to the second virial theorem with ρ_4: We write Eq. (8.11) in the form

$$V\frac{\partial\beta P(N, V)}{\partial V} + V[\beta P(N, V)]^2 = \frac{1}{\nu S}\int_S \mathbf{r}\cdot\nabla\rho_1(\mathbf{r}; N, V)\, d^{\nu-1}r + \frac{V}{S^2}\iint_S \rho_2(\mathbf{r}_1, \mathbf{r}_2; N, V)\, d^{\nu-1}r_1\, d^{\nu-1}r_2. \quad (8.13)$$

We then use the identity (8.7) to obtain

$$\begin{aligned} &V\frac{\partial\beta P(N, V)}{\partial V} + V[\beta P(N, V)]^2 \\ &= \frac{1}{\nu SR}\int_V (\nu + \mathbf{r}\cdot\nabla)(\mathbf{r}\cdot\nabla)\rho_1(\mathbf{r}; N, V)\, d^\nu r \\ &\quad + \frac{V}{R^2S^2}\iint_V (\nu + \mathbf{r}_1\cdot\nabla_1)(\nu + \mathbf{r}_2\cdot\nabla_2) \\ &\quad \times \rho_2(\mathbf{r}_1, \mathbf{r}_2; N, V)\, d^\nu r_1\, d^\nu r_2 \\ &= \beta P(N, V) - \frac{N}{V} + \frac{1}{\nu^2 V}\int_V (\mathbf{r}\cdot\nabla)^2\rho_1(\mathbf{r}; N, V)\, d^\nu r \\ &\quad + \frac{1}{V}\iint_V \rho_2(\mathbf{r}_1, \mathbf{r}_2; N, V)\, d^\nu r_1\, d^\nu r_2 \\ &\quad + \frac{1}{\nu V}\iint_V (\mathbf{r}_1\cdot\nabla_1 + \mathbf{r}_2\cdot\nabla_2)\rho_2(\mathbf{r}_1, \mathbf{r}_2; N, V)\, d^\nu r_1\, d^\nu r_2 \\ &\quad + \frac{1}{\nu^2 V}\iint_V (\mathbf{r}_1\cdot\nabla_1)(\mathbf{r}_2\cdot\nabla)\rho_2(\mathbf{r}_1, \mathbf{r}_2; N, V)\, d^\nu r_1\, d^\nu r_2 \\ &= \beta P(N, V) - \frac{N}{V} + \frac{N(N-1)}{V} \\ &\quad + 2(N-1)\left[\beta P(N, V) - \frac{N}{V}\right] \\ &\quad + \frac{1}{\nu^2 V}\left[\int_V (\mathbf{r}\cdot\nabla)^2\rho_1(\mathbf{r}; N, V)\, d^\nu r \right. \\ &\quad \left. + \iint_V (\mathbf{r}_1\cdot\nabla_1)(\mathbf{r}_2\cdot\nabla_2)\rho_2(\mathbf{r}_1, \mathbf{r}_2; N, V)\, d^\nu r_1\, d^\nu r_2\right] \end{aligned} \quad (8.14)$$

or

$$\partial/\partial V[V\beta P(N, V)] + V\left[\beta P(N, V) - \frac{N}{V}\right]^2 = \frac{1}{\nu^2 V}\left\{\int_V (\mathbf{r}\cdot\nabla)^2\rho_1(\mathbf{r}; N, V) + \iint_V (\mathbf{r}_1\cdot\nabla_1)(\mathbf{r}_2\cdot\nabla_2)\rho_2(\mathbf{r}_1, \mathbf{r}_2; N, V)\, d^\nu r_1\, d^\nu r_2\right\}. \quad (8.15)$$

For pair interaction the Yvon–Born–Green equations can be used to convert the gradients of the distribution functions. The calculation is straightforward though tedious, and leads for spherically symmetric pair interaction to the second virial theorem [Eq. (3.1)], when the second term on the left is expressed by means of the virial theorem.

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APPENDIX A

If $f(N, V)$ is any function of N and V, its correlation with N in the GCE is given by

$$\langle Nf(N, V)\rangle_z - \langle N\rangle_z\langle f(N, V)\rangle_z = \frac{\partial}{\partial\log z}\langle f(N, V)\rangle_z. \quad (A1)$$

To prove this note that by definition of $\langle\ \rangle_z$

$$\mathcal{Q}(z, V)\langle Nf(N, V)\rangle_z = \sum_0^\infty \frac{Nz^N}{N!} Z_N(V) f(N, V) = \frac{\partial}{\partial \log z}[\mathcal{Q}(z, V)\langle f(N, V)\rangle_z] \quad \text{(A2)}$$

or

$$\langle Nf(N, V)\rangle_z = \mathcal{Q}^{-1}(z, V)\frac{\partial}{\partial \log z}[\mathcal{Q}(z, V)\langle f(N, V)\rangle_z] = \langle N\rangle_z\langle f(N, V)\rangle_z + \frac{\partial}{\partial \log z}\langle f(N, V)\rangle_z. \quad \text{(A3)}$$

This is easily generalized to higher powers of N. We have

$$\langle N^m f(N, V)\rangle = \mathcal{Q}^{-1}(z, V)\frac{\partial^m}{\partial \log z^m}[\mathcal{Q}(z, V)\langle f(N, V)\rangle_z]. \quad \text{(A4)}$$

Inserting $\mathcal{Q}(z, V)\ \mathcal{Q}^{-1}(z, V)$ between the factors $\partial/\partial \log z$ one obtains

$$\langle N^m f(N, V)\rangle = \Omega^m\langle f(N, V)\rangle_z, \quad \text{(A5)}$$

where Ω is the operator $\mathcal{Q}^{-1}(z, V)(\partial/\partial \log z)\mathcal{Q}(z, V)$. Now note that

$$\Omega\Phi(z) \equiv \mathcal{Q}^{-1}(z, V)\frac{\partial}{\partial \log z}[\mathcal{Q}(z, V)\Phi(z)] = \left[\frac{\partial}{\partial \log z} + \langle N\rangle_z\right]\Phi(z), \quad \text{(A6)}$$

so that we have as generalization of Eq. (A1)

$$\langle N^m f(N, V)\rangle_z = \left[\frac{\partial}{\partial \log z} + V\rho(z, V)\right]^m \langle f(N, V)\rangle_z. \quad \text{(A7)}$$

APPENDIX B

In Appendix A we had found an exact expression for the correlation between N and any function of N relative to the probability distribution of the GCE [Eq. (A1)]. The corresponding theorem for the correlation between $P(N, V)$ and any function $f(N, V)$ is obtained as follows.

We have

$$\frac{\partial}{\partial V}[\mathcal{Q}(z, V)\langle f(N, V)\rangle_z] = \sum_{N=0}^\infty \frac{z^N}{N!}\left[\frac{\partial Z_N(V)}{\partial V} f(N, V) + Z_N(V)\frac{\partial f(N, V)}{\partial V}\right] = \sum_{N=0}^\infty \frac{z^N}{N!} Z_N(V)\left[P(N, V)f(N, V) + \frac{\partial f(N, V)}{\partial V}\right]. \quad \text{(B1)}$$

Dividing by $\mathcal{Q}(z, V)$ and writing out the left-hand side one obtains

$$\frac{\partial}{\partial V}\langle f(N, V)\rangle_z + \langle \beta P(N, V)\rangle_z\langle f(N, V)\rangle_z = \langle P(N, V)f(N, V)\rangle_z + \left\langle \frac{\partial f(N, V)}{\partial V}\right\rangle_z. \quad \text{(B2)}$$

The correlation is thus

$$\langle \beta P(N, V)f(N, V)\rangle_z - \langle \beta P(N, V)\rangle_z\langle f(N, V)\rangle_z = \frac{\partial}{\partial V}\langle f(N, V)\rangle_z - \left\langle \frac{\partial f(N, V)}{\partial V}\right\rangle_z. \quad \text{(B3)}$$

We note that both (A1) and (B3) can be applied to the correlation between N and $\beta P(N, V)$ and we obtain

$$\frac{\partial}{\partial \log z}\langle \beta P(N, V)\rangle_z = \frac{\partial}{\partial V}\langle N\rangle_z = \frac{\partial}{\partial V}\left(V\left\langle \frac{N}{V}\right\rangle_z\right) = \rho(z, V) + V\frac{\partial}{\partial V}\rho(z, V) \quad \text{(B4)}$$

or

$$\frac{\partial}{\partial \log z}\langle \beta P(N, V)\rangle_z = \frac{\partial \beta P(z, V)}{\partial \log z} + V\frac{\partial}{\partial V}\rho(z, V), \quad \text{(B5)}$$

where $P(z, V)$ is the conventional GC pressure.

On the Propagation of Gravitational Fields in Matter

PETER SZEKERES
Center for Radiophysics and Space Research, Cornell University, Ithaca, New York
(Received 14 September 1965)

A purely covariant treatment is made of those solutions of the Einstein field equations which represent pure gravitational radiation propagating in fluid and electromagnetic media. The analysis involves a discussion of the full Bianchi identities in carefully selected tetrad frames. In this way the interaction between the gravitational field and the medium is transferred to a coupling between a preferred frame for the gravitational field and one for the matter field. The gravitational radiation no longer propagates along shear-free null geodesics, as it does in vacuum, and the shear and ray curvature of the propagation vector are shown to depend directly on the properties of the medium. Some new solutions of the field equations, representing transverse gravitational waves propagating in an electromagnetic field, are exhibited and discussed in some detail. It is shown that no such solutions exist, at least in simple cases, for perfect fluids. Finally, the treatment presented here is compared with the more usual electromagnetic treatment, and it is shown why the theories require basically different approaches.

1. INTRODUCTION

A CONSIDERABLE amount has been written about the propagation of gravitational radiation in empty space.[1] These investigations rely heavily on the study of what are called *algebraically special* gravitational fields, which correspond physically to the case of "pure" radiation. The principal result is the theorem of Goldberg and Sachs (1962):

A vacuum metric is algebraically special if and only if it admits a shear-free null geodesic congruence.

Although it is possible to considerably relax the vacuum conditions[2] it is by no means true that the theorem holds in general. This paper deals with the question; what happens to the Goldberg–Sachs theorem when there are perfect fluids or electromagnetic fields present? The answer to this question should furnish clues to the following problems: (a) the interaction of gravitational fields with matter, (b) the generation of gravitational waves in physically realistic sources, (c) the establishment of criteria for the presence of gravitational radiation in matter, (d) a new function theory for nonvacuum gravitational fields.

The analysis rests upon the decomposition of the curvature tensor into the trace-free Weyl tensor and a sum of terms arising from the Ricci tensor:

$$R_{abcd} = C_{abcd} + g_{a[c}R_{d]b} + R_{a[c}g_{d]b} - \tfrac{1}{3}Rg_{a[c}g_{d]b}.^{3} \quad (1.1)$$

On account of the Einstein field equations

$$R_{ab} - \tfrac{1}{2}Rg_{ab} = -T_{ab}, \quad (1.2)$$

the Ricci terms in (1.1) can be equated with the presence of matter. The Weyl tensor, having all the symmetries of a vacuum Riemann tensor, is to be thought of as representing the *free gravitational field.* At any point of space–time the Ricci tensor and Weyl tensor are completely independent, but in a region they are connected through the differential Bianchi identities, which can be written in the following form[4]:

$$C_{abcd}{}^{;d} = R_{c[a;b]} - \tfrac{1}{6}g_{c[a}R_{,b]}. \quad (1.3)$$

The remarkable resemblance that (1.3) bears to Maxwell's equations

$$F^{ab}{}_{,b} = j^{a},$$

leads to the suggestion that the Bianchi identities represent the interaction between the gravitational and matter fields. The right-hand side J_{abc} of (1.3) is to be regarded as a *matter current*; it satisfies a "conservation equation"

$$J^{abc}{}_{;c} = 0, \quad (1.4)$$

analogous to the conservation equation of electrodynamics

$$j^{a}{}_{,a} = 0.$$

The matter current represents that part of the source which interacts with the free gravitational field. Those parts of the matter which do not contribute to J_{abc} are called *gravitationally inert*; the propagation of the free gravitational field is in no way dependent

[1] See, for example, F. A. E. Pirani, "Gravitational Radiation", article in *Gravitation, an Introduction to Current Research*, edited by L. Witten (John Wiley & Sons, Inc., New York, 1962).

[2] W. Kundt and A. Thompson, Compt. Rend. Acad. Sci. Paris **254**, 4257 (1962).

[3] Square brackets denote antisymmetrization,

$$A_{[ab]} = [1/2!](A_{ab} - A_{ba}).$$

Round brackets denote symmetrization.

[4] W. Kundt and M. Trümper, Akad. Wiss. Mainz. No. 12 (1962).

upon them. There is nothing corresponding to this in electrodynamics where, by Maxwell's equations, the electromagnetic field determines the complete charge-current distribution. The difference between the two cases can be expressed by saying that photon telescopes can be used to explore the universe completely with regard to its electric charges, but a graviton telescope may fail to detect the presence of matter in certain states.

In Sec. 2 the Bianchi identities (1.3) are considered when there is a perfect fluid present and the Weyl tensor is algebraically special. It is found that the gravitational field propagates along a null direction whose shear and refraction (as measured by the curvature of the rays) is determined completely by the dynamical and kinematical properties of the fluid. Futhermore the fluid decomposes into separate parts which interact independently with the Petrov type-N, type-III and type-D components of the gravitational field. In Sec. 3 a similar analysis is carried out for electromagnetic fields. In this case it is found that the shear and refraction of the gravitational field depend on the optical properties of the electromagnetic field.

Some exact solutions with a Petrov type N gravitational wave propagating along shear-free null geodesics in a nonnull electromagnetic field are exhibited in Sec. 4. In Sec. 5 it is shown that Petrov type N solutions cannot exist in a perfect fluid if the fluid pressure vanishes. Without the condition $p = 0$ the problem remains unsolved, but it is pointed out that "almost perfect" fluid solutions of Petrov type N may exist.

In conclusion the physical significance of the analysis is discussed, with particular emphasis on its relation with electromagnetic theory.

2. GRAVITATIONAL FIELDS IN PERFECT FLUIDS

(i) Dynamics and Kinematics of Fluids

For a perfect fluid the energy–stress tensor takes the form

$$T_{ab} = \mu u_a u_b + p h_{ab}, \tag{2.1}$$

where

$$u_a u^a = -1, \qquad h_{ab} = g_{ab} + u_a u_b.$$

The kinematics of the fluid are studied by breaking up the covariant derivative of the 4-velocity in the following way:

$$u_{a;b} = \sigma_{ab} + \omega_{ab} + \tfrac{1}{3}\theta h_{ab} - \dot{u}_a u_b, \tag{2.2}$$

where

$$\dot{u}_a = u_{a;b}u^b,$$

$$\theta = u^a{}_{;a},$$

$$\omega_{ab} = h_{[a}{}^c h_{b]}{}^d u_{c;d},$$

and

$$\sigma_{ab} = h_{(a}{}^c h_{b)}{}^d u_{c;d}.$$

With respect to a Fermi propagated frame, ω_{ab} and σ_{ab} are respectively the rates of *rotation* and *shear* of neighbouring particles of the fluid[5]; θ is the rate of *expansion* of the timelike congruence. We define shear and rotation scalars σ and ω by

$$\sigma^2 = \tfrac{1}{2}\sigma_{ab}\sigma^{ab}, \qquad \omega^2 = \tfrac{1}{2}\omega_{ab}\omega^{ab}.$$

From the field equations (1.2), we obtain the Ricci tensor

$$R_{ab} = -(p + \mu)u_a u_b + \tfrac{1}{2}(p - \mu)g_{ab}, \tag{2.3}$$

and the contracted Bianchi identities result in equations of motion for the fluid,

$$\dot{\mu} + (\mu + p)\theta = 0, \tag{2.4a}$$

$$h_a{}^b p_{,b} + (\mu + p)\dot{u}_a = 0. \tag{2.4b}$$

The full Bianchi identities (1.3) yield, on substituting (2.3),[4]

$$C_{abcd}{}^{;d} = \mu_{,[a}u_{b]}u_c + \tfrac{1}{3}\mu_{,d}h^d{}_{[a}g_{b]c} - (\mu + p)(\omega_{ab}u_c - u_{[a}\omega_{b]c} + u_{[a}\sigma_{b]c}). \tag{2.5}$$

The right-hand side of this equation is the matter current J_{abc} discussed in Sec. 1. Equations (2.4) only involve θ, $\dot{u}_a$, $\dot{\mu}$ and $h_a{}^b p_{,b}$; we say that these quantities constitute the *inert part* of the fluid since they are not connected with the propagation of the free gravitational field. J_{abc} involves essentially the shear and rotation of the fluid, and the spatial gradient of the density; these constitute the *gravitationally active part* of the fluid, the part that can be found by observing the propagation of the free gravitational field.

(ii) Algebra of the Weyl Tensor

In order to study the Weyl tensor it is convenient to set up a quasi-orthonormal tetrad of null vectors k_a, m_a, t_a, l_a satisfying

$$k_a m^a = t_a l^a = 1, \quad k_a k^a = m_a m^a = t_a t^a = k_a t^a = m_a t^a = 0. \tag{2.6}$$

Introducing three self-dual bivectors

$$V_{ab} = 2k_{[a}l_{b]}, \qquad U_{ab} = 2m_{[a}t_{b]}, \qquad M_{ab} = 2k_{[a}m_{b]} + 2l_{[a}t_{b]}, \tag{2.7}$$

[5] J. Ehlers, Akad. Wiss. Mainz. No. 11 (1961).

we can decompose the Weyl tensor into tetrad components[6]

$$C_{abcd} + iC^*_{abcd} = C_1V_{ab}V_{cd} + C_2(V_{ab}M_{cd} + M_{ab}V_{cd}) + C_3(M_{ab}M_{cd} + U_{ab}V_{cd} + V_{ab}U_{cd}) + C_4(U_{ab}M_{cd} + M_{ab}U_{cd}) + C_5U_{ab}U_{cd}, \quad (2.8)$$

where

$$C^*_{abcd} = \tfrac{1}{2}(-g)^{\frac{1}{2}}\epsilon_{abij}C^{ij}{}_{cd}. \quad (2.8)$$

The various terms in (2.8) have the following physical interpretations[7]: the C_1 term represents a transverse wave component in the k_a direction, the C_2 term a longitudinal wave component, and the C_3 term a "Coulomb" component. The C_4 and C_5 terms represent longitudinal and transverse components in the m_a direction.

(iii) Optics of Null Congruences

The principal optical properties of a null congruence having k_a as tangent can be studied from the tetrad components of the complex vector

$$L_b = k_{a;b}\bar{l}^a. \quad (2.9)$$

L_b is determined up to a phase $e^{i\theta}$, since l^a may be subjected to transformations of the form

$$l'^a = e^{i\theta}(l^a + Ak^a).$$

We shall call L_a the *optical vector* of the null congruence; its tetrad components are

$$\gamma = L_bk^b = \gamma^{(1)} + i\gamma^{(2)}, \quad \Omega = L_bm^b, \quad \sigma = L_b\bar{l}^b, \quad z = L_bt^b = \theta + i\omega. \quad (2.10)$$

γ vanishes if and only if k_a is geodesic; it measures the ray curvature or the departure from geodicity in the rays. Consequently we may think of it as representing the *refraction* of the null congruence. σ is called the *shear*, θ the *expansion*, ω the *twist*, and Ω the *angular velocity* or *rotation* of the null congruence.[6]

(iv) Propagation of the Gravitational Field

Consider now an algebraically special Weyl tensor. This means that there exists a null vector k_a, such that $C_4 = C_5 = 0$ in (2.8). The Weyl tensor is of Petrov type N if $C_2 = C_3 = 0$ for this k_a, of Petrov type III if $C_3 = 0$, and of Petrov type II or D if $C_3 \neq 0$. A simple calculation from (2.8) with these specializations yields the following relations:

In Petrov type N

$$U^{ab}V^{ce}C_{abcd}{}^{;d} = C_1(\bar{l}^e\gamma - k^e\sigma), \quad (2.11)$$

in Petrov type III

$$V^{ab}C_{abcd}{}^{;d} = 2C_2(\bar{l}_c\gamma - k_c\sigma), \quad (2.12)$$

and in Petrov type II or D

$$V^{ab}V^{ce}C_{abcd}{}^{;d} = 3C_3(\bar{l}^e\gamma - k^e\sigma). \quad (2.13)$$

When there is a fluid present with streamlines u^a, we normalize k_a to make

$$k_au^a = -1,$$

and defining $s_a = h_a{}^bk_b$ (whence $s_as^a = 1$, $s_au^a = 0$) we can choose the null vector m_a such that

$$k_a = u_a + s_a, \quad m_a = \tfrac{1}{2}(s_a - u_a). \quad (2.14)$$

Substituting the Bianchi identities (2.5) into Eqs. (2.11), (2.12), and (2.13) we find the following expressions for the shear and refraction of the principal null congruence k_a (denoted here by σ_0 and γ_0 to distinguish them from the fluid quantities):

In Petrov type N

$$3C_1\gamma_0 = \tfrac{1}{2}(\mu_{,a}\bar{l}^a - 3(\mu + p)(\omega_{ab} + \sigma_{ab})\bar{l}^as^b),$$
$$3C_1\sigma_0 = \tfrac{1}{2}(\mu_{,a}s^a - 3(\mu + p)(\omega_{ab} + \sigma_{ab})\bar{l}^a\bar{l}^b), \quad (2.15)$$

in Petrov type III

$$3C_2\gamma_0 = \tfrac{1}{2}(\mu_{,a}s^a + 3(\mu + p)(\omega_{ab} + \sigma_{ab})\bar{l}^a\bar{l}^b),$$
$$3C_2\sigma_0 = -\tfrac{1}{4}(\mu_{,a}\bar{l}^a + 3(\mu + p)(\omega_{ab} + \sigma_{ab})\bar{l}^as^b), \quad (2.16)$$

in Petrov types II or D

$$3C_3\gamma_0 = -\mu_{,b}\bar{l}^b - (\mu + p)(3\omega_{ab}\bar{l}^as^b - \sigma_{ab}\bar{l}^bs^c),$$
$$3C_3\sigma_0 = (\mu + p)\sigma_{bc}\iota^b\bar{l}^c. \quad (2.17)$$

k^a is called the *principal null direction* of the gravitational field; the field is to be regarded as propagating along this direction. Equations (2.15), (2.16), and (2.17) show that the shear and refraction of the principal null direction of an algebraically special gravitational field are determined by the tetrad components of the spacelike density gradient, the rotation and the shear of the fluid.

If the Weyl tensor is of Petrov type N we have $C_2 = C_3 = 0$, and the right-hand sides of equations (2.16) and (2.17) must vanish. It follows then from (2.15) that[4]

$$(\mu + p)\sigma_{ab} = C_1\sigma_0(3s_as_b - h_{ab}), \quad (2.18)$$

$$(\mu + p)\omega_{ab} = 2s_{[a}(\bar{l}_{b]}C_1\gamma_0 + t_{b]}\bar{C}_1\gamma_0), \quad (2.19)$$

[6] R. Sachs, Proc. Roy. Soc. (London) **A264**, 309 (1961).
[7] P. Szekeres, J. Math. Phys. **6**, 1387 (1965).

and

$$h^a{}_b\mu_{,a} = 3(C_1\gamma_0 \bar{l}_b + \bar{C}_1\bar{\gamma}_0 l_b + \sigma_0 s_b). \qquad (2.20)$$

Hence the optical shear and the refraction are directly proportional to the shear and the rotation of the fluid:

$$\sqrt{2}\,|C_1\gamma_0| = (\mu + p)\omega, \qquad (2.21)$$

$$\sqrt{3}\,|C_1\sigma_0| = (\mu + p)\sigma. \qquad (2.22)$$

From (2.22) we see that σ_0 is real if and only if C_1 is real; this means that the principal axes of the optical shear coincide with the polarization axes of the transverse gravitational field (the axes l^a, $\bar{l}^a$ which make C_1 real). Equation (2.18) shows that the fluid shear has a principal axis in the ray direction s_a and is degenerate in the transverse (l_a, $\bar{l}_a$) plane. From (2.19) and (2.21) it is seen that the refraction of the wave is determined by the rotation of the fluid. The axis of rotation of the fluid must lie in the transverse plane of the wave; if it coincides with one of the polarization directions (C_1 real and $\gamma_0^{(1)}$ or $\gamma_0^{(2)} = 0$) then the wave is reflected at right angles to it, whereas if it is at 45° to the polarization directions the wave is deflected in the direction of the rotation axis (Fig. 1).

For a type-III Weyl tensor the right-hand side of Eq. (2.17) must vanish, since $C_3 = 0$. Hence we have

$$3C_2\sigma_0 = -(\mu + p)\sigma_{bc}\bar{l}^b s^c, \qquad (2.23)$$

and k_a is shear-free if and only if s^a (the longitudinal wave direction according to an observer traveling with the fluid) is a principal axis of the fluid shear (Fig. 2). Equation (2.16) can be split up into real and imaginary parts

$$6C_2\gamma_0^{(1)} = \mu_{,a}s^a - \tfrac{1}{2}(\mu + p)\sigma_{bc}s^b s^c,$$

$$2C_2\gamma_0^{(2)} = (\mu + p)\omega_{ab}f^a e^b, \qquad (2.24)$$

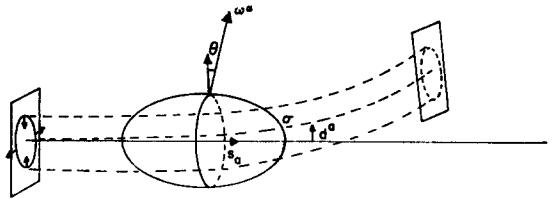

FIG. 1. Propagation of a transverse gravitational wave (type N) in a perfect fluid. The central ellipsoid represents the shear of the fluid streamlines. The broken lines denote graviton paths. They are deflected from the geodesic by a vector d^a which makes an angle $\phi = 2\theta \pm \frac{1}{2}\pi$ with the rotation axis ω^a, where θ is the angle ω^a makes with one of the polarization axes of the plane wave. The magnitude of this deflection is proportional to the angular velocity ω of the fluid. A circular cross section of gravitons is transformed into an ellipse, by an amount proportional to the fluid shear σ in the direction of wave propagation.

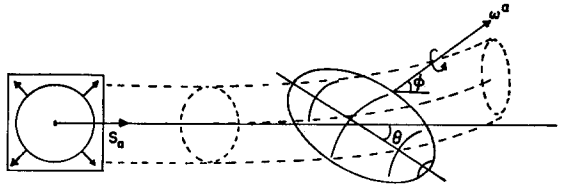

FIG. 2. Propagation of a longitudinal wave (type III) in a perfect fluid. The circle of gravitons is transformed into an ellipse, by an amount depending on the angle θ between the principal fluid shear axis and the direction of wave propagation s_a. The deflection out of the plane of the polarization is proportional to cos ϕ, the angle between s_a and the rotation axis ω^a.

where

$$l^a = (1/\sqrt{2})(e^a + if^a), \quad \bar{l}^a = (1/\sqrt{2})(e^a - if^a).$$

Hence the ray is only left undeflected in a direction orthogonal to its longitudinal plane of polarization [the (s_a, e_a) plane] if the axis of rotation of the fluid is orthogonal to the ray direction. The refraction in its own plane is determined by the components in the ray direction of the density gradient and fluid shear. It is unaffected by any rotation the fluid may have about s_a as axis.

Equations (2.15), (2.16), and (2.17) suggest that not only can the matter be split up into gravitationally inert and active parts, but the active part J_{abc} can be further split up into separate parts interacting with the transverse wave component, the longitudinal wave component and the Coulomb part of the field. For example, the shear tensor can be split up as a sum of three terms:

$$\sigma_1(s_a s_b - \tfrac{1}{3}h_{ab}), \qquad \sigma_2 s_{(a}e_{b)} + \sigma_3 s_{(a}f_{b)},$$

and

$$\sigma_4(e_a e_b - f_a f_b) + \sigma_5 e_{(a}f_{b)}.$$

From Eqs. (2.18), (2.23), and (2.17) it appears that for an algebraically special field with principal null vector $k^a = s^a + u^a$, the first term interacts with the shear of the type-III component, and the last with the Coulomb component. This splitting off is really the essence of Kundt and Thompson's statement of the Goldberg–Sachs theorem:[2]

Any two of the following imply the third:

(A) C_{abcd} *is algebraically special with* k_a *for principal null vector.*

(B) k_a *is shear-free and geodesic.*

(C) $V^{ab}V^{ce}C_{abcd}{}^{;d} = 0$

$V^{ab}C_{abcd}{}^{;d} = 0$ *for Petrov type III*

$U^{ab}V^{ce}C_{abcd}{}^{;d} = 0$ *for Petrov type N.*

From Eqs. (2.11–(2.13) it is clear that (A), (B) $\Rightarrow$ (C), and (A), (C) $\Rightarrow$ (B). The proof that (B), (C) $\Rightarrow$ (A) is less trivial.

3. INTERACTION OF GRAVITATIONAL AND ELECTROMAGNETIC FIELDS

An electromagnetic field is represented by a skew-symmetric tensor F_{ab} satisfying Maxwell's equations

$$(F_{ab} + iF^*_{ab})^{;b} = 0. \tag{3.1}$$

The energy-stress tensor is given by

$$T_{ab} = F_{ai}F_b{}^i - \tfrac{1}{4}g_{ab}F_{ij}F^{ij} = -R_{ab}. \tag{3.2}$$

(i) Null Field

The electromagnetic field is said to be *null* if there exists a null vector such that

$$(F_{ab} + iF^*_{ab})k^a = 0,$$

from which it follows that the Maxwell tensor can be written in the form

$$F_{ab} + iF^*_{ab} = V_{ab} = 2k_{[a}l_{b]}, \tag{3.3}$$

where the conventions of Sec. 2 are adopted. Maxwell's equations (3.1) now imply that

$$k_{a;b}k^b l^a = 0 \quad \text{and} \quad k_{a;b}l^a l^b = 0,$$

k_a is shear-free and geodesic. From the field equations (3.2) we have

$$R_{ab} = -\tfrac{1}{2}k_a k_b$$

and the Bianchi identities (1.3) can be written as

$$C_{abcd}{}^{;d} = R_{c[a;b]} = -\tfrac{1}{2}(k_c k_{[a;b]} + k_{c;[b}k_{a]}), \tag{3.4}$$

whence

$$V^{ce}V^{ab}C_{abcd}{}^{;d} = 0.$$

From the Goldberg–Sachs–Kundt–Thompson theorem quoted at the end of Sec. 2, it follows that the gravitational field must be algebraically special with k_a as principal null direction. This result is what we might expect intuitively—the gravitational field associated with a pure radiation electromagnetic field consists of pure gravitational radiation.

If the Weyl tensor is of Petrov type N, we can contract (3.4) with $\bar{l}^c l^b$ and find that

$$0 = k_{c;b}\bar{l}^c l^b = z = \theta + i\omega.$$

Hence the expansion and twist must vanish if the Weyl tensor represents a pure transverse gravitational wave. All solutions of the field equations representing this situation have been found by Kundt.[8]

[8] W. Kundt, Physik, **163**, 77 (1961).

(ii) Non-null Field

The Maxwell tensor has the form

$$F_{ab} + iF^*_{ab} = A(2p_{[a}q_{b]} + 2\bar{r}_{[a}r_{b]}), \tag{3.5}$$

where p_a, q_a are the principal null vectors of the electromagnetic field.[9] p_a, q_a, r_a, $\bar{r}_a$ form a quasi-orthonormal null tetrad (we call it the *electromagnetic frame*). A is the (complex) electromagnetic *amplitude* or *field strength.*

Maxwell's equations (3.1) can now be regarded as expressing the gradient of the field amplitude in terms of optical parameters of the principal null directions:

$$\tfrac{1}{2}(\ln A)_{,a} = -z^{(p)}q_a - z^{(q)}p_a + \Omega^{(p)}r_a + \Omega^{(q)}\bar{r}_a, \tag{3.6}$$

where

$$z^{(p)} = L^{(p)}_b r^b, \qquad z^{(q)} = L^{(q)}_b \bar{r}^b,$$
$$\Omega^{(p)} = L^{(p)}_b q^b, \qquad \Omega^{(q)} = L^{(q)}_b p^b,$$

$L^{(p)}_b$, $L^{(q)}_b$ being the optical vectors p_a and q_a,

$$L^{(p)}_b = p_{a;b}\bar{r}^a, \qquad L^{(q)}_b = q_{a;b}\bar{r}^a.$$

The field equations (3.2) result in

$$R_{ab} = |A|^2(2p_{(a}q_{b)} - \tfrac{1}{2}g_{ab}). \tag{3.7}$$

On substituting into the Bianchi identities we can carry out a similar analysis to that for a fluid medium. There are two cases to be distinguished:

(a) The gravitational field is algebraically special and its principal null vector k_a coincides with one of the null vectors p_a or q_a of the electromagnetic field. The two fields shall be called *aligned* in this case; it has been shown by Kundt and Trümper[4] that k_a must be shear-free and geodesic.

(b) The gravitational and electromagnetic fields are *nonaligned*; that is, k_a does not coincide with either p_a or q_a. It is possible to scale these null vectors such that

$$k_a p^a = -k_a q^a = -1.$$

By a spacelike rotation $r_a \to e^{i\theta}r_a$ we can achieve that

$$k_a = p_a - q_a + r_a + \bar{r}_a.$$

The null tetrad for the gravitational field can be completed by choosing

$$m_a = \tfrac{1}{4}(-p_a + q_a + r_a + \bar{r}_a),$$
$$t_a = \tfrac{1}{2}(p_a + q_a + \bar{r}_a - r_a).$$

This normalization amounts to a coupling of the

[9] J. L. Synge, *Relativity, the Special Theory* (North-Holland Publishing Company, Amsterdam, 1956).

gravitational and electromagnetic frames, so as best to view the interaction. Substituting (3.7) into the right-hand side of the Bianchi identities (1.3), and using the identities (2.11)–(2.13) and Maxwell's equations in the form (3.6), we arrive at the following relations:

For a type N Weyl tensor

$$\begin{aligned} C_1\gamma &= -|A|^2 (L_a^{(p)} + L_a^{(q)})m^a , \\ C_1\sigma &= \tfrac{1}{4} |A|^2 (L_a^{(p)} + L_a^{(q)})\bar{l}^a , \end{aligned} \tag{3.8}$$

for a type III Weyl tensor

$$\begin{aligned} 2C_2\gamma &= |A|^2 (L_a^{(p)} + L_a^{(q)})\bar{l}^a , \\ 2C_2\sigma &= \tfrac{1}{4} |A|^2 (L_a^{(p)} + L_a^{(q)})k^a, \end{aligned} \tag{3.9}$$

for a type II or D Weyl tensor

$$\begin{aligned} 3C_3\gamma &= 4 |A|^2 ((L_a^{(p)} + L_a^{(q)})m^a \\ &\qquad + (L_a^{(p)} - L_a^{(q)})\bar{l}^a) , \\ 3C_3\sigma &= |A|^2 (-(L_a^{(p)} + L_a^{(q)})l^a \\ &\qquad + (L_a^{(p)} - L_a^{(q)})k^a). \end{aligned} \tag{3.10}$$

Hence with this choice of tetrads, the interaction between an algebraically special gravitational field and a nonaligned electromagnetic field is completely determined by the tetrad components in the gravitational frame of the sum and difference of the two optical vectors of the electromagnetic field. If the Weyl tensor is of Petrov type N then the right-hand sides of (3.9) and (3.10) must vanish; if the principal null vector k_a of the gravitational field is to be shear-free and geodesic it is clear that the sum of the optical vectors, $L_a^{(p)} + L_a^{(q)}$, must vanish. Exact solutions representing this situation are discussed in the next section.

4. EXACT ELECTROMAGNETIC SOLUTIONS

(i) Null Solutions

In the light of the preceding analysis it would be interesting to exhibit some exact solutions representing gravitational waves propagating through various media. As a first example there exist the metrics of Kundt[8] representing a type N gravitational field having $\sigma = \theta = \omega = \Omega = 0$ (planefronted waves with parallel rays), accompanied by a plane electromagnetic wave,

$$ds^2 = \tfrac{1}{2}(dx^2 + dy^2) - 2\,du\,dr + 2U\,du^2,$$

where $U = U(x, y, u)$ satisfied

$$\partial^2 U/\partial x^2 + \partial^2 U/\partial y^2 = -\tfrac{1}{2}.$$

The coordinates are those introduced by Robinson and Trautman[10] in which $x^1 = u = \text{const}$ are null hypersurfaces

$$g^{ab}u_{,a}u_{,b} = 0.$$

The vectors $k_a = u_{,a}$, are tangent to the family of null geodesics lying in the hypersurfaces, and $x^2 = r$ is chosen as an affine parameter along these geodesics. The coordinates $x^3 = x$ and $x^4 = y$ label the geodesics on each surface $u = \text{const}$.

(ii) Nonaligned Nonnull Solutions

There also exist solutions of the field equations with a nonnull electromagnetic field and which are of Petrov type N. To find these solutions we use the relations obtained from the Bianchi identities in the previous section and put these into the Newman-Penrose formalism[11] to obtain further simplifications. Finally we set up Robinson–Trautman coordinates and use the methods of Newman, Tamburino and Unti[12,13] to obtain the exact solutions. The procedure is long and cumbersome, but fairly straightforward. The final result is the following metric:

$$\begin{aligned} ds^2 &= \tfrac{1}{2}\cos^2 \kappa r(dx^2 + dy^2) \\ &\quad - 4\,du\,dr - 2\tau(2r + \kappa^{-1}\sin 2\kappa r)\,du\,dx \\ &\quad + 4\kappa^{-2}(2\tau^2 \sin^2 \kappa r - 2e^{2u} - r\kappa\,\partial\kappa/\partial u)\,du^2, \end{aligned} \tag{4.1}$$

where

$$\begin{aligned} \tau &= \tau(u, x) = e^u \coth (e^u x + f(u)), \\ \kappa &= \kappa(u, x) = g(u)e^u \sinh (e^u x + f(u)), \end{aligned}$$

$g(u)$ and $f(u)$ are arbitrary functions of u. This metric is of Petrov type N with principal null vector pointing along $k_a \propto u_{,a} = (1, 0, 0, 0)$. k_a is geodesic, shear-free and twist-free, but it will have an expansion and a rotation. The Ricci tensor turns out to be

$$R^{ab} = 4e^{2u}(2p^{(a}q^{b)} - \tfrac{1}{2}g^{ab}),$$

where

$$\begin{aligned} p^a = (&\tfrac{1}{4}\kappa e^{-u}, -r(\tfrac{1}{2}e^{-u}\,\partial\kappa/\partial u + \tau^2 e^{-u}\tan \kappa r \\ &+ \tau \sec \kappa r), e^{-u}\tau \tan \kappa r + \sec \kappa r, 0), \end{aligned}$$

and

$$q^a = -p^a + (0, -2r\tau \sec \kappa r, 2 \sec \kappa r, 0).$$

[10] I. Robinson and A. Trautman, Phys. Rev. Letters **4**, 431 (1960).
[11] E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).
[12] E. Newman and L. Tamburino, J. Math. Phys. **3**, 902 (1962).
[13] E. Newman, L. Tamburino, and T. Unti, J. Math. Phys. **4**, 915 (1963).

p^a and q^a are a pair of null vectors satisfying $p_a q^a = 1$.

By (3.7) the metric can be considered as representing a transverse gravitational wave propagating along shear-free null geodesics through a nonnull electromagnetic field. The principal null vectors of this field are p^a and q^a, neither of which are aligned with the gravitational wave k^a, and the electromagnetic field strength is $A = 2e^u$.

The electromagnetic field has the odd character that it is not a wave field (since it is not null—the electric and magnetic fields are nowhere equal and perpendicular) yet its amplitude propagates with the velocity of light. It may be thought of as a "quasi-wave" field. For a timelike observer the passage of the field will appear like an electromagnetic sheet whose strength rises (or diminishes) exponentially without limit. We may calculate the strength C_1 of the gravitational wave in the frame $(k^a, m^a, \bar{t}^a, \bar{l}^a)$ determined from the normalizations of Sec. 3. It is

$$C_1 = \tfrac{1}{2}\kappa \tan \kappa r$$
$$= \tfrac{1}{2} g(u) e^u \sinh (e^u x + f(u)) \tan \kappa r.$$

Thus the arbitrary function $g(u)$ measures the strength of the gravitational wave, which is seen to be quite independent of the electromagnetic field strength A. The function $f(u)$ is merely a phase function on the wave hypersurfaces u-const, which can be set to zero by a coordinate transformation

$$x' = x + e^{-u} f(u).$$

It is interesting that C_1 has singularities at $r = (n + \tfrac{1}{2})\pi\kappa^{-1}$. These are real singularities of the manifold, and there is no way of avoiding them. Another way in which these singularities show up is in the expansion of the gravitational propagation vector $k_a = u_{,a}$. When there is no electromagnetic field we have that $\theta = k^a{}_{;a}$ satisfies

$$d\theta/dr = \theta^2,$$

so that

$$\theta = 1/r$$

and the waves are spherical, emanating from a source at $r = 0$. With the electromagnetic field present the equation becomes modified to read

$$d\theta/dr = \theta^2 + \kappa^2,$$

so that

$$\theta = \kappa \tan \kappa r.$$

The waves are infinitely divergent at the points $r = (n + \tfrac{1}{2})\pi\kappa^{-1}$. If we choose to restrict the manifold to the region $-\tfrac{1}{2}\pi\kappa^{-1} < r < \tfrac{1}{2}\pi\kappa^{-1}$ it will be incomplete.

(iii) Aligned Nonnull Solutions

The metric (4.1) is by no means the most general one representing a pure transverse gravitational wave in a nonnull electromagnetic field. It is not even the most general one with shear-free geodesic propagation vector k_a. The analysis in the Penrose–Newman formalism makes it clear that the electromagnetic field strength A may be variable over the hypersurfaces u = const. However it must be constant along the tangents k_a if these are to be shear-free and geodesic:

$$A_{,a} k^a \equiv \partial A/\partial r = 0.$$

The full integration of the field equations in this more general case is considerably more complicated, and a closed form for the metric has not been found.

The metric (4.1) represents the case of a type-N wave in a nonaligned electromagnetic field. There exist further solutions representing a type-N wave in an aligned field. As pointed out in Sec. 3 (ii) (a), the principal null vector k^a is shear-free and geodesic. For Petrov type N it turns out furthermore that k^a has vanishing expansion, twist and angular momentum (that is, it is a p.p. wave), and the electromagnetic field amplitude A is constant. This makes the Newman–Penrose field equations fairly straightforward to integrate. The result is

$$ds^2 = \tfrac{1}{2}P^{-2}(dx^2 + dy^2)$$
$$- 2\,du\,dr - P^{-2}(X\,du\,dx + Y\,du\,dy)$$
$$+ \{U - \tfrac{1}{2}|A|^2 r^2 + \tfrac{1}{2}P^{-2}(X^2 + Y^2)\}\,du^2 \qquad (4.2)$$

where $P = P(u, x, y)$ satisfies

$$P^2 \nabla^2 \ln P = \tfrac{1}{2}|A|^2 = \text{const.}$$

$U(x, y, u)$ satisfies

$$\nabla^2 U = -P^2,$$

and

$$Z = X + iY = f(u, z) - 4\,\partial U/\partial z,$$

where $z = x + iy$, $\nabla^2 \equiv \partial^2/\partial x^2 + \partial^2/\partial y^2$, and f is an arbitrary analytic function of z. This metric is of Petrov type N with propagation vector pointing along $k_a = u_{,a} = (1, 0, 0, 0)$. The Ricci tensor has the form

$$R^{ab} = |A|^2 (2k^{(a} m^{b)} - \tfrac{1}{2} g^{ab}), \qquad (4.3)$$

where

$$m^a = (-1, -\tfrac{1}{4}|A|^2 r^2 + U, X, Y).$$

k^a and m^a are the principal null vectors of the electromagnetic field. The null vector is neither shear-free nor geodesic. Completing the tetrad with the vectors t^a, $\bar{t}^a$, where $t^a = (0, 0, P, iP)$, we find for the shear and refraction of m^a

$$\sigma = m_{a;b}t^a t^b = P^2 ,$$

$$\gamma = m_{a;b}t^a m^b = -2P\,\partial U/\partial z.$$

In this frame the gravitational field strength C_1 can be calculated;

$$C_1 = -8\frac{\partial(P^2\,\partial U/\partial z)}{\partial z} - \frac{\partial P^2}{\partial u} - \frac{X\,\partial P^2}{\partial x} - \frac{Y\,\partial P^2}{\partial y} - P^2(|A|^2 r + 4\,\partial Z/\partial z).$$

We see that the field strength varies along the geodesics of propagation:

$$C_{1,a}k^a = \partial C_1/\partial r = 2 - P^2\,|A|^2.$$

If the null vector m^a has vanishing shear, it is clear we cannot use the metric (4.2) since $P^2 = 0$. This situation is represented by the metric

$$ds^2 = \tfrac{1}{2}P^{-2}(dx^2 + dy^2) - 2\,du\,dr + 2(U - \tfrac{1}{4}\,|A|^2 r^2)\,du^2, \qquad (4.4)$$

where

$$P^2\nabla^2 \ln P^2 = \tfrac{1}{2}\,|A|^2,$$

$$\nabla^2 U = 0.$$

The Ricci tensor is again of the form (4.3) but with $m^a = (-1, -\frac{1}{4}\,|A|^2 r^2 + U, 0, 0)$. In this case m^a is shear-free, but it is still not geodesic. The gravitational field strength is given now by

$$C_1 = -8\,\partial(P^2\,\partial U/\partial z)/\partial z,$$

and is constant along the k^a geodesics, $\partial C_1/\partial r = 0$.

(iv) A Conformally Flat Solution

The metrics (4.2), (4.3) are all the metrics representing a pure transverse gravitational wave propagating through an aligned nonnull electromagnetic field. From the metric (4.4) we can obtain an interesting case if we put $U = 0$. m^a is now geodesic, $\gamma = 0$, but also $C_1 = 0$. This means that the Weyl tensor vanishes, and there is no free gravitational field at all. That is, the metric

$$ds^2 = \tfrac{1}{2}P^{-2}(dx^2 + dy^2) - 2\,du\,dv - \tfrac{1}{2}\,|A|^2 r^2\,du^2,$$

where

$$\nabla^2 \ln P^2 = 0$$

represents a conformally flat space, with a nonnull electromagnetic field present.

5. EXACT FLUID SOLUTIONS

The question we now investigate is whether there exist any Petrov type N solutions of the field equations with a perfect fluid. A partial answer has been given by Kundt and Trümper,[4] who show that no solutions exist if $\omega = 0$ (ω = angular velocity of fluid). By Eq. (2.21) this is seen to be equivalent to the statement that no Petrov type N solutions with perfect fluids exist in which the waves are propagated along null geodesics ($\gamma = 0$). However, the case

$$p = \mu + A(t),$$

where t = const are the hypersurfaces to which the u^a are orthogonal (they exist on account of the postulate $\omega = 0$), eludes the Kundt–Trümper analysis. They discard this case as unphysical since it is usual to have $p < \frac{1}{3}\mu$. This is not totally convincing, however, since μ might be almost constant on the hypersurfaces t = const, and $A(t)$ chosen in such a way as to have $p < \frac{1}{3}\mu$ satisfied everywhere. There appears to be no straightforward way of eliminating this case, and it must remain an open question whether there exists solutions of Petrov type N with $p = \mu + A(t)$.

The more general case $\omega \neq 0$ is much harder to analyze since the fluid streamlines are no longer hypersurface-orthogonal and it is not possible to set up suitable Gaussian coordinates. We have managed to deal with the case $p = 0$, where by (2.4b) the streamlines are geodesic, $\dot{u}_a = 0$. The result, proved in the Appendix, is the following:

No solutions of Petrov type N with incoherent matter ($p = 0$) exist.

While the question of the existence of type N solutions is still not decided, we see from the above results that such solutions, if they exist, must be of a complexity considerably exceeding that of any fluid solutions that have been found to date.

To conclude this discussion, we give a simple argument to show that locally there can be a fluid present in a Petrov type N metric. Consider a conformal transformation of the metric,

$$\hat{g}_{ab} = e^{2u}g_{ab}.$$

The Ricci tensor transforms as

$$\hat{R}_{ab} = R_{ab} + 2u_{a;b} - 2u_a u_b + (2u_c u^c + u^c{}_{;c})g_{ab},$$

where

$$u_a = u_{,a}, \qquad u_{a;b} = u_{b;a}.$$

The Weyl tensor remains invariant

$$\hat{C}^a{}_{bcd} = C^a{}_{bcd},$$

so that the Petrov type of the metric is unchanged by the conformal transformation. If we consider g_{ab} to be the metric tensor for a vacuum solution $R_{ab} = 0$, and let u be a solution of the partial differential equation

$$g^{ab}u_{,a}u_{,b} = u_a u^a = -1, \tag{5.1}$$

then

$$\hat{R}_{ab} = 2\sigma_{ab} + (5\theta/3 - 2)h_{ab} - \theta u_a u_b,$$

where

$$u_{a;b} = \sigma_{ab} + \tfrac{1}{3}\theta h_{ab}.$$

Using the field equations in the new space

$$\hat{R}_{ab} - \tfrac{1}{2}\hat{R}\hat{g}_{ab} = -\hat{T}_{ab},$$

where

$$\hat{R} = \hat{R}_{ab}\hat{g}^{ab} = 6(\theta - 1)e^{-2u},$$

we find that

$$\hat{T}_{ab} = -2\sigma_{ab} + (4\theta/3 - 1)e^{-2u}\hat{h}_{ab} + (3 - 2\theta)e^{-2u}\hat{u}_a\hat{u}_b, \tag{5.2}$$

where $\hat{u}_a = e^u u_a$ is a timelike unit vector in the g_{ab} space, and $\hat{h}_{ab} = \hat{g}_{ab} + \hat{u}_a\hat{u}_b$. Thus we have generated a perfect fluid solution from the vacuum if we can find a solution of Eq. (5.1) with $\sigma_{ab} = 0$. We cannot find such a solution if the initial metric is of Petrov type N, since the fluid streamlines would be hypersurface-orthogonal ($\omega = 0$), contradicting the result of Kundt and Trümper. However it is clear that at any point of the manifold it is possible to find a solution having $\sigma_{ab} = 0$ at that point. In this way we can generate a "local fluid." But as we depart from this point we will have $\sigma_{ab} \neq 0$, and anisotropies will appear in the energy tensor. It is not inconceivable that we might find a solution in which σ remains small relative to θ at least for a sizable region of the manifold, and in this region we will have an "almost-perfect" fluid. We can obtain an upper bound for the size of the region in which T_{ab} remains physical. From (5.2) it is seen that the density and mean pressure are given by

$$\mu = e^{-2u}(3 - 2\theta),$$
$$p = e^{-2u}(4\theta/3 - 1).$$

Hence, if μ and p are both to be positive we must have

$$\tfrac{3}{4} \leq \theta < \tfrac{3}{2}.$$

Furthermore θ should be much closer to the lower value than the higher, else the pressure dominates the density. Now we can use the Ricci identities

$$R^d{}_{acd}u_d = 2u_{a;[bc]}.$$

Contracting over a and c and using the vacuum condition $R_{ab} = 0$, we find on further contracting with u^b that

$$\dot{\theta} \equiv \partial\theta/\partial u = -2\sigma^2 - \tfrac{1}{3}\theta^2.$$

If initially at $u = u_0$, $\theta = \frac{3}{4} + \epsilon$, we will have

$$\partial\theta/\partial u < -\tfrac{3}{16},$$

hence θ can only remain $> \frac{3}{4}$ until a time $u_1 = u_0 + 16\,\epsilon/3$, after which the pressure becomes negative.

6. RELATION TO ELECTROMAGNETIC THEORY

The results obtained in this paper for the propagation of gravitational waves in matter have a strangely unfamiliar ring when we try to compare them with the usual electromagnetic treatment. For example, the "refraction" discussed here is nothing like the refraction of electromagnetic waves, for there is no slowing down of the waves—there is merely a deflection from the straightest, the geodesic, path—while the other feature of the interaction, the shear of the waves, is something never discussed in electromagnetic theory. It is not hard to see where the difference between the two theories lies. We could treat the electromagnetic field in a similar way, discussing the Maxwell equations

$$F^{ab}{}_{,b} = j^a,$$

and obtaining a departure from geodicity and a shear in the electromagnetic wave coupled to the current vector j^a. But this treatment would be entirely wrong if applied, say, to light passing through a slab of glass. In this case the interesting features occur at the atomic scale, where the current j^a becomes extremely complicated. When we smooth out all these tiny currents we have $j^a = 0$, so that the field should propagate as though there was no matter present at all,

$$F^{ab}{}_{,b} = 0.$$

But at the atomic level there is the creation of a large number of oscillating dipole moments which produce their own field, out of phase with this freely propagating field in just such a way as to produce a total transmitted wave traveling with a speed less than that of light in vacuum. Feynman[14]

[14] R. Feynman, *Lectures on Physics*, Vols. I and II (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1963).

has recently given a very clear and beautiful treatment of just this problem.

There are several reasons why such a discussion would not be applicable to the gravitational case. In the first place general relativity is a continuum theory and is only valid at that scale where we can regard the matter as smoothed out into a highly regular fluid. It is very difficult to see how one could treat a system of discrete particles in the theory. This feature arises again and again, its most famous instance perhaps occurring in cosmology where the whole galactic population is smeared out into a continuum. Secondly, the principle of equivalence demands that all masses respond equally to the gravitational field, with the result that no dipole moments are created in the matter. It is true that quadrupole moments may occur, but there is still another point to bear in mind here. It is only on the astronomical scale that matter is held together by purely gravitational forces; on the terrestrial scale it is the much larger electromagnetic forces that are important. A comparable situation in the electromagnetic theory would be if the atoms were held together not by the electric forces but by some field which was stronger by a factor of about 10^{40} (even the nuclear forces pale into insignificance here). In such a case the induced dipole moments would be weaker by a corresponding factor, and the usual phenomenon of refraction would never be observed. Our analysis of refraction would then have to follow lines similar to those discussed in this paper.

The above discussion raises some inevitable queries. If large-scale gravitational waves arise, or have arisen at a more chaotic epoch of the universe, how do these propagate through the galactic system? The analysis should now follow the more familiar electromagnetic treatment, with induced quadrupole moments in the galaxies replacing atomic dipole moments. At the other end of the scale, we may ask how very short wavelength gravitational radiation (of atomic dimensions) would propagate in ordinary matter. Again, the electromagnetic treatment should be the one to adopt.

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APPENDIX: PETROV TYPE-N SOLUTIONS WITH INCOHERENT MATTER

Consider a fluid with $p = 0$. From Eqs. (2.4a, b) we have

$$\dot{\mu} = -\mu\theta,$$

$$\dot{u}_a = 0.$$

Let us assume $\omega \neq 0$. If the Weyl tensor is of Petrov type N with principal null vector $k_a = u_a + s_a$, we have from (2.21) that $\gamma \neq 0$ (k_a is not geodesic). Take r_a the unit vector pointing along $\gamma l_a + \bar{\gamma} t_a$, and q_a the unit vector pointing along $i(\gamma l_a - \bar{\gamma} t_a)$. u_a, s_a, r_a, and q_a form an orthonormal tetrad. From Eqs. (2.17) to (2.22) and (2.2) we have

$$u_{a;b} = 2\omega s_{[a} r_{b]} + 3\sigma(s_a s_b - \tfrac{1}{3} h_{ab}) + \tfrac{1}{3}\theta h_{ab} \tag{A1}$$

and

$$\mu_{,b} = \mu(3\omega r_b + \sqrt{3}\,\sigma s_b + \theta u_b). \tag{A2}$$

If we put these into the current conservation equation (1.4) we get

$$\dot{\omega} = -\tfrac{1}{3}\omega(2\theta + \sqrt{3}\,\sigma) \tag{A3}$$

and

$$\dot{s}_a q^a = \dot{r}_a q^a = 0. \tag{A4}$$

Consider the Ricci identities

$$R^a{}_{bcd} u_a = 2u_{b;[dc]}.$$

Using (1.1) and the field equations (2.3) this may be rewritten in terms of the Weyl tensor

$$C^a{}_{bcd} u_a = 2u_{b;[dc]} + \tfrac{1}{3}\mu u_{[d} g_{c]b}. \tag{A5}$$

Contracting over b and c, and a further contraction with u^d results in the well-known Raychaudhuri equation

$$\dot{\theta} = -\tfrac{1}{2}\mu + 2\omega^2 - 2\sigma^2 - \tfrac{1}{3}\theta^2. \tag{A6}$$

Using the fact that $C^a{}_{bcd}$ is of Petrov type N,

$$C^a{}_{bcd} k_a = 0, \tag{A7}$$

results in

$$\sqrt{3}\,\dot{\sigma} = \tfrac{1}{2}\omega^2 - \tfrac{2}{3}\sqrt{3}\,\sigma\theta - \sigma^2 \tag{A8}$$

and

$$\dot{s}_d r^d = 0.$$

The last equation together with (A4) gives that

$$\dot{s}_d = \dot{r}_d = 0. \tag{A9}$$

Using the Weyl tensor symmetry

$$C^{a}{}_{[bcd]} = 0,$$

and the fact that $\mu_{,a}$ is a gradient in (A2)

$$\mu_{,[a;b]} = 0,$$

we find, using (A7), that

$$s_{[b;c}r_d u_{e]} = 0.$$

That is,

$$0 = s_{a;b}q^a s^b = k_{a;b}q^a k^b = i(\gamma^2 - \bar{\gamma}^2)/\sqrt{2}\,|\gamma|.$$

Hence $\gamma^{(1)}\gamma^{(2)} = 0$, that is, either $\gamma^{(1)}$ or $\gamma^{(2)}$ is zero, which means that q_a and r_a coincide with the polarization directions of the transverse wave. This means that we can write the Weyl tensor as

$$C_{abcd} = 2C(k_{[a}r_{b]}k_{[c}r_{d]} - k_{[a}q_{b]}k_{[c}q_{d]}).$$

By (A5), (A6), and (A8) we find

$$C = 2C_{abcd}u^a r^b u^c r^d = -\omega^2. \tag{A10}$$

Now,

$$\sqrt{2}\,|\gamma| = k_{a;b}r^a k^b,$$

and by (2.21) it follows that

$$\mu = \omega(\omega - s_{a;b}r^a s^b). \tag{A11}$$

Now

$$(s_{a;b}r^a s^b)_{;c}u^c = s_{a;c;b}r^a u^c s^b + R_{dacb}s^d r^a s^b u^c.$$

From (A5) and (A7) it follows that the last term vanishes, while the second term can be written as

$$\omega s_{a;c}r^a r^c - \tfrac{1}{3}(\theta + 2\sqrt{3}\,\sigma)s_{a;c}r^a s^c.$$

If we now differentiate (A11) along u^a we find using (A3), that

$$\omega^2 s_{a;b}r^a r^c = \tfrac{1}{3}\omega^2(\sqrt{3}\,\sigma - \theta) - \mu\sqrt{3}\,\sigma.$$

A final differentiation along u^a of this equation results in

$$\mu\omega^2 = 0.$$

Hence $\omega = 0$ and our theorem is proved, since by (A10) this means $C = 0$ and the Weyl tensor vanishes.

Asymptotic Correlations of the Hamiltonian Matrix Elements

NAZAKAT ULLAH
Tata Institute of Fundamental Research, Bombay, India
(Received 20 September 1965)

The statistical correlations of the matrix elements of real symmetric Hamiltonians are studied using the assumption of representation invariance and the limit of large dimension N. The diagonal–diagonal correlation coefficient is expressed in terms of a parameter which gives the ratio of the dispersion of off-diagonal element to that of the diagonal element. It is shown that for a certain class of real-symmetric Hamiltonian ensembles in the limit $N \to \infty$, the diagonal–diagonal correlation coefficient goes as λN^{-1}, where λ is some positive constant independent of N and the correlation coefficient of two different eigenvalues is the same as the one obtained using the weak assumption of independent probabilities.

I. INTRODUCTION

THE joint probability distribution for the Gaussian ensemble of real-symmetric Hamiltonian matrices was first derived by Porter and Rosenzweig.[1] This derivation is based on the assumptions that (1) the matrix elements are distributed independently of each other, and (2) the Hamiltonian is statistically invariant under linear orthogonal transformations of the set of basic functions. The assumption (2) is a physical assumption, because this simply means that the joint probability distribution should be independent of the orientation of the base system of axes, but assumption (1) is quite unphysical.[2] It is natural to ask if there is some way of avoiding the weak assumption that the joint probability distribution of the Hamiltonian matrix elements is made up of independent distributions for the separate matrix elements. It has been shown recently[3] that the requirement of invariance under arbitrary changes of representation and the limit of large dimension are sufficient to obtain the same results for the distribution of the eigenvector components of a random Hamiltonian matrix, as those obtained by the requirements of representation invariance and the independent distribution. In this paper, we shall study the correlations of the Hamiltonian matrix elements using the assumption of representation invariance and the limit of large dimension.

Let us consider an ensemble of $N \times N$ real-symmetric Hamiltonian matrices with elements $H_{\mu\nu}$. These matrices belong to a definite value of the total angular momentum and parity and have $\frac{1}{2}N(N+1)$ different matrix elements which we take to be the diagonal plus superdiagonal matrix elements. The ensemble of matrices is described by giving the differential probability with which a matrix characterized by certain numerical values of the matrix elements $H_{\mu\nu}$ occurs. It should be pointed out here that we do not know in what representation H will be diagonal and therefore a typical member of the ensemble will have a large number of nonzero off-diagonal elements. The N eigenvalues E_λ and the eigenvector components $a_{\mu\lambda}$ of the random Hamiltonian matrix will themselves be random. They are related by

$$H_{\mu\nu} = \sum_\lambda E_\lambda a_{\mu\lambda} a_{\nu\lambda}. \tag{1}$$

The $N \times N$ matrix formed from the eigenvector components $a_{\mu\lambda}$ will be a random orthogonal matrix.

We are interested in the ensemble averages of the products of the matrix elements given by equation (1). Using the representation invariance hypotheses this averaging can be done separately over the eigenvalues and the eigenvector components.[1] The averages of the products of components of a set of orthogonal unit vectors randomly oriented in the N-dimensional space are known.[4] These known averages enable us to predict some of the correlations of the Hamiltonian matrix elements and to find relations between the correlation coefficients of the Hamiltonian matrix elements and those of its eigenvalues.

II. CORRELATIONS OF HAMILTONIAN MATRIX ELEMENTS

It has been shown earlier[4] that for any N, the representation invariance hypothesis leads to the conclusion that there are no correlations between an odd power of the off-diagonal matrix element and any power of diagonal or another off-diagonal matrix element. In this section we would like to study the correlations for large N. But before we discuss the

[1] C. E. Porter and N. Rosenzweig, Suomalaisen Tiedeakat. Toimituksia Ser. **AVI, 44** (1960).
[2] F. J. Dyson, J. Math. Phys. **3**, 140 (1962).
[3] Nazakat Ullah, J. Math. Phys. **6**, 1102 (1965).
[4] Nazakat Ullah, Nucl. Phys. **58**, 65 (1964).

case for large N, let us first give an expression for diagonal–diagonal correlation valid for all N. Using expression (1) and the known averages of the eigenvector components,[4] we can show that the diagonal–diagonal correlation coefficient is given by

$$C_{H_{\mu\mu},H_{\xi\xi}} = 1 - \beta^2, \tag{2}$$

where

$$\beta = \left[N - \frac{\langle(\mathrm{Tr}\, H)^2\rangle}{\langle \mathrm{Tr}\, H^2\rangle}\right]^{\frac{1}{2}} \times \left[(N-1) + \tfrac{1}{2}(N-1)\frac{\langle(\mathrm{Tr}\, H)^2\rangle}{\langle \mathrm{Tr}\, H^2\rangle}\right]^{-\frac{1}{2}}. \tag{3}$$

The bracket sign $\langle\ \rangle$ above denotes the ensemble average. In writing expression (2) we have taken $\langle \mathrm{Tr} H\rangle = 0$, which simply means that the mean eigenvalue is taken to be zero.

The ratio of the dispersion of the off-diagonal element to that of the diagonal element can be expressed in terms of the parameter β, which depends on N and $\langle(\mathrm{Tr}\, H)^2\rangle/\langle \mathrm{Tr}\, H^2\rangle$, as

$$\langle H_{\mu\nu}^2\rangle/\langle H_{\mu\mu}^2\rangle = \tfrac{1}{2}\beta^2. \tag{4}$$

Using the relation between the diagonal–diagonal correlation coefficient and the correlation coefficient of two different eigenvalues, the latter correlation coefficient is given by

$$C_{E_\mu,E_\xi} = -\frac{3\beta^2 - 2}{(N-1)\beta^2 + 2}. \tag{5}$$

It is interesting to note that the correlation coefficient given by expression (5) can have both positive and negative values depending on the parameter β. The results of the independent distribution immediately follow if we put $\beta^2 = 1$.

To study the correlation coefficient given by expression (2) for large values of N, we consider the ratio

$$\gamma = \langle(\mathrm{Tr}\, H)^2\rangle/\langle \mathrm{Tr}\, H^2\rangle. \tag{6}$$

We shall show that for a certain class of real-symmetric Hamiltonian ensembles, γ is of the order of N^{-1}. To show this let us denote the joint probability density function by $P_N(H_{11}, H_{12}, \cdots, H_{NN})$, then

$$\gamma = \frac{\int (\mathrm{Tr}\, H)^2 P_N(H_{11}, \cdots, H_{NN}) \prod_{\mu\le\nu} dH_{\mu\nu}}{\int \mathrm{Tr}\, H^2 P_N(H_{11}, \cdots, H_{NN}) \prod_{\mu\le\nu} dH_{\mu\nu}}. \tag{7}$$

Let us make an orthogonal transformation on N variables $H_{11}, H_{22}, \cdots, H_{NN}$

$$H'_{\mu\mu} = \sum_\nu C_{\mu\nu} H_{\nu\nu}, \tag{8}$$

such that $C_{11} = C_{12} = \cdots = C_{1N} = N^{-\frac{1}{2}}$, then

$$H'_{11} = N^{-\frac{1}{2}}\,\mathrm{Tr}\, H,$$

and since C is an orthogonal matrix, therefore

$$\sum_\mu H_{\mu\mu}^2 = \sum_\mu H_{\mu\mu}'^2, \qquad \prod_\mu dH_{\mu\mu} = \prod_\mu dH'_{\mu\mu}.$$

Expression (7) now becomes

$$\gamma = N \frac{\int H_{11}'^2 P_N(H'_{11}, H_{12}, \cdots, H'_{NN}) \prod_{\mu<\nu} dH_{\mu\nu} \prod_\mu dH'_{\mu\mu}}{\int (\sum_\mu H_{\mu\mu}'^2 + 2\sum_{\mu<\nu} H_{\mu\nu}^2) P_N(H'_{11}, H_{12}, \cdots, H'_{NN}) \prod_{\mu<\nu} dH_{\mu\nu} \prod_\mu dH'_{\mu\mu}}.$$

We now regard the matrix H as a vector in $[L = \frac{1}{2}N(N+1)]$-dimensional vector space[5] and introduce the L-dimensional spherical polar coordinates

$$H'_{11} = rq_1, \cdots, H'_{NN} = rq_N,$$
$$\sqrt{2}\, H_{12} = rq_{N+1}, \cdots, \sqrt{2}\, H_{N-1,N} = rq_L,$$

then

$$\gamma = N \frac{\int r^{L+1} q_1^2 P_N(r, q_1, \cdots, q_L)\, dr\, d\Omega_L}{\int r^{L+1} P_N(r, q_1, \cdots, q_L)\, dr\, d\Omega_L}, \tag{9}$$

where $d\Omega_L$ is the L-dimensional differential solid angle. Expression (9) can be written as

$$\gamma = N \frac{\int_0^\pi F_N(\sin\theta, \cos\theta) \cos^2\theta \sin^{L-2}\theta\, d\theta}{\int_0^\pi F_N(\sin\theta, \cos\theta) \sin^{L-2}\theta\, d\theta}, \tag{10}$$

where $F_N(\sin\theta, \cos\theta)$ is the function obtained by integrating over r and all the angular variables except θ. By a slight change of variable we can express γ as

$$\gamma = N \frac{\int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} F_N(-\sin\alpha, \cos\alpha) \sin^2\alpha \cos^{L-2}\alpha\, d\alpha}{\int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} F_N(-\sin\alpha, \cos\alpha) \cos^{L-2}\alpha\, d\alpha}. \tag{11}$$

[5] N. Rosenzweig, *Brandeis University Summer Institute Lectures in Theoretical Physics, 1962* (W. A. Benjamin, Inc., New York, 1963), Vol. 3, p. 91.

We now make the assumption that our probability function P_N is such that the function $F_N(\alpha)$ can be expanded in a convergent series around $\alpha = 0$. Therefore, most of the contribution to the integrals in the numerator and denominator of expression (11) will come from $\alpha = 0$ when L is large and the dependence of the ratio γ on N will be like N^{-1}. Expressions (2), (3), (4), and (5) show that for such ensembles in the limit of large N, the ratio of dispersion of the off-diagonal element to that of diagonal element is $\frac{1}{2}$, the diagonal–diagonal correlation goes as λN^{-1}, where λ is some positive constant independent of N and the correlation coefficient C_{E_μ, E_ξ} is given by

$$C_{E_\mu, E_\xi} = -N^{-1}. \tag{12}$$

The correlation coefficient given by expression (12) is the same as the one obtained using the assumption of independent probabilities.

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Unitary Representations of the Lorentz Group on 4-Vector Manifolds*

JONAS STASYS ZMUIDZINAS
Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California
(Received 26 July 1965; revised manuscript received 26 October 1965)

A review is presented of irreducible unitary representations of the (3 + 1)-dimensional restricted Lorentz group on manifolds of time-, light-, and spacelike 4-vectors. In each case a complete set of orthonormal (in the sense of the distribution theory) basis functions is available. The completeness relation for the nontrivial spacelike case is proved in detail. Expansion formulas, Lorentz-group analogs of the Fourier integral theorem, are given. In particular, expansions of plane-wave solutions of the Klein–Gordon equation for $-\infty < m^2 < \infty$ are worked out as an illustrative example. Possible physical applications are briefly discussed.

I. INTRODUCTION

THE mathematical theory of representations of the (1 + 3)-dimensional (restricted) Lorentz group $L_0(= L_+^\uparrow)$ has received a considerable amount of attention both in physical and mathematical literature.[1-3] The finite-dimensional nonunitary representations of this group have long been known and utilized in physical applications. The infinite-dimensional unitary representations have also been known for some time[4]; perhaps surprisingly, they have not been very widely applied in physics.[5] All irreducible unitary representations of L_0 are known and are usually explicitly constructed in terms of functions defined on complex manifolds.[2] For example, the so-called principal series representations of L_0 are constructed on the space of all complex-valued functions $f(z)$, $z = x + iy$, for which

$$\int\int_{-\infty}^{\infty} |f(z)|^2 \, dx \, dy < \infty.$$

The complex variable z has no immediate physical significance, and this is a distinct disadvantage for physical interpretability of these representations.

In practical applications, one frequently encounters situations in which functions of one or more 4-vectors transform according to the Lorentz group L_0. For example, scalar fields obey the trans-

* This work was sponsored by the National Aeronautics and Space Administration under Contract No. NAS7-100.

[1] B. L. van der Waerden, *Die gruppentheoretische Methode in der Quantentheorie* (Springer-Verlag, Berlin, 1932).

[2] M. A. Naĭmark, *Linear Representations of the Lorentz Group* (The Macmillan Company, New York, 1964).

[3] I. M. Gel'fand, R. A. Minlos, and Z. Ya. Shapiro, *Representations of the Rotation and Lorentz Groups and their Applications* (The Macmillan Company, New York, 1963).

[4] P. A. M. Dirac, Proc. Roy. Soc. (London) **A183**, 284 (1945); I. M. Gel'fand and M. A. Naĭmark, J. Phys. **10**, 93 (1946); Harish-Chandra, Proc. Roy. Soc. (London) **A189**, 372 (1947).

[5] E. M. Lifshitz, J. Phys. 10, 116 (1946); V. L. Ginzburg and I. E. Tamm, JETP **17**, 227 (1947); I. M. Gel'fand and A. M. Yaglom, JETP **18**, 703 (1948); I. S. Shapiro, Soviet Physics—Doklady 1, 91 (1956); I. S. Shapiro, Physics Letters 1, 253 (1962).

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formation law $\phi(x) \rightarrow \phi(\Lambda x)$; invariant (scattering) amplitudes of 4-momenta $p_1, p_2, \cdots$ transform as $A(p_1, p_2, \cdots) \rightarrow A(\Lambda p_1, \Lambda p_2, \cdots)$, etc. These various quantities do not transform irreducibly under L_0. One is frequently interested in expanding them in terms of functions irreducible under L_0. Thus one is faced with the problem of constructing irreducible (unitary) representations of the Lorentz group on a manifold of a single 4-vector and then with the problem of expanding arbitrary reasonably well-behaved functions defined on this manifold in terms of Lorentz-irreducible functions. The case of several 4-vectors is treated by performing expansions in each of the 4-vectors and then using the Clebsch–Gordan machinery to effect the desired reduction into irreducible components under L_0. Most of the required Clebsch–Gordan coefficients are available in the literature.[6] We shall not be concerned with the reduction part of the problem in this paper. Our goal is to examine the expansions of functions of a single 4-vector. We shall restrict our discussion to the important special case of spin zero for which G, one of the Casimir operators of L_0, vanishes. Nonzero spin requires extra variables, in addition to the 4-vector components, and is therefore beyond the scope of this article.

Our work is based on solutions of a number of second-order ordinary differential equations representing eigenvalue problems associated with certain operators constructed from the generators of L_0. Not all possible solutions of these equations are acceptable: only those which are normalizable to a constant or to a delta function. Our rather pedestrian approach to the expansion problem via differential equations has the virtue that all calculations are explicit and straightforward; a large body of results from the theory of differential equations may be utilized which would not be available with the more abstract approaches.

Irreducible unitary representations of the Lorentz group on manifolds of timelike 4-vectors have already been discussed by a number of authors.[6,7] Corresponding representations in terms of spacelike 4-vectors have also been discussed, although not in full generality; we believe that some of the results on this subject given here are new. The lightlike case does not appear to have been treated before. All three cases are reviewed here in the interest of completeness.

A summary of irreducible unitary representations of the restricted Lorentz group is presented in Sec. II. Lorentz-group expansions on manifolds of a single 4-vector are discussed in Sec. III for the timelike and spacelike cases. Expansions of functions of a lightlike 4-vector are considered in Sec. IV. A summary of results is presented in Sec. V, and possible physical applications are indicated. Finally, three appendices are devoted to detailed proofs of certain statements made in the text as well as to an illustrative example.

II. THE RESTRICTED LORENTZ GROUP

The Lie algebra $\mathfrak{L}_0$ of the restricted Lorentz group L_0 is spanned by the six (Hermitian) operators $M_{\mu\nu} = -M_{\nu\mu}$, $\mu, \nu = 0, 1, 2, 3$, obeying the commutation relations

$$[M_{\mu\nu}, M_{\rho\sigma}] = iM_{[\mu[\sigma}g_{\rho]\nu]},$$

where brackets denote antisymmetrizations as, e.g., in

$$a_{[\mu\nu]} = a_{\mu\nu} - a_{\nu\mu},$$

and the nonvanishing diagonal metric tensor components are

$$g_{00} = g^{00} = -g_{ii} = -g^{ii} = +1, \qquad i = 1, 2, 3.$$

Irreducible unitary representations of L_0 are characterized by the eigenvalues of its two Casimir operators F and G, commuting with each $M_{\mu\nu}$ and given by

$$F = -\tfrac{1}{2}M_{\mu\nu}M^{\mu\nu},$$

$$G = \tfrac{1}{2}M_{\mu\nu}\tilde{M}^{\mu\nu}.$$

Here $\tilde{M}$ is the dual tensor of M defined by

$$\tilde{M}^{\mu\nu} = \tfrac{1}{2}\epsilon^{\mu\nu\rho\sigma}M_{\rho\sigma},$$

$$\epsilon^{\mu\nu\rho\sigma} = \begin{cases} 1 \text{ if } (\mu\nu\rho\sigma) = \text{even permutation of } (0123), \\ -1 \text{ if } (\mu\nu\rho\sigma) = \text{odd permutation of } (0123), \\ 0 \text{ otherwise.} \end{cases}$$

We denote the eigenvalues of F and G by

$$f = 1 + \nu^2 - k^2,$$

$$g = 2k\nu.$$

[6] A. Z. Dolginov and I. N. Toptygin, Zh. Eksperim. i Teor. Fiz. **37**, 1441 (1959) [English transl.: Soviet Phys.—JETP **10**, 1022 (1960)]; A. Z. Dolginov and A. N. Moskaley, *ibid.* 1697 (1959) [English transl.: *ibid.* 1202 (1960)]; M. A. Naimark, Am. Math. Soc. Transl. **36**, Series 2, pp. 101–229.

[7] Chou Kuang-Chao and L. G. Zastavenko, Soviet Physics JETP **35**, 990 (1959); V. S. Popov, Soviet Physics JETP **37**, 794 (1960); N. Ya. Vilenkin and Ya. A. Smorodinskiĭ, Soviet Physics JETP **19**, 1209 (1964).

There are the following classes of irreducible unitary representations of L_0 labeled by k and ν[2,8]:

(i) $k = 0, \quad \nu = i;$

(ii) $k = 0, \quad \nu \geq 0;$

(iii) $k = 0, \quad \nu = i\nu_0, \quad 0 < \nu_0 < 1;$

(iv) $k = 1, 2, 3, \cdots, \quad -\infty < \nu < \infty;$

(v) $k = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots, \quad -\infty < \nu < \infty.$

The representation (v) is double-valued; all others are single-valued. The representation (i) with $f = g = 0$ is the trivial or identity representation of L_0.

We shall use the notation

$$\mathbf{M} = (M_1, M_2, M_3) = (M_{23}, M_{31}, M_{12}),$$

$$\mathbf{N} = (N_1, N_2, N_3) = (M_{01}, M_{02}, M_{03}).$$

The commutation relations for the M_i and N_i are

$$[M_i, M_j] = ie_{ijk}M_k,$$

$$[M_i, N_j] = ie_{ijk}N_k,$$

$$[N_i, N_j] = -ie_{ijk}M_k,$$

where

$$e_{ijk} = \epsilon^{0ijk}.$$

The M_i span the Lie algebra $\mathfrak{su}(2)$ of the two-dimensional unimodular group $SU(2)$ homomorphic to R_3, the three-dimensional rotation group.

The operators $\mathbf{M}^2$ and M_3 form a maximal abelian subalgebra of the operator algebra spanned by the six $M_{\mu\nu}$, and hence they may be diagonalized simultaneously with F and G. Thus one may introduce the vectors $|k\nu j\mu\rangle$ defined by the four eigenvalue equations

$$(F, G, M^2, M_3)\,|k\nu j\mu\rangle = (1 + \nu^2 - k^2, 2k\nu, j(j+1), \mu)\,|k\nu j\mu\rangle.$$

Here

$$j = k + n, \quad n = 0, 1, 2, \cdots,$$

$$\mu = j, \quad j - 1, \cdots, -j.$$

It is possible to choose a canonical form of the operators $M_{\mu\nu}$ and the vectors $|k\nu j\mu\rangle$ for which the following relations are valid[8]:

$$M_3\,|j\mu\rangle = \mu\,|j\mu\rangle,$$

$$(M_1 \pm iM_2)\,|j\mu\rangle = [(j \mp \mu)(j \pm \mu + 1)]^{\frac{1}{2}}\,|j\mu \pm 1\rangle,$$

$$N_3\,|j\mu\rangle = [(j+1)^2 - \mu^2]^{\frac{1}{2}}C^{k\nu}_{j+1}\,|j+1\mu\rangle + [k\nu\mu/j(j+1)]\,|j\mu\rangle + (j^2 - \mu^2)^{\frac{1}{2}}C^{k\nu}_j\,|j-1\mu\rangle,$$

$$(N_1 \pm iN_2)\,|j\mu\rangle = \mp[(j+1\pm\mu)(j+2\pm\mu)]^{\frac{1}{2}}C^{k\nu}_{j+1} \times |j+1\mu\pm1\rangle + k\nu\{[(j\mp\mu)(j+1\pm\mu)]^{\frac{1}{2}}/j(j+1)\} \times |j\mu\pm1\rangle \pm [(j\mp\mu)(j-1\mp\mu)]^{\frac{1}{2}}C^{k\nu}_j\,|j-1\mu\pm1\rangle,$$

$$C^{k\nu}_j = j^{-1}[(j^2 - k^2)(j^2 + \nu^2)/(4j^2 - 1)]^{\frac{1}{2}},$$

where we have suppressed k, ν in the vectors $|k\nu j\mu\rangle$. There is an error in Joos' coefficient of $|j\mu \pm 1\rangle$ in the expression for $(N_1 \pm iN_2)\,|j\mu\rangle$; he has $[j(j+1)]^{-\frac{1}{2}}$ instead of $[j(j+1)]^{-1}$. The vectors $|j\mu\rangle$ are just $\Phi_{m,j}$ in Joos's notation and are related to Naĭmark's[2] f^k_ν by the following substitutions:

$$|j+1\mu\rangle \to -if^{k+1}_\nu,$$

$$|j\mu\rangle \to f^k_\nu,$$

$$|j-1\mu\rangle \to if^{k-1}_\nu,$$

$$(k, \nu, j, \mu) \to (k_0, -ic, k, \nu).$$

III. LORENTZ GROUP EXPANSIONS

We consider in this section the problem of constructing irreducible unitary representations of the restricted Lorentz group L_0 in terms of functions of a single 4-vector, x. The solution of this problem shall lead us to the desired decomposition of an arbitrary reasonably well-behaved function of x into a (possibly continuous) sum of functions transforming irreducibly under L_0.

As mentioned in the Introduction, we restrict ourselves to the spinless case ($G = 0$). This means that the generators of $\mathfrak{L}_0$ may be taken of the form

$$M_{\mu\nu} = X_{[\mu}P_{\nu]},$$

where

$$[P_\mu, X_\nu] = ig_{\mu\nu}.$$

Let us immediately choose the representation

$$P_\mu = i\partial_\mu = i\partial/\partial x^\mu,$$

$$X_\mu = x_\mu,$$

$$-\infty < x_\mu < \infty, \qquad \mu = 0, 1, 2, 3.$$

Then

$$M_{\mu\nu} = ix_{[\mu}\partial_{\nu]},$$

$$F = x^2\partial^2 - 3x\cdot\partial - xx{:}\partial\partial$$

with $xx{:}\partial\partial = x^\mu x^\nu \partial_\mu\partial_\nu$. In addition to F, $\mathbf{M}^2$, and M_3, we may also diagonalize any one linear combination of the operators P^2, X^2, and $P\cdot X + X\cdot P$. We choose $P^2 = -\partial^2$, minus the d'Alembertian. Thus

$$(P^2, F, \mathbf{M}^2, M_3)\psi_{mfj\mu}(x) = (m^2, f, j(j+1), \mu)\psi_{mfj\mu}(x).$$

[8] H. Joos, Fortschr. Physik 10, 65 (1962).

The operator P^2 is extraneous to the Lorentz group and bears roughly the same relation to it as the radial part of the Laplacian to the three-dimensional rotation group. Not too much more will be said about P^2 in the following. The functions $\psi_{mfj\mu}(x)$ are expected to be concrete realizations of the abstract vectors $|kvj\mu\rangle$ of Sec. II, at least for the values of k and v satisfying $kv = 0$.

To get a more explicit form of the above eigenvalue equations, we put[9]

$$x = (x_0, x\mathbf{n}),$$
$$x = |\mathbf{x}|,$$
$$\mathbf{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta),$$

with

$$-\infty < x_0 < \infty,$$
$$0 \le x < \infty,$$
$$0 \le \theta \le \pi,$$
$$0 \le \varphi < 2\pi.$$

We find

$$-\boldsymbol{\partial} = \partial/\partial\mathbf{x} = \mathbf{n}\,\partial/\partial x - x^{-1}\mathbf{n}\times(\mathbf{n}\times\partial/\partial\mathbf{n}),$$
$$\partial/\partial\mathbf{n} = (\cos\theta\cos\varphi, \cos\theta\sin\varphi, -\sin\theta)\,\partial/\partial\theta + (-\sin\varphi/\sin\theta, \cos\varphi/\sin\theta, 0)\,\partial/\partial\varphi,$$
$$\mathbf{M} = -i\mathbf{n}\times\partial/\partial\mathbf{n},$$
$$\mathbf{N} = -i\mathbf{n}(x_0\,\partial/\partial x + x\,\partial/\partial x_0) - x_0x^{-1}\mathbf{n}\times\mathbf{M}.$$

From these results it follows that

$$-P^2 = \partial^2/\partial x_0^2 - \partial^2/\partial x^2 - 2x^{-1}\,\partial/\partial x + x^{-2}\mathbf{M}^2,$$
$$F = -(x_0\,\partial/\partial x + x\,\partial/\partial x_0)^2 - 2x_0x^{-1}(x_0\,\partial/\partial x + x\,\partial/\partial x_0) + (x_0^2 - x^2)x^{-2}\mathbf{M}^2,$$
$$-\mathbf{M}^2 = \partial^2/\partial\theta^2 + \cot\theta\,\partial/\partial\theta + (\sin\theta)^{-2}\,\partial^2/\partial\varphi^2,$$
$$M_3 = -i\,\partial/\partial\varphi.$$

It is clear that $\psi_{mfj\mu}(x)$ may be written as

$$\psi_{mfj\mu}(x) = \varphi^j_{mf}(x_0, x)a_{j\mu}(\mathbf{n}),$$

where the a's satisfy the eigenvalue equations

$$\mathbf{M}^2a_{j\mu} = j(j+1)a_{j\mu}, \qquad M_3a_{j\mu} = \mu a_{j\mu}, \tag{3.1}$$

and for integral j are just the familiar spherical harmonics[10]:

$$a_{j\mu}(\mathbf{n}) \equiv Y_{j\mu}(\theta,\varphi) = e^{i\mu\varphi}\left[\frac{2j+1}{4\pi}\frac{(j-\mu)!}{(j+\mu)!}\right]^{\frac{1}{2}}\mathsf{P}_j^\mu(\cos\theta),$$
$$\mathsf{P}_j^\mu(x) = \frac{(1-x^2)^{\mu/2}}{2^jj!}\frac{d^{j+\mu}}{dx^{j+\mu}}(x^2-1)^j.$$

We note the normalization

$$\int d\mathbf{n}a_{j\mu}(\mathbf{n})^*a_{j'\mu'}(\mathbf{n}) = \delta_{jj'}\delta_{\mu\mu'},$$
$$\int d\mathbf{n} = \int_0^\pi d\theta\sin\theta\int_0^{2\pi}d\varphi.$$

The $a_{j\mu}$ satisfy (2.4) with

$$M_1 \pm iM_2 = e^{\pm i\varphi}(\pm\partial/\partial\theta + i\cot\theta\,\partial/\partial\varphi).$$

Since

$$\mathsf{P}_j^\mu(-x) = (-)^{j+\mu}\mathsf{P}_j^\mu(x),$$
$$e^{i\mu(\varphi+\pi)} = (-)^\mu e^{i\mu\varphi},$$

we have

$$a_{j\mu}(-\mathbf{n}) = (-)^ja_{j\mu}(\mathbf{n}).$$

The completeness relations read

$$\sum_{\mu=-j}^{j}a_{j\mu}(\mathbf{n})a_{j\mu}(\mathbf{n}')^* = \frac{2j+1}{4\pi}P_j(\mathbf{n}\cdot\mathbf{n}'),$$
$$\mathbf{n}\cdot\mathbf{n}' = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi-\varphi'),$$
$$\sum_{j=0}^{\infty}(j+\tfrac{1}{2})P_j(\mathbf{n}\cdot\mathbf{n}') = \delta(1-\mathbf{n}\cdot\mathbf{n}').$$

The solutions $\mathsf{P}_j^\mu(\cos\theta)$ of (3.1) for $j = 0, 1, 2, \cdots$, and $\mu = j, j-1, \cdots, -j$ are unique, bounded, differentiable, single-valued, and normalizable on the interval $0 \le \theta \le \pi$. For half-integral j at least one of these properties fails to be true. More precisely, the following situation holds. For $j = \frac{1}{2}, \frac{3}{2}, \cdots$ and $\frac{1}{2} \le \mu \le j$ the functions $\mathsf{P}_j^{-\mu}(\cos\theta)$ are quite satisfactory. However, for negative μ and $j > \frac{1}{2}$ these functions are not square-integrable with respect to the measure $d(\cos\theta)$ and hence must be discarded. One may be tempted to use $a_{j\mu} \sim \mathsf{P}_j^{-|\mu|}(\cos\theta)$. But then a repeated application of $M_1 - iM_2$ to $\mathsf{P}_j^{-\frac{1}{2}}(\cos\theta)$ leads to the undesirable functions $\mathsf{P}_j^\nu(\cos\theta)$ with $\nu = \frac{1}{2}, \frac{3}{2}, \cdots$ Nothing new is gained by admitting Legendre functions of the second kind because of the identity

$$\mathsf{Q}_j^\mu(x) = (-)^{\mu+\frac{1}{2}}\frac{\pi}{2}\frac{(j+\mu)!}{(j-\mu)!}\mathsf{P}_j^{-\mu}(x).$$

The only admissible set of solutions is for $j = \frac{1}{2}$ for which the two functions $(\sin\theta)^{\frac{1}{2}}$ and $(\sin\theta)^{-\frac{1}{2}}\cos\theta$ are normalizable. Thus, except for this single case,

[9] Note that x is used to denote both the 4-vector (x_μ) and the magnitude of its spatial part, $|\mathbf{x}|$. The usage should be clear from context.

[10] See, e.g., M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957).

half-integral angular momentum solutions of (3.1) are pathological and will henceforth be ignored.[11]

The function φ^j_{mf} satisfies

$$(F_j, P^2_j)\varphi^j_{mf}(x_0, x) = (f, m^2)\varphi^j_{mf}(x_0, x),$$

where the subscript j indicates that $\mathbf{M}^2$ in F and P^2 has been replaced by its eigenvalue $j(j+1)$. To separate variables in the above equations, let

$$r^2 = x_0^2 - x^2 \qquad (-\infty < r^2 < \infty),$$
$$\rho = x_0/x \qquad (-\infty < \rho < \infty),$$

and assume the decomposition

$$\varphi^j_{mf}(x_0, x) = b^j_f(\rho)c^f_m(r). \tag{3.2}$$

Transforming to the new variables and substituting (3.2), we find

$$\left[(1-\rho^2)\frac{d^2}{d\rho^2} + j(j+1) + \frac{f}{1-\rho^2}\right]b^j_f(\rho) = 0, \tag{3.3}$$

$$\left(\frac{d^2}{dr^2} + \frac{3}{r}\frac{d}{dr} + \frac{f}{r^2} + m^2\right)c^f_m(r) = 0. \tag{3.4}$$

We may think of the functions $\psi_{mfj\mu}(x)$ as being the transformation coefficients between the vectors $|x\rangle$ (eigenvectors of X_μ) and $|mfj\mu\rangle$:

$$\psi_{mfj\mu}(x) = \langle x \mid mfj\mu\rangle.$$

Thus, with proper normalizations, we shall require that

$$\int dx\langle mfj\mu \mid x\rangle\langle x \mid m'f'j'\mu'\rangle = \delta(m-m')\delta(f \mid f')\delta_{jj'}\delta_{\mu\mu'}$$

and

$$\int df \int dm \sum_{j,\mu} \langle x \mid mfj\mu\rangle\langle mfj\mu \mid x'\rangle = \delta(x-x'),$$

where

$$dx = dx_0\, dx_1\, dx_2\, dx_3,$$

$$\delta(x-x') = \prod_{\mu=0}^{3} \delta(x_\mu - x'_\mu),$$

and $\delta(f|f')$ is either $\delta_{kk'}$ or $\delta(\nu-\nu')$, depending on whether f and f' are discrete or continuous; similarly, $\int df$ stands either for $\int d\nu$ or $\sum_k$.

The volume element $\int dx$ may be decomposed into three parts, each invariant under L_0:

$$\int dx = \int dx\ \theta(x^2)\theta(x_0) + \int dx\ \theta(x^2)\theta(-x_0) + \int dx\ \theta(-x^2),$$

where

$$\theta(\alpha) = \begin{cases} 0 & \alpha \le 0, \\ 1 & \alpha > 0. \end{cases}$$

In terms of the variables r^2, ρ, and $\mathbf{n}$, we have

$$\int dx\ \theta(x^2)\theta(x_0) = \int_0^\infty dr^2\, r^2 \int_1^\infty d\rho\ \tfrac{1}{2}(\rho^2-1)^{-2} \int d\mathbf{n}, \tag{3.5}$$

$$\int dx\ \theta(x^2)\theta(-x_0) = \int_0^\infty dr^2\, r^2 \int_{-\infty}^{-1} d\rho\ \tfrac{1}{2}(\rho^2-1)^{-2} \int d\mathbf{n}, \tag{3.6}$$

$$\int dx\ \theta(-x^2) = \int_{-\infty}^0 dr^2\, r^2 \int_{-1}^1 d\rho\ \tfrac{1}{2}(\rho^2-1)^{-2} \int d\mathbf{n}. \tag{3.7}$$

Our solutions will be appropriately normalized with respect to the above measures.

Let us now proceed to the solution of the eigenvalue equation $F_j b^j_f = f b^j_f$. It is easily verified that two linearly independent solutions of (3.3) are

$$(\rho^2-1)^{\frac{1}{2}}P^\alpha_j(\rho) \quad \text{and} \quad (\rho^2-1)^{\frac{1}{2}}Q^\alpha_j(\rho),$$

where P^α_j and Q^α_j are the associated Legendre functions of the first and second kinds,[12] respectively, and

$$\alpha = (1-f)^{\frac{1}{2}} = (k^2-\nu^2)^{\frac{1}{2}}.$$

The Legendre functions are single-valued and regular in the complex ρ-plane cut from $-\infty$ to 1. The timelike and spacelike solutions are quite different qualitatively and require individual discussion. We consider the timelike case first.

Timelike Case

For a timelike vector x we have $x_0^2 - x^2 = r^2 > 0$ and $\rho^2 = (x_0/x)^2 > 1$. Thus ρ falls in either of the two open intervals $(1, \infty)$ or $(-\infty, -1)$. Consider functions on $(1, \infty)$. Using the volume element (3.5), we shall require

$$\frac{1}{2}\int_1^\infty d\rho\ (\rho^2-1)^{-2} b^j_f(\rho)^* b^j_{f'}(\rho) = \delta(f \mid f'). \tag{3.8}$$

[11] See, however, the discussion of the rotation group representations for an arbitrary complex j given by V. S. Popov and E. I. Dolinskiĭ, Soviet Physics JETP 19, 1232 (1964).

[12] All formulas quoted here concerning the Legendre functions are to be found in A. Erdélyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1, pp. 120–181.

Remembering that $g = 2k\nu = 0$ and disregarding half-integral representations according to previous arguments, we have three separate cases to consider:

$$\text{(i)}\quad \alpha = \pm k, \quad k = 1, 2, 3, \cdots;$$

$$\text{(ii)}\quad \alpha = \pm i\nu, \quad \nu > 0;$$

$$\text{(iii)}\quad \alpha = \pm\nu_0, \quad 0 < \nu_0 \leq 1.$$

Since

$$P_j^\alpha(\rho) \sim \rho^j, \qquad Q_j^\alpha(\rho) \sim \rho^{-j-1},$$

for $\rho \to \infty$, it follows that for $j > 0$ only the Q_j^α can be used. Now

$$Q_j^\alpha(\rho) \sim \begin{cases} (\rho - 1)^{-\alpha/2}, & \operatorname{Re}\alpha > 0, \\ (\rho - 1)^{\alpha/2}, & \operatorname{Re}\alpha < 0, \end{cases} \tag{3.9}$$

at $\rho \sim 1$, so that for the case (i) the solutions are unnormalizable, the integrand in (3.8) behaving like $(\rho - 1)^{-1-k/2}$. Thus we are left with cases (ii) and (iii) with $j = 0, 1, 2, \cdots$. Consider the case (ii). For $j = 1, 2, 3, \cdots$ we must use $Q_j^{i\nu}$ although for $j = 0$ both $Q_0^{i\nu}$ and $P_0^{i\nu}$ are admissible. We dismiss $P_0^{i\nu}$ by requiring that the $j = 0$ solution be obtainable by means of a lowering operator from the $j = 1$ function. Thus, with a slight change in notation, we have

$$b_\nu^j(\rho) = B_\nu^j(\rho^2 - 1)^{\frac{1}{2}} Q_j^{i\nu}(\rho) \tag{3.10}$$

with the normalization constant B_ν^j to be determined next. Noting

$$Q_j^{i\nu}(\rho) \underset{\rho\to 1^+}{\to} e^{-\pi\nu}\Gamma(j + 1 + i\nu) \times \operatorname{Re}\left\{\frac{\Gamma(i\nu)}{\Gamma(j + 1 + i\nu)}\left(\frac{\rho - 1}{2}\right)^{-\frac{1}{2}i\nu}\right\}$$

we find, using asymptotic integration, that

$$\frac{1}{2}\int_1^\infty d\rho\,(\rho^2 - 1)^{-1} Q_j^{i\nu}(\rho)^* Q_j^{i\nu'}(\rho) = \frac{\pi^2 e^{-2\pi\nu}}{4\nu \sinh \pi\nu}\,\delta(\nu - \nu')$$

plus a term proportional to $\delta(\nu + \nu') = 0$ (since $\nu, \nu' > 0$). Thus we see that the solutions (3.10) are normalized to $\delta(\nu - \nu')$ with

$$|B_\nu^j| = (2/\pi)e^{\pi\nu}(\nu \sinh \pi\nu)^{\frac{1}{2}}.$$

Using well-known relations between contiguous Legendre functions, one can ascertain that the functions

$$b_\nu^j(\rho) = i^j\left[\frac{\Gamma(j + 1 - i\nu)}{\Gamma(j + 1 + i\nu)}\right]^{\frac{1}{2}} \frac{2}{\pi} e^{\pi\nu}(\nu \sinh \pi\nu)^{\frac{1}{2}} \times (\rho^2 - 1)^{\frac{1}{2}} Q_j^{i\nu}(\rho) \qquad (1 < \rho < \infty), \tag{3.11}$$

multiplied by the $a_{j\mu}(\mathbf{n})$ behave canonically under the action of $\mathbf{M}$ and

$$\mathbf{N} = i\mathbf{n}(\rho^2 - 1)\,\partial/\partial\rho - \rho\mathbf{n} \times \mathbf{M}.$$

They are thus concrete realizations of the vectors $|k = 0\nu j\mu\rangle$ on the manifold of positive timelike 4-vectors $x(x^2 > 0, x_0 > 0)$.

Taking ρ in the interval $(-\infty, -1)$, we obtain solutions on the manifold of negative timelike 4-vectors $x(x^2 > 0, x_0 < 0)$. Using the fact that $(\rho^2 - 1)^{\frac{1}{2}} = -|\rho^2 - 1|^{\frac{1}{2}}$ for $\rho < -1$ and

$$Q_\nu^\mu(-\rho) = -e^{\pm i\pi\nu} Q_\nu^\mu(\rho) \qquad (\operatorname{Im}\rho \gtrless 0),$$

we find

$$b_\nu^j(\rho) = (-)^j b_\nu^j(-\rho) \qquad (\rho < -1),$$

for both signs of $\operatorname{Im}\rho$.

The solutions (3.11) can be put into a familiar form by setting

$$\rho = \coth \xi$$

and using Whipple's formula

$$Q_\nu^\mu(z) = e^{i\pi\mu}(\pi/2)^{\frac{1}{2}}\Gamma(1 + \nu + \mu)(z^2 - 1)^{-\frac{1}{4}} \times P_{-\frac{1}{2}-\mu}^{-\frac{1}{2}-\nu}[z(z^2 - 1)^{-\frac{1}{2}}] \qquad (\operatorname{Re} z > 0).$$

We find

$$b_\nu^j(\rho) = i^j(\tfrac{1}{2}\sinh\zeta)^{-\frac{1}{2}} \prod_{n=0}^{j} (\nu^2 + n^2)^{\frac{1}{2}} P_{-\frac{1}{2}\pm i\nu}^{-\frac{1}{2}-j}(\cosh\zeta),$$

where either sign of $\pm i\nu$ is valid. Using the integral representation

$$P_\nu^\mu(\cosh\alpha) = (2/\pi)^{\frac{1}{2}}(\sinh\alpha)^\mu[\Gamma(\tfrac{1}{2} - \mu)]^{-1} \times \int_0^\alpha dv\,(\cosh\alpha - \cosh v)^{-\mu-\frac{1}{2}} \cosh(\nu + \tfrac{1}{2})v$$

valid for $\operatorname{Re}\mu < \frac{1}{2}$, we have the alternate expression[13]

$$b_\nu^j(\rho) = i^j 2\pi^{-\frac{1}{2}} \prod_{n=0}^{j} (\nu^2 + n^2)^{\frac{1}{2}}(j!)^{-1}(\sinh\zeta)^{-j-1} \times \int_0^\zeta dv\,(\cosh\zeta - \cosh v)^j \cos\nu v.$$

This can also be written as[13]

$$b_\nu^j(\rho) = -(-i)^j 2\pi^{-\frac{1}{2}} \prod_{n=0}^{j} (\nu^2 + n^2)^{-\frac{1}{2}}(\sinh\zeta)^j \times d^{j+1}\cos\nu\zeta/d(\cosh\zeta)^{j+1}.$$

As shown by Joos,[8] the following completeness relation holds for the *ab*-functions:

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[13] A. Z. Dolginov and I. N. Toptygin, reference of Footnote 6.

$$\mathcal{K}_\nu(p) = \sum_{j=0}^{\infty} \sum_{\mu=-j}^{j} a_{j\mu}(\mathbf{n}) b_\nu^j(\rho) a_{j\mu}(\mathbf{n}')^* b_\nu^j(\rho')^*$$

$$= (\nu/\pi^2)(p^2 - 1)^{-\frac{1}{2}} \sin\{\nu \log[p + (p^2 - 1)^{\frac{1}{2}}]\},$$

$$p = \hat{x}\cdot\hat{x}' = x\cdot x'(r^2 r'^2)^{-\frac{1}{2}}, \qquad (3.12)$$

valid for $x_0, x_0' > 0$ and $x_0, x_0' < 0$, hence for $p > 1$. For the mixed case, $x_0 > 0$ and $x_0' < 0$ or $x_0 < 0$ and $x_0' > 0$, one has $p < -1$ and, as one may easily trace through,

$$\mathcal{K}_\nu(p) = -(\nu/\pi^2)(p^2 - 1)^{-\frac{1}{2}}$$

$$\times \sin\{\nu \log[-p - (p^2 - 1)^{\frac{1}{2}}]\}. \qquad (3.13)$$

The formulas (3.12) and (3.13) may be combined by writing

$$\mathcal{K}_\nu(p) = \nu[\pi^2(p^2 - 1)^{\frac{1}{2}}]^{-1}$$

$$\times \sin\{\nu \log[|p| + (p^2 - 1)^{\frac{1}{2}}]\} \quad (p^2 > 1) \qquad (3.14)$$

or

$$\mathcal{K}_\nu(p) = \nu\pi^{-2} \sin\zeta/\sinh\zeta$$

with

$$|p| = \cosh\zeta, \qquad \zeta > 0.$$

As further shown by Joos,[8]

$$\int_0^\infty d\nu\ \mathcal{K}_\nu(p) = 2\,|x_0|\, r^2\, \delta(x - x') \qquad (p > 1)$$

or, in a manifestly Lorentz-invariant form,

$$\int_0^\infty d\nu\ \mathcal{K}_\nu(p) = \int_0^\infty dr'^2\, r'^2\, \delta(x - x').$$

For $p < -1$ the integral vanishes, of course. Stated in a different way, we have the following decomposition of the four-dimensional delta function:

$$\delta(x - x')$$

$$= \{\pi^2 x^2[(\hat{x}\cdot\hat{x}')^2 - 1]^{\frac{1}{2}}\}^{-1}\, \delta(x^2 - x'^2)\theta(\hat{x}\cdot\hat{x}' - 1)$$

$$\times \int_0^\infty d\nu\ \nu \sin\{\nu \log(\hat{x}\cdot\hat{x}' + [(\hat{x}\cdot\hat{x}')^2 - 1]^{\frac{1}{2}})\}. \qquad (3.15)$$

The kernel $\mathcal{K}_\nu(p)$ has the "reproducing property" expressed by the formula

$$\int d\nu\ \delta(\nu^2 - 1)\mathcal{K}_\nu(u\cdot v)\mathcal{K}_\nu(u'\cdot v)$$

$$= \delta(\nu - \nu')\mathcal{K}_\nu(u\cdot u'), \qquad u^2 = u'^2 = 1, \qquad (3.16)$$

which may be verified by substituting expansions (3.12) for the kernels in the integrand or by direct integration.

Let us finally consider the case (iii) with $\alpha = \pm\nu_0$, $0 < \nu_0 \leq 1$. As we have seen, for $j > 0$ only the Q_j^α functions behave properly at $\rho = \infty$. However, (3.9) shows that

$$Q_j^{\pm\nu_0}(\rho) \sim (\rho - 1)^{-|\nu_0|/2}$$

at $\rho = 1$; hence they must be discarded. The only remaining possibility is to use the functions $P_0^{-\nu_0}(\rho)(j = 0)$ which behave like $(\rho - 1)^{\nu_0/2}$ at $\rho = 1$:

$$P_0^{-\nu_0}(\rho) = -\frac{1}{\Gamma(1 + \nu_0)}\left(\frac{\rho - 1}{\rho + 1}\right)^{\nu_0/2}.$$

A trivial calculation shows that

$$\frac{1}{2}\int_1^\infty d\rho\ (\rho^2 - 1)^{-1} P_0^{-\nu_0}(\rho)^* P_0^{-\nu_0'}(\rho)$$

$$= [2(\nu_0 + \nu_0')\Gamma(1 + \nu_0)\Gamma(1 + \nu_0')]^{-1}.$$

Thus these solutions are *not* orthogonal for different values of ν_0. This is not at all surprising since they correspond to the so-called complementary series of irreducible unitary representations of L_0 constructed on a Hilbert space with an inner product different from that of the Hilbert space appropriate to the basic (or principal) series of representations with k and ν real. We shall not further discuss the complementary series of representations in this paper since they do not occur in expansion formulas we are going to consider. We hope to examine these representations on another occasion.

Next on our agenda is the expansion problem of functions of timelike 4-vectors. Let us suppose that the function $\varphi(x)$ is square-integrable on the manifold $x^2 = r^2 > 0$, $x_0 > 0$:

$$\int dx\ \delta(x^2 - r^2)\theta(x_0)\ |\varphi(x)|^2 < \infty,$$

We define its "Lorentz transform" $\tilde{\varphi}_{\nu j\mu}(r^2)$ by

$$\tilde{\varphi}_{\nu j\mu}(r^2) = \int dx\ (x^2)^{-1}\ \delta(x^2 - r^2)\theta(x_0)\varphi(x)$$

$$\times\ a_{j\mu}(\mathbf{n})^* b_\nu^j(\rho)^*; \qquad (3.17)$$

the inverse is given by

$$\varphi(x) = \int_0^\infty d\nu \sum_{j=0}^{\infty} \sum_{\mu=-j}^{j} \tilde{\varphi}_{\nu j\mu}(r^2) a_{j\mu}(\mathbf{n}) b_\nu^j(\rho). \qquad (3.18)$$

A rigorous proof of these formulas is beyond the scope of this work; we may only remark that it parallels the proof given by Naĭmark[2] of a general theorem on the expansion of functions defined on the group manifold of the group $SL(2, C)$ homomorphic to the Lorentz group. The analog of the Plancherel

theorem[14] of the Fourier theory is the formula

$$\int dx\,(x^2)^{-1}\,\delta(x^2-r^2)\theta(x_0)\,|\varphi(x)|^2 = \int_0^\infty d\nu \sum_{j=0}^{\infty}\sum_{\mu=-j}^{j} |\tilde{\varphi}_{\nu j\mu}(r^2)|^2.$$

Spacelike Case

For a spacelike vector x we have $x_0^2 - x^2 = r^2 < 0$ and hence $\rho^2 = (x_0/x)^2 < 1$ or $-1 < \rho < 1$. The normalization to be imposed on our solutions is, according to (3.7),

$$\frac{1}{2}\int_{-1}^{1} d\rho\,(\rho^2-1)^{-2} b_\nu^j(\rho)^* b_{\nu'}^j(\rho) = \delta(f \mid f').$$

Just as in the timelike case considered above, we have here three sets of values of $\alpha = (1-f)^{\frac{1}{2}}$ to be investigated separately. We start with the case (ii), $\alpha = i\nu$, $\nu > 0$. Let us take the solutions $b_\nu^j(\rho)$ given by (3.11) for $\rho > 1$ and try to continue them into the region $\rho < 1$. Since $b_\nu^j(\rho)$ is regular in the complex ρ-plane cut from $-\infty$ to 1, we see that we get two different continuations, depending on whether we continue along the upper or the lower edges of the cut. Thus we shall consider the two functions $b_\nu^j(\rho + i0)$ and $b_\nu^j(\rho - i0)$; note that $b_\nu^j(\rho + i0) = b_\nu^j(\rho - i0)$ for $\rho^2 > 1$. On the interval $(-1, 1)$ it is advantageous to introduce the Legendre functions on the cut, $\mathsf{P}_j^{i\nu}(\rho)$ and $\mathsf{Q}_j^{i\nu}(\rho)$. Making use of the formulas

$$e^{\mp\nu}Q_j^{i\nu}(\rho \pm i0) = e^{\mp\pi\nu/2}[\mathsf{Q}_j^{i\nu}(\rho) \mp (i\pi/2)\mathsf{P}_j^{i\nu}(\rho)],$$

$$\mathsf{P}_j^{i\nu}(-\rho) = (-)^j[\cosh\pi\nu\,\mathsf{P}_j^{i\nu}(\rho) + (2/i\pi)\sinh\pi\nu\,\mathsf{Q}_j^{i\nu}(\rho)] \qquad (0 < \rho < 1),$$

$$[(\rho \pm i0)^2 - 1]^{\frac{1}{2}} = \pm i(1-\rho^2)^{\frac{1}{2}} \qquad (\rho^2 < 1),$$

we find

$$b_\nu^j(\rho \pm i0) = \pm\mathfrak{B}_\nu^j(\rho)[e^{\pm\pi\nu/2}\mathsf{P}_j^{i\nu}(\rho) - (-)^j e^{\mp\pi\nu/2}\mathsf{P}_j^{i\nu}(-\rho)],$$

$$\mathfrak{B}_\nu^j(\rho) = i^j\left(\frac{\nu}{\sinh\pi\nu}\right)^{\frac{1}{2}}\left[\frac{\Gamma(j+1-i\nu)}{\Gamma(j+1+i\nu)}\right]^{\frac{1}{2}}(1-\rho^2)^{\frac{1}{2}}.$$

Let us define the linear combinations

$$b_\nu^{j\pm}(\rho) = 2^{-\frac{1}{2}}\begin{pmatrix}\operatorname{csch}\pi\nu/2\\ \operatorname{sech}\pi\nu/2\end{pmatrix}[b_\nu^j(\rho+i0) \pm b_\nu^j(\rho-i0)] = 2^{-\frac{1}{2}}\mathfrak{B}_\nu^j(\rho)[\mathsf{P}_j^{i\nu}(\rho) \pm (-)^j\mathsf{P}_j^{i\nu}(-\rho)]. \qquad (3.17)$$

It is clear that

$$b_\nu^{j\pm}(-\rho) = \pm(-)^j b_\nu^{j\pm}(\rho). \qquad (3.18)$$

[14] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Oxford University Press, London, 1948) 2nd ed.

A simple computation shows that

$$\frac{1}{2}\int_{-1}^{1} d\rho\,(\rho^2-1)^{-2} b_\nu^{j\pm}(\rho)^* b_{\nu'}^{j\pm}(\rho) = \delta(\nu_- - \nu').$$

The result

$$\frac{1}{2}\int_{-1}^{1} d\rho\,(\rho^2-1)^{-2} b_\nu^{j\pm}(\rho)^* b_{\nu'}^{j\mp}(\rho) = 0$$

follows from (3.18). The factor $2^{-\frac{1}{2}}$ in (3.17) is necessary for proper normalization since for the spacelike case both $\rho = +1$ and $\rho = -1$ endpoints contribute to $\delta(\nu - \nu')$.

The kernels

$$\mathcal{K}_\nu^\pm(p) = \sum_{j=0}^{\infty}\frac{2j+1}{4\pi}P_j(\mathbf{n}\cdot\mathbf{n}')b_\nu^{j\pm}(\rho)b_\nu^{j\pm}(\rho')^*$$

are evaluated in Appendix A, where it is shown that

$$\mathcal{K}_\nu^\pm(p) = \begin{cases}\mp\frac{1}{2}\mathcal{K}_\nu(p) & p > 1,\\ 0 & -1 < p < 1,\\ -\frac{1}{2}\mathcal{K}_\nu(p) & p < -1;\end{cases} \qquad (3.19)$$

here $\mathcal{K}_\nu(p)$ is given by (3.14). Note that under $p \to -p$, we have $\mathcal{K}_\nu^\pm(p) \to \pm\mathcal{K}_\nu^\pm(p)$, as necessary.

Let us next consider the case (i) with $\alpha = k$, $k = 1, 2, 3, \cdots$. It is known that the Legendre functions $\mathsf{P}_j^k(\rho)$ form an orthogonal set with respect to the weight function $(1-\rho^2)^{-1}$:

$$\int_{-1}^{1} d\rho\,(1-\rho^2)^{-1}\mathsf{P}_j^k(\rho)\mathsf{P}_j^{k'}(\rho) = \delta_{kk'}(j+k)!/k(j-k)!.$$

Thus we have the normalized solutions

$$b_k^j(\rho) = i^j\left[2k\frac{(j-k)!}{(j+k)!}\right]^{\frac{1}{2}}(1-\rho^2)^{\frac{1}{2}}\mathsf{P}_j^k(\rho), \qquad (3.20)$$

$$\frac{1}{2}\int_{-1}^{1} d\rho\,(\rho^2-1)^{-2} b_k^j(\rho)^* b_{k'}^j(\rho) = \delta_{kk'}.$$

We note that

$$\mathsf{P}_j^k(-\rho) = (-)^{j+k}\mathsf{P}_j^k(\rho).$$

The phase factor i^j has been determined by letting $i\nu \to k$ in the functions $b_\nu^{j\pm}(\rho)$ and ignoring an unimportant constant over-all phase factor. The solutions $\mathsf{Q}_j^{\pm k}$ behave as $(1-\rho)^{-k/2}$, $k = 1, 2, 3, \cdots$, for $\rho \sim 1$, and hence they are unnormalizable.

We compute next the kernel

$$\mathcal{K}_k(p) = \sum_{j=k}^{\infty}\frac{2j+1}{4\pi}P_j(\mathbf{n}\cdot\mathbf{n}')b_k^j(\rho)b_k^j(\rho')^*.$$

From (3.20) we have

$$b_k^j(\rho)b_k^j(\rho')^* = 2k\frac{(j-k)!}{(j+k)!}(1-\rho^2)^{\frac{1}{2}}(1-\rho'^2)^{\frac{1}{2}}\mathsf{P}_j^k(\rho)\mathsf{P}_j^k(\rho').$$

Using the addition theorem[15]

$$P_j(\cos\alpha) = P_j(\rho)P_j(\rho') + 2\sum_{m=1}^{j}\frac{(j-m)!}{(j+m)!}\mathsf{P}_j^m(\rho)\mathsf{P}_j^m(\rho')\cos m\omega,$$

$$\cos\alpha = \rho\rho' + (1-\rho^2)^{\frac{1}{2}}(1-\rho'^2)^{\frac{1}{2}}\cos\omega,$$

valid for $|\rho|, |\rho'| \leq 1$ of interest here, and the orthogonality relations

$$\frac{1}{\pi}\int_0^\pi d\omega \cos m\omega \cos n\omega = \begin{cases} 1 & m = n = 0, \\ \frac{1}{2} & m = n \geq 1, \\ 0 & m \neq n, \end{cases}$$

we obtain

$$\frac{(j-k)!}{(j+k)!}\mathsf{P}_j^k(\rho)\mathsf{P}_j^k(\rho') = \frac{1}{\pi}\int_0^\pi d\omega\, P_j(\cos\alpha)\cos k\omega \qquad (j \geq k \geq 1).$$

Thus

$$\mathcal{K}_k = \frac{k}{\pi^2}(1-\rho^2)^{\frac{1}{2}}(1-\rho'^2)^{\frac{1}{2}}\sum_{j=k}^{\infty}(j+\tfrac{1}{2})P_j(\mathbf{n}\cdot\mathbf{n}') \times \int_0^\pi d\omega\, P(\cos\alpha)\cos k\omega.$$

Interchanging the integration and summation and extending the latter to run from $j = 0$ at no extra cost (because of the orthogonality of $P_j(\cos\alpha)$ to $\cos k\omega$ for $j < k$), we find

$$\mathcal{K}_k = \frac{k}{\pi^2}(1-\rho^2)^{\frac{1}{2}}(1-\rho'^2)^{\frac{1}{2}} \times \int_0^\pi d\omega\, \delta(\cos\alpha - \mathbf{n}\cdot\mathbf{n}')T_k(\cos\omega),$$

where

$$T_k(\cos\omega) = \cos k\omega$$

is the kth Chebichef polynomial of the first kind.[16] Noting that

$$(1-\rho^2)^{\frac{1}{2}}(1-\rho'^2)^{\frac{1}{2}}\,\delta(\cos\alpha - \mathbf{n}\cdot\mathbf{n}') = \delta\left(\cos\omega + \frac{\rho\rho' - \mathbf{n}\cdot\mathbf{n}'}{(1-\rho^2)^{\frac{1}{2}}(1-\rho'^2)^{\frac{1}{2}}}\right) = \delta(\cos\omega + p),$$

we get

$$\mathcal{K}_k = kT_k(-p)\theta(1-|p|)/\pi^2(1-p^2)^{\frac{1}{2}}. \qquad (3.21)$$

This kernel, too, has the reproducing property

$$\int dv\, \delta(v^2+1)\mathcal{K}_k(u\cdot v)\mathcal{K}_{k'}(u'\cdot v) = \delta_{kk'}\mathcal{K}_k(u\cdot u').$$

Moreover, it is orthogonal to $\mathcal{K}_\nu^\pm$:

$$\int dv\, \delta(v^2+1)\mathcal{K}_k(u\cdot v)\mathcal{K}_\nu^\pm(u'\cdot v) = 0;$$

this follows from the easily proved orthogonality of b_k^j and $b_\nu^{j\pm}$.

As we show in detail in Appendix B, the completeness relation for spacelike solutions of (3.3) is

$$(1-\rho^2)\delta(\rho-\rho') = \frac{1}{2}\int_0^\infty d\nu\,\nu(\sinh\pi\nu)^{-1}[\mathsf{P}_j^{i\nu}(\rho)\mathsf{P}_j^{-i\nu}(\rho') + \mathsf{P}_j^{i\nu}(-\rho)\mathsf{P}_j^{-i\nu}(-\rho')] + \sum_{k=1}^{\infty}k\frac{(j-k)!}{(j+k)!}\mathsf{P}_j^k(\rho)\mathsf{P}_j^k(\rho')$$

for $j \geq 1$; when $j = 0$, the last term is omitted. Multiplying this through by

$$(-2/x^2)\,\delta(x^2-x'^2)(1-\rho^2)(2j+1)P_j(\mathbf{n}\cdot\mathbf{n}')/4\pi$$

and summing on j from 0 to ∞, we find, on interchanging j-summation with ν-integration and k-summation in the above,

$$\begin{aligned}\delta(x-x') &= -(2/x^2)\,\delta(x^2-x'^2)(1-\rho^2)^2 \times \delta(\rho-\rho')\,\delta(1-\mathbf{n}\cdot\mathbf{n}') \\ &= -(1/x^2)\,\delta(x^2-x'^2)\left\{\sum_{k=1}^{\infty}\mathcal{K}_k(p) + \int_0^\infty d\nu[\mathcal{K}_\nu^+(p)+\mathcal{K}_\nu^-(p)]\right\}, \qquad (3.22)\end{aligned}$$

where

$$\mathcal{K}_\nu^+(p) + \mathcal{K}_\nu^-(p) = -\mathcal{K}_\nu(p)\theta(-1-p)$$

and $\mathcal{K}_\nu$ is given by (3.14). The formula (3.22) is the spacelike analog of (3.15).

No continuous normalizable solutions of (3.3) can be found for the case (iii) with $\alpha = \pm\nu_0$, $0 < \nu_0 \leq 1$, because of the singular behavior of both Legendre functions at $\rho = -1$. A particular linear combinations of the two Legendre functions which is nonsingular at $\rho = -1$ becomes singular at $\rho = +1$ and vice versa. If one is prepared to accept solutions which themselves or their derivatives are discontinuous at some interior point of the interval $(-1, 1)$, then normalizable solutions may indeed be constructed. We shall not consider them.

The expansion formulas for the spacelike case are obvious analogs of those previously given for the timelike case, except that now we must include both discrete and continuous contributions.

[15] A. Erdélyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 2, p. 244.

[16] Reference of Footnote 15, p. 183.

As an application of the expansion formulas, we consider in Appendix C a decomposition of the plane-wave solutions of the Klein–Gordon equation (for positive and negative m^2) in terms of the Lorentz-irreducible functions discussed above.

IV. LIGHTLIKE SOLUTIONS

In the lightlike case we have $x_0^2 = x^2$, and hence the "spherical" and the "radial" equations, (3.3) and (3.4), are both in terms of the same independent variable. Consequently, a novel situation obtains. We write

$$|x_0| = e^u = (x_1^2 + x_2^2 + x_3^2)^{\frac{1}{2}} \qquad (-\infty < u < \infty)$$

and consider x_1, x_2, x_3 as independent variables. The expressions for $\mathbf{M}^2$ and M_3 are the same as before while those for F and P^2 are obtained by setting $\partial_0 \equiv 0$ in the corresponding expressions for the timelike and spacelike cases given in Sec. III. We find

$$P^2 = e^{-2u}(\partial^2/\partial u^2 + \partial/\partial u - \mathbf{M}^2),$$
$$F = -\partial^2/\partial u^2 - 2\partial/\partial u.$$

Diagonalization of F leads to the eigenvalue equation

$$(d^2/du^2 + 2\, d/du + f)b_f(u) = 0$$

with solutions, for $f \neq 1$,

$$b_f(u) = C_1 e^{\beta_1 u} + C_2 e^{\beta_2 u}, \tag{4.1}$$
$$\beta_{1,2} = -1 \pm (1 - f)^{\frac{1}{2}}.$$

The invariant volume element is[17]

$$\int dx\ \delta(x^2) = \frac{1}{2}\int_{-\infty}^{\infty} du\, e^{2u} \int d\mathbf{n}.$$

The only normalizable class of solutions (4.1) is that for $f = 1 + \nu^2$, $\nu > 0$. One easily verifies that the functions

$$b_\nu^\pm(u) = (-i)^j e^{(-1 \pm i\nu)u} \pi^{-\frac{1}{2}} \left[\frac{\Gamma(j + 1 \pm i\nu)}{\Gamma(j + 1 \mp i\nu)}\right]^{\frac{1}{2}}$$

satisfy

$$\frac{1}{2}\int_{-\infty}^{\infty} du\, e^{2u} b_\nu^\pm(u)^* b_{\nu'}^\pm(u) = \delta(\nu - \nu'),$$
$$\frac{1}{2}\int_{-\infty}^{\infty} du\, e^{2u} b_\nu^\pm(u)^* b_{\nu'}^\mp(u) = 0,$$

and, multiplied by $a_{j\mu}(\mathbf{n})$, behave canonically under $\mathbf{M}$ and

$$\mathbf{N} = -i(\mathbf{n}\, \partial/\partial u + \partial/\partial \mathbf{n}).$$

We also have the completeness relation

$$\int_0^\infty d\nu\, [b_\nu^+(u) b_\nu^+(u')^* + b_\nu^-(u) b_\nu^-(u')^*] = 2e^{-2u}\, \delta(u - u').$$

It should be clear that the solutions $b_\nu^\pm$ do *not* satisfy the eigenvalue equation $P^2\psi = m^2\psi$ for $m^2 \neq 0$. If $m^2 = 0$, then $P^2\psi = 0$ can be satisfied only at the expense of having $j = \pm i\nu$ or $j = -1 \pm i\nu$, of no interest to us.

From the above we see that lightlike solutions are of a rather simple nature, being pure exponentials independent of the angular momentum j. It follows that various expansion formulas are just those of the Fourier integral theory which need not be repeated here.[14]

V. DISCUSSION

The theory of decomposing functions defined on a manifold according to irreducible representations of a given group is known in the mathematical literature as harmonic analysis.[18] A familiar example is the theory of Fourier integrals connected with the group R of real numbers under addition. Viewed in this light, our work might be described as a physicist's version of harmonic analysis associated with the Lorentz group L_0. The noncompact nature of L_0 (or R) is reflected in the occurrence of delta-function normalizations for the basis functions of some of the representations. This fact does not present any great difficulty. The non-Abelian character of L_0 is, on the other hand, the real source of complications because of the appearance of associated Legendre functions with complex-valued indices, as contrasted with simple exponentials in the case of the group R.

Let us briefly summarize the results of the preceding sections. We have found that the discrete representations of L_0($\nu = 0$, $k = 1, 2, 3, \cdots$) occur only in the spacelike case. The continuous series of representations ($\nu > 0$, $k = 0$) occur in all three cases. All these representations belong to the principal series of irreducible unitary representations of L_0. Normalizable continuous solutions belonging to the complementary series of representations are available in the timelike case only. They are nonorthogonal with respect to the inner product used for the remaining solutions. Moreover, they fail to appear in expansion formulas.

A unified treatment of timelike and spacelike

[17] We omit the factor $\theta(\pm x_0)$ on the understanding that the sign of x_0 is fixed, solutions for both signs being the same.

[18] G. Bachman, *Elements of Abstract Harmonic Analysis* (Academic Press Inc., New York, 1964).

solutions is obtained if one uses the parametrization $x_0^2 - x^2 = r^2$, $x_0/x = \rho$. Then $-\infty < \rho < \infty$, and $\rho > 1$, $-1 < \rho < 1$, and $\rho < -1$ correspond to the positive timelike, spacelike, and negative timelike cases, respectively. Positive timelike solutions may be continued to the spacelike region along either the upper or the lower edges of the cut $(-1, 1)$ in the complex ρ-plane, yielding two sets of solutions with different reflection properties under $\rho \to -\rho$.

We should point out the well-known fact that the noncompact Lorentz group L_0 is very closely related to the compact group R_4 of real rotations in four dimensions. Formally, the transition from L_0 to R_4 is accomplished by letting $x_0 = ix_4$, x_4 real, or, in terms of the group generators, $(\mathbf{M}, \mathbf{N}) \to (\mathbf{M}, i\mathbf{N})$. The solutions of the eigenvalue equation $F\psi = f\psi$ for the case of R_4 may be obtained by simply continuing the solutions for L_0 in the eigenvalue f (which now takes on a discrete set of values only). Our approach based on differential equations makes the connection between R_4 and L_0 very explicit and easily tractable.

A possible physical application of our formalism would be to the treatment of the Bethe–Salpeter equation[19] dispensing with the sometimes problematical Wick's rotation[20] of momenta to the euclidian region. Another application that comes to mind is to scattering amplitudes, in the manner of Shapiro.[5] Finally, it is known that R_4 and L_0 are the symmetry groups of the nonrelativistic Coulomb field for bound and continuum states, respectively.[21–24] In view of the close connection between the two groups, as just discussed, one sees that yet another, and very important, application of the L_0-representations would be to the class of problems involving the nonrelativistic Coulomb field.

APPENDIX A

Our goal in this appendix is to calculate the sums

$$\mathcal{K}_\nu^\pm(\hat{x}\cdot\hat{x}') = \sum_{j=0}^{\infty} \frac{2j+1}{4\pi} P_j(\mathbf{n}\cdot\mathbf{n}') b_\nu^{j\pm}(\rho) b_\nu^{j\pm}(\rho')^* \quad \text{(A1)}$$

for the spacelike case $\hat{x}^2 = \hat{x}'^2 = -1$. We recall that

$$b_\nu^{j\pm}(\rho) = i^j \left(\frac{\nu}{2\sinh \pi\nu}\right)^{\frac{1}{2}} \left[\frac{\Gamma(j+1-i\nu)}{\Gamma(j+1+i\nu)}\right]^{\frac{1}{2}} \sin\theta \times [\mathsf{P}_j^{i\nu}(\cos\theta) \pm (-)^j \mathsf{P}_j^{i\nu}(-\cos\theta)],$$

where we have put

$$\rho = \cos\theta, \qquad 0 < \theta < \pi.$$

Rather than attempting to sum (A1) directly, we consider first the sums

$$\chi_\nu^\pm = \sum_{j=0}^{\infty} \frac{2j+1}{4\pi} P_j(\mathbf{n}\cdot\mathbf{n}') \left(\frac{\nu}{2\sinh \pi\nu}\right)^{\frac{1}{2}} \sin\theta \times [\mathsf{P}_j^{i\nu}(\cos\theta) \pm (-)^j \mathsf{P}_j^{i\nu}(-\cos\theta)].$$

Using the representations[25]

$$\mathsf{P}_j^{i\nu}(\cos\theta) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{(\sin\theta)^{i\nu}}{\Gamma(\frac{1}{2} - i\nu)} \times \int_0^\pi d\varphi\, (\cos\varphi - \cos\theta)_+^{-\frac{1}{2}-i\nu} \cos(j+\tfrac{1}{2})\varphi,$$

$$(-)^j \mathsf{P}_j^{i\nu}(-\cos\theta) = (-)^j [\mathsf{P}_j^{i\nu}(\cos\theta)\cos(j+i\nu)\pi - (2/\pi)\mathsf{Q}_j^{i\nu}(\cos\theta)\sin(j+i\nu)\pi] = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{(\sin\theta)^{i\nu}}{\Gamma(\frac{1}{2}-i\nu)} \int_0^\pi d\varphi\, (\cos\varphi - \cos\theta)_-^{-\frac{1}{2}-i\nu} \sin(j+\tfrac{1}{2})\varphi,$$

where

$$x_+ = \begin{cases} x & x > 0, \\ 0 & x \le 0, \end{cases} \qquad x_- = \begin{cases} 0 & x \ge 0, \\ -x & x < 0, \end{cases}$$

we have, upon interchanging summation and integration,

$$\chi_\nu^\pm = \tfrac{1}{2}(\pi^3 \sinh \pi\nu)^{-\frac{1}{2}} \frac{(\sin\theta)^{1+i\nu}}{\Gamma(\frac{1}{2}-i\nu)} \times \int_0^\pi d\varphi \sum_{j=0}^{\infty} (j+\tfrac{1}{2}) P_j(\mathbf{n}\cdot\mathbf{n}'') \times [(\cos\varphi - \cos\theta)_+^{-\frac{1}{2}-i\nu} \cos(j+\tfrac{1}{2})\varphi \pm (\cos\varphi - \cos\theta)_-^{-\frac{1}{2}-i\nu} \sin(j+\tfrac{1}{2})\varphi].$$

Let

$$S = \sum_{j=0}^{\infty} (j+\tfrac{1}{2}) P_j(\mathbf{n}\cdot\mathbf{n}'') \cos(j+\tfrac{1}{2})\varphi = \frac{1}{2i}\frac{\partial}{\partial\varphi} \sum_{j=0}^{\infty} P_j(\mathbf{n}\cdot\mathbf{n}'')[e^{\frac{1}{2}i\varphi}(e^{i\varphi})^j - e^{-\frac{1}{2}i\varphi}(e^{-i\varphi})^j].$$

To make the sums meaningful, we let $e^{i\varphi} \to e^{i(\varphi+i\epsilon)}$, $e^{-i\varphi} \to e^{-i(\varphi-i\epsilon)}$, $\epsilon > 0$. Then the two series are of the form $\sum_j P_j h^j$, $|h| < 1$, for which the following formula is valid:

$$\sum_{j=0}^{\infty} P_j(\cos\alpha) h^j = (1 - 2h\cos\alpha + h^2)^{-\frac{1}{2}}.$$

[19] E. E. Salpeter and H. A. Bethe, Phys. Rev. **84**, 1232 (1951).
[20] G. C. Wick, Phys. Rev. **96**, 1124 (1952).
[21] V. Fock, Z. Physik **98**, 145 (1935).
[22] V. Bargmann, Z. Physik **99**, 576 (1936).
[23] L. C. Biedenharn, J. Math. Phys. **6**, 433 (1965).
[24] L. C. Biedenharn and P. J. Brussaard, *Coulomb Excitation* (Oxford University Press, New York, 1965).
[25] W. Magnus and F. Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1954), pp. 66–67.

Thus we find

$$S = -i2^{-\frac{1}{2}}\frac{\partial}{\partial\varphi}\{[\cos(\varphi + i\epsilon) - \mathbf{n}\cdot\mathbf{n}'']^{-\frac{1}{2}} - [\cos(\varphi - i\epsilon) - \mathbf{n}\cdot\mathbf{n}'']^{-\frac{1}{2}}\}.$$

Noting that

$$\cos(\varphi \pm i\epsilon) \simeq \cos\varphi \mp i\epsilon\sin\varphi, \quad \sin\varphi > 0 \quad (0 < \varphi < \pi),$$

and using the formulas[26]

$$(x \pm i\epsilon)^\lambda = x_+^\lambda + e^{\pm i\pi\lambda}x_-^\lambda,$$
$$(d/dx)x_\pm^\lambda = \pm\lambda x_\pm^{\lambda-1},$$

valid for an arbitrary complex $\lambda \neq -1, -2, \cdots$ in the limit $\epsilon \to 0^+$, we find with $\lambda = -\frac{1}{2}$ that

$$S = -2^{-\frac{1}{2}}\sin\varphi(\cos\varphi - \mathbf{n}\cdot\mathbf{n}'')_-^{-\frac{1}{2}}.$$

Similarly, we obtain

$$\sum_{j=0}^{\infty}(j + \tfrac{1}{2})P_j(\mathbf{n}\cdot\mathbf{n}'')\sin(j + \tfrac{1}{2})\varphi = -2^{-\frac{1}{2}}\sin\varphi(\cos\varphi - \mathbf{n}\cdot\mathbf{n}'')_+^{-\frac{1}{2}}.$$

Thus

$$\chi_\nu^\pm = -(4\pi)^{-\frac{1}{2}}(2\nu/\sinh\pi\nu)^{\frac{1}{2}} \times (\sin\theta)^{1+i\nu}[\Gamma(\tfrac{1}{2} - i\nu)]^{-1}\int_0^\pi d\varphi\sin\varphi \times \{(\cos\varphi - \cos\theta)_+^{-\frac{1}{2}-i\nu}(\cos\varphi - \mathbf{n}\cdot\mathbf{n}'')_-^{-\frac{1}{2}} \pm (\cos\varphi - \cos\theta)_-^{-\frac{1}{2}-i\nu}(\cos\varphi - \mathbf{n}\cdot\mathbf{n}'')_+^{-\frac{1}{2}}\}.$$

The first integral is taken over the values of φ satisfying $\mathbf{n}\cdot\mathbf{n}'' > \cos\varphi > \cos\theta$, while the second over those satisfying $\cos\theta > \cos\varphi > \mathbf{n}\cdot\mathbf{n}''$. Making the substitutions

$$t = \frac{\cos\varphi - \cos\theta}{\mathbf{n}\cdot\mathbf{n}'' - \cos\theta} \quad \text{and} \quad t = \frac{\cos\varphi - \mathbf{n}\cdot\mathbf{n}''}{\cos\theta - \mathbf{n}\cdot\mathbf{n}''}$$

in the first and second integrals, respectively, we find that both integrals are multiples of the beta function $B(-\frac{1}{2}, \frac{1}{2} - i\nu)$.[27] More precisely, the result is

$$\chi_\nu^\pm(\xi) = (2\nu)^{\frac{1}{2}}[4\pi\Gamma(-i\nu)(\sinh\pi\nu)^{\frac{1}{2}}]^{-1} \times (\xi_-^{-1-i\nu} \pm \xi_+^{-1-i\nu}), \qquad \text{(A2)}$$

$$\xi = (\cos\theta - \mathbf{n}\cdot\mathbf{n}'')/\sin\theta = \sinh\zeta - \mathbf{n}\cdot\mathbf{n}''\cosh\zeta. \qquad \text{(A3)}$$

[26] I. M. Gel'fand and G. E. Shilov, *Generalized Functions* (Academic Press Inc., New York, 1964), Vol. 1.

[27] Strictly speaking, the integrals do not exist because the factors $(\cos\varphi - \mathbf{n}\cdot\mathbf{n}'')_\pm^{-\frac{1}{2}}$ are nonintegrable at the singularity. This apparent difficulty may be eliminated by writing $\partial(\cdots)_\pm^{-\frac{1}{2}}/\partial(\cos\varphi) = -\partial(\cdots)_\pm^{-\frac{1}{2}}/\partial(\mathbf{n}\cdot\mathbf{n}'')$ and then integrating over φ.

It is easy to show that $\mathcal{K}_\nu^\pm$ may be calculated by the formula

$$\mathcal{K}_\nu^\pm = \int d\mathbf{n}''\,\chi_\nu^\pm(\sinh\zeta - \mathbf{n}\cdot\mathbf{n}''\cosh\zeta) \times \chi_\nu^\pm(\sinh\zeta' - \mathbf{n}'\cdot\mathbf{n}''\cosh\zeta')^*. \qquad \text{(A4)}$$

Substituting (A2) into (A4), we find

$$\mathcal{K}_\nu^\pm = (2\pi)^{-3}\nu^2(I_{++} + I_{--} \pm I_{+-} \pm I_{-+}),$$

where

$$I_{\alpha\beta} = \int d\mathbf{n}''\xi_\alpha^{-1-i\nu}\xi_\beta'^{-1+i\nu}, \qquad \alpha, \beta = \pm.$$

Now

$$\xi_+^{-1-i\nu}\xi_\pm'^{-1+i\nu} + \xi_-^{-1-i\nu}\xi_\mp'^{-1+i\nu} = \int_0^\infty d\alpha\,\alpha^{-i\nu}\delta\left(\alpha \mp \frac{\xi}{\xi'}\right)(\pm\xi\xi')^{-1} = (2\pi i)^{-1}\int_0^\infty d\alpha\,\alpha^{-i\nu}\{\xi^{-1}[(\alpha \pm i\epsilon)\xi' \mp \xi]^{-1} - \xi^{-1}[(\alpha \pm i\epsilon)\xi' \mp \xi]^{-1}\}.$$

Thus we are called upon to compute the integrals

$$J_\pm(z) = \int d\mathbf{n}''[\xi(z\xi' \pm \xi)]^{-1},$$

where $z = \alpha \pm i\epsilon, \to 0^+$. The expressions for the $\mathcal{K}_\nu^\pm$ in terms of the $J_\pm$ are

$$\mathcal{K}_\nu^\pm = (2\pi)^{-3}\nu^2(2\pi i)^{-1}\int_0^\infty d\alpha\,\alpha^{-i\nu}\{J_-(\alpha - i\epsilon) - J_-(\alpha + i\epsilon) \pm [J_+(\alpha + i\epsilon) - J_+(\alpha - i\epsilon)]\}.$$

From (A3) we find

$$J_\pm(z) = (m\cosh\zeta)^{-1}\int d\mathbf{n}''\,(u - \mathbf{n}\cdot\mathbf{n}'')^{-1} \times (u' - \hat{\mathbf{m}}\cdot\mathbf{n}'')^{-1}, \qquad \text{(A5)}$$

$$\mathbf{m} = z\cosh\zeta'\mathbf{n}' \pm \cosh\zeta\mathbf{n},$$
$$u = \tanh\zeta,$$
$$u' = (z\sinh\zeta' \pm \sinh\zeta')/m, \qquad \text{(A6)}$$
$$\hat{\mathbf{m}} = \mathbf{m}/m.$$

The integral (A5) is well-known and is given by[28]

$$\int d\mathbf{n}''\,(u - \mathbf{n}\cdot\mathbf{n}'')^{-1}(u' - \hat{\mathbf{m}}\cdot\mathbf{n}'')^{-1} = \frac{2\pi}{\kappa}\log\frac{uu' - \hat{\mathbf{m}}\cdot\mathbf{n} + \kappa}{uu' - \hat{\mathbf{m}}\cdot\mathbf{n} - \kappa},$$

$$\kappa^2 = (uu' - \hat{\mathbf{m}}\cdot\mathbf{n})^2 - (1 - u^2)(1 - u'^2),$$

$$\hat{\mathbf{m}}\cdot\mathbf{n} = (z\cosh\zeta'\mathbf{n}\cdot\mathbf{n}' \pm \cosh\zeta)/m.$$

[28] M. L. Goldberger in *Relations de dispersion et particules élémentaires*, ed. by C. de Witt (John Wiley & Sons, Inc., New York, 1960), p. 62.

Using (A6), we find

$$(uu' - \hat{\mathbf{m}}\cdot\mathbf{n})m = (1 + pz)/\cosh\zeta,$$

$$\kappa^2 m^2 = z^2(p^2 - 1)/\cosh^2\zeta,$$

$$p = \sinh\zeta\sinh\zeta' - \cosh\zeta\cosh\zeta'\mathbf{n}\cdot\mathbf{n}' \equiv \hat{x}\cdot\hat{x}'.$$

Thus

$$J_\pm(z, p) = \frac{2\pi}{z(p^2 - 1)^{\frac{1}{2}}}\log\frac{1 + z[p + (p^2 - 1)^{\frac{1}{2}}]}{1 + z[p - (p^2 - 1)^{\frac{1}{2}}]}.$$

Let us consider the case $p > 1$. Writing $p = \cosh\rho$, $\rho > 0$, we have

$$J_+(\alpha \pm i\epsilon, p) = \frac{2\pi}{(\alpha \pm i\epsilon)\sinh\rho}\log\frac{1 - (\alpha \pm i\epsilon)e^{\rho}}{1 - (\alpha \pm i\epsilon)e^{-\rho}}.$$

Using

$$(\alpha \pm i\epsilon)^{-1} = P/\alpha \mp i\pi\delta(\alpha),$$

$$\log(\alpha \pm i\epsilon) = \log|\alpha| \pm i\pi\theta(-\alpha),$$

we obtain

$$J_+(\alpha + i\epsilon, p) - J_+(\alpha - i\epsilon, p) = -\frac{4\pi^2 i}{\sinh\rho}\frac{P}{\alpha}[\theta(\alpha - e^{-\rho}) - \theta(\alpha - e^{\rho})].$$

In a similar manner, we find

$$J_-(\alpha + i\epsilon, p) - J_-(\alpha - i\epsilon, p) = 0$$

and, performing a trivial integration,

$$\mathcal{K}_\nu^{\pm}(p) = \mp\frac{\nu}{2\pi^2}\frac{\sin\nu\rho}{\sinh\rho} = \mp\frac{\nu}{2\pi^2(p^2 - 1)^{\frac{1}{2}}} \times \sin\{\nu\log[p + (p^2 - 1)^{\frac{1}{2}}]\} \quad (p > 1).$$

For the case $p < -1$, we write $p = -\cosh\rho$, $\rho > 0$, and find

$$\mathcal{K}_\nu^{\pm}(p) = -\frac{\nu}{2\pi^2}\frac{\sin\nu\rho}{\sinh\rho} = -\frac{\nu}{2\pi^2(p^2 - 1)^{\frac{1}{2}}} \times \sin\{\nu\log[-p + (p^2 - 1)^{\frac{1}{2}}]\} \quad (p < -1).$$

Finally, it is easy to check that $\mathcal{K}_\nu^{\pm}(p) = 0$ for $|p| < 1$.

APPENDIX B

In this appendix we derive an expansion formula for functions of a spacelike 4-vector argument. It is sufficient to treat only a part of the problem, namely, that associated with the eigenvalue equation $F\psi = f\psi$. We shall use the theory, notation, and results for second-order ordinary differential operators as discussed by Titchmarsh.[29]

[29] E. C. Titchmarsh, *Eigenfunction Expansions* (Oxford University Press, London, 1962), Part I, 2nd ed.

Let us put, for fixed j,

$$\rho = \tanh\zeta \qquad (-\infty < \zeta < \infty),$$

$$b_j^j(\rho) = \operatorname{sech}\zeta\chi_\lambda(\zeta),$$

$$\lambda = j - 1.$$

Then (3.3) reads

$$L\chi_\lambda = \lambda\chi_\lambda, \tag{B1}$$

where

$$L = -d^2/d\zeta^2 + q(\zeta),$$

$$q(\zeta) = -j(j + 1)\operatorname{sech}^2\zeta.$$

Solutions of (B1) are linear combinations of $\mathsf{P}_j^\alpha(\tanh\zeta)$ and $\mathsf{Q}_j^\alpha(\tanh\zeta)$ or, equivalently, of $\mathsf{P}_j^\alpha(\tanh\zeta)$ and $\mathsf{P}_j^\alpha(-\tanh\zeta)$, where

$$\alpha = (-\lambda)^{\frac{1}{2}}.$$

Let $\theta(\zeta, \lambda)$ and $\phi(\zeta, \lambda)$ be two solutions of (B1) satisfying the boundary conditions

$$\theta'(0, \lambda) = \phi(0, \lambda) = 0,$$

$$\theta(0, \lambda) = -\phi'(0, \lambda) = 1.$$

The first pair of boundary conditions is satisfied by

$$\theta(\zeta, \lambda) = A[\mathsf{P}_j^\alpha(\tanh\zeta) + \mathsf{P}_j^\alpha(-\tanh\zeta)],$$
$$\phi(\zeta, \lambda) = B[\mathsf{P}_j^\alpha(\tanh\zeta) - \mathsf{P}_j^\alpha(-\tanh\zeta)]. \tag{B2}$$

Imposition of the second pair of conditions yields

$$A = 1/2\mathsf{P}_j^\alpha(0),$$

$$B = -1/2\mathsf{P}_j^{\alpha\prime}(0),$$

where

$$\mathsf{P}_j^{\alpha\prime}(0) = [d\mathsf{P}_j^\alpha(x)/dx]_{x=0}.$$

It is clear that θ is symmetric and ϕ antisymmetric in $\tanh\zeta$ and hence ζ. Thus we may restrict our attention to the half-interval $(0, \infty)$ in ζ. Next, we must construct a solution of (B1) which is square-integrable on $(0, \infty)$. Suppose

$$\psi(\zeta, \lambda) = \theta(\zeta, \lambda) - m(\lambda)\phi(\zeta, \lambda)$$

is this solution (there is only one because we are dealing with the limit point case, as general theorems of Ref. 29 show). Using (B2), we have

$$\psi = (A - mB)\mathsf{P}_j^\alpha(\rho) + (A + mB)\mathsf{P}_j^\alpha(-\rho).$$

Since $\mathsf{P}_j^\alpha(-\rho)$ fails to be square-integrable at $\rho = +1$ for integral values of j of sole interest to us, we must set its coefficient equal to zero; thus

$$m(\lambda) = -A/B = \mathsf{P}_j^{\alpha\prime}(0)/\mathsf{P}_j^{\alpha}(0)$$
$$= 2\tan\frac{\pi(j+\alpha)}{2} \times \frac{\Gamma(1+\frac{1}{2}j+\frac{1}{2}\alpha)\Gamma(1+\frac{1}{2}j-\frac{1}{2}\alpha)}{\Gamma(\frac{1}{2}+\frac{1}{2}j+\frac{1}{2}\alpha)\Gamma(\frac{1}{2}+\frac{1}{2}j-\frac{1}{2}\alpha)}.$$

The Legendre function $\mathsf{P}_j^{\alpha}(\tanh\zeta)$ is square-integrable on $(0, \infty)$ provided $\operatorname{Re}\alpha < 0$; we henceforth assume that this condition holds. The expansion theorem takes the form

$$f(\zeta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\sigma(\lambda)\,\theta(\zeta,\lambda)\int_{-\infty}^{\infty} d\zeta'\,\theta(\zeta',\lambda)f(\zeta') + \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau(\lambda)\,\phi(\zeta,\lambda)\int_{-\infty}^{\infty} d\zeta'\,\phi(\zeta',\lambda)f(\zeta')$$

for every $f \in L^2(-\infty, \infty)$; here

$$\sigma(\lambda) = -\lim_{\delta\to 0^+}\int_0^{\lambda} du\,\operatorname{Im}[m(u+i\delta)]^{-1},$$
$$\tau(\lambda) = +\lim_{\delta\to 0^+}\int_0^{\lambda} du\,\operatorname{Im} m(u+i\delta).$$

In other words,

$$\delta(\zeta-\zeta') = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\sigma(\lambda)\,\theta(\zeta,\lambda)\theta(\zeta',\lambda) + \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau(\lambda)\,\phi(\zeta,\lambda)\phi(\zeta',\lambda).$$

It remains to compute the spectral functions σ and τ.

With the help of Γ-function identities we obtain

$$m(\lambda) = (j+\alpha)\prod_{n=1}^{j}\frac{j+\alpha-2n}{j+\alpha+1-2n}.$$

Decomposing this expression into partial fractions, we find

$$m(\lambda) = (j+\alpha)\times\left\{1-\sum_{n=1}^{j}\frac{2n(2j-2n+1)(2n-1)^{-1}}{j+\alpha+1-2n}\,a_{jn}\right\},$$
$$a_{jn} = (2n)!\,(2j-2n)!/[2^j n!\,(j-n)!]^2.$$

To calculate $\operatorname{Im} m$, we must specify the proper branch of α as a function of λ. Let us take a cut in the complex λ-plane running from 0 to $+\infty$ and put

$$\alpha = (e^{i\pi}\lambda)^{\frac{1}{2}}.$$

Then, setting

$$\lambda = |\lambda|\,e^{i\theta}, \qquad 0 < \theta < 2\pi,$$

we have

$$\alpha = |\lambda|^{\frac{1}{2}}\,e^{\frac{1}{2}i(\pi+\theta)}$$

and

$$\operatorname{Re}\alpha = -|\lambda|^{\frac{1}{2}}\sin\theta/2 < 0$$

for $0 < \theta < 2\pi$, as required for square-integrability of P_j^{α}. Letting further

$$\lambda = u + i\delta, \qquad -\infty < u < \infty, \qquad \delta > 0,$$

we find

$$\alpha = \begin{cases} iu^{\frac{1}{2}} - \delta', & u > 0 \\ -(-u)^{\frac{1}{2}} + i\delta', & u < 0. \end{cases} \qquad (\delta' > 0)$$

Thus for $u < 0$ we have

$$\operatorname{Im}(j+\alpha+1-2n)^{-1} = -\pi\delta(j+1-2n-(-u)^{\frac{1}{2}})$$

and

$$\operatorname{Im} m(u+i0) = \pi\sum_{n=1}^{j} 2n(2j-2n+1) \times a_{jn}\delta((-u)^{\frac{1}{2}} - j - 1 + 2n).$$

In a similar manner, we find

$$\operatorname{Im}[m(u+i0)]^{-1} = -\pi\sum_{n=0}^{j} a_{jn}\delta((-u)^{\frac{1}{2}} - j + 2n).$$

For $u > 0$, only the tangent function in (B3) contributes to $\operatorname{Im} m$:

$$\operatorname{Im} m(u+i0) = 2\left|\frac{\Gamma(1+j/2+i\sqrt{u}/2)}{\Gamma(\frac{1}{2}+j/2+i\sqrt{u}/2)}\right|^2 \times \begin{cases}\tanh\pi\frac{1}{2}u^{\frac{1}{2}} & j \text{ even},\\ \coth\pi\frac{1}{2}u^{\frac{1}{2}} & j \text{ odd},\end{cases}$$
$$\operatorname{Im}[m(u+i0)]^{-1} = -[\operatorname{Im} m(u+i0)]^{-1}.$$

A somewhat lengthy but straightforward computation now yields the result

$$\delta(\zeta-\zeta') = \frac{1}{2}\int_0^{\infty} d\nu\,\nu(\sinh\pi\nu)^{-1}[\mathsf{P}_j^{i\nu}(\rho)\mathsf{P}_j^{-i\nu}(\rho') + \mathsf{P}_j^{i\nu}(-\rho)\mathsf{P}_j^{-i\nu}(-\rho')] + \sum_{k=1}^{j} k\,\frac{(j-k)!}{(j+k)!}\,\mathsf{P}_j^{k}(\rho)\mathsf{P}_j^{k}(\rho').$$

APPENDIX C

As an illustration of the theory given in Sec. III, we shall expand the exponential function $\exp(-ip\cdot x)$ in terms of the eigenfunctions of the operators F and P^2 for the timelike and spacelike cases. These expansions are four-dimensional analogs of the well-known expansion

$$\exp(i\mathbf{p}\cdot\mathbf{x}) = \sum_{l=0}^{\infty}(2l+1)i^l j_l(px)P_l(\hat{\mathbf{p}}\cdot\hat{\mathbf{x}}). \qquad \text{(C1)}$$

The role of $j_l(px)$ is played by the solutions of the "radial equation" (3.4); in place of $P_l(\hat{\mathbf{p}}\cdot\hat{\mathbf{x}})$ we have the various kernels $\mathcal{K}$ discussed in Sec. III.

The point we wish to emphasize is that (C1) provides a decomposition of $\exp(i\mathbf{p}\cdot\mathbf{x})$ into a sum of functions with arguments invariant under rotations (namely, $|\mathbf{p}||\mathbf{x}|$ and $\hat{\mathbf{p}}\cdot\hat{\mathbf{x}}$). In the same manner, the anticipated expansions of $\exp(-ip\cdot x)$ will provide a decomposition of the exponential into a sum and/or integral of functions of $(\pm p^2x^2)^{\frac{1}{2}}$ and $\hat{p}\cdot\hat{x}$, i.e., a separation of $\exp(-ip\cdot x)$ into radial and spherical parts, each invariant under Lorentz transformations. There are several ways of obtaining the desired expansions. We shall use the method of direct integration which, although not the shortest, is perhaps more illuminating, especially in the spacelike case.

We start with the timelike case. The function $\exp(-ip\cdot x)$ is square-integrable on the manifold $\mathfrak{M}_+^\uparrow = \{x: x^2 = r^2 > 0, x_0 > 0\}$ provided $\operatorname{Im} p_0 < 0$, which we assume. Thus, according to (3.16), for $x \in \mathfrak{M}_+^\uparrow$ we have

$$e^{-ip\cdot x} = \int dx'\ \delta(x - x')e^{-ip\cdot x'} = \int_0^\infty d\nu\ \nu\varphi_\nu, \tag{C2}$$

where

$$\varphi_\nu = \int dx'\ \delta(x'^2 - r^2) \times \{\pi^2 r^2[(\hat{x}\cdot\hat{x}')^2 - 1]^{\frac{1}{2}}\}^{-1}\theta(\hat{x}\cdot\hat{x}' - 1) \times \sin\{\nu \log[\hat{x}\cdot\hat{x}' + ((\hat{x}\cdot\hat{x}')^2 - 1)^{\frac{1}{2}}]\}e^{-ip\cdot x'}.$$

Since x is positive timelike, we may choose a coordinate system in which $x = (r, \mathbf{0})$, $r > 0$. Letting $x_0' = r\cosh\zeta$, $\zeta > 0$, we find

$$\varphi_\nu = (2\pi^2)^{-1}\int_0^\infty d\zeta \sinh\zeta \sin\nu\zeta e^{-ip_0 r\cosh\zeta} \times \int d\mathbf{n}'\ \exp(i\mathbf{p}\cdot\mathbf{n}' r\sinh\zeta).$$

We may extend the integration on ζ to $-\infty$ provided we halve the result. The angular integration is trivial; we get

$$\varphi_\nu = (2\pi ipr)^{-1}\int_{-\infty}^\infty d\zeta \sin\nu\zeta e^{-ip_0 r\cosh\zeta} \times (e^{ipr\sinh\zeta} - e^{-ipr\sinh\zeta}), \qquad p = |\mathbf{p}|.$$

Suppose p is timelike. Then we take $p_0 = \epsilon m\cosh\zeta'$, $p = m\sinh\zeta'$, $\epsilon = \pm 1$, $m > 0$, $\zeta' > 0$ and find

$$\varphi_\nu^\epsilon = (2\pi ipr)^{-1}\int_{-\infty}^\infty d\zeta \sin\nu\zeta\{\exp[-i\epsilon mr \times \cosh(\zeta - \epsilon\zeta')] - \exp[-i\epsilon mr\cosh(\zeta + \epsilon\zeta')]\}.$$

Letting $\zeta \mp \epsilon\zeta' = \eta$ in appropriate exponentials, we have[30]

$$\varphi_\nu^\pm = \pm\frac{\sin\nu\zeta'}{\pi ipr}\int_{-\infty}^\infty d\eta \cos\nu\eta \exp[-i(\pm m)r\cosh\eta] = -\frac{1}{mr}e^{\pm\pi\nu/2}H_{i\nu}^{(2,1)}(mr)\frac{\sin\nu\zeta'}{\sinh\zeta'} \qquad \text{for } \epsilon = \pm 1. \tag{C3}$$

Here $H_{i\nu}^{(1,2)}$ are Hankel functions of the first and second kinds of order $i\nu$. Noting that $p\cdot x = \epsilon mr\cosh\zeta'$, the expansion formula (C2) takes the manifestly invariant form

$$e^{-ip\cdot x} = -[\lambda(u^2 - 1)^{\frac{1}{2}}]^{-1}\int_0^\infty d\nu\ \nu e^{\pm\frac{1}{2}\pi\nu}H_{i\nu}^{(2,1)}(\lambda) \times \sin[\nu\log(|u| + (u^2 - 1)^{\frac{1}{2}})] \qquad (x^2, x_0, p^2 > 0, p_0 \gtrless 0, \operatorname{Im} p_0 < 0)$$

with

$$\lambda = (p^2x^2)^{\frac{1}{2}} = mr > 0, \qquad u = \hat{p}\cdot\hat{x} = p\cdot x/\lambda.$$

Using (3.14), we may write this as

$$e^{-ip\cdot x} = \int_0^\infty d\nu\ \mathfrak{R}_\nu^\pm(\lambda)\mathcal{K}_\nu(u), \tag{C4}$$

$$\mathfrak{R}_\nu^\pm(\lambda) = -\pi^2\lambda^{-1}e^{\pm\pi\nu/2}H_{i\nu}^{(2,1)}(\lambda). \tag{C5}$$

Clearly, $\mathfrak{R}_\nu^\pm$ satisfies (3.4); it should also be pointed out that $\mathfrak{R}_\nu^\pm$ is essentially the Fourier sine transform of $(u^2 - 1)^{\frac{1}{2}}e^{-ip\cdot x}$.

Next, suppose p is spacelike. Letting $m \to -i\epsilon m$, $\zeta' \to \zeta' + \frac{1}{2}i\pi$ amounts to $p_0 = \epsilon m\cosh\zeta' \to p_0 = \epsilon m\sinh\zeta'$, $p = m\sinh\zeta' \to p = m\cosh\zeta'$. With these substitutions, (C3) becomes

$$\varphi_\nu = -i(\pi mr)^{-1}K_{i\nu}(mr)\frac{\sin\nu(\zeta' + \frac{1}{2}i\pi)}{\cosh\zeta'}, \qquad K_\alpha(z) = \tfrac{1}{2}\pi ie^{\frac{1}{2}i\pi\alpha}H_\alpha^{(1)}(iz).$$

Again, one has the manifestly invariant expansion

$$e^{-ip\cdot x} = (\pi[u^2 + 1]^{\frac{1}{2}})^{-1}\int_0^\infty d\nu\ \nu K_{i\nu}(\lambda) \times \{e^{\pi\nu/2}([u^2 + 1]^{\frac{1}{2}} - u)^{i\nu} - e^{-\frac{1}{2}\pi\nu}([u^2 + 1]^{\frac{1}{2}} + u)^{i\nu}\} \qquad (x^2, x_0, -p^2 > 0),$$

[30] Reference of Footnote 25, p. 26.

where now $\lambda = (-p^2x^2)^{\frac{1}{2}}$. To assure the convergence of the above integral the variable $\zeta' = (u^2+1)^{\frac{1}{2}} + u = [(u^2+1)^{\frac{1}{2}} - u]^{-1}$ must be given a small negative imaginary part.

Expansions on the manifold $\mathfrak{M}_+^{\downarrow} = \{x: x^2 = r^2 > 0, x_0 < 0\}$ are just complex conjugates of the corresponding expansions on $\mathfrak{M}_+^{\uparrow}$ given above; this follows from

$$e^{-ip\cdot x} \to e^{-ip_0x_0} = [e^{-ip_0(-x_0)}]^*.$$

We consider next expansions of the exponential function on the manifold $\mathfrak{M}_- = \{x: x^2 = r^2 < 0\}$. Using (3.22), we get

$$e^{-ip\cdot x} = \int dx'\ \delta(x-x')e^{-ip\cdot x'} = \int_0^\infty d\nu\ \nu\varphi_\nu^{(1)} + \sum_{k=1}^\infty k\varphi_k^{(2)}$$

with

$$\varphi_\nu^{(1)} = \int dx'\ \delta(x'^2 - r^2) \times \theta(-1 - \hat{x}\cdot\hat{x}')[\pi^2r^2((\hat{x}\cdot\hat{x}')^2 - 1)^{\frac{1}{2}}]^{-1} \times \sin\{\nu \log[|\hat{x}\cdot\hat{x}'| + ((\hat{x}\cdot\hat{x}')^2 - 1)^{\frac{1}{2}}]\}e^{-ip\cdot x'},$$

$$\varphi_k^{(2)} = -\int dx'\ \delta(x'^2 - r^2)\theta(1 - |\hat{x}\cdot\hat{x}'|) \times [\pi^2r^2(1 - (\hat{x}\cdot\hat{x}')^2)^{\frac{1}{2}}]^{-1}T_k(-\hat{x}\cdot\hat{x}')e^{-ip\cdot x'}.$$

We compute $\varphi_k^{(2)}$ first. It is convenient to introduce a change of variables of integration appropriate to the spacelike case. Just as in the timelike case one integrates over the three-dimensional rotation group, the little group[31] of timelike vectors with volume element $d\mathbf{n}$, so now one may integrate over the little group of spacelike vectors, which is the three-dimensional Lorentz group. Let us compute its volume element. Choosing $\hat{x} = (0, 0, 0, 1)$, we may, in view of the restriction $|\hat{x}\cdot\hat{x}'| < 1$, introduce the following parametrization for $\hat{x}'$:

$$\hat{x}_0' = \sin\alpha\sinh\beta,$$
$$\hat{x}_1' = \sin\alpha\cosh\beta\cos\gamma,$$
$$\hat{x}_2' = \sin\alpha\cosh\beta\sin\gamma,$$
$$\hat{x}_3' = \cos\alpha,$$

where

$$0 < \alpha < \pi,$$
$$-\infty < \beta < \infty,$$
$$0 \le \gamma < 2\pi.$$

[31] E. Wigner, Ann. Math. **40**, 149 (1939).

The volume element dx' is found to be

$$dx' = \tfrac{1}{2}x'^2\,dx'^2\sin^2\alpha\,d\alpha\cosh\beta\,d\beta\,d\gamma.$$

Thus

$$\varphi_k^{(2)} = \frac{1}{\pi^2}\int_0^\pi d\alpha\sin\alpha\cos k\alpha \times \int_{-\infty}^\infty d\beta\cosh\beta\int_0^{2\pi}d\gamma\,e^{-ip\cdot x'}. \tag{C6}$$

Suppose p is spacelike. Then we write

$$p = ([-p^2]^{\frac{1}{2}}\sinh\zeta, [-p^2]^{\frac{1}{2}}\cosh\zeta\mathbf{n}),$$
$$\mathbf{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$$

and find

$$p\cdot x' = (p^2r^2)^{\frac{1}{2}}[\sinh\zeta\sin\alpha\sinh\beta - \cosh\zeta\sin\theta\sin\alpha \times \cosh\beta\cos(\gamma-\varphi) - \cosh\zeta\cos\theta\cos\alpha].$$

The integration over γ in (C6) may immediately be done:

$$\int_0^{2\pi}d\gamma\,e^{ia\cos(\gamma-\varphi)} = 2\pi J_0(a),$$
$$a = (p^2r^2)^{\frac{1}{2}}\cosh\zeta\sin\theta\sin\alpha\cosh\beta \equiv b\cosh\beta.$$

Next, we do the integral over β[32]:

$$\int_{-\infty}^\infty d\beta\cosh\beta e^{-ic\sinh\beta}J_0(b\cosh\beta) = 2\int_0^\infty dt\cos|c|\,tJ_0(b[t^2+1]^{\frac{1}{2}}) = 2\frac{\cos(b^2-c^2)^{\frac{1}{2}}}{(b^2-c^2)^{\frac{1}{2}}}\theta(b-|c|),$$
$$c = (p^2r^2)^{\frac{1}{2}}\sinh\zeta\sin\alpha. \tag{C7}$$

The result so far is

$$\varphi_k^{(2)} = 2(\pi\lambda[1-u^2]^{\frac{1}{2}})^{-1}\int_0^\pi d\alpha\cos k\alpha e^{-i\lambda u\cos\alpha} \times \cos(\lambda[1-u^2]^{\frac{1}{2}}\sin\alpha)\theta(1-u^2),$$
$$\lambda = (p^2x^2)^{\frac{1}{2}}, \qquad u = \hat{p}\cdot\hat{x}.$$

Setting $u = \cos\omega$, $0 < \omega < \pi$, combining the exponential with the second cosine function in the integrand, we get

$$\varphi_k^{(2)} = (\pi\lambda[1-u^2]^{\frac{1}{2}})^{-1}\theta(1-u^2)\int_0^\pi d\alpha\cos k\alpha \times [e^{-i\lambda\cos(\alpha+\omega)} + e^{-i\lambda\cos(\alpha-\omega)}].$$

We may extend the α-integration to 2π provided we divide the result by two. The legitimacy of this

[32] Reference of Footnote 25, p. 33.

operation becomes obvious when we remark that by letting α range from 0 to 2π, we are integrating twice over $\mathfrak{M}_-$ subject to the restriction $|\hat{x}\cdot\hat{x}'| < 1$. Letting $\alpha \pm \omega = \alpha'$, we finally find

$$\varphi_k^{(2)} = 2(\lambda[1 - u^2]^{\frac{1}{2}})^{-1}T_k(u)(-i)^k J_k(\lambda)\theta(1 - |u|) \qquad (p^2, x^2 < 0).$$

Using the identities

$$e^{iz\sin\phi} = \sum_{n=-\infty}^{\infty} e^{in\phi}J_n(z),$$

$$J_{-n}(z) = (-)^n J_n(z),$$

it is easy to verify that

$$\sum_{k=1}^{\infty} k\varphi_k^{(2)} = \sum_{k=1}^{\infty} \mathcal{R}_k(\lambda)\mathcal{K}_k(u) = e^{-i\lambda u} \quad (u^2 < 1),$$

$$\mathcal{R}_k(\lambda) = 2\pi^2 i^k \lambda^{-1} J_k(\lambda). \tag{C8}$$

If $p^2 > 0$, then $\varphi_k^{(2)} = 0$. This follows from the vanishing of the step function in (C7):

$$\theta(b - |c|) = \theta(\sinh\zeta\sin\theta - \cosh\zeta) = 0$$

with the substitutions $\cosh\zeta \leftrightarrow \sinh\zeta$ to change from spacelike to timelike $\hat{p}$.

Considering $\varphi_\nu^{(1)}$ next, we may carry out the required integrations by taking

$$\hat{x}_0' = \sinh\alpha\cosh\beta,$$

$$\hat{x}_1' = \sinh\alpha\sinh\beta\cos\gamma,$$

$$\hat{x}_2' = \sinh\alpha\sinh\beta\sin\gamma,$$

$$\hat{x}_3' = \cosh\alpha$$

with

$$-\infty < \alpha < \infty,$$

$$0 < \beta < \infty,$$

$$0 \le \gamma < 2\pi.$$

The calculations are straightforward, and so we only state the results:

$$\nu\varphi_\nu^{(1)} = \begin{cases} -\mathcal{R}_\nu^{\pm}([p^2x^2]^{\frac{1}{2}})\mathcal{K}_\nu(\hat{p}\cdot\hat{x}) & p^2 > 0, \quad -1 \pm \hat{p}\cdot\hat{x} > 0; \\ -\mathcal{R}_\nu'([-p^2x^2]^{\frac{1}{2}})\mathcal{K}_\nu'(\hat{p}\cdot\hat{x}) & p^2 < 0. \end{cases}$$

Here

$$\mathcal{R}_\nu'(\lambda) = \lambda^{-1}K_{i\nu}(\lambda), \tag{C9}$$

$$\mathcal{K}_\nu'(u) = \nu(\pi[u^2 + 1]^{\frac{1}{2}})^{-1}[e^{\frac{1}{2}\pi\nu}([u^2 + 1]^{\frac{1}{2}} - u)^{i\nu} - e^{-\frac{1}{2}\pi\nu}([u^2 + 1]^{\frac{1}{2}} + u)^{i\nu}]. \tag{C10}$$

Summarizing, we have the following expansions of the exponential function:

$$e^{-ip\cdot x} = \begin{cases} \int_0^\infty d\nu\, \mathcal{R}_\nu^{\pm}([p^2x^2]^{\frac{1}{2}})\mathcal{K}_\nu(\hat{p}\cdot\hat{x})\theta(-1\pm\hat{p}\cdot\hat{x}), & p^2, x^2 > 0; \\ \int_0^\infty d\nu\, \mathcal{R}_\nu'([-p^2x^2]^{\frac{1}{2}})\mathcal{K}_\nu'(\hat{p}\cdot\hat{x}), & p^2 < 0, \quad x^2 > 0; \\ -\int_0^\infty d\nu\, \mathcal{R}_\nu'([-p^2x^2]^{\frac{1}{2}})\mathcal{K}_\nu'(\hat{p}\cdot\hat{x}), & p^2 > 0, \quad x^2 < 0; \\ -\int_0^\infty d\nu\, \mathcal{R}_\nu^{\pm}([p^2x^2]^{\frac{1}{2}})\mathcal{K}_\nu(\hat{p}\cdot\hat{x})\theta(-1 \pm \hat{p}\cdot\hat{x}) \\ -\sum_{k=1}^{\infty} \mathcal{R}_k([p^2x^2]^{\frac{1}{2}})\mathcal{K}_k(\hat{p}\cdot\hat{x})\theta(1 - |\hat{p}\cdot\hat{x}|), & p^2, x^2 < 0; \end{cases} \tag{C11}$$

here $\mathcal{R}_\nu^{\pm}$, $\mathcal{K}_\nu$, $\mathcal{R}_\nu'$, $\mathcal{K}_\nu'$, $\mathcal{R}_k$, $\mathcal{K}_k$ are respectively given by (C5), (3.14), (C9), (C10), (C8), and (3.21). The integrands are assumed to incorporate small imaginary parts of appropriate arguments necessary for the absolute convergence of the integrals. The expansions (C11) clearly are symmetric in p and x, as they should be, except for the minus signs in the last two expansions. These minus signs may be understood by noting that for spacelike x the radial part of the volume element reads

$$\int_{-\infty}^{0} dx^2\, x^2 = \int_{\infty}^{0} d(-x^2)(-x^2) = -\int_0^\infty dy^2\, y^2.$$

We see that discrete representations of L_0 contribute only when both p and x are spacelike and then only for $-1 < \hat{p}\cdot\hat{x} < 1$. In all cases the radial parts of the expansions satisfy (C1).

It should be pointed out that (C11) has been given by Joos[8] for the case $p^2, x^2, x_0 > 0$.