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S Matrix and Low Energy Theorem in the Theory of Correlation Functions

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We have examined the current correlation functions in statistical mechanics from a scattering theory viewpoint. In the light of low energy theorems, we study the connection between the long wavelength, low-frequency correlation functions of conserved currents and the on-shell scattering matrix elements which describe the collision processes taking place in the thermodynamical system of interest. Explicit general formulas are derived for the leading correction terms to the ideal gas correlation functions. These correction terms include the effect of two-body scatterings and double scatterings in three-body events. They are expressed in terms of two-body cross section, time delay, and the quantum analog of the distance of closest approach. Their connection to the second virial coefficient is established through sum rules. Relationship between our results and the Boltzmann equation is discussed.

1. INTRODUCTION

The statistical mechanics of gaseous systems has been formulated with the dynamical information fully expressed through the on-shell S matrix.[1,2] The basic motivation, as discussed in Ref. 1, was that the S matrix as a form of dynamical information is more general and, on occasion, even more useful than the nonrelativistic interaction Hamiltonian. The S matrix was introduced through a generalized virial expansion for the grand potential. Each term in the virial series can be expressed in terms of on-shell S matrix elements. The first few terms, sufficient for describing a dilute system, involve the S matrix for collisions among a small number of particles. In this paper, we inquire into the question of introducing the S matrix in a similar fashion into the theory of correlation functions.

The correlation functions describe the fluctuations of dynamical variables and the responses of the system to weak space–time varying external fields coupled to these dynamical variables. The most often encountered dynamical variables are the local densities and fluxes of particle number, charge, spin, etc. We shall refer to them simply as *currents*. We shall write the Heisenberg operators representing them as $j^\mu(x)$, with $j^0(x)$ denoting the density at $(\mathbf{x}, t)$ and $j^i(x)$, $i = 1, 2, 3$, denoting the flux. The correlation functions are commonly expressed as Fourier transforms of grand canonical averages:

$$\int d^4x e^{ik\cdot x}\langle j^\mu(x) j^\nu(0)\rangle, \tag{1.1}$$

where $k \cdot x \equiv \omega t - \mathbf{k} \cdot \mathbf{x}$. We shall restrict our discussion to currents which are conserved in the sense that a continuity equation

$$\frac{\partial j^0}{\partial t} + \nabla \cdot \mathbf{j} = 0 \tag{1.2}$$

is satisfied. This local conservation law will play a major role in our discussion. Examples of conserved currents are the electrical current and the various particle probability currents in the nonrelativistic case. With essentially trivial modifications of the techniques developed here, one could treat conserved tensor densities $\mathcal{C}^{\mu\nu}(x)$. An important example of such an object is the energy–momentum tensor which is built out of the densities and fluxes of energy and momentum.

To introduce the S matrix into the theory of correlation functions, one can begin by writing down for any correlation function an expansion in powers of a certain fugacity z as was done for the grand potential $-pV$. The real question is whether it is possible, as it is for $-pV$, to express the expansion coefficients in terms of on-shell S-matrix elements. The answer to this question for general $\mathbf{k}$ and ω is negative as is evident in view of the following simple arguments.

Recall that, in the usual expansion for $-pV$ in powers of z, the coefficient b_n of z^n depends on the n-body dynamics through the *density of states*. The density of states depends on the boundary condition for the wavefunctions at the walls of the box in which the system is quantized. For a very large box, the asymptotic wavefunctions, which are completely determined by the S matrix, are sufficiently accurate at the walls. That is why b_n is completely determined by the n-body S matrix. In the expansion for a correlation function, the coefficient of z^n is likewise determined by the n-body dynamics. However, for an arbitrary $k = (\mathbf{k}, \omega)$, the dynamical information concerning the variation of currents over a finite distance and time interval is needed. One necessarily probes into regions where interactions take place.

The on-shell S matrix determines only the wavefunctions in the asymptotic region, i.e., far out of the region of interaction, and is therefore insufficient for determining the current correlation over a finite space–time interval.

What we have just pointed out is that the S matrix cannot be expected to provide information about correlation functions when either $|\mathbf{k}|^{-1}$ is on the order of the size D of a typical constituent gas particle or ω^{-1} is on the order of a typical interaction time τ. However, if one is studying the properties of the gas as a whole rather than the properties of individual particles, often the interesting regions are either $|\mathbf{k}|^{-1} \gg D$ or $\omega^{-1} \gg \tau$ or both. When *both* conditions $|\mathbf{k}|^{-1} \gg D$ and $\omega^{-1} \gg \tau$ are satisfied, the S matrix does determine, to a degree to be specified later, essentially all of the correlation function. This is because, in the limit of small $\mathbf{k}$ and ω, rapid variations of currents are smoothed out by the integration over a large region of order k^{-1} in size. Most of the current is carried by particles which are free before and after a collision, and the wavefunctions describing these free particles are determined by the S matrix.

It seems obvious that the leading order term in k^{-1} in the n-particle contribution to the correlation function should be determined by the S matrix. This is, in fact, true, and furthermore this leading term involves only cross sections rather than the complete scattering amplitude. However, it turns out that this leading term is not entirely adequate. For example, the f-sum rule and compressibility sum rule are not satisfied. For conserved currents of the type mentioned above, one can also compute the next to leading term in k^{-1}. This term involves not only cross sections but also the phase of the scattering amplitude. A large portion of this paper is devoted to explicitly demonstrating this in the two-body case. The improvement obtained by keeping this term is significant. Among other things, the sum rules are now satisfied.

Since the terms which are most singular in k^{-1} depend, as mentioned above, only on cross sections, the reader will probably not be surprised to learn that a correlation function computed in the approximation of keeping only the most singular terms is just what one would obtain from a linearized Boltzmann equation. The equilibrium solution to the Boltzmann equation is a perfect gas. This is why the sum rules are not satisfied by this simplest small k approximation to the correlation functions. In some sense, then, what we obtain by keeping the next terms in k^{-1} is a correction to the Boltzmann equation which takes account of finite interaction distances and times. The reader will see later that it is current conservation which allows one to take account, to first order at least, of finite interaction distances and times while still working with the strictly on-shell S matrix.

In this paper we will not actually prove all the statements made above. In fact, we will restrict ourselves to the two- and three-body contributions to the correlation functions. The generalization to n-body contributions appears to be straightforward although very difficult.

An ultimate goal of the program would be to obtain S-matrix expressions for correlation functions which are (i) accurate whenever $|\mathbf{k}|^{-1} \gg D$ and $\omega^{-1} \gg \tau$, (ii) have the correct analytic behavior for small $\mathbf{k}$ and ω, and (iii) satisfy the sum rules and other constraints which link correlation functions to equilibrium statistical mechanics which has already been formulated in terms of the S matrix. Let us look at some basic ideas as to how this might be done.

Recall that the correlation function measures the response to a weak external field coupled to the currents. Think of the external field as describing another particle, which we shall, for the simplicity of discussion, refer to as "photon" or simply "γ". It is not hard to see that the correlation function is directly related to the scattering amplitude of the process

$$\text{particles} + \gamma \rightarrow \text{particles} + \gamma.$$

For the simplest case of one particle, the amplitude is simply the "Compton scattering" amplitude. If there are two particles, the amplitude would involve the full dynamics of the two-body interaction at the presence of the photons.

At this point we recall that there are the so-called "low energy theorems" for amplitudes of scattering processes involving small k photons.[3] It was shown, for example, that, for the Bremstrahlung process

$$p_1 + p_2 \rightarrow p_1 + p_2 + \gamma$$

in which particles 1 and 2 collide and emit a photon of momentum k, the amplitude can be expressed in terms of kinematic variables of free particles and the on-shell scattering amplitude for $p_1 + p_2 \rightarrow p_1 + p_2$ to the two leading orders in k^{-1}. In the case of Compton scattering, it was shown that, to the first two orders in k^{-1}, only the charge and magnetic moment of the particle appear, no matter how complicated the structure of the particle is.[3] In proving these low energy theorems, the conservation of the electromagnetic current played an important role. The physical picture behind the low energy theorems is clearly the same as what we described above, i.e., the current, which is the source of photons, comes dominantly from the free particles before and after

the scattering. The physical reason behind the fact that the next term in k^{-1} is also determined by on-shell amplitudes is less trivial and will be discussed in detail later in the text.

The above qualitative discussion suggests that we can set up the following program for introducing the S matrix as the input of dynamical information into the theory of correlation functions:

(i) Expand the correlation function of interest in powers of z:

$$c = \text{correlation function} = \sum_n c_n z^n \qquad (1.3)$$

so that the coefficient c_n summarizes the contribution of n-particle states.

(ii) Derive an identity to relate c_n to the scattering amplitude for the schematic process

$$n \text{ particles} + \gamma \to n \text{ particles} + \gamma. \qquad (1.4)$$

(iii) Derive a low energy theorem to express the amplitude for (1.4) to some leading orders in k^{-1} in terms of the scattering amplitudes for

$$n \text{ particles} \to n \text{ particles}, \qquad (1.5)$$

i.e., the n-particle S-matrix elements.

(iv) Obtain the desired c_n by using the identity derived in (ii) and the low energy theorem (iii).

This program is clearly analogous to that in Refs. 1 and 2 for expressing the virial coefficients in terms of S-matrix elements. The structure of correlation functions is far more complex than that of virial coefficients. In practice the program is very difficult to carry out, although it makes good sense in principle. What we explicitly do in this paper is to compute the leading and next to leading term in k^{-1} for c_2 and the leading term only for c_3. From this calculation, which is itself quite difficult, the reader should be able to see the pattern suggested above beginning to emerge. Furthermore, we obtain an expression for c_2 which is quite interesting from a theoretical point of view and could have some practical application. Our expression for c_2 has all the desired properties such as satisfying the sum rules and is accurate when the above-mentioned inequalities

$$|\mathbf{k}|^{-1} \gg D, \quad \omega^{-1} \gg \tau \qquad (1.6)$$

are both satisfied. A proper quantum mechanical definition of D and τ can be given in terms of the energy ϵ and momentum transfer q derivatives of the scattering amplitude f. One defines

$$\tau \sim f^{-1}\frac{\partial}{\partial \epsilon} f, \quad D \sim f^{-1}\frac{\partial}{\partial q} f, \qquad (1.7)$$

which are known to be estimates of the interaction time and range.[4]

The practical usefulness of our result for c_2 depends, of course, on how closely c is approximated by the two terms zc_1 and z^2c_2. (The one-body term c_1 is essentially trivial to calculate.) Since (1.3) is essentially a density expansion, it is clear that the density must be low. In addition, it turns out that $|\mathbf{k}|$ and ω must not both be too small. This may be seen as follows.

In a gas the correlation function must be singular near ω and $\mathbf{k}$ equal to zero because of the possibility of exciting sound waves. Since the propagation of sound is a collective effect, an expansion to any finite order in density will never give these acoustic singularities correctly. By definition, the wavelength $2\pi/k$ of sound is long compared to the mean free path l and the period of a sound wave must be long compared to the mean free time τ_c. Evidently, to avoid the collective region where (1.3) converges slowly at best we must require that

$$|\mathbf{k}|^{-1} \ll l \sim (\bar{N}\sigma)^{-1}, \quad \omega^{-1} \ll \tau_c \sim (\bar{N}\sigma v)^{-1}, \qquad (1.8)$$

where we have used the standard estimates for l and τ_c in terms of the density $\bar{N}$, the two-body cross section σ, and the thermal velocity v. We emphasize that only one of the inequalities in (1.8) need be satisfied. Thus we have upper bounds on both $\mathbf{k}$ and ω (1.6), which are necessary in order that our expression for c_2 be valid, and a lower bound on either $|\mathbf{k}|$ or ω (1.8) which is necessary to make (1.3) converge rapidly. For a dilute system where the density of particles $\bar{N}$ is very small compared to the volume of particle D^3, the inequalities are completely compatible. One can estimate

$$D/l \sim \tau/\tau_c \sim \bar{N}D^3, \qquad (1.9)$$

where we have set $\sigma = D^2$ and $\tau = vD$. To take a physical example, for argon gas at standard temperature and pressure, we have[5]

$$D \sim 3.6 \text{ Å}, \; l \sim 700 \text{ Å}, \; \tau_c \sim 1.7 \times 10^{-10} \text{ sec}, \qquad (1.10)$$

and τ is probably of order 10^{-13} sec. Clearly, in this case there is a quite reasonable range of $\mathbf{k}$ and ω over which our result for c_2 could be useful.

It is evident that the density expansion of correlation functions is rather peculiar, especially near $\mathbf{k}$ and ω equal to zero. We would like now to give a qualitative discussion of this expansion. It turns out that the coefficient c_n of z^n in (1.3) will contain a piece which goes like k^{-n} for small k, another which behaves like k^{-n+1}, another going like k^{-n+2}, and so on. In addition, there are pieces of c_n which have

finite limits as $k \to 0$. The latter are generally outside the scope of our S-matrix formalism. Also there are almost certainly terms going like $k^{-n+2} \log k$, $k^{-n+3} \times \log^2 k$, etc. These $\log k$ terms will be ignored in the present discussion. The k^{-n} singularity in c_n can be shown to come from an n-body scattering process made up of $n-1$ successive two-body scatterings. A k^{-n+1} term in c_n can be generated by a succession of $n-2$ two-body events followed by one true three-body scattering and so on. The fact that the degree of singularity in k^{-1} increases with n suggests that the expansion in (1.3) should be rearranged so that all the terms of order $z^n k^{-n}$ are summed first, then all the terms of order $z^n k^{-n+1}$, etc. To do this, it is convenient to define

$$z' = \min\left((kl)^{-1}, (\omega\tau_c)^{-1}\right),$$
$$\zeta = \max\left(D/l, \tau/\tau_c\right) \approx \bar{N}D^3. \tag{1.11}$$

Notice that both z' and ζ are proportional to density. Evidently ζ is always small for a dilute system and never exceeds order of unity for even the most dense gas. On the other hand, for small $\mathbf{k}$ and ω, z' can become large even for the most dilute gas. Now we can write

$$z^n c_n = (z')^n c_{n0} + (z')^{n-1}\zeta c_{n1} + (z')^{n-2} \times \zeta^2 c_{n2} \cdots + z'\zeta^{n-1} c_{nn-1} + O(1), \tag{1.12}$$

where $O(1)$ means terms which are finite as $\mathbf{k}$ and ω tend to zero and, as mentioned above, we suppress possible $\log k$ terms. Note that, as it should be, each term in (1.12) contains a factor (density)^n. The term containing $(z')^{n-m}$ has a singularity like k^{m-n} for small k. Summing over n, one has

$$c = \sum_n c_n z^n = \sum_{n,m<n} (z')^{n-m}\zeta^m c_{nm} + O(1) \tag{1.13}$$

or

$$c = f_0(z') + \zeta f_1(z') + \zeta^2 f_2(z') + \cdots + O(1), \tag{1.14}$$

where

$$f_m(z') = \sum_{n>m} (z')^n c_{nm}.$$

Since ζ, unlike z', is always small, (1.14) is a more sensible density expansion than (1.3). We remind the reader that the $O(1)$ in (1.13) represents terms in c which are finite as $\mathbf{k}$ and ω go to zero and appear to be outside the scope of our S-matrix formalism.

In this language, we will explicitly compute the first three terms in the expansion of f_0 in powers of z' and the first two terms in the expansion of f_1. We are sure, but strictly speaking have not proven, that to all orders in z'

(i) f_0 is what one would obtain from the Boltzmann equation,

(ii) f_1 can be expressed in terms of strictly on-shell scattering amplitudes.

We do not know much about f_n for $n \geq 2$.

It is expected that one should be able to obtain f_1 from a generalized Boltzmann equation. There is a vast amount of literature on the subject of generalized Boltzmann equations in connection with the theory of transport coefficients, where one is interested in the limiting case $k \to 0$, i.e., $z' \to \infty$.[6] Note that the Boltzmann equation is valid for $\zeta \to 0$ and *arbitrary* z'. The task of obtaining a generalized equation valid to $O(\zeta)$ and for arbitrary z' is expected to be more difficult than that of obtaining one valid only for $z' \to \infty$. If such an equation does exist, its iteration solution must reproduce (1.13). In particular, it must reproduce c_{20}, c_{21}, and c_{30}, which will be furnished by this paper, and serve as a hint as well as a test for any proposed generalization of the Boltzmann equation.

The outline of the paper is as follows.

In Sec. 2, we summarize for later references our notation convention, well-known identities relating correlation functions of various kinds, and sum rules.

Section 3 is devoted to the steps (i) and (ii) of the S-matrix program for (1.3). Here the basic formulation and special techniques are developed.

In Sec. 4, we discuss the physical basis for the low energy theorem and the basic idea behind the mathematical technique in taking advantage of the conservation law. The low energy theorem for Compton scattering is worked out as an illustration.

In Sec. 5, we illustrate the basic idea and technique further by deriving a low energy theorem for the Bremsstrahlung process. Then the low energy theorem for the process (1.4) with $n = 2$ in (1.3) is worked out. Step (iii) is then completed for $n = 2$.

The correlation function up to terms of $n = 2$ is established in Sec. 6, completing step (iv) for $n = 2$.

In Sec. 7, we verify that our results for $n = 2$ satisfy the f-sum rule and the compressibility sum rule, and thereby establish the connection between the 2-body contribution to the correlation function and the second virial coefficient.

In Sec. 8, the three-body contribution to the correlation functions is examined, in order to gain some qualitative understanding of the role of multiparticle scattering. The leading term $O(k^{-3})$, i.e., the c_{30} term in (1.13), is evaluated. This completes the formula for the correlation functions with three correction terms to the ideal gas term in a consistent approximation.

The connection of our approach to the Boltzmann equation is studied in Sec. 9, in order to shed some light on possible improvements of the kinetic equation.

Concluding remarks are included in Sec. 10.

In this paper, generality is emphasized. Only the basic notions of scattering theory and statistical mechanics are needed for discussion and derivations. No reference is made to the interaction Hamiltonian. As a result, our conclusions will be applicable to fully relativistic problems.

2. DEFINITIONS AND IDENTITIES

In this section, we establish our notation, and list definitions and well-known general formulas for later references.

A. Basic Notations

Imagine a large uniform system in thermal equilibrium at temperature β^{-1}. Let N be a conserved extensive quantity and μ the corresponding chemical potential. For definiteness and simplicity, we consider a gas of spinless particles and N is the conserved particle number. The density matrix is

$$\rho = \{\exp[-\beta(H-\mu N)]\}/\mathrm{Tr}\{\exp[-\beta(H-\mu N)]\}. \tag{2.1}$$

Associated with N, there is the local current $j^\mu(x)$, $\mu = 0, 1, 2, 3$. $j^0(x)$ denotes the Heisenberg operator at time t for the local density at $\mathbf{x}$ so that

$$N = \int d^3x j^0(x) \tag{2.2}$$

and $j^i(x)$, $i = 1, 2, 3$, denote those for the components of the local flux. We are adapting the notational conventions in relativistic problems. We shall always use A^μ to denote $(\mathbf{A}, A^0)$, A_μ for $(-\mathbf{A}, A^0)$, $A \cdot B$ for $A_\mu B^\mu = A^0B^0 - \mathbf{A}\cdot\mathbf{B}$, in particular,

$$k^\mu = (\mathbf{k}, \omega), \quad x^\mu = (\mathbf{x}, t), \quad \partial^\mu = \left(\nabla, \frac{\partial}{\partial t}\right),$$
$$k\cdot x = \omega t - \mathbf{k}\cdot\mathbf{x}. \tag{2.3}$$

The current operators satisfy the continuity equation and the usual commutation rules:

$$\partial_\mu j^\mu(x) = 0, \quad [j^0(\mathbf{x}, t), j^0(\mathbf{x}', t)] = 0,$$
$$[j^0(\mathbf{x}, t), j^i(\mathbf{x}', t)] = i\partial_i\delta(\mathbf{x}-\mathbf{x}')j^0(\mathbf{x}, t), \tag{2.4}$$

where the commutator of j^0 and j^i given here is only correct in the nonrelativistic limit. We will not need the relativistic form which is, in any case, not known.

B. Correlation Functions

There is a whole set of functions describing the correlation of current fluctuations and responses to weak external fields coupled to the currents. They are Fourier transforms of various products of current operators averaged over the grand canonical ensemble, and are usually referred to as "correlation functions," "response functions," "structure functions," and many other names. Let us list a few. We define

$$A(k) = \int d^4x e^{ik\cdot x}A(x). \tag{2.5}$$

Let

$$S'^{\mu\nu}(x) = \langle\{j^\mu(x), j^\nu(0)\}\rangle, \quad S^{\mu\nu}(x) = \langle[j^\mu(x), j^\nu(0)]\rangle,$$
$$F^{\mu\nu}(x) = -i\langle T(j^\mu(x)j^\nu(0))\rangle, \tag{2.6}$$
$$R^{\mu\nu}(x) = -i\langle[j^\mu(x), j^\nu(0)]\rangle\theta(t),$$

where the curly bracket denotes the anticommutator. We are mainly interested in their Fourier transforms defined by (2.5). We shall refer to these four functions of k as "correlation function," "commutator," "time ordered product," and "response function," respectively. They are linearly related to each other. One verifies that

$$S^{\mu\nu}(k) = S'^{\mu\nu}(k)\tanh\tfrac{1}{2}\beta\omega,$$
$$S^{\mu\nu}(k) = i[R^{\mu\nu}(k) - R^{*\nu\mu}(k)],$$
$$S'^{\mu\nu}(k) = i[F^{\mu\nu}(k) - F^{*\nu\mu}(k)], \tag{2.7}$$
$$R^{\mu\nu}(k) = \int \frac{d\omega'}{2\pi}\frac{S^{\mu\nu}(\mathbf{k}, \omega')}{\omega - \omega'}.$$

In the dispersion integral for $R^{\mu\nu}$, ω is supposed to be immediately above the real axis. Clearly, $R^{\mu\nu}$ is well defined by the integral as a function of complex ω. On the other hand, notice that the rest in (2.7) *including* $F^{\mu\nu}$ is defined for real ω only. We shall assume the system is invariant under time and space inversion so that all the above-defined functions are symmetric in μ and ν. It follows from (2.7) that

$$S^{\mu\nu}(k) = -2\,\mathrm{Im}\,R^{\mu\nu}(k), \quad S'^{\mu\nu}(k) = -2\,\mathrm{Im}\,F^{\mu\nu}(k). \tag{2.8}$$

From the continuity equation and commutation rules (2.4), one can derive the identities

$$k_\mu S^{\mu\nu}(k) = k_\mu S'^{\mu\nu}(k) = 0,$$
$$k_\mu F'^{\mu\nu}(k) = k_\mu R'^{\mu\nu}(k) = 0, \tag{2.9}$$

where

$$F'^{0\nu}(k) = F^{0\nu}(k), \quad R'^{0\nu}(k) = R^{0\nu}(k),$$
$$F'^{ij}(k) = F^{ij}(k) + \delta^{ij}\bar{N}/m, \tag{2.10}$$
$$R'^{ij}(k) = R^{ij}(k) + \delta^{ij}\bar{N}/m,$$

where $\bar{N}$ is the average density. We shall take the volume of the system to be unity so that $\bar{N} = \langle N\rangle$.

We can also write

$$F'^{\mu\nu}(k) = -i\int e^{ik\cdot x}d^4x\langle T'(j^\mu(x)j^\nu(0))\rangle,$$

$$T'(j^0(x)j^\nu(0)) = T(j^0(x)j^\nu(0)),$$

$$T'(j^i(x)j^k(0)) = T(j^i(x)j^k(0)) + i\delta^{ik}\delta(\mathbf{x})\frac{j^0(0)}{m}. \quad (2.11)$$

The definition of T' given here is nonrelativistic. However, there is a relativistic object with the same properties, see for example the third work cited in Ref. 3.

From (2.9) and (2.10), one easily deduces the well-known f-sum rule:

$$\int\frac{d\omega}{2\pi}\omega S^{00}(k) = \mathbf{k}^2\frac{\bar{N}}{m}. \quad (2.12)$$

From the definition of the correlation function, one obtains the compressibility sum rule:

$$\lim_{\mathbf{k}\to 0}\frac{1}{2}\int\frac{d\omega}{2\pi}S'^{00}(k) = \langle(N-\bar{N})^2\rangle = z\frac{\partial\bar{N}}{\partial z}, \quad (2.13)$$

where $z = e^{\beta\mu}$ is the fugacity.

3. FUGACTITY EXPANSION AND THE SCATTERING MATRIX

A. Fugacity Expansion

We want to expand the correlation and the related functions in powers of the fugacity z in analogy to the virial expansion for the pressure p, which is

$$p = (\beta\lambda^3)^{-1}\sum_{n=1}^{\infty}b_nz^n, \quad (3.1)$$

$$\lambda^{-3}b_n = (\mathrm{Tr}\, e^{-\beta H})_{n,c}, \quad \lambda = (2\pi\beta/m)^{\frac{1}{2}}. \quad (3.2)$$

The subscripts n, c restrict the trace to states with $N = n$ and include only "connected terms." The sum of connected terms is obtained by subtracting from the full trace all those traces where there are no interactions between two or more clusters of particles. Indeed, if one goes through a counting procedure similar to that leading to (3.1) and (3.2), one obtains analogous expansions for the correlation and related functions. It is sufficient to discuss one of the functions. We have, for $F'^{\mu\nu}$ defined by (2.10) and (2.11),

$$F'^{\mu\nu} = \sum_{n=1}^{\infty}z^nF_n'^{\mu\nu}, \quad (3.3)$$

$$F_n'^{\mu\nu} = -i\int d^4xe^{ik\cdot x}(\mathrm{Tr}\, e^{-\beta H}T'(j^\mu(x)j^\nu(0)))_{n,c}. \quad (3.4)$$

Equation (3.4) shows that the dynamics of n particles in an infinite volume must be known to determine $F_n'^{\mu\nu}$.

In the Introduction, we have examined the question whether the (on-shell) S-matrix elements between states of $N = n$ supply sufficient dynamical information for determining $F_n'^{\mu\nu}$. It was concluded from qualitative arguments that, for small k, the leading term in k^{-1} is completely determined by the S matrix. In fact, the next leading term is also determined by the S matrix. To verify these statements explicitly, we need the low energy theorems, which we shall discuss in detail in Secs. 4 and 5. We now devote the remainder of this section to transform (3.4) into a form suitable for the application of scattering theory.

B. Small Angle Limit

For reasons which will be apparent shortly, we state

$$(\mathrm{Tr}\, e^{-\beta H}j^\nu(0))_{n,c} = \lim_{\theta\to 0}(\mathrm{Tr}\, e^{-\beta H}j^\nu(0)e^{iJ_3\theta})_{n,c}, \quad (3.5)$$

$$(\mathrm{Tr}\, e^{-\beta H}j^\mu(x)j^\nu(0))_{n,c} = \lim_{\theta\to 0}(\mathrm{Tr}\, e^{-\beta H}j^\mu(x)j^\nu(0)e^{iJ_3\theta})_{n,c}, \quad (3.6)$$

where J_3 is the angular momentum operator along the z axis or any other axis through the origin. Intuitively, (3.5) and (3.6) are obviously true, since $j^\nu(0)$ measures the current at the origin only. Rotating the wavefunction around the origin cannot have much effect. Rigorous proof follows the steps in Appendix A of Ref. 2. It is also true that

$$\int d^4xe^{ik\cdot x}(\mathrm{Tr}\, e^{-\beta H}j^\mu(x)j^\nu(0))_{n,c} = \lim_{\theta\to 0}\int d^4xe^{ik\cdot x}(\mathrm{Tr}\, e^{-\beta H}j^\mu(x)j^\nu(0)e^{iJ_3\theta})_{n,c} \quad (3.7)$$

if, as we shall assume, the integrand falls off (except for a constant term irrelevant for $k \neq 0$) fast enough for $x \to \infty$. We can therefore rewrite (3.4) as

$$F_n'^{\mu\nu} = \lim_{\theta\to 0} -i\int d^4xe^{ik\cdot x}(\mathrm{Tr}\, e^{-\beta H}[T'(j^\mu(x)j^\nu(0))]\times e^{i\theta J_3})_{n,c}. \quad (3.8)$$

C. Photon Scattering Amplitude

We want to write the trace in (3.8) as a sum over a complete set of eigenstates of H. Scattering theory tells us that the set of "in states" form such a set and so does the set of "out states":

$$\sum_a|a\ \mathrm{in}\rangle\langle a\ \mathrm{in}| = 1, \quad (3.9)$$

$$\sum_b|b\ \mathrm{out}\rangle\langle b\ \mathrm{out}| = 1, \quad (3.10)$$

where a and b label the momenta of the incoming and outgoing particles. The S-matrix elements are given by

$$\langle b|\,S\,|a\rangle = \langle b\ \mathrm{out}\,|\,a\ \mathrm{in}\rangle. \quad (3.11)$$

Writing the trace of (3.8) as a sum over in states and inserting a sum over out states to the left of $e^{-\beta H}$, we obtain

$$F_n'^{\mu\nu} = \lim_{\theta\to 0} \sum_{a,b} (e^{-\beta E_a} \langle a|\, S^\dagger\, |b\rangle \langle b|\, T^{\mu\nu}(kk')\, |a'\rangle)_c, \tag{3.12}$$

where E_a is the energy of $|a \text{ in}\rangle$ and it is understood that a and b are states with $N = n$, and

$$\langle b|\, T^{\mu\nu}(k, k')\, |a'\rangle = -i \int d^4x\, e^{ik\cdot x} \langle b \text{ out}|\, T'(j^\mu(x) j^\nu(0))\, |a' \text{ in}\rangle \tag{3.13}$$

and

$$|a' \text{ in}\rangle \equiv e^{i J_3 \theta}\, |a \text{ in}\rangle. \tag{3.14}$$

The matrix element (3.13) is formally identical to the amplitude for the scattering process $a' \to b$ with an additional "photon," i.e., for the process

$$a' + \gamma' \to b + \gamma \tag{3.15}$$

via the coupling $-ej_\mu A^\mu + (e^2/2m)\mathbf{A}^2 j^0$ to $O(e^2)$. The polarizations and momenta for γ' and γ are, respectively, (k', ν) and (k, μ), with k' fixed by over all momentum conservation. Of course, even though we use the word "photon," we do not have $\omega = c\,|\mathbf{k}|$ here. The components of k are completely arbitrary.

Since $[J_3, H] = 0$, it follows that $E_a = E_{a'}$. The S matrix conserves energy. Therefore, in (3.12), we have

$$E_a = E_b = E_{a'}, \quad \omega = \omega'. \tag{3.16}$$

Owing to the rotation, we have,

$$\mathbf{p}_b = \mathbf{p}_a \neq \mathbf{p}_{a'}, \quad \mathbf{k} \neq \mathbf{k}', \tag{3.17}$$

where $\mathbf{p}_a$ is the total momentum of $|a \text{ in}\rangle$, etc. We now see the purpose of the rotation by θ. Without it, (3.12) would be undefined in the momentum representation because of the singularity in the forward amplitudes, which was studied in detail in Refs. 1 and 2 for the virial coefficients. The simplest example of singular terms is shown in Fig. 1, where, including the photon, there are three particles. The p_1'' energy denominator would vanish owing to momentum conservation if $\theta = 0$. For finite θ, no such problem occurs.

The next step is to see how the photon scattering amplitude given by (3.13) can be expressed in terms of $\langle b|\, S\, |a'\rangle$ for small k. This is the subject of low energy theorems, which we shall study in the next two sections.

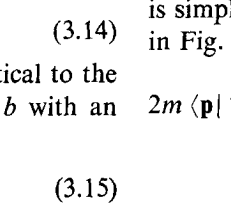


FIG. 1. A term in $T^{\mu\nu}$ given by (3.13). If $k = k'$, $p_1 = p_1'$, and $p_2 = p_2'$, then $p_1'' = p_1$ and the energy denominator for p_1'' will vanish.

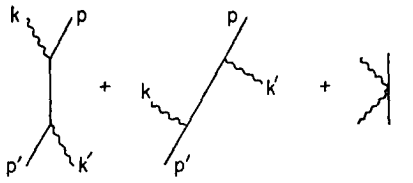


FIG. 2. Compton scattering by a point particle.

D. The Case $n = 1$

Let us apply our results to the trivial case of $n = 1$, i.e., to the ideal gas. The S matrix is simply unity, and we may set $\theta = 0$ from the start. The amplitude (3.13) is simply the "Compton scattering" amplitude shown in Fig. 2. We have, for arbitrary p, p', and k,

$$2m \langle \mathbf{p}|\, T^{\mu\nu}(k, k')\, |\mathbf{p}'\rangle = \frac{(2p + k)^\mu (2p' + k')^\nu}{2p\cdot k + k^2} + \frac{(2p - k')^\nu (2p' - k)^\mu}{-2p'\cdot k + k^2} - 2g^{\mu\nu}. \tag{3.18}$$

The 4-vector p^μ will always denote the energy–momentum of a free particle. A positive infinitesimal imaginary part is understood in the denominators. $g^{00} = -g^{ii} = 1$, 0 otherwise. Substituting (3.18) in (3.12), we obtain $F_1'^{\mu\nu}$. The correlation function $S'^{\mu\nu}$ for an ideal gas can thus be obtained by taking the imaginary part of $F_1'^{\mu\nu}$ [see (2.8) and (2.10)]:

$$S'^{\mu\nu} = zS_1'^{\mu\nu} + O(z^2), \tag{3.19}$$

$$S_1'^{\mu\nu} = -2 \operatorname{Im} F_1'^{\mu\nu}, \tag{3.20}$$

$$F_1'^{\mu\nu} = \int d^3p (2\pi)^{-3} \frac{m}{\epsilon} \langle \mathbf{p}|\, T^{\mu\nu}(k, k)\, |\mathbf{p}\rangle e^{-\beta\epsilon}, \quad \epsilon = (p^2 + m^2)^{\frac{1}{2}}. \tag{3.21}$$

The general formula for $S_1'^{\mu\nu}$ is complicated. The nonrelativistic limit is quite manageable. We have, after a little algebra,

$$\begin{aligned} S_1'^{00}(k) &= (m^2/\pi\beta\,|\mathbf{k}|) e^{-\beta m\omega^2/2\mathbf{k}^2} (e^{-\beta\mathbf{k}^2/8m} \cosh \tfrac{1}{2}\beta\omega), \\ S_1'^{03} &= S_1'^{30} = (\omega/|\mathbf{k}|) S_1'^{00}, \\ S_1'^{33} &= (\omega^2/\mathbf{k}^2) S_1'^{00}, \\ S_1'^{11} &= S_1'^{22} = (m/\beta) S_1'^{00}. \end{aligned} \tag{3.22}$$

All other components of $S_1'^{\mu\nu}$ vanish. The third axis is taken to point in the direction of $\mathbf{k}$.

4. LOW ENERGY THEOREMS

In this section and the next, we consider the scattering amplitude

$$T^{\mu\nu} \equiv \langle b|\, T^{\mu\nu}(k, k')\, |a'\rangle = -i \int d^4x e^{ik\cdot x} \langle b \text{ out}|\, T'(j^\mu(x) j^\nu(0))\, |a' \text{ in}\rangle \tag{4.1}$$

with small k and k' and arbitrary b and a'.

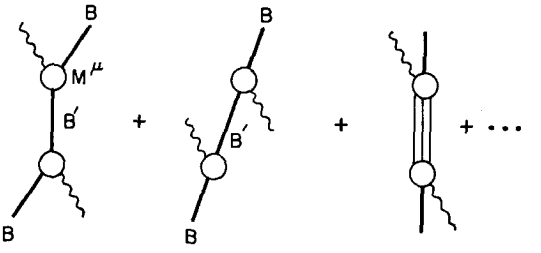


FIG. 3. Compton scattering by a bound state. The intermediate state can either be a bound state or a state in a continuum.

In order to illustrate the basic idea and technique without getting involved in too much algebra right at the beginning, we shall first obtain $T^{\mu\nu}$ for the case of a bound state, i.e., the case

$$|a' \text{ in}\rangle = |B, \mathbf{p}'\rangle, \quad |b \text{ out}\rangle = |B, \mathbf{p}\rangle. \tag{4.2}$$

$T^{\mu\nu} = T_B^{\mu\nu}$ is thus the "Compton scattering" amplitude for a composite particle B. The diagrams are shown in Fig. 3. The intermediate state can be the same bound state, or another bound state, or a multiparticle state in the continuum. To obtain the full amplitude, one would have to sum over all these intermediate states. However, for very small k, the dominant contribution comes from $|B\rangle$ itself and other bound states $|B'\rangle$ with the same binding energy, and has the form

$$A^{\mu\nu}/(2p \cdot k + k^2) + A'^{\mu\nu}/(-2p \cdot k' + k'^2), \tag{4.3}$$

where p is the momentum of the bound state. $A^{\mu\nu}$ and $A'^{\mu\nu}$ will be discussed later. The contribution from all other intermediate states are of $O(1)$ as $k \to 0$ since there is an energy gap between these states and $|B\rangle$ and the energy denominator will not vanish as $k \to 0$. Now comes the important observation that $T_B^{\mu\nu}$ satisfies the conservation law

$$k_\mu T_B^{\mu\nu} = k'_\nu T_B^{\mu\nu} = 0. \tag{4.4}$$

Suppose one finds an amplitude $T_B'^{\mu\nu}$ which includes the singular term (4.3) and which also satisfies the conservation law, i.e.,

$$k_\mu T_B'^{\mu\nu} = k'_\nu T_B'^{\mu\nu} = 0. \tag{4.5}$$

Write

$$T_B^{\mu\nu} = T_B'^{\mu\nu} + r^{\mu\nu}, \tag{4.6}$$

where the remainder $r^{\mu\nu}$ is nonsingular and is of $O(1)$ as $k \to 0$. By (4.4) and (4.5), we have

$$k_\mu r^{\mu\nu} = k'_\nu r^{\mu\nu} = 0. \tag{4.7}$$

Since $r^{\mu\nu}$ is independent of k as $k \to 0$, we conclude therefore that $r^{\mu\nu}$ must vanish as $k \to 0$. Thus,

$$T_B^{\mu\nu} = T_B'^{\mu\nu} + O(k), \tag{4.8}$$

i.e., $T_B'^{\mu\nu}$ not only counts for the leading term, but also the next leading term, the $O(1)$ term. Therefore, if we add to (4.3) some nonsingular term so that it satisfies the conservation law exactly, we will have found the $T_B'^{\mu\nu}$ in (4.8). To accomplish this, let us evaluate the numerators in (4.3) first. Let the first photon vertex in Fig. 3 be

$$M^\mu_{BB'}(p, p + k) = n(2p + k)^\mu \delta_{BB'} + M'^\mu_{BB'}, \tag{4.9}$$

$$M'^\mu_{BB'} = \int e^{-i\mathbf{k}\cdot\mathbf{x}} \langle B| j^\mu(\mathbf{x}) |B'\rangle \, d^3x - n\delta^\mu_0 \delta_{BB'}, \tag{4.10}$$

where n is the number of particles making up the bound state. Equation (4.10) is evaluated in the center of mass frame of the composite particle and $|B\rangle$ and $|B'\rangle$ are the bound state wavefunctions. Thus,

$$A^{\mu\nu} = \sum_{B'} M^\mu_{BB'}(p, p + k) M^\nu_{B'B}(p + k, p'), \tag{4.11}$$

and a similar expression can be written down for $A'^{\mu\nu}$ in (4.3). For small k, (4.10) gives

$$\begin{aligned} M'^0_{BB'} &= O(k^2), \\ M'^i_{BB'} &= nk_j \sigma^{ji}_{BB'} + O(k^2), \end{aligned} \tag{4.12}$$

where

$$\begin{aligned} n\sigma^{ji}_{BB'} &= i \int d^3x \, \langle B| x^j j^i(\mathbf{x}) |B'\rangle \\ &= \tfrac{1}{2} i \int d^3x \, \langle B| [x^j j^i(\mathbf{x}) - x^i j^j(\mathbf{x})] |B'\rangle, \end{aligned} \tag{4.13}$$

may be interpreted as the matrix element of the "magnetic moment." If we define $\sigma^{\mu 0} = \sigma^{0\mu} = 0$, we have a simple expression for (4.9):

$$\begin{aligned} &M^\mu_{BB'}(p, p + k) \\ &\quad = n[(2p + k)^\mu \delta_{BB'} + k_\lambda \sigma^{\lambda\mu}_{BB'}] + O(k^2). \end{aligned} \tag{4.14}$$

Note that $\sigma^{\mu\nu} = -\sigma^{\nu\mu}$ so that $k_\mu k_\lambda \sigma^{\lambda\mu} = 0$. Substituting (4.14) in (4.11), one can calculate $A^{\mu\nu}$ and $A'^{\mu\nu}$. Finally, we have for (4.3)

$$T_B'^{\mu\nu} = (n^2/2M)(\tilde{C}^{\mu\nu} + k_\lambda \sigma^{\lambda\mu} \tilde{A}^\nu - k'_\lambda \sigma^{\lambda\nu} \tilde{B}^\mu), \tag{4.15}$$

where

$$\begin{aligned} \tilde{C}^{\mu\nu} = &\frac{(2p + k)^\mu (2p' + k')^\nu}{2p \cdot k + k^2} \\ &+ \frac{(2p - k')^\nu (2p' - k)^\mu}{-2p \cdot k' + k'^2} - 2g^{\mu\nu} \end{aligned} \tag{4.16}$$

is the Compton amplitude for a point particle,

$$\begin{aligned} \tilde{B}^\mu &= \frac{(2p + k)^\mu}{2p \cdot k + k^2} + \frac{(2p' - k)^\mu}{-2p' \cdot k + k^2}, \\ \tilde{A}^\nu &= \frac{(2p' + k')^\nu}{2p' \cdot k' + k'^2} + \frac{(2p - k')^\nu}{-2p \cdot k' + k'^2}, \end{aligned} \tag{4.17}$$

and we have added the $-2g^{\mu\nu}$ term to (4.3) so that the conservation law is satisfied exactly. We have also written $\sigma^{\lambda\mu}$ for $\sigma^{\lambda\mu}_{BB}$. Nondiagonal matrix elements do not contribute to this order. We have thus arrived at the well-known conclusion that the two leading terms in the Compton scattering amplitude depend only on the mass, the "charge" n, and the "magnetic moment" $n\sigma^{\mu\nu}$, in suitable units.

What we have demonstrated is that, by using the conservation law, one is able to obtain the next leading term by considering the leading diagrams only. The same idea and technique can be applied when the in and out states involve more than one particle, as we shall see in the next section, although the algebra will be more involved.

5. LOW ENERGY THEOREMS, TWO PARTICLES

A. Bremsstrahlung

The main result of this section will be a low energy theorem for the amplitude $T^{\mu\nu}$ defined by (4.1) with two particles in the incoming and outgoing states. For clarity of presentation and better understanding of the physical meaning of various terms, we shall first look at a simpler problem, that is, the bremsstrahlung amplitude T^{μ} shown in Fig. 4, i.e., the amplitude for emitting a photon by one of the colliding particles. As Fig. 4 indicates, the photon can be emitted by one of the external lines, i.e., by the initial or the final free particles, or emitted when 1 and 2 are interacting. Clearly, only the diagrams (a) and (b) contribute to $O(k^{-1})$. In terms of two-body T-matrix elements, we have

$$\begin{aligned} T^{\mu} = {} & [(2p_1 + k)^{\mu}/2p_1 \cdot k + k^2] \langle p_1 + k, p_2 | T | p_1' p_2' \rangle \\ & + \langle p_1 p_2 | T | p_1' - k, p_2' \rangle \\ & \times [(2p_1' - k)^{\mu}/-2p_1' \cdot k + k^2] \\ & + \text{diagram (c)} + (1 \leftrightarrow 2), \end{aligned} \tag{5.1}$$

where $(1 \leftrightarrow 2)$ denotes the same diagrams with particle labels 1 and 2 interchanged to account for the case where the photon is emitted by particle 2 instead of 1. The contribution of (c) is of $O(1)$ and nonsingular as $k \to 0$. We now parametrize the two-body T-matrix elements in the usual relativistic terminology:

$$\langle pq | T | p'q' \rangle = f(p^2, q^2, p'^2, s, t), \tag{5.2}$$

where

$$s = (p + q)^2, \quad t = (p - p')^2, \quad u = (p' - q)^2. \tag{5.3}$$

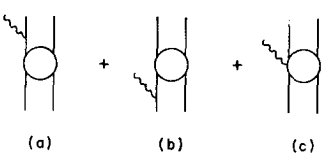


FIG. 4. Bremsstrahlung amplitude T^{μ}.

The u variable turned out to be irrelevant. When the T matrix is "on-shell," we must have

$$p^2 = q^2 = p'^2 = m^2.$$

We define the on-shell matrix elements by

$$f(s, t) = f(m^2, m^2, m,^2 s, t). \tag{5.4}$$

In this case

$$\begin{aligned} t &= -(\mathbf{p} - \mathbf{p}')^2 \\ s &= \epsilon^2, \text{ in c.m. frame,} \end{aligned} \tag{5.5}$$

where ϵ is the c.m. energy of the two-body system. Now let us look at the 2-body T-matrix elements in (5.1). For the first one, we have

$$\begin{aligned} & \langle p_1 + k_1 p_2 | T | p_1' p_2' \rangle \\ & = f((p_1 + k)^2, m^2, m^2, (p_1 + p_2 + k)^2, (p_2 - p_2')^2) \\ & = f(s, t) + \frac{\partial f}{\partial s} [2(p_1 + p_2) \cdot k + k^2] + O(b_1), \end{aligned} \tag{5.6}$$

where

$$b_1 \equiv 2p_1 \cdot k + k^2. \tag{5.7}$$

The $O(b_1)$ term in (5.6) contributes an $O(1)$ *nonsingular* term to T^{μ}. Note that the second term contribution to T^{μ} is formally $O(1)$ but is singular as $k \to 0$, i.e., it can have a value from $-\infty$ to ∞ depending how k approaches zero. Similar arguments apply to the second two-body T-matrix in (5.1); we obtain

$$\langle p_1 p_2 | T | p_1' - k, p_2' \rangle = f(s, t) + O(a_1), \tag{5.8}$$

$$a_1 \equiv -2p_1' \cdot k + k^2. \tag{5.9}$$

Again, the $O(a_1)$ term contributes a nonsingular $O(1)$ term to T^{μ}. Substituting (5.8) and (5.6) in (5.1), we have

$$\begin{aligned} T^{\mu} = {} & \tilde{B}_1^{\mu} f(s, t) + \frac{(2p_1 + k)^{\mu}}{2p_1 \cdot k + k^2} [2(p_1 + p_2) \cdot k + k^2] \frac{\partial f}{\partial s} \\ & - [2(p_1 + p_2) + k]^{\mu} \frac{\partial f}{\partial s} + r^{\mu} + (1 \leftrightarrow 2), \end{aligned} \tag{5.10}$$

where

$$\begin{aligned} \tilde{B}^{\mu} = {} & (2p + k)^{\mu}/(2p \cdot k + k^2) \\ & + (2p' - k)^{\mu}/(-2p' \cdot k + k^2), \end{aligned} \tag{5.11}$$

which appeared earlier in (4.17). We have introduced a term $-[2(p_1 + p_2) + k]^{\mu} \partial f/\partial s$ so that T^{μ} satisfies the conservation law $k_{\mu} T^{\mu} = 0$ without the remainder r^{μ}. In arriving at (5.10) we have left out terms of $O(1)$ as $k \to 0$. However, since $k_{\mu} r^{\mu} = 0$ and r^{μ} must be independent of k, we conclude that

$$r^{\mu} = O(k). \tag{5.12}$$

Let the antisymmetric tensor $\beta_1^{\lambda\mu}$ be defined as

$$\beta_1^{\lambda\mu} = \frac{(2P + k)^\lambda (2p_1 + k)^\mu - (2P + k)^\mu (2p_1 + k)^\lambda}{2p_1 \cdot k + k^2},$$
$$P \equiv p_1 + p_2. \tag{5.13}$$

Then (5.10) has the form

$$T^\mu = \tilde{B}_1^\mu f(s, t) + k_\lambda \beta_1^{\lambda\mu} \frac{\partial f}{\partial s} + (1 \leftrightarrow 2) + O(k). \tag{5.14}$$

This is the low energy theorem for bremsstrahlung. We have thus demonstrated that the on-shell two-body scattering amplitudes are sufficient to determine the two leading terms in T^μ.

B. Physical Interpretation of the Bremsstrahlung Low Energy Theorem

The amplitude $\tilde{B}_1^\mu$, as shown in (5.11) has two terms. The first is the amplitude for photon emission by the outgoing plane wave p_1 which is switched on at time $t = 0$, and the second is that by the incoming plane wave p_1' switched off at $t = 0$. The two-body amplitude f in the first term of (5.10) is the probability amplitude for switching off p_1' and switching on p_1. The meaning of the second term in (5.10) is less transparent. It can be understood if we construct a wavepacket to describe particle 1. The effect of $\partial f/\partial s \sim \partial f/\partial \epsilon$ is a modification of the shape and a delay in the switching on time of the outgoing wavepacket.[4] Notice that $\partial f/\partial \epsilon$ here is taken at constant momentum transfer. Classically, we are fitting the exact trajectory of particle 1 by two straight paths which agree with the asymptotic parts of the exact trajectory, with the delay of the appearance of the final path counted for. In fixing up the time delay, one has to patch up the paths so that there is a continuous current going when the initial path is off and the final path is not on yet. The third term of (5.10) does this job. One moment of reflection shows that the $O(1)$ term in T^μ is just the space–time integral of the current. A trajectory patched up with straight lines having the right asymptotic behavior and conserving the current therefore describes correctly the process to $O(k^{-1})$ *and* to $O(1)$.

C. Emission and Absorption, Asymptotic Amplitudes

We now proceed to derive a low energy theorem for $T^{\mu\nu}$ defined by (4.1) for $n = 2$. The diagrams for $T^{\mu\nu}$ are shown in Fig. 5. In order to make the physical meaning of our formulas explicit and also to save writing, we introduce the following notation.

1. *Absorption of the Photon* (k', ν)

A^ν is the amplitude for absorption by the *outgoing* plane wave p, and A'^ν is that by the *incoming* plane wave p':

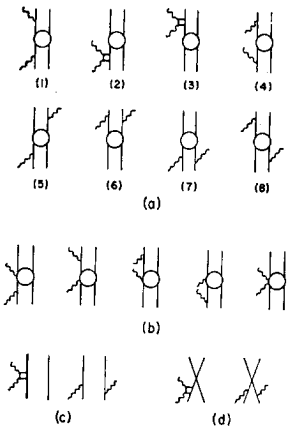


FIG. 5. Diagrams for $T^{\mu\nu}$ with $n = 2$. The small square with two photon lines attached denotes the Compton scattering amplitude $C^{\mu\nu}$ or $C'^{\mu\nu}$ defined by (5.19). (a) Photon lines attached to external particle lines only. (b) One or both photon lines attached to internal particle line. (c) Disconnected terms in $T^{\mu\nu}$. (d) Exchange diagrams due to the identity of the two particles.

$$A^\nu = \frac{(2p - k')^\nu}{-2p \cdot k' + k'^2}, \quad A'^\nu = \frac{(2p' + k')^\nu}{2p' \cdot k' + k'^2}, \tag{5.15}$$
$$a \equiv -2p \cdot k' + k'^2, \quad a' \equiv 2p' \cdot k' + k'^2,$$
$$\alpha^{\lambda\nu} \equiv (2P - k')^\lambda A^\nu - (2P - k')^\nu A^\lambda. \tag{5.16}$$

We shall always associate primed quantities with incoming plane waves and unprimed ones with outgoing plane waves. The vector P is always the total momentum $p_1 + p_2$.

2. *Bremsstrahlung, Emission of the Photon* (k, μ)

B^μ is the amplitude for emission by the outgoing p and B'^μ is that by the incoming p':

$$B^\mu = \frac{(2p + k)^\mu}{2p \cdot k + k^2}, \quad B'^\mu = \frac{(2p' - k)^\mu}{-2p' \cdot k + k^2}, \tag{5.17}$$
$$b \equiv 2p \cdot k + k^2, \quad b' \equiv -2p' \cdot k + k^2,$$
$$\beta^{\lambda\mu} \equiv (2P + k)^\lambda B^\mu - (2P + k)^\mu B^\lambda. \tag{5.18}$$

3. *Compton Scattering, Emission of* (k, μ), *and Absorption of* (k', ν)

$C^{\mu\nu}$ is the amplitude for Compton scattering by the outgoing wave p and $C'^{\mu\nu}$ is that by the incoming wave p':

$$cC^{\mu\nu} = \frac{(2p + k)^\mu (2p + 2k - k')^\nu}{2p \cdot k + k^2} + \frac{(2p - k')^\nu (2p + k - 2k')^\mu}{-2p \cdot k' + k'^2} - 2g^{\mu\nu},$$
$$c'C'^{\mu\nu} = \frac{(2p' + k')^\nu (2p' + 2k' - k)^\mu}{2p' \cdot k' + k'^2} + \frac{(2p' - k)^\mu (2p' + k' - 2k)^\nu}{-2p' \cdot k + k^2} - 2g^{\mu\nu}, \tag{5.19}$$
$$c \equiv 2p \cdot (k - k') + (k - k')^2,$$
$$c' \equiv -2p' \cdot (k - k') + (k - k')^2. \tag{5.20}$$

4. Particle Labels

Note that the letters A, B, C, a, b, and c used above remind us of the names of the processes. The particle labels will be carried explicitly as subscripts, for example,

$$a_2' \text{ means } p_2' \cdot k' + k'^2. \tag{5.21}$$

5. Conservation Laws

The above defined A, B, and C amplitudes satisfy

$$\begin{aligned} k_\nu' A^\nu &= -1, & k_\nu' A'^\nu &= 1, \\ k_\mu B^\mu &= 1, & k_\mu B'^\mu &= -1, \\ k_\mu C^{\mu\nu} &= A^\nu, & k_\nu' C^{\mu\nu} &= -B^\mu, \\ k_\mu C'^{\mu\nu} &= -A'^\nu, & k_\nu' C'^{\mu\nu} &= B'^\mu. \end{aligned} \tag{5.22}$$

These equations may be interpreted as the "divergence" or the "source" of the photon amplitudes owing to the switch on and off of the outgoing and incoming plane waves.

D. Matrix Elements

Clearly the eight diagrams in Fig. 5(a) are of $O(k^{-2})$. The leading terms are proportional to

$$(ba')^{-1}, (c'a')^{-1}, (c'b')^{-1}, \text{ etc.}$$

The first four diagrams in Fig. 5(b) are of $O(k^{-1})$, proportional to

$$a'^{-1}, a^{-1}, b^{-1}, b'^{-1}. \tag{5.23}$$

The last diagram in Fig. 5(b) is of $O(1)$. The disconnected terms in Fig. 5(c) will be discussed later. It is not hard to notice that c^{-1} and c'^{-1} never appear alone. They are always accompanied by the a and b denominators in $C^{\mu\nu}$ and $C'^{\mu\nu}$. We also notice that a^{-1} and a'^{-1} are singular in k' but nonsingular in k since they do not depend on k. Likewise b^{-1} and b'^{-1} are singular in k but not in k'.

Suppose that a certain quantity $r^{\mu\nu}$ is of $O(a^{-1}, a'^{-1}, b^{-1}, b'^{-1})$, i.e., it is of $O(k^{-1})$ and it contains terms singular in either k or in k' but none in both. Suppose further that $r^{\mu\nu}$ satisfies the conservation law in both k and k', i.e.,

$$k_\mu r^{\mu\nu} = 0, \quad k_\nu' r^{\mu\nu} = 0. \tag{5.24}$$

Then we must have

$$r^{\mu\nu} = O(1), \quad \text{as } k \to 0, \tag{5.25}$$

instead of $O(k^{-1})$. Therefore, if we find the contribution to $T^{\mu\nu}$ which includes all terms singular in both k and k' and satisfies the conservation law in both k and k', then we will have found $T^{\mu\nu}$ to the first two leading orders in k^{-1}. This is the same situation as that in the low energy theorems we discussed previously. We have to consider only the leading diagrams (1)–(8) in Fig. 5 which contain terms singular in both k and k'.

Similar to (5.6) and (5.8), the eight two-body T-matrix elements in (1)–(8) are found to be

$$\begin{aligned} &(1)\ f(s,t'') + \eta \frac{\partial f}{\partial s} + O(b,a'), \\ &(2)\ f(s,t'') + O(c'), \\ &(3)\ f(s,t'') + \lambda \frac{\partial f}{\partial s} + O(c), \\ &(4)\ f(s,t'') - \eta' \frac{\partial f}{\partial s} + O(a,b'), \\ &(5)\ f(s,t') + \eta \frac{\partial f}{\partial s} + O(b,a'), \\ &(6)\ f(s,t') + \lambda \frac{\partial f}{\partial s} + O(b,a), \\ &(7)\ f(s,t') + O(b',a'), \\ &(8)\ f(s,t') - \eta' \frac{\partial f}{\partial s} + O(b',a), \end{aligned} \tag{5.26}$$

where

$$\begin{aligned} \eta &\equiv 2P \cdot k + k^2, \quad \eta' \equiv 2P \cdot k' - k'^2, \\ \lambda &\equiv 2P \cdot (k - k') + (k - k')^2, \\ t' &\equiv (p_1 - p_1' - k')^2, \quad t'' \equiv (p_1 - p_1' + k - k')^2. \end{aligned} \tag{5.27}$$

Since only $O(k)$ terms in these matrix elements are of interest, we set

$$\begin{aligned} f(s,t') &= f(s,t) - 2k' \cdot (p_1 - p_1') \frac{\partial f}{\partial t}, \\ f(s,t'') &= f(s,t) + 2(k - k') \cdot (p_1 - p_1') \frac{\partial f}{\partial t}, \\ t &\equiv (p_1 - p_1')^2. \end{aligned} \tag{5.28}$$

We see that we have not only the derivative of f with respect to energy appearing, but also that with respect to the momentum transfer. While the former gives the effect of time delay in switching on the outgoing wave, the latter counts for besides a distortion also a space displacement of the outgoing wave. The vector $2(p_1 - p_1')\partial\chi/\partial t$ plays the role of the distance of closest approach in a classical description.[7] Qualitatively, the derivative term will count for the fact that the outgoing particles are created at a delayed time and at a distance apart instead of at the space time origin. Now it is a matter of writing down the A, B, and C amplitudes for the outgoing and incoming plane waves and substituting (5.26) for the two-body matrix elements. Collecting terms, we

obtain

$$T^{\mu\nu} = M^{\mu\nu} f + N^{\mu\nu} \frac{\partial f}{\partial s} + Q'^{\mu\nu} \frac{\partial f}{\partial t} + r^{\mu\nu}, \quad (5.29)$$

where $M^{\mu\nu}$, $N^{\mu\nu}$, and $Q'^{\mu\nu}$ depend only on the kinematic variables k, k', p, and p'. All the relevant dynamical information is summarized in the on-shell amplitude and its derivatives. $M^{\mu\nu}$ is the total amplitude for the absorption and bremsstrahlung by the incoming and the (undelayed, unshifted) outgoing waves. We have

$$M^{\mu\nu}(p, p') = (A_1 + A_1' + A_2 + A_2')^\nu (B_1 + B_1' + B_2 + B_2')^\mu + [C_1^{\mu\nu} - B_1^\mu A_1^\nu + C_1'^{\mu\nu} - B_1'^\mu A_1'^\nu + (1 \leftrightarrow 2)], \quad (5.30)$$

where the first term is the product of absorption and that of emission, as if these two processes were independent, and the second term corrects for the deviation of the Compton scattering by a plane wave from the absorption and emission by the same plane wave taken as independent processes. The second term of (5.29) corrects for the delay of switching on the outgoing waves. We have

$$N^{\mu\nu}(p, p') = k_\lambda(\beta_1 + \beta_2)^{\lambda\mu}(A_1 + A_2 + A_1' + A_2')^\nu - k_\lambda(\alpha_1 + \alpha_2)^{\lambda\nu}(B_1 + B_2 + B_1' + B_2')^\mu + (C_1^{\mu\nu} - A_1^\nu B_1^\mu + C_2^{\mu\nu} - A_2^\nu B_2^\mu)(k - k') \cdot 2P. \quad (5.31)$$

Finally, the third term in (5.29) counts for the effect of a displacement of the outgoing waves, i.e., the fact that they are created at a distance apart:

$$\begin{aligned} Q'^{\mu\nu} &= Q''^{\mu\nu} + Q'''^{\mu\nu}, \\ Q''^{\mu\nu} &= -2(A_1 + A_1')^\nu \times (B_2 + B_2')^\mu k' \cdot (p_1 - p_1') + (1 \leftrightarrow 2), \quad (5.32) \\ Q'''^{\mu\nu} &= 2[A_1^\nu B_1'^\mu + A_1'^\nu B_1^\mu + C_1^{\mu\nu} + C_1'^{\mu\nu}] \times (k - k') \cdot (p_1 - p_1') + (1 \leftrightarrow 2). \end{aligned}$$

Similar to the third term in (5.10), there are terms in (5.31) which are added in by hand so that $T^{\mu\nu}$ without the remainder $r^{\mu\nu}$ satisfies

$$k_\mu T^{\mu\nu} = k_\nu' T^{\mu\nu} = 0.$$

Thus $r^{\mu\nu}$ satisfies (5.24), and we conclude that

$$r^{\mu\nu} = O(1). \quad (5.33)$$

Equation (5.29) is thus the desired low energy theorem. Note that each of $M^{\mu\nu}$, $N^{\mu\nu}$, and $Q'^{\mu\nu}$ satisfies the conservation law in both k and k'.

The disconnected terms in Fig. 5(c) and the exchange terms in Fig. 5(d) are trivial. They will play a part in the correlation function as will be seen shortly.

6. CORRELATION FUNCTION, EFFECT OF TWO-BODY INTERACTION

With the low energy theorems (4.15) and (5.29), we are now in a position to calculate the two leading terms of $F_n'^{\mu\nu}$ in k^{-1} for $n = 2$. The imaginary part of $F_2'^{\mu\nu}$ then gives the two-body contribution to the correlation function $S'^{\mu\nu}$:

$$S_2'^{\mu\nu}(k) = -2 \operatorname{Im} F_2'^{\mu\nu}(k), \quad (6.1)$$

$$S'^{\mu\nu} = zS_1'^{\mu\nu} + z^2 S_2'^{\mu\nu} + O(z^3), \quad (6.2)$$

where $zS_1'^{\mu\nu}$ is the ideal gas approximation given by (3.22). For quicker reference, let us write (3.12) here:

$$F_2'^{\mu\nu} = \lim_{\theta \to 0} \sum_{r,s} e^{-\beta E_r} \langle r | S^\dagger | s \rangle \langle s | T^{\mu\nu}(k, k') | r' \rangle, \quad |r'\rangle = e^{iJ_3\theta} |r\rangle. \quad (6.3)$$

A. Two-Body Bound States

According to the low energy theorem (4.15), a two-body bound state acts just like a point particle with "charge" 2 and a "magnetic moment" as far as the $O(k^{-1})$ and $O(1)$ terms in $T^{\mu\nu}$ are concerned. Only the $O(k^{-1})$ term is of interest here since only the contributions $O(k^{-2})$ and $O(k^{-1})$ are kept in the low energy theorem for two-body scattering states. The magnetic moment term, which is of $O(1)$ (and in fact zero when all orientations of the moment are counted), will be ignored. We have

$$S_2'^{\mu\nu}(\text{bound states}) = 4S_1'^{\mu\nu}(m \to 2m) \sum_B e^{-\beta E_B} + O(1), \quad (6.4)$$

where $S_1'^{\mu\nu}$ is the one-particle contribution given by (3.22) and $-E_B$ is the binding energy of the state B.

B. Exchange Diagrams

The diagrams shown in Fig. 5(d), coming from the identity of particles, give rise to the following terms to $\langle \mathbf{p}_1 \mathbf{p}_2 | T^{\mu\nu}(k, k) | \mathbf{p}_1 \mathbf{p}_2 \rangle$:

$$\pm(1/2m)\bar{C}_1^{\mu\nu}(2\pi)^3 \delta(\mathbf{p}_1 - \mathbf{p}_2)(\epsilon_2/m) \quad (6.5)$$

and

$$\pm[-2\pi i \delta(2p_1 \cdot k + k^2)(2p_1 + k)^\mu (2p_1 + k)^\nu \times (1/2m)(\epsilon_2/m)\delta(\mathbf{p}_1 + \mathbf{k} - \mathbf{p}_2)], \quad (6.6)$$

where the $\pm$ signs refer to the cases of bosons and fermions, respectively, and $\bar{C}^{\mu\nu}$ is the forward Compton scattering amplitude

$$\bar{C}^{\mu\nu} = \frac{(2p + k)^\mu (2p + k)^\nu}{2p \cdot k + k^2} + \frac{(2p - k)^\mu (2p - k)^\nu}{-2p \cdot k + k^2} - 2g^{\mu\nu}. \quad (6.7)$$

Note that $\bar{C}^{\mu\nu}$ is the same as $C^{\mu\nu}$ with $k = k'$ *except* for a factor of c [see (5.19)]. Integrating (6.5) and (6.6) over $d^3p_1\, d^3p_2(2\pi)^{-6}(m^2/\epsilon_1\epsilon_2)e^{-\beta(\epsilon_1+\epsilon_2)}$, we obtain

$$S_2'^{\mu\nu}(\text{exchange}) = \pm S_1'^{\mu\nu}(\beta \to 2\beta) + O(1). \quad (6.8)$$

C. Scattering States

In (6.3), we make the replacements $r \to \mathbf{p}_1\mathbf{p}_2$, $s \to \mathbf{q}_1\mathbf{q}_2$. Similarly to $\epsilon_{1,2}$, let us define

$$\nu_1 = q_1^0 = (\mathbf{q}_1^2 + m^2)^{\frac{1}{2}}. \quad (6.9)$$

To simplify the notation, let

$$E = \epsilon_1 + \epsilon_2, \quad P = p_1 + p_2 = q_1 + q_2. \quad (6.10)$$

For the frequently occurring phase space integrals, we write

$$d\mathbf{p} = d^3p_1\, d^3p_2(2\pi)^{-6}(m^2/\epsilon_1\epsilon_2),$$
$$dq = d^3q_1\, d^3q_2(2\pi)^{-6}(m^2/\nu_1\nu_2)(2\pi)^4\delta(\nu_1 + \nu_2 - \epsilon_1 - \epsilon_2) \times \delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{q}_1 - \mathbf{q}_2). \quad (6.11)$$

Then (6.3) has the form (see Fig. 6)

$$F_2'^{\mu\nu} = \lim_{\theta\to 0} \tfrac{1}{2}\int d\mathbf{p}\, e^{-\beta E}\Big(\langle \mathbf{p}_1\mathbf{p}_2|\, T^{\mu\nu}(kk')\, |\mathbf{p}_1'\mathbf{p}_2'\rangle + \tfrac{1}{2}i\int dq\, f^*(s,t)\,\langle \mathbf{q}_1\mathbf{q}_2|\, T^{\mu\nu}(kk')\, |\mathbf{p}_1'\mathbf{p}_2'\rangle\Big)_c, \quad (6.12)$$

where the factors $\frac{1}{2}$ in front of $d\mathbf{p}$ and dq are to count for the identity of the two particles.

The next step is to substitute the expression (5.29) and the disconnected terms in Fig. 5(c) for $T^{\mu\nu}$ in (6.12), simplify, and carry out the limit $\theta \to 0$.

D. Small Angle Limit

Since $\mathbf{p}_1'$ and $\mathbf{p}_2'$ are obtained by rotating $\mathbf{p}_1$ and $\mathbf{p}_2$, it is obvious that

$$\mathbf{p}_1'^2 = \mathbf{p}_1^2, \quad \mathbf{p}_2^2 = \mathbf{p}_2'^2, \quad \omega = \omega'. \quad (6.13)$$

Notice that $\omega = \omega'$ does not imply $|\mathbf{k}| = |\mathbf{k}'|$. The vector $\mathbf{k}'$ is completely determined by momentum conservation. The geometry is shown in Fig. 7.

Evidently, as $\theta \to 0$, $k \to k'$. The only terms in $T^{\mu\nu}$ which are not defined for $k = k'$ are the Compton amplitudes $C_{1,2}^{\mu\nu}$ and $C_{1,2}'^{\mu\nu}$ as is shown clearly by (5.20).

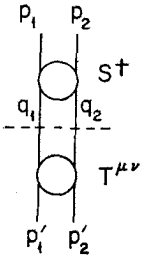


FIG. 6. Kinematic variables in the product $S^\dagger T^{\mu\nu}$. The photon lines are not shown. The horizontal dashed line indicates a factor of energy conservation δ function.

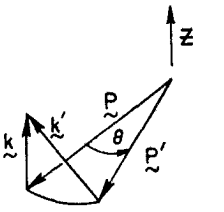


FIG. 7. Geometry for $\mathbf{k}$, $\mathbf{k}'$, $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$ and $\mathbf{P}' = \mathbf{p}_1' + \mathbf{p}_2'$. The z-components of $\mathbf{P}$, $\mathbf{P}'$ are not shown. The axis of rotation points along $\mathbf{k}$.

These amplitudes appear in $M^{\mu\nu}$ and in $Q'''^{\mu\nu}$ [see (5.30) and (5.32)]. Those in (5.31) are suppressed by the condition $\omega = \omega'$ and the fact that $\mathbf{k} - \mathbf{k}'$ is perpendicular to $\mathbf{P}$ to the order of interest.

We now concentrate on the contribution of these Compton amplitudes to $F_2'^{\mu\nu}$. Consider the terms in $M^{\mu\nu}$ first:

$$F_C'^{\mu\nu}(\theta) = \int d\mathbf{p}\, e^{-\beta E}\Big((C_1^{\mu\nu} + C_1'^{\mu\nu})f(s,t) + \tfrac{1}{2}i\int dq\, |f(s,t')|^2 (C^{\mu\nu}(q_1) + C_1'^{\mu\nu})\Big). \quad (6.14)$$

Figure 8(a) shows the corresponding diagrams. The meaning of $C^{\mu\nu}(q_1)$ is clear: The p_1 in the $C_1^{\mu\nu}$ defined before is replaced by q_1. Notice that the last diagram in Fig. 8(a) vanishes since energy–momentum conservation is violated. Keeping in mind that the rotation operator $e^{iJ_3\theta}$ commutes with the T matrix and applying the optical theorem, we can reduce (6.14) down to the diagrams shown in Fig. 8(b).

$$F_C'^{\mu\nu}(\theta) = \int d\mathbf{p}\, e^{-\beta E}(C_1^{\mu\nu} + C_1'^{\mu\nu})f^*(s,t). \quad (6.15)$$

The axis of rotation is entirely arbitrary. We shall

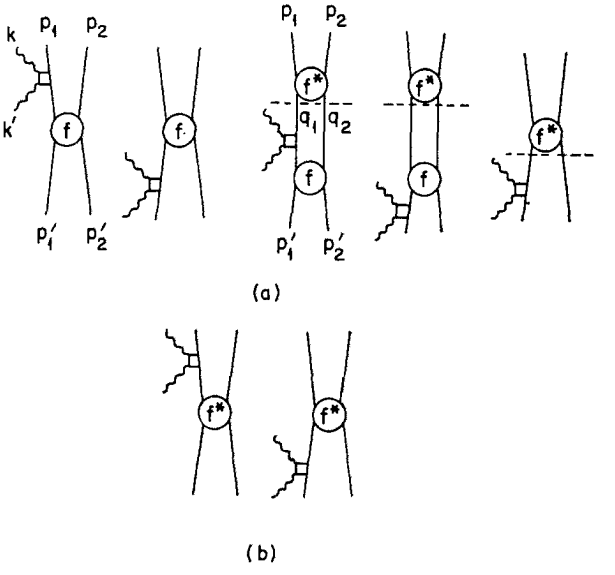


FIG. 8. (a) Contribution of the Compton amplitude to $\langle \mathbf{p}|\, S^\dagger T^{\mu\nu}\, |\mathbf{p}'\rangle$. The last diagram comes from a disconnected term in $T^{\mu\nu}$. It vanishes by kinematical constraints. (b) The diagrams in (a) reduce down to these two terms.

choose the axis along $\mathbf{k}$ (see Fig. 7). It follows that

$$p_1 \cdot k = p_1' \cdot k, \quad p_2 \cdot k = p_2' \cdot k. \tag{6.16}$$

We define

$$\xi = k - k'. \tag{6.17}$$

Then

$$\xi = (\mathbf{k} - \mathbf{k}', 0), \quad k \cdot \xi = 0, \quad k'^2 = k^2 + \xi^2. \tag{6.18}$$

To see explicitly how $C_1^{\mu\nu}$ and $C_1'^{\mu\nu}$ behave, we go back to (5.19) and (5.20). In terms of ξ, we have

$$\begin{aligned} &c_1 = 2p_1 \cdot \xi + \xi^2, \quad c_1' = -2p_1' \cdot \xi + \xi^2, \\ &2p_1' \cdot k' + k'^2 = 2p_1 \cdot k + k^2 + c_1', \\ &-2p_1 \cdot k' + k'^2 = -2p_1 \cdot k + k^2 + c_1. \end{aligned} \tag{6.19}$$

All the other factors of k' can be expressed in terms of k and ξ. We now change the integration variable $\mathbf{p}_1$ in the second term of (6.15) so that

$$\mathbf{p}_1' \to \mathbf{p}_1 + \boldsymbol{\xi}. \tag{6.20}$$

Under this change of variable,

$$\begin{aligned} &c_1' \to -c_1, \quad \mathbf{p}_1^2 \to (\mathbf{p}_1 + \boldsymbol{\xi})^2 = \mathbf{p}_1^2 - c_1, \\ &\epsilon_1^2 = m^2 + \mathbf{p}_1^2 \to \epsilon_1^2 - c_1. \end{aligned} \tag{6.21}$$

The integrand of (6.15) now becomes

$$\begin{aligned} &(2p_1 + k + \xi)^\nu (2p_1 + k)^\mu \\ &\quad \times \left(\frac{Y(\epsilon_1^2)}{2p_1 \cdot k + k^2} - \frac{Y(\epsilon_1^2 - c_1)}{2p_1 \cdot k + k^2 - c_1} \right) c_1^{-1} \\ &\quad + (2p_1 - k + 2\xi)^\mu (2p_1 - k + \xi)^\nu \\ &\quad \times \left(\frac{Y(\epsilon_1^2)}{-2p_1 \cdot k + k^2 + c_1} - \frac{Y(\epsilon_1^2 - c_1)}{-2p_1 \cdot k + k^2} \right) c_1^{-1} \\ &\quad - 2g^{\mu\nu}[Y(\epsilon_1^2) - Y(\epsilon_1^2 - c_1)]c_1^{-1}, \end{aligned} \tag{6.22}$$

where $Y(\epsilon_1^2)$ is the part of the integrand that depends on ϵ_1 including the factor $1/\epsilon_1$ in $d\mathbf{p}$ [see (6.11)]:

$$Y(\epsilon_1^2) \propto (1/\epsilon_1) f^* e^{-\beta E}. \tag{6.23}$$

In (6.22), we have ignored terms of $O(\omega/m)$, i.e., the frequency is assumed to be small compared to the mass of the particle. Now the limit $\theta \to 0$ can be taken easily in (6.22). We simply let ξ, c_1, and t approach zero and obtain

$$\begin{aligned} F_C'^{\mu\nu} &= \lim_{\theta \to 0} F_C'^{\mu\nu}(\theta) \\ &= \int d\mathbf{p} \Big(-e^{-\beta E} (B_1^\mu A_1'^\nu + B_1'^\mu A_1^\nu)_{p=p'} f^*(s, 0) \\ &\quad + \bar{C}_1^{\mu\nu} \frac{\partial}{\partial \epsilon_1} [e^{-\beta E} (m/\epsilon_1) f^*(s, 0)] \Big), \end{aligned} \tag{6.24}$$

where $\bar{C}^{\mu\nu}$ is the forward Compton scattering amplitude defined by (6.7).

Next, we consider the contribution of $C_1^{\mu\nu}$ and $C_1'^{\mu\nu}$ in $Q'''^{\mu\nu}$ [see (5.32)]. Similar to (6.14), we have

$$\begin{aligned} F_C'''^{\mu\nu}(\theta) = \int d\mathbf{p}\, e^{-\beta E} \Big(&(C_1^{\mu\nu} + C_1'^{\mu\nu}) \left(\frac{\partial f}{\partial t} \right)_{t=0} 2(p_1 - p_1') \cdot \xi \\ &+ \tfrac{1}{2} i \int dq\, f^*(s, t) \frac{\partial}{\partial t} f(s, t) \\ &\times [C^{\mu\nu}(q_1) + C_1'^{\mu\nu}] 2(q_1 - p_1') \cdot \xi \Big), \end{aligned}$$

$$t = (q_1 - p_1')^2. \tag{6.25}$$

In the limit $\theta \to 0$, by (6.7), (6.19), and (5.20), we have

$$\begin{aligned} &2(C^{\mu\nu}(q_1) + C_1'^{\mu\nu})(q_1 - p_1') \cdot \xi \\ &\quad = \bar{C}^{\mu\nu}(q_1) \frac{(q_1 - p_1) \cdot \xi}{q_1 \cdot \xi} + \bar{C}_1^{\mu\nu} \frac{(q_1 - p_1) \cdot \xi}{-p_1 \cdot \xi} \end{aligned} \tag{6.26}$$

and the first term of (6.25) vanishes. Taking advantage of the $p \leftrightarrow q$ symmetry in (6.25), we have

$$\begin{aligned} \lim_{\theta \to 0} F_C'''^{\mu\nu}(\theta) = i \int d\mathbf{p}\, e^{-\beta E} \tfrac{1}{2} \int dq\, f^* \frac{\partial f}{\partial t} \\ \times \bar{C}_1^{\mu\nu} \frac{2(p_1 - q_1) \cdot \xi}{p_1 \cdot \xi}. \end{aligned} \tag{6.27}$$

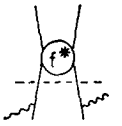
Recall that $\xi = (\boldsymbol{\xi}, 0)$ and, in the $\tilde{\theta} \to 0$ limit, the vector $\boldsymbol{\xi}$ is perpendicular to $\mathbf{k}$ and $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$. Thus, in (6.27), we may write

$$\boldsymbol{\xi} = \mathbf{k} \times \mathbf{P}, \quad p_1 \cdot \xi = \tfrac{1}{2}(p_1 - p_2) \cdot \xi. \tag{6.28}$$

Clearly, only the values of p_1 and q_1 in the c.m. frame are relevant in evaluating the last factor of (6.27). The dependence on ξ can be removed by further exploiting the symmetries. In all the other terms of $T^{\mu\nu}$, θ can be set to zero directly. Multiplying $T^{\mu\nu}$ by $S^\dagger$ and taking into account the diagram in Fig. 9, we obtain

$$\begin{aligned} F_2'^{\mu\nu} = \tfrac{1}{2} i \int d\mathbf{p}\, e^{-\beta E} dq \Big(&|f(s,t)|^2 [\bar{M}^{\mu\nu}(q, p) - \bar{M}^{\mu\nu}(p, p)] \\ &+ N^{\mu\nu}(q, p) f^* \frac{\partial}{\partial s} f + Q^{\mu\nu}(q, p) f^* \frac{\partial}{\partial t} f \Big) \\ &+ \int d\mathbf{p} \Big[e^{-\beta E} \Big(\lambda^\mu(p_1) \lambda^\nu(p_2) f^*(s, 0) \\ &+ N^{\mu\nu}(p, p) \frac{\partial f(s, 0)}{\partial s} \Big) \\ &+ \bar{C}^{\mu\nu}(p_1) \frac{\partial}{\partial \epsilon_1} \left(\frac{m}{\epsilon_1} f^*(s, 0) e^{-\beta E} \right) \\ &+ (2m)^{-1} (2\pi)^2 \delta(a_1) \delta(b_2) \\ &\times (2p_1 + k)^\nu (2p_2 - k)^\mu f^*(s, 0) e^{-\beta E} \Big] + O(1), \end{aligned} \tag{6.29}$$

FIG. 9. A term in $S^\dagger T^{\mu\nu}$ contributed by a disconnected term in $T^{\mu\nu}$, the last one in Fig. 5(c).



where

$$Q^{\mu\nu}(q, p) = Q''^{\mu\nu}(q, p) + 2(\bar{C}_1^{\mu\nu}\{[(p_1 - q_1)\cdot\xi]/(p_1\cdot\xi)\} + (1 \leftrightarrow 2)) \quad (6.30)$$

[see (6.27) and (5.32)] and $\bar{M}^{\mu\nu}$ is given by the first term of $M^{\mu\nu}$ [see (5.30)], i.e., it is simply the product of total absorption amplitude and the total emission amplitude:

$$\bar{M}^{\mu\nu} = (A_1 + A_2 + A_1' + A_2')^\nu (B_1 + B_2 + B_1' + B_2')^\mu, \quad (6.31)$$

and λ^μ is the forward absorption or emission amplitude

$$\begin{aligned}\lambda^\mu(p) &= (2p + k)^\mu/(2p\cdot k + k^2) \\ &\quad + (2p - k)^\mu/(-2p\cdot k + k^2) \\ &= B^\mu(p) + B'^\mu(p) \\ &= A^\mu(p) + A'^\mu(p). \end{aligned} \quad (6.32)$$

$N^{\mu\nu}$ and $\bar{C}^{\mu\nu}$ are, respectively, defined by (5.31) and (6.7).

E. Summary of the Two-Body Terms

What is left to be done is to take the imaginary part of (6.29) to obtain $S_2'^{\mu\nu}$. Since the result contains many terms, it may be more instructive to present them term by term, and discuss their origin and implication in each case.

(*i*) *Terms of* $O(k^{-2})$:

$$-\int d\mathbf{p}\, e^{-\beta E}(v\, d\sigma) 4\,\mathrm{Re}\left[\frac{p_1^\mu p_1'^\nu}{d_1 d_1'} - \frac{p_1^\mu p_1^\nu}{d_1^2} + \frac{p_1^\mu p_2'^\nu}{d_1 d_2'} - \frac{p_1^\mu p_2^\nu}{d_1 d_2}\right]. \quad (6.33)$$

Here $v\, d\sigma = \frac{1}{2}dp'|f(s, t)|^2$ [see (6.11) for the abbreviation dp'] is the rate of the transition $\mathbf{p}_1' + \mathbf{p}_2' \to \mathbf{p}_1 + \mathbf{p}_2$. The first two terms in the square bracket come from the diagrams (1)–(4) in Fig. 5(a) and the other two from (5)–(8). The symbol d will always denote the denominator

$$d = p\cdot k. \quad (6.34)$$

A positive infinitesimal imaginary part in d is understood. Equation (6.33) has a simple classical interpretation. Notice that (in the nonrelativistic case, for simplicity)

$$\frac{p^\mu}{d} = -i\int d^4x e^{ik\cdot x}\frac{p^\mu}{m}\,\delta\left(\mathbf{x} - t\frac{\mathbf{p}}{m}\right)\theta(t) \quad (6.35)$$

describes the photon emission amplitude by a point charge created at $x = 0$ going out with velocity $\mathbf{p}/m$. Equation (6.33) may be interpreted as owing to particles coming with momenta $p_1'p_2'$ and making a sudden change at $x = 0$ to p_1, p_2 and then moving out. The effect of a decrease in the intensity of forward moving particles is counted for by the two negative terms.

(*ii*) *Terms of* $O(k^{-1})$, *energy derivatives of the scattering amplitudes, "time delay" terms:* Define $f = |f|\,e^{i\chi}$. We have[7]

$$\begin{aligned}&-\int d\mathbf{p}\, e^{-\beta E}(v\, d\sigma)\frac{\partial\chi}{\partial s} \\ &\quad\times 8\,\mathrm{Im}\left[P\cdot k\,\frac{p_1^\mu}{d_1}\left(\frac{p_1'^\nu}{d_1'} + \frac{p_2'^\nu}{d_2'}\right) - \frac{2}{d_1}(P^\mu p_1^\nu + P^\nu p_1^\mu)\right], \\ &-\left(\frac{4}{m^2}\right)\int d\mathbf{p}\, e^{-\beta E} 2\,\mathrm{Re}\frac{\partial f(s, 0)}{\partial s} \\ &\quad\times \mathrm{Im}\left[P\cdot k\,\frac{p_1^\mu}{d_1}\left(\frac{p_1^\nu}{d_1} + \frac{p_2^\nu}{d_2}\right) - \frac{2}{d_1}(P^\mu p_1^\nu + P^\nu p_1^\mu)\right]. \end{aligned} \quad (6.36)$$

As was mentioned before, the derivative $\partial\chi/\partial s \sim \partial\chi/\partial\epsilon$ can be interpreted as a "time delay." The real part of $f(s, 0)$ describes the energy shift of a particle due to scattering with other particles in the medium. Its derivative describes the time delay in forward scattering.

(*iii*) *Terms of* $O(k^{-1})$, *derivative of the amplitude with respect to momentum transfer:*

$$\int d\mathbf{p}\, e^{-\beta E}(v\, d\sigma)\frac{\partial\chi}{\partial t} 8\,\mathrm{Im}\left((p_1 - p_1')\cdot k\,\frac{p_1^\mu p_2'^\nu}{d_1 d_2'} + \frac{1}{d_1}\left(\frac{2t}{s - 4m^2}\right)[p_1^\mu p_1^\nu + \tfrac{1}{2}(p_1^\mu p_2^\nu + p_2^\mu p_1^\nu)]\right], \quad (6.37)$$

where $2t/(s - 4m^2)$ is just $(1 - \cos\theta)$ in the c.m. frame. The fact that (6.37) satisfies the conservation law can be shown in a few steps although they are not directly obvious.

(*iv*) *Terms of* $O(k^{-1})$, *involving no derivative of* f: First, there is a term from (1)–(4) in Fig. 5(a):

$$\left(\frac{2}{m}\right)\int d\mathbf{p}\,\frac{\partial}{\partial\epsilon_1}\left(\frac{m}{\epsilon_1}\,\mathrm{Re}\, f(s, 0)e^{-\beta E}\right)2\pi\delta(d_1)p_1^\mu p_1^\nu. \quad (6.38)$$

The differentiation operator is easily removed by integrating by parts. Then there is a term from (5)–(8) in Fig. 5(a):

$$\begin{aligned}&-2\int d\mathbf{p}\, e^{-\beta E}\,\mathrm{Im}\,[\lambda^\mu(p_1)\lambda^\nu(p_2)]\,\mathrm{Re}\, f(s, 0) \\ &\quad = \int d\mathbf{p}\, e^{-\beta E}\,\mathrm{Re}\, f(s, 0) 2\pi\delta(d_1) \\ &\qquad\times\left((p_1^\mu k^\nu + p_1^\nu k^\mu)\frac{\mathcal{P}}{d_2} + 2k^2(p_1^\mu p_2^\nu + p_1^\nu p_2^\mu)\mathcal{P}'\frac{1}{d_2}\right), \end{aligned} \quad (6.39)$$

where $\mathcal{P}$ denotes the principal part and $\mathcal{P}'$ its derivative.

These two terms (6.38) and (6.39) are the only terms in the weakly interacting limit in the sense that if we keep only the *first order* in the two-body coupling constant, all other terms would not appear, since they are at least second order.

(v) *The bound state contribution* (6.4) *and exchange term* (6.8)*:* To sum up, we have

$$S_2'^{\mu\nu} = (6.33) + (6.36) + (6.37) + (6.38) + (6.39) + (6.4) + (6.8) + O(1). \quad (6.40)$$

This is the z^2 correction term to the ideal gas term. Before discussing three-body terms, we shall examine $S_2'^{\mu\nu}$ in more detail.

7. SUM RULES AND CONNECTIONS TO THE SECOND VIRIAL COEFFICIENT

To gain further insight into our results, let us examine how $S_2'^{\mu\nu}$ satisfies a couple of nontrivial sum rules and establish its connection to the second virial coefficient.

By the nature of our approach, the conservation law

$$k_\mu S_2'^{\mu\nu} = k_\nu S_2'^{\mu\nu} = 0 \quad (7.1)$$

is satisfied at every stage of calculation. It is easily verified that each term in (6.40) satisfies (7.1) separately.

A. Sum Rules and the Virial Coefficients

Recall that the coefficients b_n are defined by

$$p = (\beta\lambda^3)^{-1} \sum_{n=1}^{\infty} b_n z^n. \quad (7.2)$$

For the average density $\bar{N}$ and the average density fluctuation, we have

$$\bar{N} = \beta z \frac{\partial p}{\partial z} = \lambda^{-3} \sum_n n b_n z^n,$$

$$\langle (N - \bar{N})^2 \rangle = z \frac{\partial \bar{N}}{\partial z} = \lambda^{-3} \sum_n n^2 b_n z^n. \quad (7.3)$$

Therefore, the f-sum rule and the compressibility sum rule [see (2.12) and (2.13)], written as expansions in powers of z, have the form

$$\int \frac{d\omega}{2\pi} \omega S_n^{00}(k) = \mathbf{k}^2 \int \frac{d\omega}{2\pi} \frac{S_n^{33}(k)}{\omega} = \lambda^{-3} n b_n \left(\frac{\mathbf{k}^2}{m}\right), \quad (7.4)$$

$$\lim_{\mathbf{k}\to 0} \int \frac{d\omega}{2\pi} S_n'^{00}(k) = 2\lambda^{-3} n^2 b_n, \quad (7.5)$$

where $S_n'^{\mu\nu}$ and $S_n^{\mu\nu}$ are defined in the sense of (3.3). The third axis is taken along $\mathbf{k}$. Using the first identity of (2.7), we can write the f-sum rule (7.4) as

$$\lambda^{-3} n b_n = \tfrac{1}{2} m\beta \int \frac{d\omega}{2\pi} S_n'^{33}(k) + O(|\mathbf{k}|) = \tfrac{1}{2} m\beta \int \frac{d\omega}{2\pi} S_n'^{00}(k) \frac{\omega^2}{\mathbf{k}^2} + O(|\mathbf{k}|). \quad (7.6)$$

Notice that $S_n'^{\mu\nu}$ as a function of ω falls off rapidly when $\omega/kv \gg 1$, where v estimates the average velocity of a particle, $v \sim (m\beta)^{-\frac{1}{2}}$. These sum rules relate the moments of the correlation functions to the virial coefficients. They also provide rather nontrivial tests for the validity of formulas for the correlation functions.

We recall that a two-particle bound state is equivalent here to a point particle of mass $2m$ and "charge" 2. Since the correlation functions of free particles satisfy both sum rules, the bound state contribution to these sum rules is trivial and will be ignored for simplicity.

B. The Compressibility Sum Rule

Let us check (7.5) for $n = 2$ with $S_2'^{00}$ given by (6.40). For simplicity, let us discuss the nonrelativistic case. For $\mu = \nu = 0$, we set $p^0 = m$ and obtain

$$\begin{aligned} S_2'^{00}(k) &= 4m^2 \int d\mathbf{p}\, e^{-\beta E}(v\, d\sigma) \\ &\times \left[-\mathrm{Re}\left(\frac{1}{d_1 d_1'} - \frac{1}{d_1^2} + \frac{1}{d_1 d_2'} - \frac{1}{d_1 d_2}\right) \right. \\ &+ \mathrm{Im}\left(\frac{\omega}{d_1 d_1'} + \frac{\omega}{d_1 d_2'} - \frac{4}{d_1}\right)\frac{\partial \chi}{\partial \epsilon} \\ &\left. + 2\,\mathrm{Im}\left((p_1 - p_1')\cdot k \frac{1}{d_1 d_2'} + \frac{2}{d_1}(1 - \cos\theta)\right)\frac{\partial \chi}{\partial t}\right] \\ &- 2m^2 \int d\mathbf{p} \left[e^{-\beta E}\, \mathrm{Re}\frac{\partial f}{\partial \epsilon} \right. \\ &\times 2\pi\left(\omega\delta'(d_1) + \omega \frac{1}{\pi}\,\mathrm{Im}\frac{1}{d_1 d_2} + \frac{4}{m}\delta(d_1)\right) \\ &\left. - \frac{\partial}{\partial \epsilon} e^{-\beta E}\, \mathrm{Re}\, f(\epsilon, 0) \frac{2\pi}{m} \delta(d_1)\right] \\ &- 2\int d\mathbf{p}\, e^{-\beta E}\, \mathrm{Im}\,[\lambda^0(p_1)\lambda^0(p_2)]\, \mathrm{Re}\, f(\epsilon, 0) + O(1), \end{aligned} \quad (7.7)$$

where the exchange term (6.8) is left out for simplicity, ϵ is now the c.m. *kinetic energy*, and θ the c.m. scattering angle. Again notice that there is no k dependence in the scattering amplitudes, which contains all the dynamics in the problem. The k dependence only appears in kinematical factors $d_{1,2}$

and $d'_{1,2}$. Since

$$m^2 \operatorname{Im}\int_{-\infty}^{\infty} d\omega \frac{\omega}{d_1 d_1'} = -\pi, \quad \int_{-\infty}^{\infty} d\omega \frac{1}{d_1 d_1'} = 0, \quad (7.8)$$

the ω integration (7.5) can be performed easily. Also, under the $1 \leftrightarrow 2$ symmetry, we have, writing u for $\hat{\mathbf{k}} \cdot \mathbf{p}/m$,

$$\operatorname{Im}[\lambda^0(p_1)\lambda^0(p_2)] = -2\pi\delta(d_1)\mathcal{P}(u_1 - u_2)^{-2} + O(1). \quad (7.9)$$

It follows from (7.9) that

$$\int \frac{d\omega}{2\pi}\int d\mathbf{p}\, e^{-\beta E} \operatorname{Im}[\lambda^0(p_1)\lambda^0(p_2)] \operatorname{Re} f(\epsilon, 0)$$
$$= -\int d\mathbf{p}\, e^{-\beta E}[\hat{\mathbf{k}} \cdot (\mathbf{p}_1 - \mathbf{p}_2)]^{-2} \operatorname{Re} f(\epsilon, 0) 2m$$
$$= -\int d\mathbf{p} \frac{\partial}{\partial \epsilon}[e^{-\beta E} \operatorname{Re} f(\epsilon, 0)]. \quad (7.10)$$

The contribution of the $\partial\chi/\partial t$ term in (7.7) is interesting. After the ω integration, we have, for the $\partial\chi/\partial t$ term in the integrand of (7.7),

$$-8m(1 - \cos\theta)\frac{\partial \chi}{\partial t}, \quad (7.11)$$

since

$$m\int \frac{d\omega}{2\pi} \operatorname{Im}\frac{1}{d} = -\pi. \quad (7.12)$$

Since

$$t = -2m\epsilon(1 - \cos\theta), \quad (7.13)$$

we have

$$-2m(1 - \cos\theta)\frac{\partial \chi}{\partial t} = \frac{\partial \chi}{\partial t}\left(\frac{\partial t}{\partial \epsilon}\right)_\theta = \left(\frac{\partial \chi}{\partial \epsilon}\right)_{s,\theta}, \quad (7.14)$$

which combines with the contribution of the $\partial\chi/\partial\epsilon$ term in (7.7) to give $(\partial\chi/\partial\epsilon)_0$. Putting terms together, we obtain

$$\int \frac{d\omega}{2\pi} S_2'^{00}(k)$$
$$= \left[-\int d\mathbf{p}\, e^{-\beta E}\epsilon^{-\frac{1}{2}} \operatorname{Re}\frac{\partial}{\partial \epsilon}\epsilon^{\frac{1}{2}} f(\epsilon, 0)\right.$$
$$\left. + \int d\mathbf{p}\, e^{-\beta E}(v\, d\sigma)\left(\frac{\partial \chi}{\partial \epsilon}\right)_\theta\right] \times 4 + O(|\mathbf{k}|). \quad (7.15)$$

It can be verified easily that the quantity in the square bracket of (7.15) is just $2\lambda^{-3}b_2$ in view of the formula[1]

$$\lambda^{-3}b_2 = \tfrac{1}{2}\int dE(4\pi i)^{-1} \operatorname{Tr}\left(S^{-1}(E)\frac{\overleftrightarrow{\partial}}{\partial E} S(E)\right),$$
$$S(E) = 1 - 2\pi i\delta(E - H_0)T(E), \quad (7.16)$$

where the trace is taken over two-body states.

C. The f-Sum Rule

We now proceed to verify (7.6) for $n = 2$ with $S_2'^{00}$ given by (7.7). We want to carry out the integral

$$\int \frac{d\omega}{2\pi} S_2'^{00}(k)\frac{\omega^2}{\mathbf{k}^2}. \quad (7.17)$$

In spite of the two extra powers of ω, the integral is well defined. This is easily seen if we use $S_2'^{33}(k)$ instead of $S_2'^{00}(k)$.

Again, one finds that the first term in (7.7), i.e., the $O(k^{-2})$ term, does not contribute to the ω-integral. The other terms can be integrated easily but the combination of the integrated terms is somewhat delicate. We shall show a few less trivial steps.

Let us define the quantities u_1, u_2, u_1', and u_2' by

$$u = \hat{\mathbf{k}} \cdot \mathbf{p}/m, \quad u' = \hat{\mathbf{k}} \cdot \mathbf{p}'/m, \quad (7.18)$$

i.e., the component of the velocity along $\mathbf{k}$. Consider the last term of (7.7). We have, using (7.9) and under the $1 \leftrightarrow 2$ symmetry,

$$I \equiv \int \frac{d\omega}{2\pi} \operatorname{Im}[\lambda^0(p_1)\lambda^0(p_2)]\frac{\omega^2}{\mathbf{k}^2}$$
$$= -4u_1^2(u_1 - u_2)^{-2}(2m)^{-1}$$
$$= [-(u_1 + u_2)^2(u_1 - u_2)^{-2} - 1] \cdot (2m)^{-1}. \quad (7.19)$$

Now we notice that $u_1 + u_2$ is a conserved quantity in two-body scattering by momentum conservation. Therefore, we may replace $(u_1 + u_2)^2$ in (7.19) by its average value, i.e.,

$$(u_1 + u_2)^2 \to \langle (u_1 + u_2)^2 \rangle = 2/(m\beta), \quad (7.20)$$

where the last step is obvious in view of the equipartition law. Similar to (7.10), we obtain from (7.19)

$$-2\int d\mathbf{p}\, e^{-\beta E} \operatorname{Re} f(\epsilon, 0) I$$
$$= (m\beta)^{-1}\int d\mathbf{p} \frac{\partial}{\partial \epsilon}[e^{-\beta E} \operatorname{Re} f(\epsilon, 0)]$$
$$+ m^{-1}\int d\mathbf{p}\, e^{-\beta E} \operatorname{Re} f(\epsilon, 0) \quad (7.21)$$

for the last term of (7.7). We see that the u variables have disappeared. Next we consider the term preceding the one we just considered in (7.7), i.e.,

$$2\int d\mathbf{p} \operatorname{Re}\frac{\partial}{\partial \epsilon} e^{-\beta E} f(\epsilon, 0)\int \frac{d\omega}{2\pi} 2\pi\delta(d_1)\frac{\omega^2}{\mathbf{k}^2}$$
$$= 2\int d\mathbf{p} \frac{\partial}{\partial \epsilon}[e^{-\beta E} f(\epsilon, 0)] \cdot u_1^2. \quad (7.22)$$

Again, by $1 \leftrightarrow 2$ symmetry and by (7.20), we write

$$u_1^2 = \tfrac{1}{4}(u_1 + u_2)^2 + \tfrac{1}{4}(u_1 - u_2)^2 = (2m\beta)^{-1} + \tfrac{1}{4}(u_1 - u_2)^2. \quad (7.23)$$

By the spherical symmetry in the c.m. frame, we have

$$\tfrac{1}{4}(u_1 - u_2)^2 = (1/3m)\epsilon. \quad (7.24)$$

Furthermore, we have

$$\int d\mathbf{p} \tfrac{1}{3}\epsilon \frac{\partial}{\partial \epsilon} \operatorname{Re} f(\epsilon, 0) e^{-\beta\epsilon} = -\tfrac{1}{3}\int d\mathbf{p}(1 + \tfrac{1}{2}) \operatorname{Re} f(\epsilon, 0) e^{-\beta\epsilon}, \quad (7.25)$$

where we have integrated ϵ by parts and noted the $\epsilon^{\frac{1}{2}}$ dependence of $d\mathbf{p}$. Substituting (7.25) and (7.23) in (7.22), we have

$$(m\beta)^{-1}\int d\mathbf{p} \frac{\partial}{\partial \epsilon} [\operatorname{Re} e^{-\beta E} f(\epsilon, 0)] - m^{-1}\int d\mathbf{p} \operatorname{Re} e^{-\beta E} f(\epsilon, 0), \quad (7.26)$$

for the next to the last term in (7.7). We see that the second term in (7.26) cancels the second term in (7.21) while the first terms add. There is no such nontrivial cancellation for the other terms in (7.7). Using the fact that

$$u_1 + u_2 = u_1' + u_2', \quad (7.27)$$

we can always combine the u variables to form $(u_1 + u_2)^2$, which can be replaced by $2/m\beta$. The net effect may be summarized as replacing u_1^2, u_2^2, u_1u_2, u_1u_2' by $\frac{1}{4}(u_1 + u_2)^2 = \frac{1}{4}(2/m\beta)$. Our results can be summed up as

$$\int \frac{d\omega}{2\pi} S_2'^{00}(k) \frac{\omega^2}{\mathbf{k}^2} = (2m\beta)^{-1}\int \frac{d\omega}{2\pi} S_2'^{00}(k) = \frac{4}{m\beta}\lambda^{-3} b_2. \quad (7.28)$$

We have thus verified that our result (6.40) satisfies the two sum rules in the nonrelativistic case, which are rather nontrivial tests for (6.40).

8. THREE-BODY TERMS

The results obtained above for the case $n = 2$ could be trivially generalized to $n \geq 3$ if the scattering amplitudes for multiparticle processes were well-behaving functions like the two-body amplitude. One would conclude that $T^{\mu\nu}$ is of $O(k^{-2})$ always. The low energy theorems and the correlation functions would appear just like the $n = 2$ case with more particle labels. However, in real life the multiparticle scattering amplitudes have various singularities. These singularities invalidate a naive extension of the $n = 2$ results. Physically this is easy to understand. In the above study of the two-body low energy theorems and correlation functions, the size of the space–time region of interaction is considered as small compared to k^{-1}, so that the currents carried by the incoming and outgoing plane waves dominate. However, a multiparticle scattering event may take place in an infinitely extended space–time, as indicated mathematically by the singularities of the amplitudes. For example, the double- and triple-scattering, and the rescattering process shown in Fig. 10 are not localized when the incoming and outgoing momenta are such that the intermediate particles become real on-shell particles instead of just transient intermediate states.

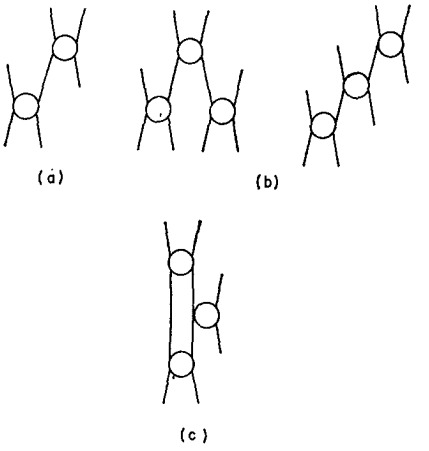


FIG. 10. (a) A double-scattering event in three-body scattering. (b) Triple-scattering events in four-body scattering. (c) Rescattering in three-body scattering.

To understand the main features of multiparticle contribution to correlation functions, let us study the three-body terms in some detail. After a qualitative discussion, we shall evaluate the leading three-body contribution to $S'^{\mu\nu}$. Then the next leading terms will be examined qualitatively.

A. Disconnected Terms and Double-Scattering Terms

Before we begin, let us be reminded of the simple fact that, in the theory of multiparticle scattering, the disconnected terms of the scattering amplitude play an important role. For example, the n-particle unitarity relation is not satisfied by the connected n-particle amplitude alone. It is satisfied only when both disconnected and connected terms are included. The interference of disconnected and connected terms is the quantum mechanical description of damping. Generally, in calculating physical quantities such as the correlation functions, one computes the products of full T matrices and then takes the connected part of the product. Figure 11 shows some examples of disconnected terms in $T^{\mu\nu}$.

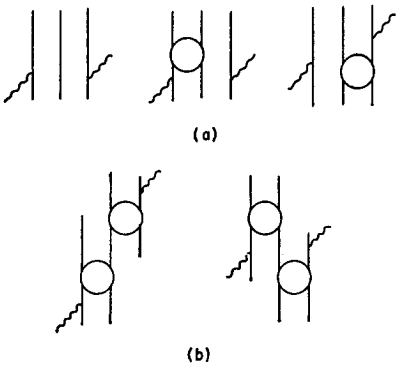


FIG. 11. (a) Some disconnected terms in the three-body contribution to $T^{\mu\nu}$.
(b) Some double-scattering contribution to $T^{\mu\nu}$.

The most serious singularity of the connected three-body amplitude comes from the double-scattering diagram, as shown in Fig. 10(a). Figure 11(a) shows the corresponding $T^{\mu\nu}$. The amplitude is infinite whenever the intermediate particle is on-shell.[8]

Figure 12 shows some of the diagrams of the

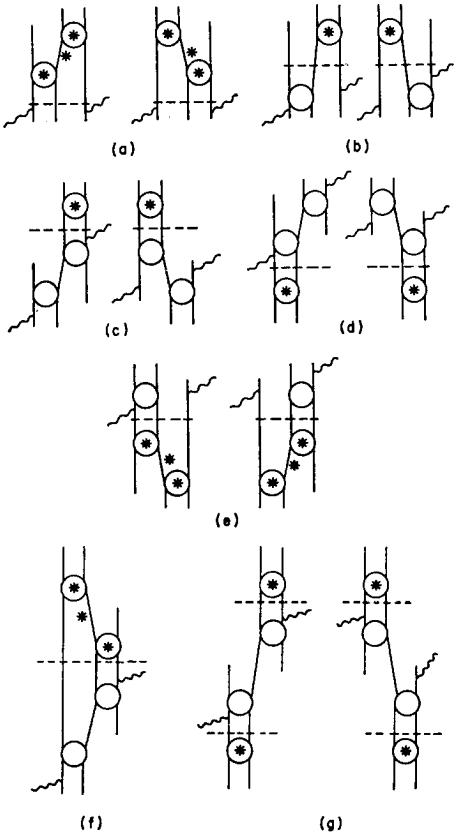


FIG. 12. Some of the diagrams for $S^{\dagger}T^{\mu\nu}$ contributing to the $O(k^{-3})$ term in $F_3'^{\mu\nu}$. The symbol * indicates the Hermitian conjugate of the T matrix or propagator. These diagrams and others obtained from them by moving photon lines to different external lines all have a factor k^{-1} from the intermediate state propagator. We have moved around the T matrices in some of the diagrams when allowed by cyclic permutations under trace. The $O(k^{-3})$ part of (f) is given by the first diagram of (g). We put (f) here only to remind the reader where (g) comes from.

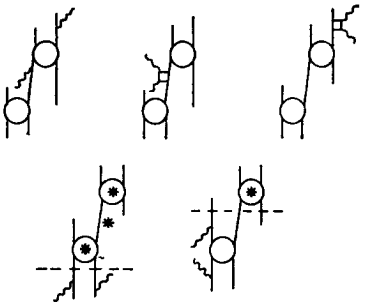


FIG. 13. Some of the diagrams for $S^{\dagger}T^{\mu\nu}$ contributing to the $O(k^{-3})$ term in $F_3'^{\mu\nu}$.

product $S^{\dagger}T^{\mu\nu}$ contributing to $F_3'^{\mu\nu}$. It is not difficult to see that their contribution is of $O(k^{-3})$. Each photon on an external line gives rise to a factor k^{-1}, and the propagator in the intermediate particle is of $O(k^{-1})$ forced by momentum conservation. The extra k^{-1} coming from a propagator is a new feature not found in two-body terms. Evidently, for n-body terms, there will be contribution of $O(k^{-n})$.

There are other terms contributing to $O(k^{-3})$. Figure 13 shows some of them. They count for, besides other effects, the emission and absorption of photons by the intermediate particles, which can propagate over a long distance. These terms are necessary to assure the conservation of currents to the leading order, i.e., $O(k^{-3})$. One may view these terms as the correction to the Compton amplitude and the two-body $T^{\mu\nu}$ due to the presence of other particles in the medium, i.e., some kind of "self-energy" correction to the external lines. By using the small angle limit technique used in Sec. 6, one can show easily that the leading contribution of these terms is of $O(k^{-3})$, being the second derivative of the Compton amplitude and the first derivative of the two-body $T^{\mu\nu}$ with respect to k.

B. Evaluation of the Leading Terms

We proceed to evaluate the leading term in $S_3'^{\mu\nu}$. The result, together with the $S_2'^{\mu\nu}$ in (6.40), completes the approximation to $S'^{\mu\nu}$ up to the $c_{30}z'^3$ term discussed in the Introduction.

There are a large number of diagrams contributing to $O(k^{-3})$. Instead of evaluating all of them, we shall again exploit the conservation law so that we only have to evaluate a fraction of them. Let us observe the following facts. $F_3'^{\mu\nu}(k)$ is an integral over momenta. The $O(k^{-3})$ terms in the integrand always appear in the form

$$\frac{p^{\mu}}{d}\frac{p'^{\nu}}{d'}\frac{1}{d''} \times O(1), \tag{8.1}$$

where the denominators are given by $d = p \cdot k$, $d' = p' \cdot k$, and $d'' = p'' \cdot k$. $O(1)$ is a sum of products of scattering amplitudes and the Boltzmann factor.

There are terms where two or all of the three denominators in (8.1) are equal, i.e., terms proportional to

$$p^\mu p'^\nu/d^2d', \quad p^\mu p^\nu/d^3, \tag{8.2}$$

which come mainly from diagrams in Fig. 13 and also from other diagrams. By suitable change of integration variables, any subsum of terms of the type (8.2) in the integrand for $F_3'^{\mu\nu}$ can be written as

$$r^{\mu\nu} = r^{\nu\mu} = (p^\mu p'^\nu/d^2d' + p^\nu p'^\mu/d^2d')r_1(p, p', p'', \cdots) + (p^\mu p^\nu/d^3)r_2(p, p', p'', \cdots). \tag{8.3}$$

It follows that

$$k_\mu r^{\mu\nu} = (1/d)(p'^\nu/d' + p^\nu/d)r_1 + (p^\nu/d^2)r_2. \tag{8.4}$$

Suppose that we know also that this subsum of terms satisfies the conservation law

$$k_\mu r^{\mu\nu} = 0, \tag{8.5}$$

for arbitrary momenta; then we must have

$$r_1 = r_2 = r^{\mu\nu} = 0. \tag{8.6}$$

In other words, it is not possible to have a conserving $r^{\mu\nu}$ of $O(k^{-3})$ with only two different denominators d and d'.

Now let $I^{\mu\nu}$ be the integrand for $F_3'^{\mu\nu}$. Let

$$I^{\mu\nu} = I_1^{\mu\nu} + r^{\mu\nu}, \tag{8.7}$$

where $I_1^{\mu\nu}$ includes all terms in $I^{\mu\nu}$ with three different denominators. Furthermore, $I_1^{\mu\nu}$ satisfies

$$k_\mu I_1^{\mu\nu} = 0. \tag{8.8}$$

Of course, $I_1^{\mu\nu}$ may also have to include some terms of type (8.2) in order to satisfy the conservation law (8.8). It then follows that the $r^{\mu\nu}$ in (8.7) satisfies (8.5). Since it has no term with three different denominators, it must vanish by the above reasoning. In short, if we find a conserving $I_1^{\mu\nu}$ including all terms of three different denominators, we will have found $I^{\mu\nu}$.

With this conclusion in mind, we proceed to find the sum of diagrams giving three different denominators and then patch it up so that the conservation law is observed. The relevant diagrams are simply those in Fig. 12 with the photon lines attached on various lines in such a way that the momentum k is passed through three particle lines of different momenta. We have thus by-passed the analysis of other diagrams such as those in Fig. 13. Although the cancellations among the terms with three different denominators are very delicate, it is a straightforward algebraic task to collect terms. The main instructive feature in going through the calculation is seeing how various interference terms between connected and disconnected pieces combine to give cross sections. Here we shall simply give the answer:

$$S_3'^{\mu\nu}(k) = \int d\mathbf{p}\, e^{-\beta E}(v\, d\sigma_{12})(v\, d\sigma_{23}) \times \frac{2}{m^2}\,\mathrm{Im}\left[\left(\frac{p_1'}{d_1'} + \frac{p_2'}{d_2'} - \frac{p_1}{d_1} - \frac{p_1''}{d_2''}\right)^\mu \frac{1}{d_2''} \times \left(\frac{p_3}{d_3} + \frac{p_2}{d_2} - \frac{p_3'}{d_3'} - \frac{p_2''}{d_2''}\right)^\nu\right] + O(k^{-2}), \tag{8.9}$$

where

$$\begin{aligned} d\mathbf{p} &= d^3p_1\, d^3p_2\, d^3p_3(2\pi)^{-9}(m^3/\epsilon_1\epsilon_2\epsilon_3), \\ E &= \epsilon_1 + \epsilon_2 + \epsilon_3, \\ v\, d\sigma_{12} &= v\, d\sigma(1' + 2' \to 1 + 2''), \\ v\, d\sigma_{23} &= v\, d\sigma(2'' + 3' \to 2 + 3). \end{aligned} \tag{8.10}$$

The notation should be otherwise self-explanatory. Note that in (8.9) only the two-body cross sections appear. As we shall show later, (8.9) can also be obtained by iterating the Boltzmann equation.

C. The Rescattering Singularity

Let us take a brief look at the $O(k^{-2})$ terms. They come from two sources: first, from the derivative of the scattering amplitudes in the diagrams contributing to $O(k^{-3})$ and, second, from the three-body T-matrix diagrams with at least one closed loop and with photons attached to external lines. In principle, one can show by the low energy theorem technique that the $O(k^{-2})$ terms can be expressed in terms of on-shell two-body and three-body amplitudes and their derivatives. This is a very tedious task in practice, and we shall not go into it here. However, one does have to notice that the three-body T-matrix elements in the second source mentioned above are not free of singularities. It is known that the one-loop triangular rescattering diagram [see Fig. 10(c)] does blow up for certain external momenta. Let us examine this singularity.

The rescattering amplitude blows up whenever the external and intermediate momenta are such that energy–momentum conservation is observed at each of the three two-body T matrices, i.e., when the internal lines are on-shell so that the intermediate particles can traverse an infinite distance. When the loop integral over the internal momentum is performed, the singularity is smoothed out, except for a limited set of external momenta. It has been shown[9] that if

$$|\mathbf{p}_3 - \mathbf{p}_3'| = |\mathbf{p}_1 - \mathbf{p}_1'| + |\mathbf{p}_2 - \mathbf{p}_2'|, \tag{8.11}$$

then the rescattering amplitude T_{rs} blows up. It is not difficult to demonstrate that, near the singularity

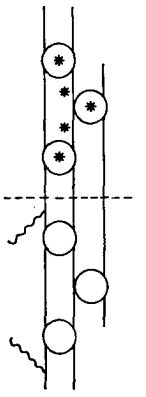


FIG. 14. A term in $F_3'^{\mu\nu}$ containing the square of the rescattering amplitude. This term is of $O(k^{-2} \ln k)$ in two dimensions and $O(k^{-2})$ in three dimensions.

given by (8.11),

$$T_{rs} \sim \ln (|\mathbf{p}_3 - \mathbf{p}_3'| - |\mathbf{p}_1 - \mathbf{p}_1'| - |\mathbf{p}_2 - \mathbf{p}_2'|) \quad (8.12)$$

for $p_i \neq p_i'$. There is no singularity for forward scattering. Thus, T_{rs} and $|T_{rs}|^2$ are integrable over momenta. No additional singularity in k will be introduced to $S_3'^{\mu\nu}$ by this singularity in the amplitude.

On the other hand, in a two-dimensional world, the rescattering singularity is more severe:

$$T_{rs} \sim [|\mathbf{p}_3 - \mathbf{p}_3'| - |\mathbf{p}_1 - \mathbf{p}_1'| - |\mathbf{p}_2 - \mathbf{p}_2'|]^{-\frac{1}{2}}. \quad (8.13)$$

Thus $|T_{rs}|^2$ is not integrable. In Fig. 14 if we ignore the k dependence of the amplitudes for the triangular T-matrix elements, we would get a logarithmic divergence. It is evident then there are terms of $O(k^{-2} \ln k)$ in the correlation function for a two-dimensional gas if no cancellation occurs.

9. HIGHER-ORDER TERMS AND KINEMATIC EQUATIONS

We shall comment briefly on the connection between our results and the kinetic equation in transport theory.

Having examined the two-body and three-body contributions to the correlation functions, let us return to the over-all picture of the expansion (1.13), which is

$$S'^{\mu\nu} = \sum_{n,m<n} z'^{n-m} \zeta^m c_{nm} + O(1), \quad (9.1)$$

where z' and ζ are defined by (1.11). This expansion is well defined if z' and ζ are both very small.

In transport theory, one is interested in correlation functions with very small k, i.e., with large z' in (9.1). Clearly, if z' is not small, (9.1) must be summed formally first in order to be meaningful. One does not start with an expansion like (9.1) in transport theory, but with a kinetic equation, which generates an expansion when it is iterated. The (nonrelativistic) Boltzmann equation is the kinetic equation at the low density limit:

$$\frac{\partial f}{\partial t} + \frac{\partial H}{\partial \mathbf{p}} \cdot \frac{\partial f}{\partial \mathbf{x}} - \frac{\partial H}{\partial \mathbf{x}} \cdot \frac{\partial f}{\partial \mathbf{p}} = \int \frac{d^3q}{(2\pi)^3} (v\, d\sigma)[f(\mathbf{p})f(\mathbf{q}) - f(\mathbf{p}')f(\mathbf{q}')], \quad (9.2)$$

where the notation is standard and the $\mathbf{x}$, t dependence of the distribution function f is implicit. Since we now have explicit formulas for c_{20}, c_{21}, and c_{30}, it should be instructive to compare them with those which we now proceed to obtain from the Boltzmann equation (9.2).

Consider a weak external (momentum-dependent) potential

$$H' = \lambda p_\nu \phi^\nu e^{-ik\cdot x}, \quad H = \mathbf{p}^2/2m + H'. \quad (9.3)$$

Let $f_0(p)$ be the Maxwell distribution and define

$$f = f_0(\mathbf{p}) + \lambda \delta f(\mathbf{p}) e^{-ik\cdot x}, \quad (9.4)$$

$$f_0(\mathbf{p}) = z \exp(-\beta \mathbf{p}^2/2m). \quad (9.5)$$

To $O(\lambda)$, the average current is, by the definition of the response function $R^{\mu\nu}$ and by (9.4),

$$\langle j^\mu(x) \rangle = \lambda R^{\mu\nu}(k)\phi_\nu e^{-ik\cdot x} = \lambda \int \frac{d^3p}{(2\pi)^3} \frac{p^\mu}{m} \delta f(\mathbf{p}) e^{-ik\cdot x}. \quad (9.6)$$

The response function is related to the correlation function $S'^{\mu\nu}$ via the identities (2.7) and (2.8):

$$S'^{\mu\nu} = -2 \operatorname{Im} R^{\mu\nu} \coth \tfrac{1}{2}\beta\omega. \quad (9.7)$$

Substituting (9.4) in (9.2) and keeping only $O(\lambda)$ terms, we obtain a linearized Boltzmann equation:

$$\delta f(\mathbf{p}) = \frac{1}{d}\Big(\frac{-\mathbf{k}\cdot\mathbf{p}}{m} \beta f_0(\mathbf{p}) p_\nu \phi^\nu + i \int d^3q (2\pi)^{-3} (v\, d\sigma) \times [f_0(\mathbf{p})\delta f(\mathbf{q}) + f_0(\mathbf{q})\delta f(\mathbf{p}) - f_0(\mathbf{p}')\delta f(\mathbf{q}') - f_0(\mathbf{q}')\delta f(\mathbf{p}')] \Big), \quad (9.8)$$

where $d = p \cdot k$ as before. Substituting (9.8) in (9.6), we find

$$R^{\mu\nu}\phi_\nu = -\beta \int d^3p (2\pi)^{-3} f_0(\mathbf{p}) \Big(\frac{\mathbf{k}\cdot\mathbf{p}}{m} \Big) \frac{p^\nu}{d} \phi_\nu + i \int d^3p_1\, d^3p_2 (2\pi)^{-6} (v\, d\sigma) \times \Big(\frac{p_1^\mu}{d_1} - \frac{p_1'^\mu}{d_1'} + \frac{p_2^\mu}{d_2} - \frac{p_2'^\mu}{d_2'} \Big) f_0(\mathbf{p}_1)\delta f(\mathbf{p}_2), \quad (9.9)$$

where the first term is the free-particle contribution. For the second iteration term, we substitute the first term in (9.8) for δf into the second term of (9.9) and

obtain the $O(z^2)$ term for $R^{\mu\nu}$:

$$z^2 R_{zB}^{\mu\nu} = -i\beta\omega z^2 \int d^3p_1\, d^3p_2 (2\pi)^{-6} (v\, d\sigma) e^{-\beta E} \times \left(\frac{p_1^\mu}{d_1} - \frac{p_1'^\mu}{d_1'} + \frac{p_2^\mu}{d_2} - \frac{p_2'^\mu}{d_2'}\right)\frac{p_2^\nu}{d_2}. \quad (9.10)$$

In view of (9.7), it is evident that the function

$$S_{2B}'^{\mu\nu} \equiv -\frac{4}{\beta\omega} \operatorname{Im} R_{2B}^{\mu\nu} \quad (9.11)$$

is the same as (6.33) for the $O(k^{-2})$ term of $S_2'^{\mu\nu}$.

For the third iteration, we first get the second iteration of δf from (9.8) and substitute it in the second term of (9.9). We obtain the $O(z^3)$ term for $R^{\mu\nu}$:

$$\begin{aligned} z^3 R_{3B}^{\mu\nu} = {} & -2\beta\omega z^3 \int d^3p_1\, d^3p_2\, d^3p_3 (2\pi)^{-9} \\ & \times e^{-\beta E} (v\, d\sigma_{12})(v\, d\sigma_{23}) \\ & \times \left(\frac{p_1^\mu}{d_1} - \frac{p_1'^\mu}{d_1'} + \frac{p_2^\mu}{d_2} - \frac{p_2'^\mu}{d_2'}\right) \\ & \times \frac{1}{d_2}\left(\frac{p_3^\nu}{d_3} + \frac{p_2^\nu}{d_2} - \frac{p_2''^\nu}{d_2''} - \frac{p_3'^\nu}{d_3'}\right), \end{aligned}$$

$$E = \epsilon_1 + \epsilon_2 + \epsilon_3, \quad d\sigma_{12} = d\sigma(1'2' \to 1\,2), \quad d\sigma_{23} = d\sigma(2\,3 \to 2''3'). \quad (9.12)$$

Like (9.11), $z^3 S_3'^{\mu\nu}$ can be obtained from (9.7) and (9.12). It is obvious that the result is the same as (8.9), at least in the nonrelativistic limit.

What we have just demonstrated is that the leading terms in $S_2'^{\mu\nu}$ and $S_3'^{\mu\nu}$ [i.e. the c_{20} and c_{30} terms in (9.1)] are in fact the same as the iteration solution of a Boltzmann equation. Clearly the next leading term in $S_2'^{\mu\nu}$ is completely missed by the Boltzmann equation. Notice that, as we have shown, the next leading term in $S_3'^{\mu\nu}$ hears the full information concerning the second virial coefficient, whereas the Boltzmann equation contains no information concerning equilibrium properties of the system.

At this point, it seems very reasonable to assert that the $O(k^{-n})$ term in $S_n'^{\mu\nu}$ is in fact the nth-iteration term obtained from the Boltzmann equation. It is natural to expect that the c_{n1} terms in (9.1) should turn out to be the nth iteration from a more general kinetic equation. In view of our result for c_{21} and qualitative discussions on c_{31}, we expect that a modified Boltzmann equation should contain terms depending on derivatives of two-body amplitudes as well as two-body and three-body cross sections. Unfortunately, the first correction term, i.e., c_{21} in (9.1) is already very complicated according to our formula. Therefore, a more general kinetic equation may not be very simple.

10. GENERAL REMARKS

It seems evident in view of the above analysis that a concise general S matrix formula for the expansion coefficients for correlation functions does not exist, in contrast to the case of virial coefficients, where a concise formula does exist formally. We have elucidated the basic limitations of an S-matrix approach to correlation functions. The most general result one can hope to achieve seems to be a kinetic equation whose kernal is expanded in terms of S-matrix elements. It would be ideal if the first few terms for the kernal are simple. Much labor is needed in this direction.

Here we have succeeded in obtaining the leading corrections to the conserved current correlation functions of an ideal gas. These corrections are unfortunately not expressible in very short formulas. Let us sum them up as

$$S'^{\mu\nu}(k) - S'^{\mu\nu}(k)_{\text{ideal gas}} = (6.40) + (8.9) + O(z'^2\zeta) + O(z'^4) + O(1), \quad (10.1)$$

with z' and ζ defined by (1.11). Equation (10.1) is a formula fully expressed in terms of on-shell two-body S-matrix elements (even though it involves three-body scattering) and is the formula corresponding to the phase shift formula for the second virial coefficient.

The fact that (10.1) is obtained from a very general analysis should be emphasized more than the details of the formula. We notice that kinetics of free particles, on-shell S-matrix elements, and conservation laws are the only concepts appearing in our discussion besides thermodynamics. A link between the concept of S matrix and that of correlation function in statistical mechanics is thus established on firm grounds.[10]

It is evident that the conservation of currents is essential in our analysis. This requirement on the currents limits the generality of our results somewhat, since not all currents are conserved. However, there are many cases where the currents of physical interest are strictly or approximately conserved. Let us comment briefly on two examples as an illustration.

(i) Consider the spin correlation in a nonrelativistic gas. The spin current is conserved only if no spin–orbit force is involved in collisions. This condition is met to a very good approximation for example when the atomic spin is zero while the nuclear spin is not, e.g., He^3. If there is an external uniform magnetic field, there will be a net average spin density. There is then an additional chemical potential ($\sim$magnetic field) associated with the spin, as well as a conserved spin (vector) current.

(ii) Consider a gas of strongly interacting baryons. The current of baryon number and the current of

isotopic spin are conserved. Our results can thus be generalized to apply to the study of baryon number correlation and isotopic spin correlation in such a gas and to obtain information concerning responses to electromagnetic and weak perturbations. When there is a net average isotopic spin density, we have to introduce a chemical potential for the total isotopic spin in addition to the chemical potential for the baryon number. Evidently, this case is very much the same as the previous example, where the atom number and the ordinary spin are conserved, except that in this case the baryon number is allowed to be negative.

In conclusion, we hope that our results will also find applications to cases where the systems are not dilute but special features would allow useful extrapolation and where the generality emphasized in this paper is not of primary importance.

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[7] We denote the phase of the scattering amplitude by χ to conform to the notation of Ref. 4.

[8] The details concerning this kind of singularity in connection with virial coefficients can be found in Refs. 1 and 2.

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Quantum Operator Ordering and the Feynman Formulation*

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A functional integral representation for the quantum Hamiltonian propagator is obtained from the Feynman formulation. It is shown that operator ordering arbitrariness in the quantum Hamiltonian is directly related to arbitrariness in the algorithmic definition of the functional integral. Examples are cited which demonstrate this fact.

INTRODUCTION

In the Feynman formulation of quantum mechanics,[1] the linear character of the system dynamics is exploited by the use of the propagator representation

$$\psi(q'', t'') = \int K(q'', q', t'' - t')\psi(q', t')\, dq', \quad (1)$$

where $K(q'', q', t'' - t')$ is the propagation kernel and dq is the volume element in q-space. The propagation kernel must satisfy the semigroup composition law

$$K(q'', q', t'' - t') = \int K(q'', q, t'' - t)K(q, q', t - t')\, dq \quad (2)$$

for $t' \leq t \leq t''$, together with the initial condition

$$\lim_{t \to 0} K(q'', q', t) = \delta(q'' - q'). \quad (3)$$

From this one can easily show that

$$i\hbar \frac{\partial \psi}{\partial t''}(q'', t'') = \int \Lambda(q'', q')\psi(q', t'')\, dq',$$

where

$$\Lambda(q'', q') \equiv i\hbar \lim_{t \to 0} \left(\frac{\partial K(q'', q', t)}{\partial t} \right). \quad (4)$$

A representation for the propagation kernel may be constructed in either of two ways. The first or "Feynman[1,2] way" is to postulate the form of the

isotopic spin are conserved. Our results can thus be generalized to apply to the study of baryon number correlation and isotopic spin correlation in such a gas and to obtain information concerning responses to electromagnetic and weak perturbations. When there is a net average isotopic spin density, we have to introduce a chemical potential for the total isotopic spin in addition to the chemical potential for the baryon number. Evidently, this case is very much the same as the previous example, where the atom number and the ordinary spin are conserved, except that in this case the baryon number is allowed to be negative.

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A representation for the propagation kernel may be constructed in either of two ways. The first or "Feynman[1,2] way" is to postulate the form of the

infinitesimal propagation kernel and then to use (2) and (3) to obtain an algorithm for computing

$$K(q'', q', t'' - t').$$

By virtue of (4), the "Feynman way" is tantamount to postulating the form of the quantum Hamiltonian operator or, equivalently, the kernel $\Lambda(q'', q')$, which clearly contains operator ordering arbitrariness.[3] The second or "alternative way" to secure a functional integral "sum over histories" representation for the propagation kernel is to put

$$K(q'', q', t'' - t') \equiv \int_{\mathcal{C}} \exp \frac{i}{\hbar} \int_{t'}^{t''} \left(p \cdot \frac{dq}{dt} - H \right) dt D(q, p),$$

where

$$\mathcal{C} \equiv \{q(t), p(t): q(t') = q', q(t'') = q'', t \in [t', t'']\}$$

and

$$D(q, p) \equiv \prod_{t' < t < t''} dq(t) \prod_{t' \leq t \leq t''} dp(t)/(2\pi\hbar)^n \qquad (5)$$

for all finite positive values of $(t'' - t')$. In (5), p and q denote n-tuples, and H is the classical Hamiltonian.

Naively, it would appear that quantum operator ordering arbitrariness is completely avoided in the functional integral representation since only c-number functions appear. However, we show in the present paper that different algorithms for computing the functional integral in the propagation kernel yield different Hermitian orderings for the quantum Hamiltonian. Recently, other authors have purported to show that the functional integral representation yields a preferred Hermitian ordering for the quantum Hamiltonian associated with a given classical Hamiltonian.[4,5] Their error lies in not taking proher account of the fact that the number of functional integration variables remains infinite for arbitrarily small $(t'' - t')$. It is shown by the work which follows that one cannot approximate the functional integral in $K(q'', q', t)$ for small t by a finite number of integrations and assume that the errors (in such a drastic approximation) will tend to zero as $t \to 0$.

CALCULATION OF $\Lambda(q'', q')$

To simplify the calculation of $\Lambda(q'', q')$ defined by (4) and to avoid the error mentioned above, we introduce the variable $u \equiv (t - t')/(t'' - t')$ which gives

$$\int_{t'}^{t''} \left(p \cdot \frac{dq}{dt} - H \right) dt = \int_0^1 p \cdot \frac{dq}{du} du - (t'' - t') \int_0^1 H \, du$$

and thus, by substitution into (5),

$$K(q'', q', t) = \int_{\mathcal{C}_u} \exp \left(\frac{i}{\hbar} \int_0^1 p \cdot \frac{dq}{du} du \right) \exp \left(- \frac{it}{\hbar} \int_0^1 H \, du \right) D_u(q, p),$$

where

$$\mathcal{C}_u \equiv \{q(u), p(u): q(0) = q', q(1) = q'', u \in [0, 1]\}$$

and

$$D_u(q, p) \equiv \prod_{0 < u < 1} dq(u) \prod_{0 \leq u \leq 1} dp(u)/(2\pi\hbar)^n. \qquad (6)$$

Partitioning the unit interval for the u integration into N cells, we obtain

$$D_u(q, p) = \lim_{N \to \infty} \prod_{k=1}^{N-1} dq_k \prod_{k=1}^{N} \frac{dp_k}{(2\pi\hbar)^n}, \qquad (7)$$

where $q_0 = q'$, $q_N = q''$. To approximate the integral $\int_0^1 p \cdot dq/du \, du$ for finite N by a Riemann sum, dq/du and p must be taken over a uniform lattice of points on the unit interval. By symmetry and the fact the (6) must satisfy the semigroup composition law, we obtain the prescription

$$q_k = q(k/N), \quad p_k = p((k - \tfrac{1}{2})/N). \qquad (8)$$

Note that p_k is halfway in between q_k and q_{k-1} on the unit interval. We must now represent (dq/du) and p_k at the same value of the parameter u by using a finite difference approximation for $(dq/du)_k$. Clearly, any such representation must be subject to the constraint implied by (3). Consider the finite difference approximation

$$\left(\frac{dq}{du} \right)_k \equiv \frac{(q_k - q_{k-1})}{N^{-1}} = N(q_k - q_{k-1}). \qquad (9)$$

Using (6), we obtain

$$\lim_{t \to 0} K(q'', q', t) = K(q'', q', 0) = \int_{\mathcal{C}_u} \exp \left(\frac{i}{\hbar} \int_0^1 p \cdot \frac{dq}{du} du \right) D_u(q, p)$$

which, by virtue of (7), (8), and (9), yields

$$\lim_{t \to 0} K(q'', q', t) = \lim_{N \to \infty} \int \exp \left(\frac{i}{\hbar} \sum_{k=1}^{N} p_k \cdot (q_k - q_{k-1}) \right) \prod_{k=1}^{N-1} dq_k \prod_{k=1}^{N} \frac{dp_k}{(2\pi\hbar)^n} = \delta(q'' - q')$$

as required. Next, we make use of (4) and (6) to obtain the functional integral representation of $\Lambda(q'', q')$:

$$\Lambda(q'', q') = \int_{\mathcal{C}_u} \exp \left(\frac{i}{\hbar} \int_0^1 p \cdot \frac{dq}{du} du \right) \int_0^1 H \, du D_u(q, p). \qquad (10)$$

Using Riemann sums in place of integrals as before, from (10) we obtain

$$\Lambda(q'', q') = \lim_{N\to\infty} \int \exp\left(\frac{i}{\hbar}\sum_{k=1}^{N} p_k \cdot (q_k - q_{k-1})\right) \times N^{-1} \sum_{m=1}^{N} H_m \prod_{k=1}^{N-1} dq_k \prod_{k=1}^{N} \frac{dp_k}{(2\pi\hbar)^n}, \quad (11)$$

where H_k is H evaluated at some point in the kth subdivision of the unit interval. Clearly, since q_k and p_k refer to $q(u)$ and $p(u)$ at different points on the interval, the approximation to H_k must be made subject to the condition

$$\lim_{N\to\infty} N^{-1} \sum_{m=1}^{N} H_m = \int_0^1 H\, du \quad (12)$$

for any path $q(u), p(u)$. Further evaluation of (11) can be effected by employing the Taylor series expansion of the classical Hamiltonian

$$H = H(q, p) = \sum_{l=0}^{\infty} A_l(q) p^l. \quad (13)$$

Substituting the expansion (13) into (11) yields

$$\Lambda(q'', q') = \lim_{N\to\infty} N^{-1} \int \sum_{m=1}^{N} \sum_{l=0}^{\infty} A_{ml} \times \prod_{k=1}^{N} \exp\left(\frac{i}{\hbar} p_k \cdot (q_k - q_{k-1})\right) \times p_m^l \frac{dp_k}{(2\pi\hbar)^n} \prod_{k=1}^{N-1} dq_k, \quad (14)$$

in which

$$A_{ml} \equiv \frac{1}{l!}\left(\frac{\partial^l H_m}{\partial p_m^l}\right)_{p=0}$$

so that

$$H_m \equiv \sum_{l=0}^{\infty} A_{ml} p_m^l.$$

After performing the integrations in (14), we obtain

$$\Lambda(q'', q') = \lim_{N\to\infty} N^{-1} \sum_{m=1}^{N} \sum_{l=0}^{\infty} \tilde{A}_{ml} \delta^{(l)}(q'' - q') \left(\frac{\hbar}{i}\right)^l, \quad (15)$$

where a superscript in parentheses denotes differentiation with respect to the argument and where

$$\tilde{A}_{ml} \equiv [A_{ml}]_{\substack{q_i = q', i < m \\ q_i = q'', i \geq m}}.$$

Since the quantum Hamiltonian must be Hermitian, we require

$$\Lambda(q'', q') = \Lambda^*(q', q''). \quad (16)$$

Hence, from (15) we obtain the condition

$$\tilde{A}_{ml}(q'', q') = \tilde{A}_{ml}(q', q''),$$

which, in addition to condition (12), must be satisfied by the quantities A_{ml}. To obtain the form of the quantum Hamiltonian, we evoke the Schrödinger equation:

$$i\hbar \frac{\partial \psi(q'', t)}{\partial t} \equiv \hat{H}\psi(q'', t) = \int \Lambda(q'', q')\psi(q', t)\, dq'.$$

Substitution of (15) yields

$$\hat{H}\psi(q'', t) = \lim_{N\to\infty} N^{-1} \sum_{m=1}^{N} \sum_{l=0}^{\infty} \left(\frac{\hbar}{i}\frac{\partial}{\partial q'}\right)^l [\tilde{A}_{ml}\psi(q', t)]_{q'=q''}. \quad (17)$$

If $\tilde{A}_{ml}$ does not depend upon m, we then obtain

$$\hat{H}\psi(q'', t) = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \binom{k}{l} \left(\frac{\hbar}{i}\right) \left(\frac{\partial^l \tilde{A}_k}{\partial q'^l}\right)_{q'=q''} \left(\frac{\partial^{k-l}\psi(q', t)}{\partial q'^{k-l}}\right)_{q'=q''},$$

where

$$\binom{k}{l} \equiv \frac{k!}{l!\,(k-l)!} \quad \text{and} \quad \tilde{A}_k \equiv \tilde{A}_{mk}.$$

Hence, we find the quantum Hamiltonian

$$\hat{H}\left(q, \frac{\hbar}{i}\frac{\partial}{\partial q}\right) = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \binom{k}{l} \left[\left(\frac{\hbar}{i}\frac{\partial}{\partial q'}\right)^l \tilde{A}_k\right]_{q'=q''=q} \left(\frac{\hbar}{i}\frac{\partial}{\partial q}\right)^{k-l}, \quad (18)$$

where we have assumed that $\tilde{A}_k$ is independent of m. Because the quantum Hamiltonian in (18) possesses a degree of arbitrariness in the approximation A_{mk}, distinct q–p operator orderings are associated with different assignments for A_{mk}. Suppose, for example, we take $A_{mk} = A_k(\frac{1}{2}(q_m + q_{m+1}))$; then we obtain $\tilde{A}_k = A_k(\frac{1}{2}(q'' + q'))$, which together with (18) gives

$$\hat{H}\left(q, \frac{\hbar}{i}\frac{\partial}{\partial q}\right) = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \binom{k}{l} \left(\frac{\hbar}{2i}\right)^l \frac{\partial^l A_k(q)}{\partial q^l} \left(\frac{\hbar}{i}\frac{\partial}{\partial q}\right)^{k-l}, \quad (19)$$

a quantum Hamiltonian prescribed by the Weyl–McCoy ordering rule. As a second example, suppose we take $A_{mk} = \frac{1}{2}[A_k(q_m) + A_k(q_{m-1})]$; then we obtain $\tilde{A}_k = \frac{1}{2}[A_k(q'') + A_k(q')]$ which together with (18) gives

$$\hat{H}\left(q, \frac{\hbar}{i}\frac{\partial}{\partial q}\right) = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \binom{k}{l} \left(\frac{\hbar}{i}\right)^l \frac{\partial^l A_k(q)}{\partial q^l} \frac{\delta_{l_0} + 1}{2} \left(\frac{\hbar}{i}\frac{\partial}{\partial q}\right)^{k-l}, \quad (20)$$

a quantum Hamiltonian prescribed by the symmetrized ordering rule. It is apparent that there are an infinite number of admissible expressions for A_{mk}, and each admissible expression gives a distinct Hermitian ordering for the generic quantum Hamiltonian H. We have shown that this ordering arbitrariness in the quantum Hamiltonian is directly related to arbitrariness in the algorithmic definition of the functional integral (5), and we conclude that the two ways of prescribing the Feynman formulation are

equivalent with regard to operator ordering arbitrariness.

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[1] R. Feynman, Rev. Mod. Phys. **20**, 367 (1948).
[2] See, for example, G. Rosen, *Formulations of Classical and Quantum Dynamical Theory* (Academic, New York, 1969), pp. 22–41.
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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 8 AUGUST 1971

Formal Equivalence of the Hydrogen Atom and Harmonic Oscillator and Factorization of the Bethe–Salpeter Equations

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We investigate the possible factorizations of the confluent hypergeometric equation and show that this leads to a formal equivalence of the usual hydrogen atom problem with that of a set of multidimensional harmonic oscillators of appropriate classical frequency in a space of varying (even) dimensionality ranging from $4l + 4$ to 2. We next use this method to investigate the solutions of some relativistic bound-state equations. As specific examples we consider Goldstein's eigenvalue problem and the Wick–Cutkosky scalar meson equation. A formal similarity also exists between the Goldstein problem and the scalar meson equation in the zero binding limit. The factorization of either of these equations leads to an infinite ladder of nonsquare integrable solutions. On the other hand, for arbitrary nonvanishing binding energies a complete solution of the scalar meson problem has been obtained by investigating the zero-energy factorization of the equation.

1. INTRODUCTION

A wide variety of physical problems in relativistic and nonrelativistic quantum mechanics can be formulated in terms of linear second order differential equations. The factorization method originated by Schrödinger[1] and Infeld and Hull[2] provides a powerful technique for treating a class of such problems. In the factorization method a single second-order linear differential equation is replaced, if possible, by an equivalent pair of first-order differential-difference equations of the form

$$D_n^{\pm} f_n = f_{n\pm 1},$$

where $D_n^{\pm}$ are first-order differential operators. Thus, if we have one solution, we can use these operators to go up or down to other solutions and continuing this procedure we can obtain a ladder of such solutions. Recently Humi[3] has shown that it is also possible to extend the formalism of the factorization method for arbitrary displacements in the spectrum space of any second order differential equation. In recent years it has been possible to identify the operators with a Lie algebra, and the possible factorizations can be classified according to these Lie algebras. Many of the properties of the special functions can be obtained in this way. This approach has been thoroughly investigated by Miller[4] and Kaufman.[5]

The factorization method is especially suited for problems involving bound states. Once the proper factorization is found, the eigenvalue solutions, if they exist, follow as a necessary condition which determines the "top" or the "bottom" of the ladder of solutions depending upon the nature of the specific problem. The successive solutions can then be easily generated by going up or down the ladder. Another distinctive feature of the method is that it provides a unified technique for treating a large class of such problems. Since the various factorizations corresponding to definite pair of $D_n^{\pm}$ are interrelated,[6] the investigation of the possible factorizations of a particular equation which appears in various physical problems may lead to an understanding of the possible interrelationships, if any, between two or more apparently unrelated problems.

In the present paper we concentrate our attention on these two particular aspects of the factorization method. First, we show that the factorization of the confluent hypergeometric equation[7] leads to a formal equivalence between the hydrogen atom and a multidimensional harmonic oscillator in a space of even

equivalent with regard to operator ordering arbitrariness.

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A wide variety of physical problems in relativistic and nonrelativistic quantum mechanics can be formulated in terms of linear second order differential equations. The factorization method originated by Schrödinger[1] and Infeld and Hull[2] provides a powerful technique for treating a class of such problems. In the factorization method a single second-order linear differential equation is replaced, if possible, by an equivalent pair of first-order differential-difference equations of the form

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The factorization method is especially suited for problems involving bound states. Once the proper factorization is found, the eigenvalue solutions, if they exist, follow as a necessary condition which determines the "top" or the "bottom" of the ladder of solutions depending upon the nature of the specific problem. The successive solutions can then be easily generated by going up or down the ladder. Another distinctive feature of the method is that it provides a unified technique for treating a large class of such problems. Since the various factorizations corresponding to definite pair of $D_n^{\pm}$ are interrelated,[6] the investigation of the possible factorizations of a particular equation which appears in various physical problems may lead to an understanding of the possible interrelationships, if any, between two or more apparently unrelated problems.

In the present paper we concentrate our attention on these two particular aspects of the factorization method. First, we show that the factorization of the confluent hypergeometric equation[7] leads to a formal equivalence between the hydrogen atom and a multidimensional harmonic oscillator in a space of even

dimensionality. We start from Kummer's differential equation for the function ${}_1F_1(a; c; z)$; the first two factorizations of the equation lead to simple recurrence relations between the contiguous hypergeometric functions. However, there exists still another factorization which corresponds to simultaneously raising a by one unit and c by two units so that $(c - 2a)$ is held fixed. The transformations involved in obtaining such a factorization correspond to transforming an equation resembling that of a harmonic oscillator to an equation resembling that for a hydrogen atom. This suggests a formal equivalence between these two problems. A closer inspection shows that the lth eigenstate of the hydrogen atom is equivalent to any of the $n = 0, 1, 2, \cdots, (2l + 1)$th eigenstates of a harmonic oscillator of appropriate classical frequency in a space of $(4l + 4 - 2n)$ dimensions. Such a connection between these two apparently unrelated problems was pointed out earlier by Bergmann and Frishman[8] and recently by Cisneros and McIntosh[9] using different arguments.

We next use this method to investigate the solutions of some relativistic bound state equations. Although the formulation of the Bethe–Salpeter equation[10] has solved the fundamental problem of constructing a fully relativistic two-body equation in the framework of quantum mechanics, the equation exhibits several unfamiliar features which are not encountered in the nonrelativistic Schrödinger equation. The use of the factorization method leads to an understanding of some of these unfamiliar features. A typical example of such a problem is Goldstein's eigenvalue problem,[11] which is known to lead to a continuous spectrum rather than a discrete one. A variety of explanations of this paradox have been offered, blaming mostly the highly singular nature of the relativistic interaction function. However, once the singularities of the interaction kernel are removed by Wick rotation,[12] both the Goldstein problem and the Wick–Cutkosky scalar meson equation[13] can be treated on an equal footing within this framework. Unlike the scalar meson equation, however, the factorization of Goldstein's eigenvalue equation corresponds to an infinite ladder of solutions without any bottom, thereby leading to a continuous spectrum unless some extra boundary conditions which are not manifestly contained in the Wick-rotated integral equation are imposed.

Using the bipolar transformations,[14,15] the scalar meson equation can also be factorized in the limits of vanishing total center of mass energy ($\epsilon = 0$) and vanishing binding energy ($\epsilon = 1$). For $\epsilon = 0$, a top of the ladder of square integrable solutions actually does exist and leads to all the results of $O(5)$ symmetry which have been obtained previously by several authors[16] using different methods. We also show how one can obtain exact eigenvalue solutions for arbitrary nonvanishing energies once the zero-energy factorization is known, and the subsequent solutions agree with the results obtained in an earlier paper.[17] In the limit of vanishing binding energy, however, the factorization of the equation leads to an infinite ladder of nonsquare integrable solutions, a situation similar to the one encountered in Goldstein's problem. Consequently, extra boundary conditions are again required to reproduce a discrete spectrum. These extra boundary conditions implicitly enter into the problem whenever one adopts Wick's method of matching[18] the so-called "internal" and "external" solutions and may be held responsible for the abnormal eigenvalues ($\lambda = \frac{1}{4}$) which do not possess a nonrelativistic limit.

2. FACTORIZATION OF THE CONFLUENT HYPERGEOMETRIC EQUATION AND FORMAL EQUIVALENCE OF THE HYGROGEN ATOM AND HARMONIC OSCILLATOR

A differential equation of the form

$$\frac{d^2y}{dx^2} + r(x, m)y + \lambda y = 0, \tag{2.1}$$

where $m = m_0, m_0 + 1, \cdots$, is said to be factorizable provided it can be replaced by each of the following two equations:

$$\begin{aligned} D^+_{m+1}D^-_{m+1}y^m_\lambda(x) &= [\lambda - L(m + 1)]y^m_\lambda(x), \\ D^-_m D^+_m y^m_\lambda(x) &= [\lambda - L(m)]y^m_\lambda(x), \end{aligned} \tag{2.2}$$

where

$$D^\pm_m = k(x, m) \pm \frac{d}{dx}.$$

A large class of differential equations of the Sturm–Liouville type are reducible to the standard from (2.1) by appropriate transformations.[19]

We start from the confluent hypergeometric equation

$$z\frac{d^2F}{dz^2} + (c - z)\frac{dF}{dz} - aF = 0. \tag{2.3}$$

To reduce it to the standard form, we introduce

$$x = z^{\frac{1}{2}}, \quad F = x^{-c+\frac{1}{2}}e^{x^2/2}y. \tag{2.4}$$

Equation (2.3) is then transformed into

$$\frac{d^2y}{dx^2} - \left[\frac{(c - \frac{1}{2})(c - \frac{3}{2})}{x^2} + x^2 - 2c + 4a\right]y = 0. \tag{2.5}$$

We now replace c by $c + m$ in the above equation, which resembles that for a harmonic oscillator; the

subsequent equation admits of a factorization

$$D_m^{\pm} = \frac{c+m-\frac{3}{2}}{x} + x \pm \frac{d}{dx}, \quad L(m) = -4(c+m). \tag{2.6}$$

The equivalent pair of first-order differential-difference equations now easily follows from Theorem 1 (see Appendix), and these lead to the recurrence relations

$$F(a; c+1; z) = \frac{c}{c-a}\left[1 - \frac{d}{dz}\right]F(a; c; z),$$
$$F(a; c-1; z) = \left[1 + \frac{z}{c-1}\frac{d}{dz}\right]F(a; c; z). \tag{2.7}$$

To obtain the a-changing recurrence relations, we regard the term $(c-1)^2$ in (2.5) as the eigenvalue parameter to be held constant in the ladder. For this we introduce the transformation

$$x = e^u, \quad y = e^{u/2}\varphi.$$

Equation (2.5) with a replaced by $(a+m)$ is transformed into

$$\frac{d^2\varphi}{du^2} - [e^{4u} + 4(m + a - \tfrac{1}{2}c)e^{2u}]\varphi = 0.$$

The factorization of this equation is given by

$$D_m^{\pm} = c + 1 - 2m - 2a - e^{2u} \pm \frac{d}{du},$$
$$L(m) = -(2m - c + 1),$$

and this leads to the recurrence relations

$$F(a+1; c; z) = \left[1 + \frac{z}{a}\frac{d}{dz}\right]F(a; c; z),$$
$$F(a-1; c; z) = \left[1 - \frac{z}{c-a} + \frac{z}{c-a}\frac{d}{dz}\right]F(a; c; z). \tag{2.8}$$

So far we have obtained the basic factorizations determining the fundamental recurrence relations which may be used to construct all the recurrence relations given by Erdélyi *et al.*[20] We shall now show that there is another new factorization (i.e., a new operator pair $D_n^{\pm}$) which simultaneously raises a by one unit and c by two units so that $(c-2a)$ is held fixed. We therefore consider Eq. (2.5) with c replaced by $(c+2m)$ and a by $(a+m)$:

$$\frac{d^2y}{dx^2} - \left[\frac{(c+2m-\frac{1}{2})(c+2m-\frac{3}{2})}{x^2} + x^2 - 2(c-2a)\right]y = 0. \tag{2.9}$$

Although this equation does not admit of a direct factorization, by a suitable change of variables,[21] namely,

$$x = \{4/(c-2a)\}^{\frac{1}{2}}\rho^{\frac{1}{2}}, \quad \psi = \rho^{\frac{1}{4}}y,$$

it can be recast into the factorizable form

$$\frac{d^2\psi}{d\rho^2} + \left[\frac{2}{\rho} - \frac{(m + c/2 - 1)(m + c/2)}{\rho^2} - \left(\frac{2}{c-2a}\right)^2\right]\psi = 0. \tag{2.10}$$

The factorization of the above equation is given by

$$D_m^{\pm} = \frac{m + \frac{1}{2}c - 1}{\rho} - \frac{1}{m + \frac{1}{2}c - 1} \pm \frac{d}{d\rho},$$
$$L(m) = -(m + \tfrac{1}{2}c - 1)^{-2}.$$

Without elaborating any further on the subsequent recurrence relations which are not important, we note that Eq. (2.10) becomes that for a hydrogen atom if we identify

$$m + \tfrac{1}{2}c = l + 1, \quad \left(\frac{2}{c-2a}\right)^2 = -\lambda_h,$$

where λ_h is negative. With this identification, the Eq. (2.9), which is equivalent to (2.10), becomes

$$\frac{d^2y}{dx^2} - \left[\frac{(2l+\frac{1}{2})(2l+\frac{3}{2})}{x^2} + x^2 - 4|-\lambda_h|^{-\frac{1}{2}}\right]y = 0. \tag{2.11}$$

The hydrogen atom equation is thus equivalent to an equation resembling closely that of a harmonic oscillator and we are led to suspect an interconnection between them. As we shall see presently, Eq. (2.11) represents the nth eigenstate of a harmonic oscillator in a space of $(4l + 4 - 2n)$ dimensions. To show this, we consider the radial equation of a p-dimensional harmonic oscillator:

$$\frac{d^2\psi}{dx^2} + \frac{(p-1)}{x}\frac{d\psi}{dx} - \left[\frac{n(n+p-2)}{x^2} + x^2 - \lambda_0\right]\psi = 0,$$

which on the substitution

$$y = x^{(p-1)/2}\psi$$

reduces to

$$\frac{d^2y}{dx^2} - \left[\frac{(n+\frac{1}{2}p-\frac{1}{2})(n+\frac{1}{2}p-\frac{3}{2})}{x^2} + x^2 - \lambda_0\right]y = 0. \tag{2.12}$$

This equation reduces to (2.11) on setting

$$p/2 = (2l + 2 - n), \quad \lambda_0 = 4\,|-\lambda_h|^{-\frac{1}{2}},$$

and, since $n \geq 0$, $p > 0$, we have $2 \leq p \leq 4l + 4$ according as $2l + 1 \geq n \geq 0$. Thus Eq. (2.11), which is equivalent to that of a hydrogen atom, represents a harmonic oscillator in a space of varying dimensionality ranging from $4l + 4$ to 2. From this we can immediately infer that the lth eigenstate of the hydrogen atom corresponding to the eigenvalue parameter λ_h, $\lambda_h < 0$, is equivalent to any of the $n = 0, 1, \cdots (2l + 1)$th eigenstates of a harmonic oscillator corresponding to the eigenvalue parameter $\lambda_0 = 4\,|-\lambda_h|^{-\frac{1}{2}}$ in a $(4l + 4 - 2n)$-dimensional space.

3. FACTORIZATION OF THE BETHE-SALPETER EQUATIONS

A. Goldstein's Eigenvalue Problem

The integral equation considered by Goldstein[11] [Goldstein's Eq. (9)] for the singlet state of a pair of fermions bound to zero total mass by a massless scalar boson after Wick rotation can be written as

$$\psi(\rho) = (1 + \rho^2)\varphi(\rho) = \frac{\lambda}{\pi^2}\int d^4\rho' \frac{\varphi(\rho')}{(\rho - \rho')^2}, \quad (3.1)$$

where we have written $\rho_\mu = m\rho_\mu$. Using the identity[22]

$$\Box_\rho^2(\rho - \rho')^{-2} = -4\pi^2\delta(\rho - \rho'),$$

we obtain from (3.1) the following differential equation:

$$\Box_\rho^2\psi(\rho) = -4\lambda\psi(\rho)/(1 + \rho^2).$$

This differential equation is equivalent to (3.1) provided that

$$\psi(0) \text{ is finite, and } \lim_{\rho\to\infty}\rho^2\psi(\rho) \text{ is finite.} \quad (3.2)$$

Separating the four-dimensional spherical harmonics, we obtain from the above

$$\frac{1}{\rho^3}\frac{d}{d\rho}\rho^3\frac{du_n}{d\rho} - \frac{n(n+2)u_n}{\rho^2} + \frac{4\lambda u_n}{(1+\rho^2)} = 0, \quad (3.3)$$

where $u_n(\rho)$ is the radial part of $\psi(\rho)$. We first reduce it to the standard form (2.1) by means of the transformations

$$\rho = \sinh x, \quad y_n(x) = \sinh^{\frac{3}{2}} x \cosh^{-\frac{1}{2}} x u_n.$$

By virtue of the boundary conditions (3.2) the function $y_n(x)$ defined in this fashion vanishes at the end points of the interval $0 \leq x \leq \infty$ corresponding to $0 \leq p \leq \infty$, and is therefore square integrable. Equation (3.3) is now transformed into

$$\frac{d^2y_n}{dx^2} + \left[\frac{\frac{3}{4}}{\cosh^2 x} - \frac{(n+\frac{1}{2})(n+\frac{3}{2})}{\sinh^2 x}\right]y_n + \lambda' y_n = 0, \quad (3.4a)$$

where $\lambda' = 4\lambda - (n+1)^2$. To investigate the square-integrable solutions of (3.4a), we introduce a function $y_n(\mu; x)$ depending on an auxiliary parameter μ which satisfies

$$\frac{d^2y_n(\mu)}{dx^2} + \left[\frac{(n-\mu+\frac{1}{2})(n-\mu+\frac{3}{2})}{\cosh^2 x} - \frac{(n+\frac{1}{2})(n+\frac{3}{2})}{\sinh^2 x}\right]y_n(\mu) + \lambda'(\mu)y_n(\mu) = 0. \quad (3.4b)$$

The required solution is then merely $y_n(n; x)$. Part of the dependence of this solution on n will be provided by the ladder operators while the remainder of this dependence will be introduced at the end of the ladder operations by setting $\mu = n$. The factorization of the above equation is given by

$$D_n^{\pm} = (n + \tfrac{1}{2})\coth x + (n - \mu + \tfrac{1}{2})\tanh x \pm \frac{d}{dx},$$
$$L(n) = -(2n - \mu + 1)^2,$$

since $L(n)$ is a decreasing function of n, by Theorem 2 (see Appendix) the bottom of the ladder of eigensolutions, if it exists, is determined by

$$D_N^+ y_N = 0,$$

and, since this condition is necessary, any ladder of square integrable solutions must satisfy this requirement. However, as can be readily verified, the above equation does not admit of a square-integrable solution consistent with the boundary conditions (3.2). We are therefore confronted with an infinite ladder of solutions without any bottom leading to a continuous spectrum unless some other boundary conditions which are not contained in the integral equation are imposed.

B. Factorization of the Wick–Cutkosky Equation

In this section we proceed to show that the factorization of the Wick–Cutkosky equation

$$\psi(p) = [(p^2 + 1 - \epsilon^2)^2 + 4\epsilon^2 p_4^2]\varphi(p) = \frac{\lambda}{\pi^2}\int d^4p' \frac{\varphi(p')}{(p - p')^2} \quad (3.5)$$

leads to a complete solution of the problem. Here 2ϵ is the total center-of-mass energy in units of m, m being the mass of the interacting particles assumed

equal. The differential equation equivalent to (3.5) is given by

$$\left[\frac{\partial^2}{\partial p_4^2} + \nabla^2\right]\psi(p) = -4\lambda\varphi(p), \tag{3.6}$$

and this is subject to the boundary conditions similar to (3.2). This equation can be recast into a separable form by using the bipolar transformations[14,15]

$$p_1 = p_s \sin\theta\cos\varphi, \quad p_2 = p_s \sin\theta \sin\varphi,$$
$$p_3 = p_s\cos\theta, \quad p_s = \omega \sin\beta/(\cosh\xi - \cos\beta),$$
$$p_4 = \omega \sinh\xi/(\cosh\xi - \cos\beta), \ \omega = (1-\epsilon^2)^{\frac{1}{2}},$$

so that Eq. (3.6) takes the form

$$\left[\frac{\partial}{\partial\xi^2} + \frac{\partial^2}{\partial\beta^2} - \frac{l(l+1)}{\sin^2\beta}\right](p_s\psi) = -\frac{\lambda(p_s\psi)}{\omega^2\cosh^2\xi + \epsilon^2\sinh^2\xi}.$$

The above equation, on separating the variables, leads to

$$\frac{d^2g_\nu^l}{d\beta^2} + \left[\nu^2 - \frac{l(l+1)}{\sin^2\beta}\right]g_\nu^l = 0, \quad 0 \le \beta \le \pi, \tag{3.7a}$$

$$\frac{d^2f_\lambda^\nu}{d\xi^2} - \left[\nu^2 - \frac{\lambda}{\omega^2\cosh^2\xi + \epsilon^2\sinh^2\xi}\right]f_\lambda^\nu = 0, \quad -\infty \le \xi \le \infty. \tag{3.7b}$$

By virtue of the boundary conditions, the functions $g(\beta)$ and $f(\xi)$ are square integrable in the domains $0 \le \beta \le \pi$ and $-\infty \le \xi \le \infty$, respectively. As we shall see presently, unlike the Goldstein problem, solutions satisfying this boundary condition actually do exist whenever $0 \le \epsilon < 1$.

We first consider the factorization of the equation (3.7a). If we regard ν^2 as the eigenvalue parameter to be held constant in the ladder, the factorization of the equation is given by

$$D_l^{\pm} = l\cot\beta \pm \frac{d}{d\beta}, \quad L(l) = l^2.$$

Since $L(l)$ is an increasing function of l by Theorem 2, the ladder of square integrable solutions, if it exists, must have a top given by

$$D_{n+1}^- g_{\nu(n)}^n = \left[(n+1)\cot\beta - \frac{d}{d\beta}\right]g_{\nu(n)}^n = 0, \tag{3.8a}$$

so that

$$\nu^2 = \nu^2(n) = L(n+1) = (n+1)^2, \tag{3.8b}$$

where $n = l + \kappa$, $\kappa = 0, 1, 2 \cdots n$. The square-integrable solutions of (3.8a),

$$g_n^n(\beta) = \Lambda_n^n \sin^{n+1}\beta,$$

where Λ_n^n is a suitable normalization constant, can be used to generate the successive ladder of solutions through the recurrence relation

$$g_n^l(\beta) = [(n-l)(n+l+2)]^{-\frac{1}{2}} \times \left[(l+1)\cot\beta + \frac{d}{d\beta}\right]g_n^{l+1}, \tag{3.9a}$$

which follows from Theorem 1. In the above we have relabeled the functions g in terms of the quantum number n. The corresponding l-raising recurrence relation is given by

$$g_n^{l+1}(\beta) = [(n-l)(n+l+2)]^{-\frac{1}{2}} \times \left[(l+1)\cot\beta - \frac{d}{d\beta}\right]g_n^l(\beta). \tag{3.9b}$$

The eigenfunctions g_n^n, g_n^{n-1}, g_n^{n-2}, etc., corresponding to $l = n, n-1, n-2$, are found to be expressible in terms of Gegenbauer polynomials, and we can easily show by induction that the κth step of the ladder from the top is given by

$$g_n^{n-\kappa}(\beta) = \Lambda_n^{n-\kappa}\sin^{n-\kappa+1}\beta C_\kappa^{n-\kappa+1}(\cos\beta). \tag{3.10}$$

That this is true for $\kappa = 0, 1, 2, 3$ can be verified directly. Let us therefore assume that this is true for $\kappa = k$. If we now use (3.9a) to obtain the next step down the ladder and use the recurrence relation

$$(2\alpha-2)\sin^2\beta\frac{d}{d(\cos\beta)}C_k^\alpha(\cos\beta) = (2\alpha-2)(2\alpha-1)\cos\beta C_k^\alpha(\cos\beta) - (2\alpha+k-1)(k+1)C_{k+1}^{\alpha-1}(\cos\beta),$$

we easily obtain

$$g_n^{n-k-1}(\beta) = \Lambda_n^{n-k-1}\sin^{n-k}\beta C_{k+1}^{n-k}(\cos\beta).$$

Thus, if solution (3.10) is true for $\kappa = k$, it is also true for $\kappa = k+1$ and therefore it is true in general. Finally, setting $\kappa = n - l$ in (3.10), we obtain

$$g_n^l(\beta) = \Lambda_n^l \sin^{l+1}\beta C_{n-l}^{l+1}(\cos\beta). \tag{3.11}$$

We can also obtain n-changing recurrence relations by substituting (3.8b) in (3.7a) and regarding $\lambda_l = l(l+1)$ as the eigenvalue term to be held constant in the ladder. For this we introduce

$$x = \ln\tan(\beta/2), \quad y_n^l = \cosh^{\frac{1}{2}} x g_n^l,$$

so that $-\infty \le x \le \infty$ corresponds to $0 \le \beta \le x$. The function y_n^l defined in this fashion satisfies

$$\frac{d^2y_n^l}{dx^2} + \frac{(n+\frac{1}{2})(n+\frac{3}{2})}{\cosh^2 x}y_n^l - (\lambda_l + \tfrac{1}{4})y_n^l = 0.$$

This equation admits of a factorization

$$D_n^{\pm} = (n + \tfrac{1}{2}) \tanh x \pm \frac{d}{dx}, \quad L(n) = -(n + \tfrac{1}{2})^2.$$

The subsequent recurrence relations can be expressed in terms of g and β and is given by

$$g_{n+1}^l(\beta) = [(n - l + 1)(n + l + 2)]^{-\frac{1}{2}} \times \left[-(n + 1)\cos\beta - \sin\beta \frac{d}{d\beta}\right] g_n^l(\beta)$$

$$g_n^l(\beta) = [(n - l + 1)(n + l + 2)]^{-\frac{1}{2}} \times \left[-(n + 1)\cos\beta + \sin\beta \frac{d}{d\beta}\right] g_{n+1}^l(\beta).$$

Having obtained the complete solution of Eq. (3.7a), we now investigate the factorization of Eq. (3.7b) corresponding to $\epsilon = 0$. The subsequent equation takes the form

$$\frac{d^2 f_\lambda^n}{d\xi^2} - \left[(n + 1)^2 - \frac{\lambda}{\cosh^2 \xi}\right] f_\lambda^n = 0. \quad (3.12)$$

If we regard λ as the eigenvalue term to be held constant in the ladder, the required transformation is

$$x = 2 \tan^{-1}(e^{\xi}), \quad y_\lambda^n = \sin^{\frac{1}{2}} x f_\lambda^n, \quad (3.13)$$

so that, by virtue of the boundary conditions, y_λ^n is square integrable in the interval $0 \leq x \leq n$ corresponding to $-\infty \leq \xi \leq \infty$ and satisfies

$$\frac{d^2 y_\lambda^n}{dx^2} - \frac{(n + \frac{1}{2})(n + \frac{3}{2})}{\sin^2 x} y_\lambda^n + \lambda' y_\lambda^n = 0,$$

where $\lambda' = \lambda + \frac{1}{4}$. The factorization of the above equation is given by

$$D_n^{\pm} = (n + \tfrac{1}{2}) \cot x \pm \frac{d}{dx}, \quad L(n) = (n + \tfrac{1}{2})^2. \quad (3.14)$$

Again $L(n)$ is an increasing function of n and the top of the ladder of square integrable eigenfunctions are given by

$$D_{N+1}^{-} y_N^N = \left[(N + \tfrac{3}{2}) \cot x \pm \frac{d}{dx}\right] y_N^N = 0, \quad (3.15a)$$

$$\lambda' = \lambda_N' = L(N + 1) = (N + \tfrac{3}{2})^2,$$

$$\therefore \quad \lambda = (N + 1)(N + 2), \quad (3.15b)$$

$$N = n + x, \quad x = 0, 1, 2 \cdots N.$$

The recurrence relations[23]

$$f_N^{n+1} = [(N + n + 3)(N - n)]^{-\frac{1}{2}} \times \left[(n + 1)\cot x - \frac{d}{dx}\right] f_N^n, \quad (3.16a)$$

$$f_N^n = [(N + n + 3)(N - n)]^{-\frac{1}{2}} \times \left[(n + 1)\cot x + \frac{d}{dx}\right] f_N^{n+1}, \quad (3.16b)$$

in conjunction with the solution of (3.15a), can be used to generate the ladder of eigenfunctions as before. These eigenfunctions are again expressible in terms of Gegenbauer polynomials, and, repeating the previous arguments, we can show that the $(N - n)$th step of the ladder from the top is given by

$$f_N^n = \sin^{-\frac{1}{2}} x y_N^n = \Gamma_N^n \sin^{n+1} x C_{N-n}^{n+\frac{3}{2}}(\cos x), \quad (3.17)$$

where Γ_N^n is a suitable normalization constant. To obtain the N-changing ladder operators, we substitute $\lambda = (N + 1)(N + 2)$ in (3.12) and regard the term $(n + 1)^2$ as the eigenvalue. The factorization of the equation is then given by

$$D_N^{\pm} = (N + 1) \tanh \xi \pm \frac{d}{d\xi}, \quad L(N) = -(N + 1)^2,$$

and this leads to the recurrence relations

$$f_{N+1}^n = [(N - n + 1)(N + n + 3)]^{-\frac{1}{2}} \times \left[(N + 2)\cos x + \sin x \frac{d}{dx}\right] f_N^n,$$

$$f_N^n = [(N - n + 1)(N + n + 3)]^{-\frac{1}{2}} \times \left[(N + 2)\cos x - \sin x \frac{d}{dx}\right] f_{N+1}^n. \quad (3.18)$$

We shall now show how one can obtain exact eigenvalue solutions of (3.7b) for arbitrary nonvanishing energies ($0 \leq \epsilon < 1$) once the zero-energy factorization is known. If we introduce the transformation (3.13), Eq. (3.7b) can be rewritten in terms of the zero-energy factorization as

$$\lambda y_\lambda^n - (\omega^2 + \epsilon^2 \cos^2 x)[D_{n+1}^{+} D_{n+1}^{-} + L(n + 1) - \tfrac{1}{4}] y_\lambda^n = 0, \quad (3.19)$$

where $D_n^{\pm}$ and $L(n)$ are given by (3.14).

We now attempt a solution in the form

$$y_\lambda^n(x) = \sum_k a_k y_{N+k}^n(x), \quad (3.20)$$

where the functions y_{N+k}^n appearing in the sum are the zero-energy eigenfunctions given by (3.17). The invariance of (3.19) under reflection $x \to \pi - x$ further ensures that summation runs over even or odd values of k only. The solution (3.19) satisfies the boundary conditions (i.e., square integrability) provided $\sum_k |a_k|^2 < \infty$. This condition, as we shall see presently, can be satisfied whenever $0 \leq \epsilon < 1$.

From the fundamental equations of factorization, namely, Eqs. (2.2) and our previous discussions of the zero-energy solutions, it is apparent that the functions y_N^n appearing in (3.20) are eigenfunctions of the operator $D_{n+1}^{+} D_{n+1}^{-} + L(n + 1)$ with the eigenvalue given by (3.15b). Thus, if we substitute (3.20) in

(3.19) and use the recurrence relations (3.18), we obtain (3.20) as a solution of (3.19) provided the coefficients satisfy

$$A_k a_{k+2} + B_k a_k + C_k a_{k-2} = 0, \qquad (3.21)$$

where A_k, B_k, C_k depend on energy. The condition for the existence of nontrivial solutions to this difference equation determines the eigenvalue problem. Following the method developed in an earlier paper,[17] the difference equation can be solved and one can show that there exists a fundamental system of solutions of (3.21) for which $\lim_{k\to\infty}|a_{k+2}/a_k| < 1$ whenever $0 \leq \epsilon < 1$; the condition $\sum |a_k|^2 < \infty$, necessary for square integrability, is therefore satisfied. The subsequent eigenvalue condition can be expressed in terms of an infinite continued fraction

$$B_0/A_0 = \cfrac{C_2/A_2}{B_2/A_2 - \cfrac{C_4/A_4}{\ddots}}.$$

For $\epsilon = 1$, $\omega = 0$ which corresponds to vanishing binding energy, the solution (3.20) is not valid since the convergence criteria $\lim_{k\to\infty}|a_{k+2}/a_k| < 1$ cannot be satisfied. The point $\epsilon = 1$, therefore, needs a separate investigation. Since, for this particular value of energy, the differential equation (3.7b) develops an extra singularity at the midpoint $\xi = 0$ which is absent when $\epsilon < 1$, it is necessary to investigate the solutions of the equation

$$\frac{d^2 f_\lambda^n}{d\xi^2} - \left[(n+1)^2 - \frac{\lambda}{\sinh^2 \xi}\right] f_\lambda^n = 0 \qquad (3.22)$$

separately in the region $0 \leq \xi \leq \infty$ and $-\infty \leq \xi \leq 0$. However, owing to the invariance of the equation under reflection $\xi \to -\xi$, it is sufficient to investigate the solutions in the domain, say $0 \leq \xi \leq \infty$. For $0 \leq \xi \leq \infty$ we introduce the transformations

$$x = \ln \coth (\xi/2), \quad y_\lambda^n = \sinh^{-\frac{1}{2}} \xi f_\lambda^n,$$

so that $\infty \geq x \geq 0$ corresponding to $0 \leq \xi \leq \infty$. Equation (3.22) is now transformed into

$$\frac{d^2 y_\lambda^n}{dx^2} - \frac{(n+\frac{1}{2})(n+\frac{3}{2})}{\sinh^2 x} y_\lambda^n + (\lambda - \tfrac{1}{4}) y_\lambda^n = 0.$$

The factorization of this equation is given by

$$D_n^{\pm} = (n+\tfrac{1}{2}) \coth x \pm \frac{d}{dx}, \quad L(n) = -(n+\tfrac{1}{2})^2.$$

$L(n)$ is thus a decreasing function of n and, as there is no square-integrable solution of the equation

$$D_N^+ y_N^N = 0,$$

we are again led to an infinite ladder of solutions without any bottom. However, it should be emphasized that, for $\epsilon = 1$, the requirement of square integrability, namely,

$$\int [y_\lambda^n(x)]^2 \, dx = \int d\xi [f_\lambda^n(\xi)]^2 / \sinh^2 \xi < \infty,$$

involves an extra condition which demands that $f_\lambda^n(\xi)$ should behave at least as $\sinh \xi$ in the vicinity of $\xi = 0$. Unlike the previous cases, therefore, the square integrability is not a boundary condition guaranteed by the integral equation.[24] There may be other boundary conditions which can lead to the discrete values of λ. Precisely it is these extra boundary conditions which may be held responsible for the abnormal eigenvalues which do not possess a nonrelativistic limit. These boundary conditions implicitly enter into the problem, through the substitution $\tanh \xi = z = \omega x$ in the vincinity of $z = 0$ (which requires that $z \to 0$ in the same way as $\omega \to 0$) and in the subsequent matching of the so-called "internal" and "external" solutions.

4. CONCLUSION

We have seen that the correspondence between the hydrogen atom and the harmonic oscillator is one of a homomorphism: Corresponding to a particular angular momentum state l of the hydrogen atom, a set of equivalent multidimensional oscillators, in varying angular-momentum states ranging from 0 to $2l + 1$ in spaces of correspondingly varying dimensions ranging from $4l + 4$ to 2, is obtained. Such a connection may be attributed to the fact that the hydrogen atom and harmonic oscillator problems of quantum mechanics may be regarded as two possible factorizations of the same equation, namely, the confluent hypergeometric equation, the factorizations themselves being interrelated. A group theoretic explanation of this interconnection has been recently provided by Cisneros and McIntosh,[9] who showed that a class of levels of the hydrogen atom which ordinarily transform according to an orthogonal group may form an irreducible representation of the unitary group which is the symmetry group of the harmonic oscillator.[25] The factorization of the Bethe–Salpeter equations on the other hand reveals a formal similarity between Goldstein's eigenvalue problem and the relativistic scalar meson equation for zero binding. In either of these cases we obtain an infinite ladder of nonsquare integrable solutions without any bottom. This similarity may again be attributed to the fact that both of these problems correspond to the same factorization of the hypergeometric equation.

Thus, unlike the nonrelativistic Schrödinger equation, the square integrability may not always be a realizable boundary condition for the covariant wave equations. Our observation is similar to that of Keam,[26] who showed that the solutions to the ladder approximation Bethe–Salpeter equation for the fermion–antifermion system bound to zero total mass by a massless vector or axial vector particle do not satisfy a set of integrability criteria. Some extra boundary conditions which are not manifestly contained in the integral equation may therefore be necessary to obtain an eigenvalue of the coupling constant. Precisely such extraboundary conditions were previously used by Biswas and Green,[27] who were able to obtain some radially symmetric solutions to the relativistic nucleon–nucleon problem by demanding that the wavefunction together with its spatio-temporal derivatives should be finite and continuous everywhere and particularly on the light cone. The abnormal eigenvalues ($\lambda = \frac{1}{4}$) of the Wick–Cutkosky equation corresponding to zero binding, as we have argued, also originate from such an extra requirement which implicitly enters into the problem through the matching of the "internal" and "external" solutions. The factorization of the scalar meson equation for $\epsilon = 0$ (maximal binding), on the other hand, leads to a complete solution of the problem: Here, unlike the previous cases, a ladder of square-integrable solutions which is truncated at the top does exist. The solutions are expressible in terms of $O(5)$ polynomials, and the various ladder operators obtained by us may be used to construct the Lie algebra of the $O(5)$ group. The zero-energy factorization once known, the exact eigenvalue solutions for arbitrary nonvanishing energies, $\epsilon < 1$, easily follow by rewriting the subsequent equation in terms of the zero-energy factorization. The corresponding eigenfunctions are expressible as infinite sums of the zero-energy eigenfunctions and the eigenvalue condition is expressible in terms of an infinite continued fraction.

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APPENDIX: FUNDAMENTAL THEOREMS OF FACTORIZATION

Theorem 1: If $y_\lambda^n(x)$ is a solution of the differential equation (2.1) for $m = n$, then

$$a_\lambda^n y_\lambda^{n+1}(x) = D_{n+1}^- y_\lambda^n(x),$$
$$b_\lambda^n y_\lambda^{n-1}(x) = D_n^+ y_\lambda^n(x) \tag{A1}$$

are also solutions corresponding to the same value of λ and $m = n + 1$ and $m = n - 1$, respectively. Here a and b are appropriate normalization constants.

Theorem 2: If $L(n)$ is an increasing function of n for $0 \leq n \leq k$ and $\lambda \leq$ the larger of $L(k)$, $L(k+1)$, then a necessary condition for quadratically integrable solutions is that

$$D_{N+1}^- y_\lambda^N(x) = 0, \tag{A2}$$

so that

$$\lambda = \lambda_N = L(N+1), \tag{A3}$$

where N is an integer and $n = 0, 1, 2 \cdots N$.

If $L(n)$ is a decreasing function of n, the corresponding requirement for the existence of square-integrable solutions is

$$D_N^+ y_\lambda^N(x) = 0, \tag{A4}$$

so that

$$\lambda = L(N), \tag{A5}$$

where N is an integer and $n = N, N+1, \cdots$.

Since these conditions are necessary, the nonexistence of square-integrable solutions of (A2) or (A4) which determines the top or the bottom of the ladder is equivalent to the nonexistence of square-integrable solutions of the original differential equation. The proof of these theorems can be found in the original paper of Infeld and Hull (Ref. 2).

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$$W_{k,m}(z) = \frac{z^{m+\frac{1}{2}}}{\Gamma(m-k+\frac{1}{2})} e^{-z/2} U(m-k+\tfrac{1}{2}; 2m+1; z),$$

where

$$U(a; c; z) = \frac{\Gamma(a)\Gamma(1-c)}{\Gamma(1+a-c)} {}_1F_1(a; c; z) + \Gamma(c-1) z^{1-c} {}_1F_1(1+a-c; 2-c; z).$$

However, we factorize the differential equation for ${}_1F_1$ function directly; much simplification results and this leads to the recurrence relations between the contiguous hypergeometric functions which cannot be obtained by factorizing Whittaker's equation.
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$$\int \{f_\lambda^n(\xi)\}^2/(\omega^2 \cosh^2 \xi + \epsilon^2 \sinh^2 \xi) < \infty,$$

follows immediately from the boundary condition $f(\pm\infty) = 0$ since the denominator is necessarily nonvanishing.
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Functions Whose Poisson Brackets Are Constants

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A local normal form under canonical transformation is found for n independent functions of $2n$ variables, with the condition that the Poisson bracket of each pair of the functions be constant. The normal form, closely related to work of Lie, is used to prove a conjecture of Avez on 1-forms in involution and to obtain a criterion for n independent functions of $2n$ variables to be extendable to a canonical coordinate system. The last result has been obtained in different ways by Lie and Kruskal.

INTRODUCTION

The book of Abraham and Marsden[1] on the foundations of mechanics attributes to Avez the following conjecture which we have reworded in local form. (The global form admits simple counter-examples.)

Conjecture: Let $f_1, \cdots, f_n$ be functions on a $2n$-dimensional symplectic manifold (M, ω) such that $\{df_i, df_j\} = 0$ for all i, j and, at a point $x \in M$, $df_1, \cdots, df_n$ are linearly independent. Then there exist functions $g_1, \cdots, g_n$, defined in a neighborhood U of x, such that $f_1, \cdots, f_n, g_1, \cdots, g_n$ form a coordinate system on U and such that following formulas are satisfied:

$$\{dg_i, dg_j\} = 0, \quad \text{for all } i, j;$$
$$\{df_i, dg_j\} = 0, \quad \text{for } i \neq j;$$
$$\{df_i, dg_i\} \text{ vanishes nowhere, for all } i.$$

In this paper, we first show that the truth of Avez's conjecture follows from a theorem of Lie on "function groups." We then present a simple proof of that case of Lie's theorem (Theorem 1) which is necessary for the proof of the conjecture. In fact, we found Theorem 1 in the effort to solve Avez's problem, and it was only later that we found out about the result of Lie. (One of the authors[2] has obtained a generalization of Theorem 1 which extends part of Lie's result to infinite-dimensional manifolds and unifies many local equivalence theorems in symplectic geometry.) In the last section, we present an application of Theorem 1 to systems of functions which satisfy the Poisson bracket relations of "half" of a canonical coordinate system.

1. DEFINITIONS, NOTATION, AND BASIC FORMULAS

We follow, with slight variations, the notation of Godbillon,[3] which may be converted into that of other authors by the judicious insertion of minus signs and the factor $\frac{1}{2}$.

Recall that a symplectic manifold is a pair (M, ω), where M is a $2n$-dimensional manifold and ω is a

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Functions Whose Poisson Brackets Are Constants

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A local normal form under canonical transformation is found for n independent functions of $2n$ variables, with the condition that the Poisson bracket of each pair of the functions be constant. The normal form, closely related to work of Lie, is used to prove a conjecture of Avez on 1-forms in involution and to obtain a criterion for n independent functions of $2n$ variables to be extendable to a canonical coordinate system. The last result has been obtained in different ways by Lie and Kruskal.

INTRODUCTION

The book of Abraham and Marsden[1] on the foundations of mechanics attributes to Avez the following conjecture which we have reworded in local form. (The global form admits simple counter-examples.)

Conjecture: Let $f_1, \cdots, f_n$ be functions on a $2n$-dimensional symplectic manifold (M, ω) such that $\{df_i, df_j\} = 0$ for all i, j and, at a point $x \in M$, $df_1, \cdots, df_n$ are linearly independent. Then there exist functions $g_1, \cdots, g_n$, defined in a neighborhood U of x, such that $f_1, \cdots, f_n, g_1, \cdots, g_n$ form a coordinate system on U and such that following formulas are satisfied:

$$\{dg_i, dg_j\} = 0, \quad \text{for all } i, j;$$
$$\{df_i, dg_j\} = 0, \quad \text{for } i \neq j;$$
$$\{df_i, dg_i\} \text{ vanishes nowhere, for all } i.$$

In this paper, we first show that the truth of Avez's conjecture follows from a theorem of Lie on "function groups." We then present a simple proof of that case of Lie's theorem (Theorem 1) which is necessary for the proof of the conjecture. In fact, we found Theorem 1 in the effort to solve Avez's problem, and it was only later that we found out about the result of Lie. (One of the authors[2] has obtained a generalization of Theorem 1 which extends part of Lie's result to infinite-dimensional manifolds and unifies many local equivalence theorems in symplectic geometry.) In the last section, we present an application of Theorem 1 to systems of functions which satisfy the Poisson bracket relations of "half" of a canonical coordinate system.

1. DEFINITIONS, NOTATION, AND BASIC FORMULAS

We follow, with slight variations, the notation of Godbillon,[3] which may be converted into that of other authors by the judicious insertion of minus signs and the factor $\frac{1}{2}$.

Recall that a symplectic manifold is a pair (M, ω), where M is a $2n$-dimensional manifold and ω is a

closed nondegenerate 2-form on M. Darboux's theorem (Ref. 3, Chap. VII, 1.10) asserts that, about each point of M, there is a coordinate system $p_1, \cdots, p_n$, $q_1, \cdots, q_n$ such that $\omega = \sum_{i=1}^n dp_i \wedge dq_i$. Such a coordinate system will be called canonical.

Associated with any 1-form α on M, there is a vector field X_α defined by the equation $\alpha = i_{X_\alpha}\omega = \omega(X_\alpha, \cdot)$. If f is a real-valued function on M, we will write X_f instead of X_{df}. Since df is closed, the Lie derivative $L_{X_f}\omega$ is zero, i.e., X_f is a Hamiltonian vector field. This fact can also be seen in canonical coordinates because

$$df = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial p_i} dp_i + \frac{\partial f}{\partial q_i} dq_i \right)$$

so that

$$X_f = \sum_{i=1}^{n} \left(-\frac{\partial f}{\partial p_i}\frac{\partial}{\partial q_i} + \frac{\partial f}{\partial q_i}\frac{\partial}{\partial p_i} \right),$$

which is clearly the vector field associated with the Hamiltonian function $-f$. The *Poisson bracket* $\{\alpha, \beta\}$ of the 1-forms α and β is defined as $i_{[X_\alpha, X_\beta]}\omega$ ($[\ ,\ ]$ is the Lie bracket), and the Poisson bracket $\{f, g\}$ of the functions f and g is the function $-\omega(X_f, X_g)$. These operations satisfy, among others, the following relations:

$$d\{f, g\} = \{df, dg\}, \tag{1}$$

$$X_{\{f,g\}} = [X_f, X_g], \tag{2}$$

$$\{f, g\} = X_f \cdot g = -X_g \cdot f. \tag{3}$$

2. LIE'S THEOREM AND AVEZ'S CONJECTURE

A k-tuple $(f_1, \cdots, f_k)$ of functions on the symplectic manifold (M, ω) is called *complete* if the differentials $df_1, \cdots, df_k$ are linearly independent and if there exist functions $U_{ij}: \mathbb{R}^k \to \mathbb{R}$ $(1 \leq i, j \leq k)$ such that

$$\{f_i, f_j\} = U_{ij}(f_1, \cdots, f_k), \quad 1 \leq i, j \leq k.$$

The matrix (U_{ij}) of functions is called the *structural matrix* of $(f_1, \cdots, f_k)$, and it is evidently determined by $(f_1, \cdots, f_k)$.

Lie's Theorem: Let $(f_1, \cdots, f_k)$ and $(f_1', \cdots, f_k')$ be complete k-tuples on the symplectic manifolds (M, ω) and (M', ω'), respectively. Suppose that $f_i(x) = f_i'(x')$ for some points $x \in M$ and $x' \in M'$. Then there exists a diffeomorphism φ from a neighborhood of x onto a neighborhood of x' such that $\varphi^*\omega' = \omega$ and $\varphi^* f_i' = f_i$ if and only if $(f_1, \cdots, f_k)$ and $(f_1', \cdots, f_k')$ have the same structural matrix and dim M = dim M'.

The "only if" part of Lie's theorem follows immediately from the uniqueness of the structural matrix and the fact that the action of diffeomorphisms such that $\varphi^*\omega' = \omega$ commutes with the Poisson bracket operation on functions. The "if" part is proven by Lie.[4] For the proof of Avez's conjecture, we only need the following corollary of Lie's theorem, which is essentially the special case in which $k = n$ and the entries in the structural matrix are constants. (The case in which the entries in the structural matrix are nonhomogeneous linear functions, with no restriction on the relation between k and n, is treated by one of the authors.[2])

Theorem 1: Let $(f_1, \cdots, f_n)$ be a n-tuple of functions on the $2n$-dimensional symplectic manifold (M, ω) such that the differentials df_i are linearly independent at a point $x \in M$ and such that $\{df_i, df_j\} = 0$, $1 \leq i, j \leq n$. Then

(i) there exists an antisymmetric matrix (b_{ij}) of constants such that $\{f_i, f_j\} = b_{ij}$, and

(ii) there exists a canonical coordinate system $(p_1, \cdots, p_n, q_1, \cdots, q_n)$ about x such that, for $1 \leq i \leq n$,

$$f_i = q_i - \tfrac{1}{2}\sum_{j=1}^{n} b_{ij} p_j. \tag{4}$$

In the following section, we present a direct proof of Theorem 1 which we feel may have some value for explicit computations. First, though, we give a proof of Avez's conjecture.

Theorem 2: Avez's conjecture (see the Introduction) is true.

Proof: Choose canonical coordinates as given by Theorem 1. Let $g_i = p_i + \frac{1}{2}p_i^2$. Direct computation shows that $\{g_i, g_j\} = 0$, $\{f_i, g_j\} = \delta_{ij}(p_i + 1)$, and the differentials are independent in a neighborhood of the origin. With the aid of (1), this implies that $\{dg_i, dg_j\} = 0$ and $\{df_i, dg_j\} = \delta_{ij}\, dp_i$, which is identically zero for $i \neq j$ and nowhere zero for $i = j$. QED

3. PROOF OF THEOREM 1

Assertion (i) follows immediately from (1) and the antisymmetry of the Poisson bracket operation. To prove (ii), we will make much use of the vector fields $X_{f_1}, \cdots, X_{f_n}$, for which we use the abbreviated notation $X_1, \cdots, X_n$. Our hypotheses and the definition of the Poisson bracket imply that $i_{[X_i, X_j]}\omega = 0$, and the nondegeneracy of ω implies that $[X_i, X_j] = 0$. By application of the Frobenius theorem,[5] we can find a coordinate system $(w_1, \cdots, w_n, z_1, \cdots, z_n)$ about x such that $\partial/\partial w_i = X_i$. By Proposition 1 in Sec. 4, with $X_i(x)$ taken for ξ_i, there exists a Lagrangian submanifold through x which can be defined by

equations $w_i = \theta_i(z_1, \cdots, z_n)$. [A Lagrangian submanifold is characterized by $\omega(X, Y) = 0$ for every pair X and Y of vectors tangent to the submanifold.] If we let $y_i = w_i - \theta_i(z_1, \cdots, z_n)$, then $(y_1, \cdots, y_n, z_1, \cdots, z_n)$ is a coordinate system, $\partial/\partial y_i = X_i$, and the manifold defined by the equations $y_i = 0$ is Lagrangian.

Let us express the 2-form ω in the coordinates $(y_1, \cdots, y_n, z_1, \cdots, z_n)$. We write y for $(y_1, \cdots, y_n)$ and z for $(z_1, \cdots, z_n)$. There exist functions $A_{ij}(y, z)$, $B_{ij}(y, z)$, and $C_{ij}(y, z)$ such that $A_{ij} = -A_{ji}$, $B_{ij} = -B_{ji}$, and

$$\omega = \tfrac{1}{2}\sum_{i,j} A_{ij}(y, z)\, dz_i \wedge dz_j - \tfrac{1}{2}\sum_{i,j} B_{ij}(y, z)\, dy_i \wedge dy_j + \sum_{i,j} C_{ij}(y, z)\, dy_i \wedge dz_j.$$

Now the function B_{ij} is equal to $-\omega(\partial/\partial y_i, \partial/\partial y_j) = -\omega(X_i, X_j) = \{f_i, f_j\} = b_{ij}$. The fact that $L_{\partial/\partial y_i}\omega = L_{X_i}\omega = 0$ implies that A_{ij} and C_{ij} are actually functions of z alone. Finally, since the manifold defined by the equations $y_i = 0$ is Lagrangian, the functions A_{ij} are actually zero. We have, therefore,

$$\omega = \sum_{i,j} dy_i \wedge (C_{ij}(z)\, dz_j - \tfrac{1}{2} b_{ij}\, dy_j).$$

Since ω is closed, so is the 2-form $\sum_{i,j} dy_i \wedge C_{ij}(z)\, dz_j$, and so are the 1-forms $\alpha_i = \sum_j C_{ij}(z)\, dz_j$. By the Poincaré lemma, there exist functions $u_1, \cdots, u_n$ such that $du_i = \alpha_i$ and $u_i(x) = f_i(x)$. If $p_1, \cdots, p_n$ are the functions such that $dp_i = dy_i$, $p_i(x) = 0$, and $q_i = u_i - \frac{1}{2}\sum_j b_{ij} p_j$, then

$$\omega = \sum dp_i \wedge dq_i.$$

A computation shows that, in the canonical coordinates $(p_1, \cdots, p_n, q_1, \cdots, q_n)$,

$$\frac{\partial}{\partial y_i} = X_i = \frac{\partial}{\partial p_i} - \tfrac{1}{2}\sum_{j=1}^{n} b_{ji} \frac{\partial}{\partial q_j},$$

so that

$$df_i = dq_i - \tfrac{1}{2}\sum_{j=1}^{n} b_{ij}\, dp_j.$$

Since $f_i(x) = q_i(x)$ and $p_i(x) = 0$, we must have

$$f_i = q_i - \tfrac{1}{2}\sum_{j=1}^{n} b_{ij} p_j. \qquad \text{QED}$$

Remark: The proof above does not give the simplest construction of the coordinates $p_1, \cdots, p_n, q_1, \cdots, q_n$ for purposes of explicit computation, but it does produce the normal form (4) by means of a fairly natural sequence of operations. If one wishes to find the (p, q) coordinates explicitly, once he has the (y, z) coordinates, it suffices to define $p_1, \cdots, p_n$ by setting $p_i = y_i - y_i(x)$ and then to *define* $q_1, \cdots, q_n$ by (4). (One can verify by direct calculation that the coordinates so obtained are canonical—this gives an alternate ending to the proof of Theorem 1.) It turns out, therefore, that the operations required for the determination of the (p, q) coordinates are : (a) One integrates the vector fields X_i to obtain the (w, z) coordinates; (b) one finds a Lagrangian subspace Λ of the tangent space to M at x complementary to the space spanned by $X_1(x), \cdots, X_n(x)$, by the method of Lemma 2 in Sec. 4; (c) one finds a Lagrangian submanifold tangent to Λ (a trivial operation, once one has any system of canonical coordinates); (d) the foregoing gives you y_i and then p_i as functions of the original coordinates, and then

$$q_i = f_i + \tfrac{1}{2}\sum_{j=1}^{n} b_{ij} p_j.$$

An alternative to doing (b) and (c) would be to find the functions $\theta_i(z_1, \cdots, z_n)$ by setting to zero the terms in $dz_i \wedge dz_j$ in ω.

4. LAGRANGIAN SUBSPACES AND SUBMANIFOLDS

If (M, ω) is a $2n$-dimensional symplectic manifold, a Lagrangian submanifold of M is an n-dimensional submanifold $L \subseteq M$ such that $\omega(X, Y) = 0$ when every X and Y are tangent to L. If V is a $2n$-dimensional vector space carrying a nondegenerate antisymmetric bilinear form Ω (such a space will be called *symplectic*), an n-dimensional subspace $W \subseteq V$ is called Lagrangian if $\Omega(\xi, \eta) = 0$ whenever ξ and η are in W. Since the tangent spaces to M are symplectic, a Lagrangian submanifold may be defined as a submanifold, all of whose tangent spaces are Lagrangian subspaces of the appropriate tangent spaces of M.

The following proposition is the goal of this section.

Proposition 1: If $\xi_1, \cdots, \xi_n$ are linearly independent tangent vectors to M at the point x, then there exists a piece of Lagrangian submanifold through x whose tangent space at p is complementary to the space spanned by $\xi_1, \cdots, \xi_n$.

The proposition follows immediately from two lemmas.

Lemma 1: Any Lagrangian subspace of the tangent space to M at x is tangent to a piece of Lagrangian submanifold.

Proof: In any system of canonical coordinates, the submanifold tangent to the given subspace and defined by linear equations in the coordinates is

necessarily Lagrangian. (The tangent spaces of such a submanifold are spanned by constant vector fields in the canonical coordinates. The coefficients of ω are also constant in these coordinates.)

Lemma 2: If $\xi_1, \cdots, \xi_n$ are linearly independent vectors in a $2n$-dimensional symplectic space (V, Ω), then there exists a Lagrangian subspace $W \subset V$ which is complementary to the space U spanned by $\xi_1, \cdots, \xi_n$.

Proof: The space U is the Ω-orthogonal direct sum of a space rad U on which Ω reduces to zero and a space W on which Ω is nonsingular (Ref. 6, p. 116). First W is the orthogonal sum of hyperbolic planes (Ref. 6, Theorem 3.7); its basis $(\eta_1, \cdots, \eta_r, \zeta_1, \cdots, \zeta_r)$ is such that $\Omega(\eta_i, \eta_j) = \Omega(\zeta_i, \zeta_j) = 0$ and $\Omega(\eta_i, \zeta_j) = \delta_{ij}$. Let T be the orthogonal complement of W; this space is nonsingular (Ref. 6, Theorem 3.5). In T, rad U is isotropic and spanned by $\zeta_{r+1}, \cdots, \zeta_{n-r}$, so that there exist, in T, $(n - 2r)$ vectors $\eta_{r+1}, \cdots, \eta_{n-r}$ such that $\Omega(\eta_i, \eta_j) = 0$ and $\Omega(\eta_i, \zeta_j) = \delta_{ij}$ (Ref. 6, Theorem 3.8). Finally, the Ω-orthogonal complement of the space spanned by $(\zeta_1, \cdots, \zeta_{n-r}, \eta_1, \cdots, \eta_{n-r})$ is nonsingular and therefore is the orthogonal sum of hyperbolic planes. In summary, we find in this way a basis of U, $(\eta_1, \cdots, \eta_r, \zeta_1, \cdots, \zeta_{n-r})$, which extends to a basis of V, $(\eta_1, \cdots, \eta_n, \zeta_1, \cdots, \zeta_n)$, with $\Omega(\eta_i, \eta_j) = \Omega(\zeta_i, \zeta_j) = 0$ and $\Omega(\eta_i, \zeta_j) = \delta_{ij}$ for all i, j such that $1 \leq i, j \leq n$. Now let Λ be spanned by $\eta_{r+1}, \cdots, \eta_{n-r}, \eta_1 + \eta_{n-r+1}, \zeta_1 - \zeta_{n-r+1}, \eta_2 + \eta_{n-r+2}, \zeta_2 - \zeta_{n-r+2}, \cdots, \eta_r + \eta_n, \zeta_r - \zeta_n$. Λ has dimension n, and it is easily seen to be complementary to U. Finally, Ω annihilates any pair of basis elements. In fact, $\Omega(\eta_i + \eta_{r+s+i}, \zeta_i - \zeta_{r+s+i}) = \Omega(\eta_i, \zeta_i) - \Omega(\eta_{r+s+i}, \zeta_{r+s+i}) = 1 - 1 = 0$, and the other pairs are obviously Ω-orthogonal. It follows that Ω annihilates any pair of elements of Λ, so that Λ is Lagrangian. QED

5. SEMICANONICAL SYSTEMS OF FUNCTIONS

If n functions are selected from a canonical coordinate system on a $2n$-dimensional symplectic manifold, they may be labeled as $(g_1, \cdots, g_k, h_1, \cdots, h_l)$ in such a way that

$$\{g_i, g_j\} = \{h_i, h_j\} = 0, \tag{5}$$

$$\{g_i, h_j\} = -\delta_{ij}. \tag{6}$$

We call any n-tuple $(g_1, \cdots, g_k, h_1, \cdots, h_l)$ of functions having linearly independent differentials and satisfying (5) and (6) a semicanonical system. The name is justified by the following consequence of Theorem 1.

Corollary 1: Any semicanonical system $(g_1, \cdots, g_k, h_1, \cdots, h_l)$ on M can be extended, locally, to a canonical coordinate system $(g_1, \cdots, g_n, h_1, \cdots, h_n)$.

Remark: A similar result was obtained by Kruskal.[7]

Proof: Let $u_1, \cdots, u_n, v_1, \cdots, v_n$ be canonical coordinates on $\mathbb{R}^{2n}$, with the usual symplectic structure. Write $(f_1, \cdots, f_n)$ for

$$(g_1, \cdots, g_k, h_1, \cdots, h_l)$$

and $(f'_1, \cdots, f'_n)$ for $(u_1, \cdots, u_k, v_1, \cdots, v_l)$. Then $(f_1, \cdots, f_n)$ and $(f'_1, \cdots, f'_n)$ have the same matrix (b_{ij}) of constant Poisson brackets. By Theorem 1, one can find, locally, canonical coordinate systems $(p_1, \cdots, p_n, q_1, \cdots, q_n)$ and $(p'_1, \cdots, p'_n, q'_1, \cdots, q'_n)$ on M and $\mathbb{R}^n$, respectively, such that $f_i = q_i - \frac{1}{2}\sum b_{ij}p_j$ and $f'_i = q'_i - \frac{1}{2}\sum b_{ij}p'_j$. Let φ be that local diffeomorphism from M to $\mathbb{R}^n$ for which $p'_i \circ \varphi = p_i$ and $q'_i \circ \varphi = q_i$. Since φ maps a canonical coordinate system into a canonical coordinate system, it is a symplectic diffeomorphism, and the functions $(u_1 \circ \varphi, \cdots, u_n \circ \varphi, v_1 \circ \varphi, \cdots, v_n \circ \varphi)$ form a canonical coordinate system as well. But $f'_i \circ \varphi = (q'_i - \frac{1}{2}\sum b_{ij}p'_j) \circ \varphi = q'_i \circ \varphi - \frac{1}{2}\sum b_{ij}(p'_j \circ \varphi) = q_i - \frac{1}{2}\sum b_{ij}p_j = f_i$, so that $(g_1, \cdots, g_n, h_1, \cdots, h_n)$, where $g_i = u_i \circ \varphi$ and $h_i = v_i \circ \varphi$, is a canonical coordinate system extending $(g_1, \cdots, g_k, h_1, \cdots, h_l)$. QED

Remarks:

(1) A well-known special case of Theorem 1 is that of n functions in involution. (See, for instance, the papers of the authors[8,9] or the book of Caratheodory.[10])

(2) Corollary 1 is a consequence of Lie's theorem, but, in fact, Lie proves the result independently, without the restriction $k + l = n$, and uses it as a *lemma* in the proof of his general theorem.[4]

(3) The coordinates $p'_1, \cdots, p'_n, q'_1, \cdots, q'_n$ on $\mathbb{R}^{2n}$ depend only on the matrix $\{b_{ij}\}$, which in turn depends only on the integers k and l. For applications, therefore, it is worthwhile to compute these coordinates once and for all. Here is an example, which illustrates the use of Theorem 1.

With $n = 2$, $k = l = 1$ (we will omit the primes from our notation), we have $\omega = du_1 \wedge dv_1 + du_2 \wedge dv_2$, $f_1 = u_1$, and $f_2 = v_1$. Then $df_1 = du_1$ and $df_2 = dv_1$, so that $X_1 = -\partial/\partial v_1$ and $X_2 = \partial/\partial u_1$. Integration of these constant vector fields is trivial; the system $(-v_1, u_1, v_2, u_2)$ of coordinates serves as the (w, z) system of the theorem.

Next, to find the Lagrangian submanifold, we go through the procedure of Lemma 2. The space U

spanned by X_1 and X_2 is nonsingular—we may take $\eta_1 = \partial/\partial u_1$ and $\zeta_1 = \partial/\partial v_1$ as a symplectic basis. The ω-orthogonal complement has $\eta_2 = \partial/\partial u_2$ and $\zeta_2 = \partial/\partial v_2$ as a symplectic basis. The Lagrangian subspace is spanned, therefore, by $\eta_1 + \eta_2 = \partial/\partial u_1 + \partial/\partial u_2$ and $\zeta_1 - \zeta_2 = \partial/\partial v_1 - \partial/\partial v_2$, which satisfy the equations $du_1 - du_2 = 0$ and $dv_1 + dv_2 = 0$. The requisite Lagrangian submanifold may be defined, therefore, by the equations $u_1 - u_2 = 0$ and $v_1 + v_2 = 0$, and the functions θ_1 and θ_2 are given by $w_1 = -v_1 = \theta_1(z_1, z_2) = v_2$ and $w_2 = u_1 = \theta_2(z_1, z_2) = u_2$. Now $y_1 = w_1 - \theta_1 = -v_1 - v_2$ and $y_2 = w_2 - \theta_2 = u_1 - u_2$. So $p_1 = y_1 = -v_1 - v_2$ and $p_2 = y_2 = u_1 - u_2$. Since $b_{12} = \{u_1, v_1\} = -1$, we have $q_1 = f_1 + \frac{1}{2}b_{12}p_2 = u_1 - \frac{1}{2}(u_1 - u_2) = \frac{1}{2}(u_1 + u_2)$ and $q_2 = f_2 + \frac{1}{2}b_{21}p_1 = v_1 + \frac{1}{2}(-v_1 - v_2) = \frac{1}{2}(v_1 - v_2)$. In summary, therefore, $(p_1, p_2, q_1, q_2) = (-v_1 - v_2, u_1 - u_2, \frac{1}{2}(u_1 + u_2), \frac{1}{2}(v_1 - v_2))$, and the inverse transformation, useful to calculate directly f_i' by a product of two transformations, is $(u_1, v_1, u_2, v_2) = (q_1 + \frac{1}{2}p_2, q_2 - \frac{1}{2}p_1, q_1 - \frac{1}{2}p_2, -q_2 - \frac{1}{2}p_2)$.

Finally we can extend the Liouville theorem:

Theorem 3: If a semicanonical system of integrals is known for a Hamiltonian system and if k Poisson brackets are 1, then the system can be reduced to k degrees of freedom.

Proof: If we have $g_1 = \alpha_1, \cdots, g_k = \alpha_k$ and $h_1 = \beta_1, \cdots, h_k = \beta_k, \cdots, h_l = \beta_l (k + l = n)$, we can do a canonical transformation such that we have the new variables $u_1 = \alpha_1, \cdots, u_k = \alpha_k$ and $v_1 = \beta_1, \cdots, v_k = \beta_k, \cdots, v_l = \beta_l$. As they are integrals, the new Hamiltonian function is independent of

$$u_1, \cdots, u_k, \cdots, u_l, v_1, \cdots, v_k$$

and we have the Hamiltonian $H(u_{l+1}, \cdots, u_n, v_{k+1}, \cdots, v_n)$. Finally, as $v_{k+1}, \cdots, v_l$ are constants of motion, we are reduced to a Hamiltonian system in the $2k$ variables $u_{l+1}, \cdots, u_n, v_{l+1}, \cdots, v_n$ and $(n - 2k)$ integrals.

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Linear Spin Chain with Nearest and Next-Nearest Neighbor Interactions

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We study the properties of a linear chain of spins governed by the Hamiltonian

$$H = J_1 \sum_{j=1}^{N} \mathbf{S}_j \cdot \mathbf{S}_{j+1} + J_2 \sum_{j=1}^{N} \mathbf{S}_j \cdot \mathbf{S}_{j+2}$$

and derive equations for an upper bound of the free energy by means of a temperature dependent Hartree–Fock approximation. These equations can be solved at zero temperature, yielding an approximate wavefunction for the ground state, of which the energy is an upper bound for the exact ground state energy. The upper bounds obtained are improvements of the results of Majumdar and Ghosh. There are several different cases to be considered, depending on the relative values of J_1 and J_2. In none of these is there a gap between the ground state and the first excited state in the thermodynamic limit. Finally, correlation functions are shortly discussed in connection with spiral structures in classical spin systems.

1. INTRODUCTION

We consider the following model of spin–spin interactions in one dimension, described by the Hamiltonian

$$H = J_1 \sum_{j=1}^{N} \mathbf{S}_j \cdot \mathbf{S}_{j+1} + J_2 \sum_{j=1}^{N} \mathbf{S}_j \cdot \mathbf{S}_{j+2}, \qquad (1)$$

where S_j^i is the component in the i direction of the spin operator at the jth site and cyclic boundary conditions have been taken. The case of $J_2 = 0$ is well known and has been the subject of many investigations[1]; it is relevant not only in the study of magnetism (for $J_1 > 0$ it is the isotropic linear antiferromagnetic chain) but also for the description of quantum lattice gases[2] and critical phenomena in liquid–gas transitions.[3] The case $J_2 \neq 0$ has been studied by Majumdar and Ghosh[4]; they determined some properties of finite chains and derived upper and lower bounds for the ground state energy per spin of (1) as N tends to infinity. The Hamiltonian (1) is also relevant to the study of polymers,[5] where one considers Hamiltonians of the type

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \qquad (2)$$

Hamiltonians of the type of (1) are especially important in the theory of helimagnetism,[6] where it is essential that the localized spins of the lattice do not only interact with their nearest neighbors but also with the next-nearest neighbors. When trying to determine properties of such systems, one usually makes the simplifying assumption that these properties do not change essentially when the spin operators in the Hamiltonian are replaced by classical vectors. In Refs. 6–10 for example, the ground state and its properties are determined in this approximation and ordering properties are discussed on the basis of this classical picture. In this approximation (1) simply becomes an expression for the energy

$$E = J_1 \sum_{j=1}^{N} S^2 \cos \theta_{j,j+1} + J_2 \sum_{j=1}^{N} S^2 \cos \theta_{j,j+2}, \qquad (3)$$

where S is the length of the classical spin vector, $\theta_{j,j+1}$ is the angle between the spins at sites j and $j+1$, and $\theta_{j,j+2}$ the angle between the spins at sites j and $j+2$. One easily finds for the ground state energy per spin

$$E_0 = \begin{cases} -S^2(J_1^2/8J_2 + J_2) & \text{if } J_2 > 0 \\ & \text{and } |J_1| \leq 4|J_2| \qquad (4) \\ S^2(\pm J_1 + J_2) & \text{all other cases} \qquad (5) \end{cases}$$

where the + and − signs refer to ferromagnetism and antiferromagnetism, respectively. For $J_2 > 0$ and $|J_1| \leq 4|J_2|$ the classical spin chain has a spiral structure at $T = 0$ as illustrated in Fig. 1. The ground state energy, when plotted as a function of J_2 for fixed value of J_1, has a kink at $J_2 = \frac{1}{4}J_1$.

2. EQUATIONS FOR THE EXTREMUM OF THE FREE ENERGY

We now turn to the quantum mechanical problem posed by (1) for the case of spins $\frac{1}{2}$, the S's being the Pauli matrices. This is an extremely difficult problem since, even for the case $J_2 = 0$, only the ground state and a few excited states are known. So we have to resort to approximate methods and shall employ a temperature dependent Hartree–Fock approximation, making use of the fact that for spins $\frac{1}{2}$ the Hamiltonian (1) can be expressed in Fermi operators.

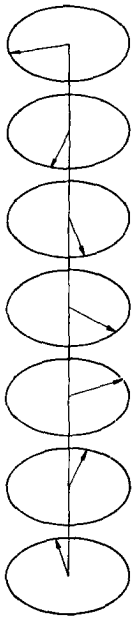

FIG. 1. Spiral structure in a classical chain.

Performing the transformations

$$S_j^x = (a_j^* + a_j)/2, \quad S_j^y = (a_j^* - a_j)/2i,$$
$$S_j^z = \tfrac{1}{2} - a_j^* a_j \tag{6}$$

and

$$a_j = \exp\left[-\pi i \sum_{k=1}^{j-1} c_k^* c_k\right] c_j,$$
$$a_j^* = c_j^* \exp\left[\pi i \sum_{k=1}^{j-1} c_k^* c_k\right], \tag{7}$$

where the c's and c^*'s are Fermi operators

$$\{c_i, c_j^*\} = \delta_{ij}, \quad \{c_i, c_j\} = \{c_i^*, c_j^*\} = 0, \tag{8}$$

we obtain (1) in the form

$$\begin{aligned} H = \sum_{j=1}^{N} [&\tfrac{1}{2}(J_1 c_j^* c_{j+1} + J_2 c_j^* c_{j+2} + \text{H.c.}) \\ &- (J_1 + J_2) c_j^* c_j + J_1 c_j^* c_j c_{j+1}^* c_{j+1} \\ &+ J_2 c_j^* c_j c_{j+2}^* c_{j+2} \\ &- J_2 (c_j^* c_{j+1}^* c_{j+1} c_{j+2} + \text{H.c.}) + \tfrac{1}{4} J_1 + \tfrac{1}{4} J_2]. \end{aligned} \tag{9}$$

After a Fourier transformation

$$c_j = N^{-\frac{1}{2}} \sum_{k=1}^{N} e^{i\phi_k j} \eta_k, \quad c_j^* = N^{-\frac{1}{2}} \sum_{k=1}^{N} e^{-i\phi_k j} \eta_k^*, \tag{10}$$

where

$$\phi_k = k2\pi/N, \qquad k = 1, \cdots, N, \tag{11}$$

to a new set of Fermi operators η and η^*, we have

$$\begin{aligned} H = \sum_{k=1}^{N} &[J_1(\cos\phi_k - 1) + J_2(\cos 2\phi_k - 1)] \eta_k^* \eta_k \\ &+ \tfrac{1}{4}(J_1 + J_2) + \frac{1}{N} \sum_{k_1 k_2 k_3 k_4} [J_1 \cos(\phi_{k_1} - \phi_{k_4}) \\ &+ J_2 \cos 2(\phi_{k_1} - \phi_{k_4}) - 2J_2 \cos(\phi_{k_1} + \phi_{k_4})] \\ &\times \bar{\Delta}(\phi_{k_1} + \phi_{k_2} - \phi_{k_3} - \phi_{k_4}) \eta_{k_1}^* \eta_{k_2}^* \eta_{k_3} \eta_{k_4}, \end{aligned} \tag{12}$$

where $\bar{\Delta}(\phi) = 1$ if $\phi = n2\pi$, $n = 0, \pm 1, \cdots$ and zero otherwise. We now introduce a so-called trial Hamiltonian H_0:

$$H_0 = \sum_{k=1}^{N} \epsilon(k) \eta_k^* \eta_k. \tag{13}$$

Bogoliubov's inequality[10] states that the trial free energy, defined by

$$F_t = \langle H \rangle_0 - TS_0, \tag{14}$$

where

$$\langle H \rangle_0 = (\text{Tr}\, e^{-\beta H_0} H)/\text{Tr}\, e^{-\beta H_0}, \quad \text{with} \quad \beta = 1/kT, \tag{15}$$

and S_0 is the entropy of the system described by (13), is an upper bound to the exact free energy F, i.e.,

$$F_t \geq F. \tag{16}$$

By varying the one-particle energies $\epsilon(k)$, one can minimize this upper bound.

Using the relation

$$\begin{aligned} \langle \eta_{k_1}^* \eta_{k_2}^* \eta_{k_3} \eta_{k_4} \rangle_0 &= (\text{Tr}\, e^{-\beta H_0} \eta_{k_1}^* \eta_{k_2}^* \eta_{k_3} \eta_{k_4})/\text{Tr}\, e^{-\beta H_0} \\ &= n_{k_1} n_{k_2} (\delta_{k_1 k_4} \delta_{k_2 k_3} - \delta_{k_1 k_3} \delta_{k_2 k_4}), \end{aligned} \tag{17}$$

where

$$n_k = \langle \eta_k^* \eta_k \rangle_0 = (1 + e^{\beta\epsilon(k)})^{-1}, \tag{18}$$

one easily finds that

$$\begin{aligned} \frac{\langle H \rangle_0}{N} = &\frac{1}{N} \sum_{k=1}^{N} \epsilon_0(k) n_k + (J_1 + J_2) \left[\frac{1}{N} \sum_{k=1}^{N} n_k\right]^2 \\ &- (J_1 - 2J_2) \left[\frac{1}{N} \sum_{k=1}^{N} n_k \cos\phi_k\right]^2 \\ &- J_2 \left[\frac{1}{N} \sum_{k=1}^{N} n_k \cos 2\phi_k\right]^2 \\ &- 2J_2 \left[\frac{1}{N} \sum_{k=1}^{N} n_k\right] \left[\frac{1}{N} \sum_{k=1}^{N} n_k \cos 2\phi_k\right] \\ &- (J_1 + 2J_2) \left[\frac{1}{N} \sum n_k \sin\phi_k\right]^2 \\ &- J_2 \left[\frac{1}{N} \sum_{k=1}^{N} n_k \sin 2\phi_k\right]^2 + \tfrac{1}{2} J_1 + \tfrac{1}{2} J_2, \end{aligned} \tag{19}$$

where

$$\epsilon_0(k) = J_1(\cos\phi_k - 1) + J_2(\cos 2\phi_k - 1). \tag{20}$$

We now assume that

$$\epsilon(\pi - k) = \epsilon(\pi + k), \tag{21}$$

and we shall show a little further on that this assumption is consistent.

Equation (21) implies

$$\sum_{k=1}^{N} n_k \sin\phi_k = \sum_{k=1}^{N} n_k \sin 2\phi_k = 0,$$

so that

$$\frac{\langle H\rangle_0}{N} = \frac{1}{N}\sum_{k=1}^{N}\epsilon_0(k)n_k + (J_1 + J_2)\left[\frac{1}{N}\sum_{k=1}^{N}n_k\right]^2 - (J_1 - 2J_2)\left[\frac{1}{N}\sum_{k=1}^{N}n_k\cos\phi_k\right]^2 - J_2\left[\frac{1}{N}\sum_{k=1}^{N}n_k\cos 2\phi_k\right]^2 - 2J_2\left[\frac{1}{N}\sum_{k=1}^{N}n_k\right]\left[\frac{1}{N}\sum_{k=1}^{N}n_k\cos 2\phi_k\right] = E_t. \quad (22)$$

For noninteracting fermions described by the Hamiltonian (13), one has for the entropy:

$$S_0 = -\frac{1}{N}\sum_{k=1}^{N} n_k \ln n_k + (1 - n_k)\ln(1 - n_k). \quad (23)$$

Using this and (22) in (14), we obtain for the extremum condition $\partial F_t/\partial n_k = 0$ [rather than $\partial F_t/\partial\epsilon(k) = 0$] the equation

$$\epsilon(k) = 4J_2(s - q)\cos^2\phi_k + [(J_1 - 2J_2)p + 2J_2] \times \cos\phi_k - 2s(J_1 + 2J_2), \quad (24)$$

where

$$s = \tfrac{1}{2} - \frac{1}{N}\sum_{k=1}^{N} n_k, \quad (25)$$

i.e., the magnetic moment per spin in the z direction,

$$p = 1 - \frac{2}{N}\sum_{k=1}^{N} n_k\cos\phi_k, \quad (26)$$

$$q = \frac{1}{N}\sum_{k=1}^{N} n_k\cos 2\phi_k. \quad (27)$$

In the limit $N \to \infty$ these sums become integrals. Boltzmann's constant has been set equal to unity. From (24) it can be seen that the assumption $\epsilon(\pi - k) = \epsilon(\pi + k)$ is consistent with the results. Equation (24) is the basic nonlinear integral equation for $\epsilon(k)$ in this approximation.

3. SOLUTION FOR $T = 0$

Exact results can be obtained for $T = 0$, since then we have the simplification

$$n_k = \begin{cases} 0 & \text{if } \epsilon(k) > 0 \\ 1 & \text{if } \epsilon(k) < 0 \end{cases}. \quad (28)$$

Now the upper bound for the free energy becomes an upper bound for the ground state energy, i.e., (16) becomes

$$E_t \geq E_0. \quad (29)$$

We are interested in the case where $N \to \infty$, so that the expressions (25), (26), and (27) become integrals. Equations (24)–(27) are now solved as follows: Determine an interval I in $[0, 2\pi]$, symmetric with respect to the point π, such that when

$$s = \tfrac{1}{2} - \frac{1}{2\pi}\int_I d\phi, \quad (25')$$

$$p = 1 - \frac{1}{\pi}\int_I \cos\phi\, d\phi, \quad (26')$$

$$q = \frac{1}{2\pi}\int_I \cos 2\phi\, d\phi \quad (27')$$

are substituted in (24), one has $\epsilon(k) > 0$ when $\phi_k \subset I$ and $\epsilon(k) < 0$ when $\phi_k \notin I$.

We have to consider four different cases, viz.: (a) $J_1 < 0, J_2 < 0$, i.e., all interactions are ferromagnetic; (b) $J_1 < 0, J_2 > 0$, and nearest neighbors interact ferromagnetically, the tendency to align is opposed by the fact that next-nearest neighbors interact antiferromagnetically; (c) $J_1 > 0$, $J_2 < 0$, nearest neighbors tend to be antiparallel, and this tendency is enhanced by the ferromagnetic next-nearest neighbor interaction; (d) $J_1 > 0$, $J_2 > 0$, i.e., all interactions are antiferromagnetic. The tendency for nearest neighbors to be antiparallel is opposed by the fact that also next-nearest neighbors tend to be antiparallel.

In the following we shall take $J_1 = 1$ when $J_1 > 0$ and $J_1 = -1$ when $J_1 < 0$; this clearly is no lin itation. Since the strength of the interaction betwe n next-nearest neighbors is likely to be smaller than between nearest neighbors, we take $J_2 = \alpha$ with $-1 < \alpha < 1$.

(a) $J_1 = -1$, $-1 < \alpha < 0$: One readily verifies that $I = 0$ is the solution, and so $s = \frac{1}{2}$, which means that this state is totally ordered. This state actually, of course, is the true ground state. With $p = 1$ and $q = 0$ one finds from (24)

$$\epsilon(k) = 2\alpha\cos^2\phi_k - \cos\phi_k - 2\alpha - 1. \quad (30)$$

The ground state energy is

$$E_t = E_0 = -\tfrac{1}{4}(1 + \alpha). \quad (31)$$

(b) $J_1 = -1$, $0 < \alpha < 1$: In the region $0 < \alpha < \frac{1}{4}$ the solution is still given by $I = 0$. For $\alpha > \frac{1}{4}$ part of the elementary excitation spectrum becomes negative (see Fig. 2) and I now is the interval $[\phi_{k_0}, \phi_{k_1}]$ (we restrict ourselves to the interval $[0, \pi]$ since everything is symmetric with respect to π). Now ϕ_{k_0} and ϕ_{k_1} have to be determined from the equations

$$\epsilon(k_0) = \epsilon(k_1) = 0, \quad (32)$$

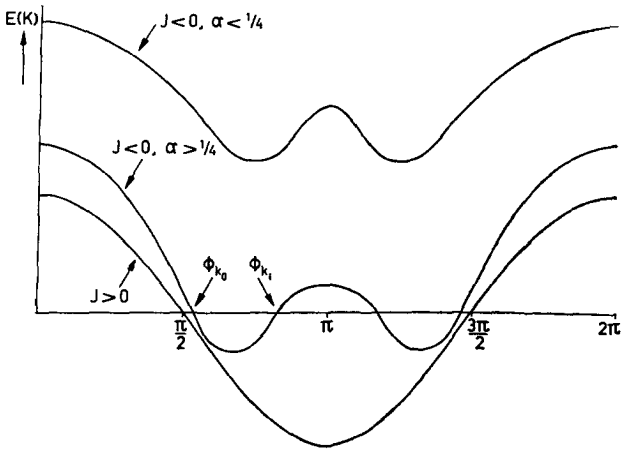

FIG. 2. Elementary excitation spectra for several cases that are examined.

or from Eqs. (24)–(27)

$$f_1(\phi_{k_0}, \phi_{k_1}) \cos^2 \phi_{k_0} + f_2(\phi_{k_0}, \phi_{k_1}) \cos \phi_{k_0} + f_3(\phi_{k_0}, \phi_{k_1}) = 0 \quad (33)$$

and

$$f_1(\phi_{k_0}, \phi_{k_1}) \cos^2 \phi_{k_1} + f_2(\phi_{k_0}, \phi_{k_1}) \cos \phi_{k_1} + f_3(\phi_{k_0}, \phi_{k_1}) = 0,$$

with

$$\begin{aligned} f_1(\phi_{k_0}, \phi_{k_1}) &= (\alpha/\pi)[2\pi + 4(\phi_{k_0} - \phi_{k_1}) \\ &\quad + 2(\sin 2\phi_{k_0} - \sin 2\phi_{k_1})], \\ f_2(\phi_{k_0}, \phi_{k_1}) &= (2/\pi)(1 + 2\alpha)(\sin \phi_{k_1} - \sin \phi_{k_0}), \quad (34) \\ f_3(\phi_{k_0}, \phi_{k_1}) &= (1 - 2\alpha)[1 - (2/\pi)(\phi_{k_1} - \phi_{k_0})]. \end{aligned}$$

The coupled transcendental equations (33) have been solved numerically for several values of α. With the resulting ϕ_{k_0} and ϕ_{k_1} one can then calculate the upper bound for the ground state energy (22). A number of results is given in Table I.

TABLE I. Numerical solutions of Eqs. 33 for several values of α with corresponding E_t.

α	ϕ_{k_0}	ϕ_{k_1}	E_t
0.30	0.46910	0.65490	−0.17550
0.35	0.63280	1.0284	−0.16617
0.40	0.69578	1.3074	−0.16108
0.45	0.71914	1.4711	−0.15942
0.50	0.73654	1.5708	−0.15982
0.55	0.75250	1.6390	−0.16251
0.60	0.76714	1.6897	−0.16493
0.65	0.78041	1.7295	−0.16735
0.70	0.79237	1.7619	−0.17113
0.75	0.80311	1.7891	−0.17532
0.80	0.81279	1.8123	−0.17986
0.85	0.82153	1.8325	−0.18468
0.90	0.82945	1.8501	−0.18973
0.95	0.83616	1.8663	−0.19499
1.00	0.84323	1.8798	−0.20043

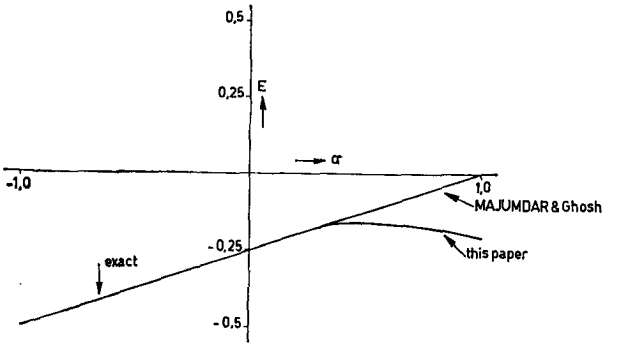

FIG. 3. Upper bounds for the ground state energy per spin for infinite chains, $J_1 < 0$, as a function of α.

In Fig. 3 the upper bound for the ground state energy is plotted as a function of α. We have also plotted as comparison the upper bound given by Majumdar and Ghosh,[4] namely $E = -\frac{1}{4}(1 + \alpha)$ (their definition of J_2 and α differs slightly from ours). For $\alpha < 0$ both approximations give the exact ground state energy, for $0 < \alpha < \frac{1}{4}$ the same upper bound, but for $\alpha > \frac{1}{4}$ our upper bound is much better. A remarkable feature is that there is a kink in the upper bound for the ground state energy for exactly the same value of α, viz., $\alpha = \frac{1}{4}$, as it is found in the classical chain. It is precisely the point at which the ferromagnetic state becomes unstable with respect to spin waves. It may well be an exact result.

(c, d) $J_1 = 1$, $-1 < \alpha < 1$: In this case the solution of the extremum equations is given by the interval $I = [\pi/2, \pi]$. The elementary excitation spectrum now is

$$\epsilon(k) = [1 + (2/\pi)(1 - \alpha)] \cos \phi_k \quad (35)$$

and the upper bound for the ground state energy is

$$E_t = -1/\pi - 1/\pi^2 + 2\alpha/\pi^2. \quad (36)$$

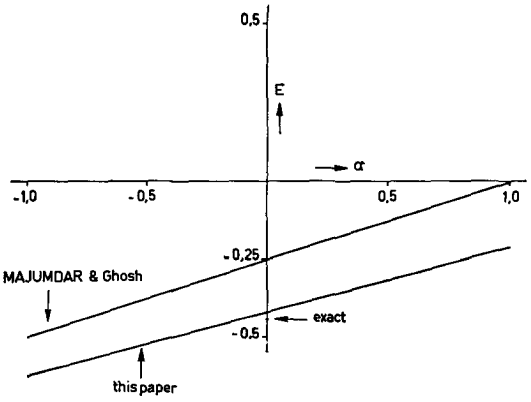

FIG. 4. Upper bounds for the ground state energy per spin for infinite chains, $J_1 > 0$, as a function of α.

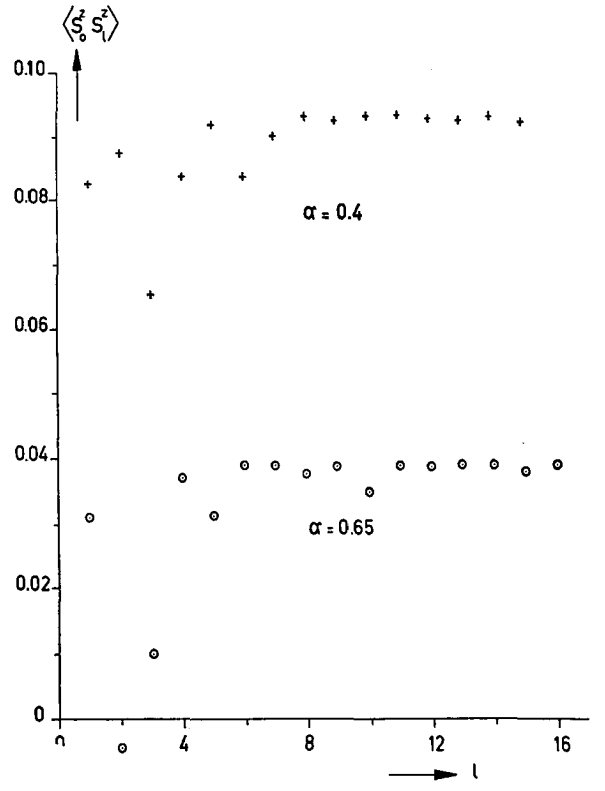

FIG. 5. The correlation functions between the z components if spins separated by l lattice sites a function of l for two values of $\alpha, J_1 < 0$.

For $\alpha = 0$ this is $E_t \simeq -0.4193$ and coincides with the result of Bulaevskii.[11] The well-known exact result due to Hulthén[1] is $E_0\ (\alpha = 0) = \ln 2 + \frac{1}{4} \simeq -0.44315$. E_t has been plotted as a function of α in Fig. 4 and again the upper bound of Ref. 4 is plotted for comparison. It is seen that the upper bound for the ground state energy lies far below the upper bound derived by Majumdar and Ghosh.

These calculations can be quite easily extended to the case when there is a magnetic field in the z direction present.

4. CORRELATION FUNCTIONS

The spiral structure of the classical spin chain is clearly reflected in the correlation functions $\langle S_0^z S_l^z \rangle$ of the quantum mechanical model. They can easily be evaluated.

(a) $J_1 = -1$, $\alpha = \frac{1}{4}$: In this case we readily find for the wavefunction that we have constructed

$$\langle S_0^z S_l^z \rangle = S^z - [(1/\pi l)(\sin l\phi_{k_1} - \sin l\phi_{k_0})]^2. \quad (37)$$

We have plotted this correlation function as a function of the distance l between the spins for several values of α. It can be seen to oscillate and for $l \to \infty$ goes to the limit of the square of the magnetization. The oscillations are the reflections of the classical spiral structure. As in the classical case, the onset of these oscillations is exactly at $\alpha = \frac{1}{4}$.

(b) $J_1 = 1$: Now one finds from (37), with $\phi_{k_0} = \pi/2$ and $\phi_{k_1} = \pi$,

$$\langle S_0^z S_l^z \rangle = S^z - [(\sin \pi l/z)/\pi l]^2. \quad (38)$$

This is in agreement with Bulaevskii's result. Equation (38) shows the same qualitative behavior as the preceding case and has not been plotted. In contradistinction to the preceding case there is not the analogy with the classical chain of spins that the onset of the oscillating behavior of the correlation function occurs at the value $\alpha = \frac{1}{4}$; the oscillations are present in the whole range $-1 < \alpha < 1$. This is probably due to the fact that the classical antiferromagnetic chain is ordered for $J_2 = 0$ whereas its quantum mechanical analog most probably is not.

ACKNOWLEDGMENT

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Specific Heat and Entropy Bounds for Ising Spin Systems*

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For quite general Ising spin systems of arbitrary dimensionality and with ferromagnetic interactions of arbitrary range, an entropy lower bound is obtained from Griffiths' inequalities and convexity relations. The bound is valid for nonnegative magnetic fields which may vary from site to site. The specific heat computed from the bound is shown to be an upper bound for the exact specific heat. If the magnetic field is taken to be zero, the entropy bound is shown to be tighter than that obtained previously by truncating a cumulantlike entropy expansion at second order. The present lower bound achieves *equality* with the exact entropy of the nearest-neighbor, N-spin, Ising ring as $N \to \infty$ for zero field and positive temperatures. An interpretation of the entropy bound is that if in the truncated expansion only binary terms arising from primary correlation are retained, the result is, nevertheless, an overestimate of the order.

1. INTRODUCTION

For some quite general Ising systems of any dimensionality it was shown[1] that the first two terms in a cumulantlike entropy expansion provide a lower bound for the exact entropy. The primary motivation for the cited work was to obtain some insight into the connection between entropy and various types of statistical association among spins, and it was the sense of the bound rather than the sharpness which was of interest.

A purpose of this paper is to present a similar entropy lower bound which is sharper than the previous one. The present bound, valid for n-dimensional Ising spin systems with arbitrary-range ferromagnetic interactions and for nonnegative magnetic fields, achieves *equality* with the exact entropy for the nearest-neighbor, N-spin, Ising ring as $N \to \infty$ for zero field and positive temperatures.

It is also shown that the specific heat computed from the entropy bound is an upper bound for the exact specific heat.

An interpretation of the entropy bound is that if in the truncated expansion one retains only primary correlation contributions in the binary term, one, nevertheless, overestimates the order.

2. DEFINITIONS AND THEOREM

The Hamiltonian for the N-spin Ising system is

$$H = -\sum_{i<j} J_{ij} s_i s_j, \tag{2.1}$$

where

$$s_i = \pm 1, \quad i = 1, 2, \cdots, N,$$

$$s_i = +1, \quad i = 0,$$

and

$$J_{ij} \geq 0, \quad 1 \leq i < j \leq N,$$

$$J_{ij} = h_j \geq 0, \quad i = 0, j = 1, 2, \cdots, N.$$

In the Hamiltonian, the symbol $\sum_{i<j}$ denotes the sum over all spin pairs i, j for which $0 \leq i < j \leq N$. The ghost spin[2] s_0 was introduced by Griffiths and constrained to have the value $+1$ so that the Hamiltonian could be associated with an Ising ferromagnet of N spins, each of magnitude $\frac{1}{2}$ and subjected to a nonnegative magnetic field which is not necessarily the same for each spin.

With $\epsilon = 0$ or 1, let $\{\epsilon, N\}$ denote the set of spin pairs i, j for which $\epsilon \leq i < j \leq N$ *and* $J_{ij} > 0$. In the following, the Boltzmann constant will be suppressed and β will denote the inverse temperature, ψ_N the entropy per spin, and $\langle \cdots \rangle$ the average in the canonical ensemble for H; then one has the following theorem.

Theorem:

$$\psi_N \geq \ln 2 - (1/2N) \times \sum_{\{0,N\}} [(1 + \langle s_i s_j \rangle) \ln (1 + \langle s_i s_j \rangle) + (1 - \langle s_i s_j \rangle) \ln (1 - \langle s_i s_j \rangle)]. \tag{2.2}$$

From the above lower bound, denoted by $\bar{\psi_N}$, one obtains an upper bound for the specific heat:

$$T \frac{\partial}{\partial T} \bar{\psi_N} = \frac{T}{2N} \sum_{\{0,N\}} [\ln (1 + \langle s_i s_j \rangle) - \ln (1 - \langle s_i s_j \rangle)] \times \left(- \frac{\partial}{\partial T} \langle s_i s_j \rangle \right),$$

but[2] from Griffiths' work $\langle s_i s_j \rangle \geq \tanh \beta J_{ij}$ and $(\partial / \partial T) \langle s_i s_j \rangle \leq 0$, and we know that $\ln (1 + x) - \ln (1 - x)$ is monotone increasing for increasing x, where $0 \leq x < 1$; therefore, the right side of the above equation is

$$\geq \frac{T}{2N} \sum_{\{0,N\}} [\ln (1 + \tanh \beta J_{ij}) - \ln (1 - \tanh \beta J_{ij})] \times \left(- \frac{\partial}{\partial T} \langle s_i s_j \rangle \right),$$

which is

$$= -\frac{T\beta}{N} \sum_{\{0,N\}} J_{ij} \frac{\partial}{\partial T} \langle s_i s_j \rangle.$$

The latter quantity is the exact specific heat c_N for the system with Hamiltonian H in Eq. (2.1); thus,

$$T \frac{\partial}{\partial T} \psi_N^- \geq c_N. \tag{2.3}$$

The proof of the theorem is also based on Griffiths' inequalities[2] and some convexity relations, and will be discussed in the next section. It should be noticed that integration of Eq. (2.3) yields Eq. (2.2) but not the condition for equality provided by Eq. (3.8). At this point it seems worthwhile to clarify the connection between the theorem and previous results.[1]

The one-spin and the two-spin marginal probabilities[3] are, respectively,

$$p(s_j) = \tfrac{1}{2}(1 + \langle s_j \rangle s_j), \quad j = 1, 2, \cdots, N, \tag{2.4}$$

$$p(s_i, s_j) = \tfrac{1}{4}(1 + \langle s_i \rangle s_i + \langle s_j \rangle s_j + \langle s_i s_j \rangle s_i s_j), \quad 1 \leq i < j \leq N. \tag{2.5}$$

Introduce the cumulant-like quantities[1]

$$\langle \hat{S}_j \rangle_c = -\langle \ln p(s_j) \rangle, \quad j = 1, 2, \cdots, N, \tag{2.6}$$

$$\langle \hat{S}_{ij} \rangle_c = -\langle \ln p(s_i, s_j) - \ln [p(s_i)p(s_j)] \rangle, \quad 1 \leq i < j \leq N, \tag{2.7}$$

and recall that $\langle \hat{S}_j \rangle_c \geq 0$ whereas[4] $\langle \hat{S}_{ij} \rangle_c \leq 0$. Specifically,

$$\langle \hat{S}_j \rangle_c = -\sum_{s_j} p(s_j) \ln p(s_j)$$
$$= \ln 2 - \tfrac{1}{2}[(1 + \langle s_j \rangle) \ln (1 + \langle s_j \rangle) + (1 - \langle s_j \rangle) \ln (1 - \langle s_j \rangle)], \tag{2.8}$$

so that the theorem may alternatively be written

$$\psi_N \geq (1/N) \sum_{j=1}^{N} \langle \hat{S}_j \rangle_c - (1/2N) \times \sum_{\{1,N\}} [(1 + \langle s_i s_j \rangle) \ln (1 + \langle s_i s_j \rangle) + (1 - \langle s_i s_j \rangle) \ln (1 - \langle s_i s_j \rangle)]. \tag{2.9}$$

Now for the case in which all $h_j = 0$, the right side of (2.9) is equal to

$$(1/N) \sum_{j=1}^{N} \langle \hat{S}_j \rangle_c + (1/N) \sum_{\{1,N\}} \langle \hat{S}_{ij} \rangle_c \geq (1/N) \sum_{j=1}^{N} \langle \hat{S}_j \rangle_c + (1/N) \sum_{1 \leq i < j \leq N} \langle \hat{S}_{ij} \rangle_c, \tag{2.10}$$

since $\langle \hat{S}_{ij} \rangle_c \leq 0$. With the right side of Eq. (2.10) denoted by $\psi_N^{(1)} + \psi_N^{(2)}$, we have

$$\psi_N \geq \psi_N^- \geq \psi_N^{(1)} + \psi_N^{(2)}. \tag{2.11}$$

The weaker lower bound is the one obtained in Ref. 1; thus, retaining only primary correlation contributions in the binary term tightens the bound but still leads to an *over*estimate of the order.

If one considers the nearest-neighbor, N-spin Ising ring in zero external field and positive temperatures, one easily verifies that the sharper bound $\psi_N^- \to \psi_N$ in the limit $N \to \infty$, whereas the weaker bound $\psi_N^{(1)} + \psi_N^{(2)}$ was shown[1] numerically to provide a close approximation to the exact entropy for that model only at sufficiently high temperatures. A deficiency of both bounds is that they are not, in general, nonnegative nor do they satisfy the third law.[5] Nevertheless, they provide nontrivial formal statements about the perturbation expansion for ψ_N, which is bounded[6] above by the sum over $\langle \hat{S}_j \rangle_c / N$.

3. PROOF OF THE THEOREM

The Hamiltonian

$$H = -\sum_{i<j} J_{ij} s_i s_j \tag{3.1}$$

defined in the previous section has an average value $\langle H \rangle$ in terms of which we may write the free energy F and the entropy per spin:

$$-\beta F = N \ln 2 - \int_0^\beta d\beta' \langle H \rangle \tag{3.2}$$

$$\psi_N = \ln 2 + \beta \langle H/N \rangle - \int_0^\beta d\beta' \langle H/N \rangle. \tag{3.3}$$

Notice that

$$\beta J_{ij} = \tfrac{1}{2}[\ln (1 + \tanh \beta J_{ij}) - \ln (1 - \tanh \beta J_{ij})]. \tag{3.4}$$

Therefore,

$$\beta \langle H \rangle = -\tfrac{1}{2} \sum_{i<j} [\ln (1 + \tanh \beta J_{ij}) - \ln (1 - \tanh \beta J_{ij})] \langle s_i s_j \rangle \tag{3.5}$$

and

$$-\int_0^\beta d\beta' \langle H \rangle = \sum_{i<j} J_{ij} \int_0^\beta d\beta' (\langle s_i s_j \rangle - \tanh \beta' J_{ij}) + \sum_{i<j} J_{ij} \int_0^\beta d\beta' \tanh \beta' J_{ij}; \tag{3.6}$$

however,

$$J_{ij} \int_0^\beta d\beta' \tanh \beta' J_{ij} = \ln \cosh \beta J_{ij} = -\tfrac{1}{2}[\ln (1 + \tanh \beta J_{ij}) + \ln (1 - \tanh \beta J_{ij})]. \tag{3.7}$$

Combining these relations gives the exact expression

$$\psi_N = \ln 2 - (1/2N) \times \sum_{i<j} [(1 + \langle s_i s_j \rangle) \ln (1 + \tanh \beta J_{ij}) + (1 - \langle s_i s_j \rangle) \ln (1 - \tanh \beta J_{ij})] + (1/N) \sum_{i<j} J_{ij} \int_0^\beta d\beta' (\langle s_i s_j \rangle - \tanh \beta' J_{ij}). \quad (3.8)$$

Since[2] $\langle s_i s_j \rangle \geq \tanh \beta J_{ij}$, the integrand is nonnegative[7] for all pairs i, j such that $0 \leq i < j \leq N$; consequently,

$$\psi_N \geq \ln 2 - (1/2N) \times \sum_{\{0,N\}} [(1 + \langle s_i s_j \rangle) \ln (1 + \tanh \beta J_{ij}) + (1 - \langle s_i s_j \rangle) \ln (1 - \tanh \beta J_{ij})]. \quad (3.9)$$

The double sum over $i < j$ has been replaced by the sum over the set $\{0, N\}$ since for $i, j \notin \{0, N\}$, $J_{ij} = 0 = \ln (1 \pm \tanh \beta J_{ij})$. The proof is now completed by using the fact that, for $0 \leq u \leq v < 1$,

$$f(u, v) \equiv -[(1 + u) \ln (1 + v) + (1 - u) \ln (1 - v) \geq f(u, u). \quad (3.10)$$

The latter inequality is obtained by adding the convexity relations[6]

$$p_i \ln p_i - p_i \ln q_i - p_i + q_i \geq 0,$$

for $i = 1, 2$, with $p_1 = 1 + u$, $p_2 = 1 - u$, $q_1 = 1 + v$, and $q_2 = 1 - v$.

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Motion of a Particle in a Random Field*

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(Received 4 February 1971)

The motion of a particle in a random force field is investigated using the diffusion approximation.

1. INTRODUCTION

In this note we extend the analysis of Frisch[1] and others,[2–7] concerning the motion of a particle in a random field. We use the diffusion approximation, which is based on the assumption that the fluctuations of the field are weak and that they are weakly correlated at widely separated points. The equations of the diffusion approximation have been derived using a two-time method in[8] which, in addition, some other applications are given. The results in this note can be viewed as a generalization of the Ornstein–Uhlenbeck theory of Brownian motion.[9] Here the starting point is a stochastic equation much more complicated than Langevin's equation which is the basis of that theory. Consequently, the analysis must be confined to suitable approximations.

2. FORMULATION AND ANALYSIS OF THE PROBLEM

Let $\mathbf{r}(t)$ be the position vector at time t of a particle of unit mass in space. We shall assume that its motion for $t > 0$ is governed by the equations

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}(t), \qquad \mathbf{r}(0) = \mathbf{r}_0,$$

$$\frac{d\mathbf{v}}{dt} = \epsilon \mathbf{F}(\mathbf{r}) - \epsilon^2 \beta \mathbf{v}, \quad \mathbf{v}(0) = \mathbf{v}_0. \quad (2.1)$$

Combining these relations gives the exact expression

$$\psi_N = \ln 2 - (1/2N) \times \sum_{i<j} [(1 + \langle s_i s_j \rangle) \ln (1 + \tanh \beta J_{ij}) + (1 - \langle s_i s_j \rangle) \ln (1 - \tanh \beta J_{ij})] + (1/N) \sum_{i<j} J_{ij} \int_0^\beta d\beta' (\langle s_i s_j \rangle - \tanh \beta' J_{ij}). \quad (3.8)$$

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$$\frac{d\mathbf{v}}{dt} = \epsilon \mathbf{F}(\mathbf{r}) - \epsilon^2 \beta \mathbf{v}, \quad \mathbf{v}(0) = \mathbf{v}_0. \quad (2.1)$$

Here $\mathbf{v}(t)$ is the velocity vector, $\mathbf{F}(\mathbf{r})$ is a random force field, ϵ is a small parameter characterizing the size of the fluctuations, and β is a parameter characterizing the frictional forces. The random force field is assumed to have mean zero and a homogeneous and isotropic covariance tensor:

$$E\{\mathbf{F}(\mathbf{r})\} = 0, \tag{2.2}$$

$$E\{F_i(\mathbf{r})F_j(\mathbf{r}')\} = \delta_{ij}N(|\mathbf{r} - \mathbf{r}'|), \quad i,j = 1,2,3. \tag{2.3}$$

The symbol $E\{\ \}$ denotes ensemble averaging.

Let us introduce the function ρ defined by

$$\rho(t, \mathbf{r}, \mathbf{v}, \mathbf{r}_0, \mathbf{v}_0) = \delta(\mathbf{r} - \mathbf{r}(t))\delta(\mathbf{v} - \mathbf{v}(t)). \tag{2.4}$$

Then ρ satisfies the stochastic Liouville equation

$$\frac{\partial \rho}{\partial t} + \mathbf{v}\cdot\nabla_r\rho + (\epsilon\mathbf{F}(\mathbf{r}) - \epsilon^2\beta\mathbf{v})\cdot\nabla_v\rho = 0,$$
$$\rho(0, \mathbf{r}, \mathbf{v}, \mathbf{r}_0, \mathbf{v}_0) = \delta(\mathbf{r} - \mathbf{r}_0)\delta(\mathbf{v} - \mathbf{v}_0). \tag{2.5}$$

Here ∇_r and ∇_v denote the gradient operator on the space and velocity variables, respectively.

We shall consider $E\{\rho(t, \mathbf{r}, \mathbf{v}, \mathbf{r}_0, \mathbf{v}_0)\}$, which is the transition probability density in phase space at time t. To find it, we shall follow[1,4,8] and use the diffusion approximation. This approximation is valid provided that ϵ is small, t is large, and $N(r)$ decays rapidly with increasing r. Let us denote the approximate transition probability density by f. Then, as is shown in the above mentioned works and with some minor modifications due to the friction term in (2.1), f satisfies the equation

$$\frac{\partial f}{\partial \tau} = \frac{1}{2}\frac{\partial^2}{\partial v^2}\left(\frac{1}{v}f\right) - \frac{\partial}{\partial v}\left[\left(\frac{1}{2v^2} - \alpha v\right)f\right], \quad v \geq 0, \quad \tau > 0, \tag{2.6}$$

$$f(0, v, v_0) = \delta(v - v_0), \quad v = |\mathbf{v}|, \quad v_0 = |\mathbf{v}_0|, \tag{2.7}$$

$$D = 2\int_0^\infty N(r)\,dr, \quad \alpha = \frac{\beta}{D}, \quad \tau = \epsilon^2 Dt. \tag{2.8}$$

The fact that f is only a function of the modulus of the velocity is a consequence of the homogeneity and isotropy condition (2.3). In the remainder of this paper we shall solve (2.6) and discuss briefly the result.

Let us observe that (2.6) is a forward or Fokker–Plank equation in $v \geq 0$ with diffusion constant $1/v$ and drift constant $(1/2v^2) - \alpha v$. According to Feller's theory of boundary conditions,[10] both 0 and ∞ are not regular, and therefore there exists exactly one fundamental solution common to both the forward and backward equation. Moreover, no boundary conditions are necessary. We shall therefore analyze the backward equation corresponding to (2.6), which is

$$\frac{\partial f}{\partial \tau} = \frac{1}{2}\frac{1}{v_0}\frac{\partial^2 f}{\partial v_0^2} + \frac{1}{2}\frac{1}{v_0^2}\frac{\partial f}{\partial v_0} - \alpha v_0\frac{\partial f}{\partial v_0}, \quad v_0 \geq 0,$$
$$f(0, v, v_0) = \delta(v - v_0). \tag{2.9}$$

Let us introduce new variables as follows:

$$\zeta_0 = e^{-3\alpha\tau}\tfrac{2}{3}v_0^{\frac{2}{3}}, \quad \sigma = (1 - e^{-3\alpha\tau})/3\alpha. \tag{2.10}$$

Then our equation transforms to

$$\frac{\partial f}{\partial \sigma} = \frac{1}{2}\left(\frac{\partial^2 f}{\partial \zeta_0^2} + \frac{1}{\zeta_0}\frac{\partial f}{\partial \zeta_0}\right). \tag{2.11}$$

The solution of (2.11) can be obtained readily by using the Hankel transform or observing that it corresponds to radial Browning motion in two dimensions. After reverting to the original variables, we obtain the following result:

$$f(\tau, v, v_0) = \frac{2\alpha v^2}{1 - e^{-3\alpha\tau}}\exp\left(\frac{-\frac{2}{3}\alpha(v^3 + v_0^3e^{-3\alpha\tau})}{1 - e^{-3\alpha\tau}}\right) \times I_0\left(\frac{\frac{4}{3}\alpha v^{3\alpha/2}v_0^{3\alpha/2}e^{-3\alpha\tau/2}}{1 - e^{-3\alpha\tau}}\right), \quad v, v_0 \geq 0. \tag{2.12}$$

Here I_0 is the modified Bessel function of the first kind. The expression (2.12) is the diffusion approximation to the transition probability density of the velocity modulus, given the initial velocity modulus at time zero. As we have pointed out, this approximation is vaild for t large and ϵ small, with τ arbitrary but finite. It is the main result of this paper.

If $\alpha\tau$ is also large, then (2.12) can be approximated further by the following density function:

$$f_\infty(v) = 2\alpha v^2\exp(-\tfrac{2}{3}\alpha v^3), \quad v \geq 0. \tag{2.13}$$

The transition density (2.12) can be thought of as an equilibrium density for the original problem and so can (2.13) if, in addition, $\tau\alpha \gg 1$. The difference between the two is important because the second is independent of the initial velocity modulus v_0, while the first does depend on v_0 and also on the parameter τ.

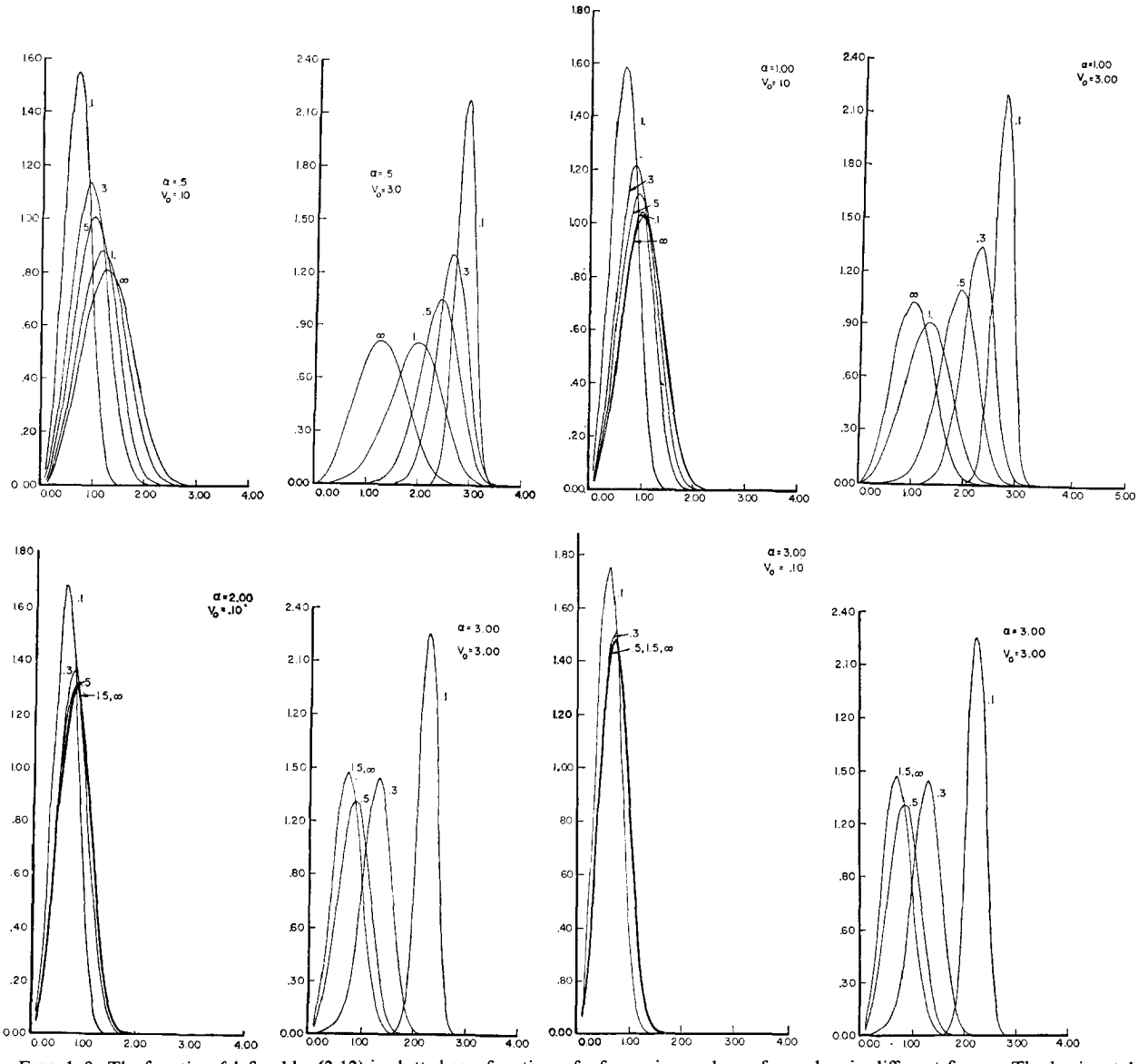
Let us compute the mean square of the velocity modulus $E\{v^2\}$. For this purpose let u and ψ be defined by

$$u = (v_0^3e^{-3\alpha\tau})^{\frac{1}{2}}, \quad \psi = (1 - e^{-3\alpha\tau})/3\alpha. \tag{2.14}$$

Then we have

$$E\{v^2\} = \int_0^\infty v^2 f(\tau, v, v_0)\,dv$$
$$= (\tfrac{2}{3})^{\frac{4}{3}}(2\psi)^{\frac{2}{3}}\Gamma(\tfrac{5}{3})e^{-u^2/2\psi}\,{}_1F_1(\tfrac{5}{3}, 1, u^2/2\psi). \tag{2.15}$$

Here ${}_1F_1(a; b; z)$ denotes the confluent hypergeometric function, and we have used a result of Ref. 11,



FIGS. 1–8. The function f defined by (2.12) is plotted as a function of v for various values of α and v_0 in different figures. The horizontal axis denotes the values of v and the vertical axis the values of $f(v)$. In each figure the curves are labeled by the value of τ for which they are computed. The value $\tau = \infty$ yields, of course, the same curve as (2.13). Thus the passage from (2.12) to (2.13) for large $\tau\alpha$ is clearly illustrated.

p. 72. Finally, in the approximation $\tau\alpha \gg 1$, (2.15) reduces to

$$E_\infty\{v^2\} = (3/2\gamma)^{\frac{2}{3}}\Gamma(\tfrac{5}{3}). \tag{2.16}$$

This last result can also be obtained from (2.13) directly.

In Figs. 1–8 we have plotted $f(v)$ from (2.12) and $f_\infty(v)$ from (2.13) for various values of α, v_0, and τ.

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Poincaré-Irreducible Tensor Operators for Positive-Mass One-Particle States. II*

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The present communication studies relations between the two classes of Poincaré-irreducible tensor operators which were constructed in a previous paper. The tensor operators of the first class transform according to those representations of the Poincaré group that are induced by the one-valued irreducible unitary representations of $SU(1, 1)$ which belong to the continuous and the discrete principal series. The tensor operators of the second class transform according to the Poincaré group representations that are induced by the irreducible unitary principal series representations of $SL(2, C)$. The Poincaré-irreducible tensor operators of the second class are decomposed into Lorentz-irreducible tensor operators which transform by the irreducible unitary $SL(2, C)$ representations of the principal series. The expansions of a spin density matrix describing a statistical ensemble of wavepackets into Poincaré- and Lorentz-irreducible components are derived. The infinite-dimensional associative algebra for the Poincaré-irreducible tensor operators of the second class is constructed. No such algebra exists for the Poincaré-irreducible tensor operators of the first class. The operator product of these tensors can only be represented as a linear superposition of the first class tensors in the limit of vanishing 4-momentum. In this limit, however, the first class tensors are no longer irreducible.

MOTIVATION AND OUTLINE

In a previous communication[1] two classes of Poincaré-irreducible tensor operators for positive mass one-particle states have been constructed. The two classes correspond to spacelike and to zero 4-momentum transfer. The tensor operators associated with a spacelike 4-momentum transfer are constructed by means of those (one-valued) unitary irreducible representations of the group $SU(1, 1)$ for which the Plancherel measure does not vanish. The construction of the tensor operators for zero 4-momentum transfer is based on the unitary irreducible representations of the group $SL(2C)$ which belong to the principal series.

The present work implements the program outlined at the end of Ref. 1. A small number of basic relations which frequently recur in the subsequent sections are introduced in Sec. 1. In Sec. 2 we establish the connection between the tensor operators of the first class in the limit of vanishing 4-momentum transfer and the irreducible tensor operators of the second class. It is emphasized that the first class tensor operators cease to be Poincaré-irreducible as the 4-momentum transfer vanishes. In this section we also present the decomposition into its Poincaré-irreducible components of a one-particle spin density matrix which corresponds to a finite-momentum spread rather than to a state with sharp particle momentum. In Sec. 3 we define Lorentz-irreducible tensor operators that transform according to those unitary irreducible representations of the group $SL(2C)$ which belong to the principal series. We then expand the Poincaré-irreducible tensor operators of the second class in terms of these Lorentz-irreducible tensor operators. This expansion reflects the fact that the tensor operators which are irreducible under the Poincaré group are reducible with respect to the (homogeneous) Lorentz group. Furthermore, we decompose a spin density matrix into its Lorentz-irreducible components and indicate how the connection between the two classes of Poincaré-irreducible tensor operators may be established through the intermediary of the Lorentz-irreducible tensor operators. In Sec. 4 we derive a relativistic generalization of a relation obtained by Biedenharn for $SO(3)$-irreducible spin tensor operators. This generalization corresponds to the relation defining the (infinite-dimensional) associative algebra for the Poincaré-irreducible tensor operators of the second class. No associative algebra exists for the Poincaré-irreducible tensor operators of the first class.

1. DEFINITIONS

The two classes of Poincaré-irreducible tensors to be defined in the following section operate on the carrier space of the irreducible unitary Poincaré group representations for a timelike orbit. Constructing the two classes of tensor operators causes two types of vector bases to emerge. These can be realized as the two sets of momentum-helicity eigenvectors [Eqs. (2.25) and (2.26) of Ref. 1]

$$|p_\lambda^s; 0\rangle = |(\phi, \theta, \gamma)^{[ms]}_\lambda\rangle \overset{\text{DEF}}{=} T(\Omega_0(\phi, \theta, \gamma))\, |m_\lambda^s\rangle \tag{1.1}$$

and

$$|p_\lambda^s; 3\rangle = |(\phi, \alpha, \zeta)^{[ms]}_\lambda\rangle \overset{\text{DEF}}{=} T(\Omega_3(\phi, \alpha, \zeta))\, |m_\lambda^s\rangle. \tag{1.2}$$

The orbiting transformations $\Omega_0(\phi, \theta, \gamma)$ and $\Omega_3(\phi, \alpha, \zeta)$ are defined as the three-parameter Lorentz transformations

$$\Omega_0(\phi, \theta, \gamma) = \exp(-i\phi j_{12}) \exp(-i\theta j_{31}) \exp(-i\gamma j_{03}) \tag{1.3}$$

and

$$\Omega_3(\phi, \alpha, \zeta) = \exp(-i\phi j_{12}) \exp(-i\alpha j_{01}) \exp(-i\zeta j_{03}). \tag{1.4}$$

We denote by $j_{\mu\nu}$, $\mu, \nu = 0, 1, 2, 3$, the Minkowski space realizations of the Lorentz group generators and by $J_{\mu\nu}$ the corresponding Hermitian operator realizations.

$$T(\Omega_0(\phi, \theta, \gamma)) = \exp(-i\phi J_{12}) \exp(-i\theta J_{31}) \times \exp(-i\gamma J_{03}) \tag{1.5}$$

and

$$T(\Omega_3(\phi, \alpha, \zeta)) = \exp(-i\phi J_{12}) \exp(-i\alpha J_{01}) \times \exp(-i\zeta J_{03}) \tag{1.6}$$

are then the unitary operator realizations of the orbiting transformations (1.3) and (1.4).

In the expressions (1.1) and (1.2) the parameters are restricted to the domains

$$0 \leq \phi < 2\pi, \quad 0 \leq \theta \leq \pi, \quad 0 \leq \gamma, \alpha < \infty, \quad -\infty < \zeta < \infty. \tag{1.7}$$

We normalize the set of state vectors for a particle of mass m and spin s in its rest frame,

$$\left\{ |m^s_\lambda\rangle: \quad -s \leq \lambda \leq s, \qquad \mathbf{J}^2 |m^s_\lambda\rangle = s(s+1) |m^s_\lambda\rangle \right.$$
$$\left. P^\mu |m^s_\lambda\rangle = \pm\delta^\mu{}_0 m |m^s_\lambda\rangle, \quad J_{12} |m^s_\lambda\rangle = \lambda |m^s_\lambda\rangle \right\}, \tag{1.8}$$

according to

$$\langle m^{\lambda'}_s \mid m^s_\lambda\rangle = 2m\delta^{\lambda'}{}_\lambda. \tag{1.9}$$

The P^μ, $\mu = 0, 1, 2, 3$, are the Hermitian operator realizations for the contravariant components p^μ of the 4-momentum $p = (p^0, \mathbf{p})$. For the basis vectors (1.1) and (1.2), the 4-momentum p is restricted to the timelike orbit which is characterized by

$$(p)^2 = p^\mu g_{\mu\nu} p^\nu = (p^0)^2 - (\mathbf{p})^2 = m^2 > 0. \tag{1.10}$$

The constructs (1.1) and (1.2) form two *improper* bases in the carrier space $\mathcal{H}[ms]$ of the irreducible unitary Poincaré group representations for the orbit (1.10), since they are not normalizable but fulfill the orthogonality relation

$$\langle p'^{\lambda'}_s; \omega \mid p^s_\lambda; \omega\rangle = 2 |p^0| \, \delta^3(\mathbf{p}' - \mathbf{p}) \delta^{\lambda'}{}_\lambda, \quad \omega = 0 \text{ or } 3. \tag{1.11}$$

Under the restricted Poincaré group, which is isomorphic to the inhomogeneous pseudo-orthogonal group $ISO(3, 1)$, the basis vectors (1.1) and (1.2) transform according to the irreducible unitary $ISO(3, 1)$ representation characterized by m and s, namely according to

$$T(a, \Lambda) |p^s_\lambda; \omega\rangle = \exp(-ia \cdot \Lambda p) \sum_{\lambda'=-s}^{s} |\Lambda p^s_{\lambda'}; \omega\rangle \, D^s[R_\omega(\Lambda, p)]^{\lambda'}{}_\lambda, \tag{1.12}$$

where

$$(a, \Lambda) \in ISO(3, 1): x \to \Lambda x + a, \quad x, a \in E_{3,1} \qquad (\Lambda x)^\mu = x^\nu \Lambda_\nu{}^\mu, \quad \Lambda \in SO(3, 1). \tag{1.13}$$

$E_{3,1}$ denotes the $(3 + 1)$-dimensional pseudo-Euclidean space with the metric defined by (1.10) (Minskowski space).

$$T(a, \Lambda) = \exp(-ia_\mu P^\mu) \exp(-\tfrac{1}{2} i\omega^{\mu\nu} J_{\mu\nu}) \tag{1.14}$$

is the unitary operator realization of the restricted Poincaré transformation (a, Λ). The Wigner rotations $R_\omega(\Lambda, p)$ are defined by

$$R_\omega(\Lambda, p) = \Omega_\omega^{-1}(\Lambda p) \Lambda \Omega_\omega(p). \tag{1.15}$$

D^s denotes the $(2s + 1)$-dimensional irreducible unitary matrix realization of the three-dimensional rotation group. The bases (1.1) and (1.2) are connected through the helicity rearrangement transformations (Ref. 2 and Appendix of Ref. 1)

$$|p^s_\lambda; \omega'\rangle = \sum_{\nu=-s}^{s} |p^s_\nu; \omega\rangle \, D^s(R_{\omega'\omega}(p))^\nu{}_\lambda, \tag{1.16a}$$

$$R_{\omega'\omega}(p) = \Omega_{\omega'}^{-1}(p) \Omega_\omega(p). \tag{1.16b}$$

For those momentum-helicity states (1.1) and (1.2) which are defined by means of the particular orbiting transformations

$$\Omega_0(\phi, \pi/2, \gamma = \alpha) \quad \text{and} \quad \Omega_3(\phi, \alpha, 0),$$

the transformation (1.16) simplifies to the equation

$$|p^s_\lambda; 3\rangle = \sum_{\nu=-s}^{s} |p^s_\nu; 0\rangle \, d^s(-\pi/2)^\nu{}_\lambda \tag{1.17}$$

or to its inverse, since

$$R_{30}(p) = \Omega_0^{-1}(\phi, \pi/2, \alpha) \Omega_3(\phi, \alpha, 0) = \exp(\tfrac{1}{2} i\pi j_{31}). \tag{1.18}$$

The relation (1.17) will be utilized in Sec. 2. In general, the rotation functions appearing in (1.16) are of the form

$$D^s(R_{\omega'\omega}(p))^\nu{}_\lambda = d^s[\theta_{\omega'\omega}(p)]^\nu{}_\lambda = \langle^\nu_s| \exp(-i\theta_{\omega'\omega} J_{31}) |^s_\lambda\rangle. \tag{1.19}$$

By means of the definitions (1.3), (1.4), and (1.16b) one finds that

$$\cos[\theta_{30}(p)] = \cos\theta\cosh\alpha, \tag{1.20}$$

where

$$p^\lambda = \pm m\Omega_0(\phi,\theta,\gamma)_0{}^\lambda = \pm m\Omega_3(\phi,\alpha,\zeta)_0{}^\lambda. \tag{1.21}$$

2. POINCARÉ-IRREDUCIBLE TENSOR OPERATORS. DEFINITIONS AND SELECTED APPLICATIONS

The carrier space $\mathfrak{K}[ms]$ for the unitary irreducible positive mass representations of the Poincaré group admits two classes of tensor operators which transform irreducibly with respect to this group. The two classes correspond to spacelike (Q) and zero (0) 4-momentum transfer. In Sec. 4 of Ref. 1 the Q class was constructed as the set of unitary irreducible tensor operators

$$(Q,\tau[ms]\omega)^{\tilde\kappa=\nu-\nu'}{}_\kappa = U(\Omega_\omega(Q))P[\tau]^{\tilde\kappa}{}_\kappa\,|q^s_\nu\rangle\langle q'^{\nu'}_s|, \tag{2.1a}$$

where

$$\kappa = 0,\pm1,\pm2,\cdots, \quad \text{for} \quad \tau = -\tfrac12 + i\sigma, \quad -\infty<\sigma<\infty, \tag{2.1b}$$

or

$$\left.\begin{aligned}\kappa,\tilde\kappa &= k, k+1,\cdots \quad \text{for} \quad k^+\\ \kappa,\tilde\kappa &= -k,-(k+1),\cdots \quad \text{for} \quad k^-\end{aligned}\right\} \qquad \tau = k^\pm,\ k = 1,2,3,\cdots \tag{2.1c}$$

The dyadic in (2.1a) is defined by means of the equations

$$|q^s_\nu\rangle = e^{-i\zeta J_{03}}|m^s_\nu\rangle, \quad -\infty<\zeta<\infty,$$
$$\langle m^{\nu'}_s \mid m^s_\nu\rangle = 2m\delta^{\nu'}{}_\nu \tag{2.2a}$$
$$P^\mu|m^s_\nu\rangle = \delta^\mu{}_0\, m\,|m^s_\nu\rangle, \quad J_{12}|m^s_\nu\rangle = \nu|m^s_\nu\rangle, \quad -s\le\nu\le s, \tag{2.2b}$$
$$q^2 = q'^2 = (q^0)^2-(q^3)^2 = m^2,\ q=(q^0,0,0,q^3),\ q'=(q^0,0,0,-q^3),$$
$$q^0 = q_0 = m\cosh\zeta, \quad q^3 = -q_3 = -m\sinh\zeta. \tag{2.2c}$$

The spacelike 4-momentum transfer Q is obtained from the standard 4-vector

$${}^\circ Q = q - q' = (0,0,0,\sqrt{-t}),\ t = {}^\circ Q^2 = -4(q^3)^2 \tag{2.3}$$

by means of the orbiting transformation $\Omega_\omega(Q)$:

$$Q^\mu_\omega = \Omega_\omega(Q)^\mu{}_\nu\,{}^\circ Q^\nu, \quad \omega = 0,3,$$
$$\Omega_\omega(Q)^\mu{}_3 = (-t)^{-\frac12}Q^\mu{}_\omega, \quad Q^2 = t<0, \tag{2.4}$$

$$(Q^\mu_{\omega=0}) = (\sqrt{-t})(-\sinh\gamma,\cos\phi\sin\theta\cosh\gamma,\ \sin\phi\sin\theta\cosh\gamma,\cos\theta\cosh\gamma)$$
$$-\infty<\gamma<\infty, \quad 0\le\phi<2\pi, \quad 0\le\theta\le\pi \tag{2.5a}$$

$$(Q^\mu_{\omega=3}) = (\sqrt{-t})(-\cosh\alpha\sinh\zeta,\cos\phi\sinh\alpha\sinh\zeta,\ \sin\phi\sinh\alpha\sinh\zeta,\cosh\zeta)$$
$$0\le\alpha<\infty, \quad -\infty<\zeta<\infty, \quad 0\le\phi<2\pi. \tag{2.5b}$$

$U(\Omega_\omega(Q))$ denotes the unitary operator realizing the orbiting transformation Ω_ω on the vector spaces $\mathfrak{K}[t,\tau]$ spanned by the tensorial sets (2.1). The projection operators in (2.1a) are defined by the relations

$$P[\tau]^{\tilde\kappa}{}_\kappa = \rho[\tau]\int d\lambda(\phi,\alpha,\psi)D([\tau]\phi,\alpha,\psi)^{\dagger\tilde\kappa}{}_\kappa T(\phi,\alpha,\psi), \tag{2.6a}$$

$$\rho[\sigma] = \sigma\tanh\pi\sigma, \quad \rho[k] = 2k-1, \tag{2.6b}$$

$$d\lambda(\phi,\alpha,\psi) = (1/8\pi^2)\,d\phi\sinh\alpha\,d\alpha\,d\psi, \quad 0\le\phi,\psi<2\pi,\ 0\le\alpha<\infty. \tag{2.6c}$$

The functions

$$D([\tau]\phi,\alpha,\psi)^{\lambda'}{}_\lambda = \langle{}^{\lambda'}_\tau|\,T(\phi,\alpha,\psi)\,|{}^\tau_\lambda\rangle, \tag{2.7a}$$

with

$$T(\phi,\alpha,\psi) = e^{-i\phi J_{12}}e^{-i\alpha J_{01}}e^{-i\psi J_{12}}, \tag{2.7b}$$

are the components of the matrix realizations for the one-valued unitary irreducible representations of $SU(1,1)$ that belong to the continuous principal series ($\tau=-\frac12+i\sigma$) or the discrete principal series ($\tau=k^\pm$).[2-5] There is a two-to-one homomorphism from $SU(1,1)$ to $SO(2,1)$; $SU(1,1)$ is not the universal covering group of $SO(2,1)$ since it is not simply connected.[6] We refer to the tensorial set (2.1) as the set of $ISO(3,1)\uparrow SO(2,1)$-irreducible tensor operators, since the $(2+1)$-dimensional Lorentz group, which leaves the standard spacelike 4-vectors (2.3) invariant, is isomorphic to the group $SO(2,1)$. The orthogonality and completeness relations for the functions (2.7a) [Eqs. (4.3a), (4.3b), and (4.4) of Ref. 1] are, for integral or half-integral $\lambda,\mu,\lambda',\mu'$,

$$\int d\lambda(\phi,\alpha,\psi)D([\tau']\phi,\alpha,\psi)^{*\lambda'}{}_{\mu'}D([\tau]\phi,\alpha,\psi)^\lambda{}_\mu = (1/\rho[\tau])\delta(\tau',\tau)\delta^{\lambda'\lambda}\delta_{\mu'\mu},$$

$$\delta(\tau',\tau) = \begin{cases}\delta(\sigma'-\sigma), & \text{if} \quad \tau' = -\tfrac12+i\sigma',\ \tau = -\tfrac12+i\sigma,\\ \delta_{k'k}, & \text{if} \quad \tau' = k'^\pm,\ \tau = k^\pm,\\ 0, & \text{otherwise,}\end{cases} \tag{2.8}$$

and

$$\int_{-\infty}^{\infty}\rho[\sigma,\epsilon]\,d\sigma\sum_{\lambda,\lambda'=-\infty}^{\infty}D([\sigma]\phi,\alpha,\psi)^{\lambda'}{}_{\lambda}\,D([\sigma]\phi',\alpha',\psi')^{*\lambda'}{}_{\lambda}$$
$$+\sum_{\eta=+,-}\sum_{k=1+\epsilon}\rho[k]\sum_{\mu,\mu'=\eta k}^{\eta\infty}D([k^{\eta}]\phi,\alpha,\psi)^{\mu'}{}_{\mu}$$
$$\times D([k^{\eta}]\phi',\alpha',\psi')^{*\mu'}{}_{\mu}$$
$$=\delta[\lambda(\phi,\alpha,\psi)-\lambda(\phi',\alpha',\psi')],$$
$$\delta[\lambda(\phi,\alpha,\psi)]=8\pi^2\delta(\phi)\delta(\cosh\alpha)\delta(\psi), \tag{2.9}$$

where, for the continuous principal series

$$\tau=-\tfrac{1}{2}+i\sigma,\quad -\infty<\sigma<\infty,$$

we have

$$\lambda=0,\pm1,\pm2,\cdots,\ \rho[\tau]=\rho[\sigma,0]=\rho[\sigma]$$
$$=\sigma\tanh\pi\sigma,\quad\text{for }\epsilon=0,$$
$$\lambda=\pm\tfrac{1}{2},\pm\tfrac{3}{2},\cdots,\ \rho[\tau]=\rho[\sigma,\tfrac{1}{2}]=\sigma\coth\pi\sigma,$$
$$\text{for }\epsilon=\tfrac{1}{2},$$

and, for the discrete principal series

$$\tau=\kappa^{\eta},\quad \rho[\tau]=\rho[k^{\eta}]=\rho[k]=2k-1,$$

we have

$$\left.\begin{aligned}\lambda&=k,k+1,\cdots\quad\text{for }\eta=(+)\\ \lambda&=-k,-k-1,\cdots\quad\text{for }\eta=(-)\end{aligned}\right\}$$
$$\begin{cases}\epsilon=0,\ k=1,2,\cdots\\ \epsilon=\tfrac{1}{2},\ k=\tfrac{3}{2},\tfrac{5}{2},\cdots.\end{cases} \tag{2.10}$$

The particular representation of the discrete series which is characterized by $k=\frac{1}{2}$ has been excluded, since $\rho\,[k=\frac{1}{2}]=0$. Those functions (2.7a) which appear in the expression (2.6a) for the projection operators used in the definition of the tensorial set (2.1) belong to the representations with $\epsilon=0$, because $\tilde{\kappa}=\nu-\nu'$ is always an integer.

If $t\to 0$, that is, in the limit of vanishing 4-momentum transfer, the orbiting transformation realized in the expression (2.10) by the operator $U(\Omega_{\omega}(Q))$ is obviously no longer determined by (2.4). In this limit the tensorial set (2.1) ceases to be irreducible and can be decomposed into the $[ISO(3,1)\uparrow SO(3,1)]$-irreducible tensor operators which are introduced in the latter part of this section. We now parametrize the orbiting transformation $\Omega_{\omega}(Q)$ by means of the parameter set

$$v\overset{\text{DEF}}{=}(\phi',\theta,\gamma)\quad\text{if}\quad\omega=0, \tag{2.11a}$$
$$v\overset{\text{DEF}}{=}(\phi',\alpha',\zeta')\quad\text{if}\quad\omega=3, \tag{2.11b}$$

and write for the tensorial set (2.1) [see Eqs. (4.37) and (4.38) of Ref. 1]

$$(Q,\tau[ms]\omega)^{\nu-\nu'}{}_{\kappa}$$
$$=(v,t\tau[ms])^{\nu-\nu'}{}_{\kappa}$$
$$=\rho[\tau]\int d\lambda(\phi,\alpha)D([\tau]\phi,\alpha,0)^{\dagger\nu-\nu'}{}_{\kappa}\sum_{\lambda,\lambda'=-s}^{s}|p^{s}_{\lambda};3\rangle$$
$$\times D^{s}[R(v;\phi,\alpha;t)]^{\lambda}_{\nu}\,D^{s}[R'(v;\phi,\alpha;t)]^{\dagger\nu'}{}_{\lambda'}\,\langle p'^{\lambda'}_{s};3|, \tag{2.12}$$

where

$$d\lambda(\phi,\alpha)=(1/4\pi)\,d\phi\sinh\alpha\,d\alpha, \tag{2.13}$$
$$p=\Omega(v)\Omega_3(\phi,\alpha,0)q,\quad p'=\Omega(v)\Omega_3(\phi,\alpha,0)q', \tag{2.14}$$
$$R(v;\phi,\alpha;t)=\Omega_3^{-1}(p)\Omega(v)\Omega_3(\phi,\alpha,\zeta(t)), \tag{2.15a}$$
$$R'(v;\phi,\alpha;t)=\Omega_3^{-1}(p)\Omega(v)\Omega_3(\phi,\alpha,-\zeta(t)), \tag{2.15b}$$

with

$$\zeta(t)=\pm\sinh^{-1}\left(\frac{\sqrt{-t}}{2m}\right)$$
$$=\pm\log\left(\frac{\sqrt{-t}+(-t+4m^2)^{\frac{1}{2}}}{2m}\right), \tag{2.16}$$

and

$$t=4m^2-(p+p')^2=4[m^2-(q^0)^2]. \tag{2.17}$$

For any pair of 4-vectors p,p', $p^2=p'^2=m^2>0$, there exists, in accordance with (2.17), $t\le 0$ where $t=0$ if and only if $p=p'$. Any such pair p,p' can be parametrized by means of the relations (2.14). With the definitions (2.2c) for q and q', the relations (2.14) can be written as

$$p^{\lambda}=m\Lambda(\phi,\alpha,\zeta(t);v)_0{}^{\lambda},\quad p'^{\lambda}=m\Lambda(\phi,\alpha,-\zeta(t);v)_0{}^{\lambda},$$
$$\Lambda(\phi,\alpha,\zeta(t);v)_0{}^{\lambda}=\Omega_3(\phi,\alpha,\zeta(t))_0{}^{\mu}\,\Omega(v)_{\mu}{}^{\lambda}. \tag{2.18}$$

The Lorentz-invariant measure on the mass shell

$$d\mu(p,p';m)\overset{\text{DEF}}{=}\delta_{\pm}(p^2-m^2)d^4p\,\delta_{\pm}(p'^2-m^2)d^4p'$$
$$=\frac{d^3\mathbf{p}}{2\,|p^0|}\frac{d^3\mathbf{p}'}{2\,|p'^0|},$$
$$\delta_{\pm}(p^2-m^2)=\tfrac{1}{2}\left(1\pm\frac{p^0}{|p^0|}\right)\delta(p^2-m^2) \tag{2.19}$$

can be expressed as

$$d\mu(p,p';m)=\tfrac{1}{2}\pi[(4m^2-t)/-t]^{\frac{1}{2}}d^4Q\,d\lambda(\phi,\alpha) \tag{2.20}$$

or, according to the parametrization (2.18), as

$$d\mu(p,p';m)=2\pi^2\,d\lambda(v,t)\,d\lambda(\phi,\alpha), \tag{2.21a}$$
$$d\lambda(v,t)=d\lambda(v)\,d\lambda(t)=d\lambda(v)(t^2-4m^2)^{\frac{1}{2}}\,dt, \tag{2.21b}$$
$$d\lambda(v)=d\lambda(\phi',\theta,\gamma)=(1/8\pi)\,d\phi'\sin\theta$$
$$\times\,d\theta(\cosh\gamma)^2\,d\gamma, \tag{2.21c}$$

$$d\lambda(v) = d\lambda(\phi', \alpha', \zeta') = (1/8\pi)\, d\phi' \sinh \alpha' \times d\alpha' (\sinh \zeta')^2\, d\zeta', \quad (2.21d)$$

$$0 \le \phi, \phi' < 2\pi, 0 \le \theta \le \pi, 0 \le \alpha, \alpha' < \infty, -\infty < \gamma, \zeta' < \infty, -\infty < t \le 0. \quad (2.21e)$$

By virtue of the Lorentz invariance of the measure (2.19), the derivation of the relation (2.20) can be conveniently carried out in the brick wall frame, for which Q reduces to ${}^{\circ}Q$. Once the relation (2.20) has been established, the relations (2.21) are easily arrived at by evaluating the Jacobians $\partial(Q^{\mu}_{\omega})/\partial(v, t)$ from Eqs. (2.5a) and (2.5b) together with the definitions (2.11a) and (2.11b).

A spin-momentum density operator accounts in general for a certain space localization and consequently for a certain finite momentum spread. Thus, it describes a statistical ensemble of wavepackets. Its matrix realization in the $\omega = 3$ momentum-helicity basis is

$$\rho([ms]a) = \int d\mu(p, p'; m) \sum_{\lambda,\lambda'=-s}^{s} |p^{s}_{\lambda}; 3\rangle \times a(p, p')^{\lambda}{}_{\lambda'} \langle p'^{\lambda'}_{s}; 3|. \quad (2.22)$$

The decomposition of the spin-momentum density matrix (2.22) into its Poincaré-irreducible components can now be derived by utilizing the relations (2.9), (2.12), and (2.21). We obtain

$$\begin{aligned}\rho([ms]\Delta) = 2\pi^2 \int d\lambda(\phi, \alpha) \int d\lambda(v) \int_{-\infty}^{0} (t^2 - 4m^2 t)^{\frac{1}{2}}\, dt \\ \times \sum_{\nu,\nu',\lambda,\lambda'=-s}^{s} D^{s}[R(v; \phi, \alpha; t)]^{\dagger}{}_{\nu\lambda} \\ \times \Delta(v; \phi, \alpha, t)^{\lambda}{}_{\lambda'}\, D^{s}[R'(v; \phi, \alpha; t)]^{\lambda'}{}_{\nu'} \\ \times \Big\{ \int_{-\infty}^{\infty} d\sigma \sum_{\kappa=0,\pm1,\pm2,\cdots} (v, t, \sigma[ms])^{\nu-\nu'}{}_{\kappa} \\ \times D([\sigma]\phi, \alpha, 0)^{\kappa}{}_{\nu-\nu'} \\ + \sum_{\eta=\mathrm{sgn}(\nu-\nu')} \sum_{k=1}^{|\nu-\nu'|\eta\infty} \sum_{\kappa=\eta k} (v, t, k^{\eta}[ms])^{\nu-\nu'}{}_{\kappa} \\ \times D([k^{\eta}]\phi, \alpha, 0)^{\kappa}{}_{\nu-\nu'} \Big\}. \end{aligned} \quad (2.23)$$

In accordance with the parametrization (2.18) we write

$$a(p, p')^{\lambda}{}_{\lambda'} = \Delta(v; \phi, \alpha; t)^{\lambda}{}_{\lambda'}. \quad (2.24)$$

Since the measure $d\lambda(v, t)$ vanishes at $t = 0$, the tensor operators (2.1) that contribute to the expansion (2.23) are all irreducible.

We now define the set of the unitary irreducible tensor operators on $\mathcal{H}[ms]$ which correspond to zero 4-momentum transfer. According to Eq. (5.31) of Ref. 1, this class can be realized by the tensorial set

$$(j_0 \boldsymbol{j}[ms])^{\sigma}{}_{j\mu} = \sum_{\kappa=-\min(\sigma,j)}^{\min(\sigma,j)} \hat{P}[j_0 \boldsymbol{j}]^{\sigma\kappa}{}_{j\mu} (ms)_{\sigma\kappa}, \quad (2.25a)$$

$\boldsymbol{j}$ imaginary continuous, $0 \le \boldsymbol{j}/i < \infty$,

$$-\min(j, \mathcal{A}) \le j_0 \le \min(j, \mathcal{A}), 0 \le \mathcal{A} \le 2s, \quad j = 0, 1, 2, \cdots; -j \le \mu \le j, \quad (2.25b)$$

where

$$(ms)_{\sigma\kappa} = \sum_{\lambda,\lambda'=-s}^{s} |m^{s}_{\lambda'}\rangle \left\langle {}^{\lambda' s}_{s\ \lambda} \middle|\, {}^{\sigma}_{\kappa} \right\rangle \langle m^{\lambda}_{s}|,$$

with

$$\left\langle {}^{\lambda' s}_{s\ \lambda} \middle|\, {}^{\sigma}_{\kappa} \right\rangle = (-1)^{s-\lambda} \left\langle {}^{\lambda'}_{s}, {}^{-\lambda}_{s} \middle|\, {}^{\sigma}_{\kappa} \right\rangle, \quad (2.26)$$

are the matrix realizations of the $SO(3)$-irreducible tensor operators associated with the particle $[m, s]$ (spin tensor operators) and where

$$\hat{P}[j_0 \boldsymbol{j}]^{\sigma\kappa}{}_{j\mu} = \rho_{\sigma}[j_0 \boldsymbol{j}] \int d\mu(\hat{\Lambda}) D([j_0 \boldsymbol{j}]\hat{\Lambda})^{\dagger\sigma\kappa}{}_{j\mu} T(\hat{\Lambda}), \quad (2.27a)$$

with

$$\rho_{\sigma}[j_0 \boldsymbol{j}] = 4(j_0^2 - \boldsymbol{j}^2)/[\pi(2\mathcal{A} + 1)], \quad (2.27b)$$

$$\hat{\Lambda} = R(\phi, \theta, \psi) B(\gamma), R(\phi, \theta, \psi) = \exp(-i\phi j_{12}) \times \exp(-i\theta j_{31}) \exp(-i\psi j_{12}),$$

$$B(\gamma) = \exp(-i\gamma j_{03}), 0 \le \phi, \psi < 2\pi, 0 \le \theta \le \pi, 0 \le \gamma < \infty, \quad (2.27c)$$

$$d\mu(\hat{\Lambda}) = (d\phi/2\pi)\, \tfrac{1}{2}\sin\theta\, d\theta (d\psi/2\pi) \tfrac{1}{2} (\sinh\gamma)^2\, d\gamma, \quad (2.27d)$$

$$T(\hat{\Lambda}) = \exp(-i\phi J_{12}) \exp(-i\theta J_{31}) \exp(-i\psi J_{12}) \times \exp(-\gamma J_{03}), \quad (2.27e)$$

$$D([j_0 \boldsymbol{j}]\hat{\Lambda})^{j'\mu'}{}_{j\mu} = \langle {}^{j'\mu'}_{j_0 \boldsymbol{j}}|\, T(\hat{\Lambda})\, |{}^{j_0 \boldsymbol{j}}_{j\mu}\rangle. \quad (2.27f)$$

More generally, the components of the unitary irreducible matrix realizations of $SO(3, 1)$ which belong to the principal series are[7-11]

$$D([j_0 \boldsymbol{j}]\Lambda)^{j'\mu'}{}_{j\mu} = \langle {}^{j'\mu'}_{j_0 \boldsymbol{j}}|\, T(\Lambda)\, |{}^{j_0 \boldsymbol{j}}_{j\mu}\rangle, \quad (2.28a)$$

where, $\boldsymbol{j}$ = imaginary continuous, $0 \le \boldsymbol{j}/i < \infty$,

$$j_0 = \begin{cases} 0, \pm1, \pm2, \cdots, \\ \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \cdots, \end{cases}$$

$$j, j' = |j_0|, |j_0| + 1, |j_0| + 2, \cdots, \quad \begin{matrix} -j' \le \mu' \le j', \\ -j \le \mu \le j, \end{matrix} \quad (2.28b)$$

$$\Lambda = \hat{\Lambda} R(0, \hat{\theta}, \hat{\psi}), 0 \le \hat{\psi} < 2\pi, 0 \le \hat{\theta} \le \pi, \quad (2.28c)$$

$$T(\Lambda) = T(\hat{\Lambda}) \exp(-i\hat{\theta} J_{31}) \exp(-i\hat{\psi} J_{12}) = T(R) T(B) T(\hat{R}). \quad (2.28d)$$

The tensorial set (2.25) is defined for integral values of j_0 only, since $\mathcal{A}$ is always an integer. In Sec. 5 of Ref. 1, the realization (2.25a) was arrived at by applying the general $SO(3, 1)$-projection operator

$$P[j_0 \boldsymbol{j}]^{\omega\kappa}{}_{j\mu} = \rho[j_0 \boldsymbol{j}] \int d\mu(\Lambda) D([j_0 \boldsymbol{j}]\Lambda)^{\dagger\omega\kappa}{}_{j\mu} T(\Lambda), \quad (2.29a)$$

with

$$\rho[j_0\mathbf{j}] = (4/\pi)(j_0^2 - \mathbf{j}^2), \tag{2.29b}$$

$$d\mu(\Lambda) = d\mu(\hat{\Lambda})\, \tfrac{1}{2}\sin\hat{\theta}\, d\hat{\theta}\, d\hat{\psi}/2\pi, \tag{2.29c}$$

to the spin tensor operators (2.26). We refer to (2.25) as the set of the $ISO(3,1)\uparrow SO(3,1)$-irreducible tensor operators, since the $(3+1)$-dimensional Lorentz group, which leaves the zero 4-vector invariant, is isomorphic to $SO(3,1)$. The parametrization according to (2.27c) and (2.28c) of the unitary operator $T(\Lambda)$ appearing in (2.28a) entails the matrix decompositions

$$D([j_0\mathbf{j}]\Lambda)^{j'\mu'}{}_{j\mu} = \sum_{\nu=-\min(j',j)}^{\min(j',j)} D([j_0\mathbf{j}]\hat{\Lambda})^{j'\mu'}{}_{j\nu}\, D([j]\hat{R})^{\nu}{}_{\mu}, \tag{2.30a}$$

$$D([j_0\mathbf{j}]\hat{\Lambda})^{j'\mu'}{}_{j\nu} = D([j']R)^{\mu'}{}_{\nu}\, D([j_0\mathbf{j}]B)^{j'\nu}{}_{j\nu}, \tag{2.30b}$$

where

$$D([j]R)^{\mu'}{}_{\mu} = D^{j}(R)^{\mu'}{}_{\mu} = \langle {}^{\mu'}_{j}|\, T(R)\, |{}^{j}_{\mu}\rangle \tag{2.30c}$$

are the ordinary rotation functions and

$$D([j_0\mathbf{j}]B)^{j'\nu}{}_{j\nu} = d_{\nu}([j_0\mathbf{j}]B)^{j'}{}_{j} = \langle {}^{j'\nu}_{j_0 j}|\, T(B)\, |{}^{j_0 j}_{j\nu}\rangle \tag{2.30d}$$

are the boost functions.

The orthogonality and completeness relations for the unitary irreducible matrix realizations

$$D([j]R),\ D([j_0\mathbf{j}]B),\ D([j_0\mathbf{j}]\Lambda),\ D([j_0\mathbf{j}]\hat{\Lambda})$$

are expressed by Eqs. (5.6) and (5.7), (5.9) and (5.10), (5.15) and (5.14), (5.17) and (5.18) of Ref. 1. From Eqs. (2.25a) and (2.27a) and from

$$\begin{aligned} T(\hat{\Lambda})(ms)_{\sigma\kappa} &= e^{-i\nu\psi}T(\Omega_0(\phi,\theta,\gamma))(ms)_{\sigma\kappa} \\ &= e^{-i\nu\psi}([ms]\phi,\theta,\gamma)_{\sigma\kappa}, \end{aligned} \tag{2.31}$$

where

$$\begin{aligned} ([ms]\phi,\theta,\gamma)_{\sigma\kappa} &= ([ms]p;0)_{\sigma\kappa} \\ &= \sum_{\lambda,\lambda'=-s}^{s} |p^s_{\lambda'};0\rangle \langle {}^{s\,\lambda'}_{s\,\lambda}\,|\, {}^{\sigma}_{\kappa}\rangle \langle p^{\lambda}_{s};0|, \\ |p^s_{\lambda};0\rangle &= T(\Omega_0(\phi,\theta,\gamma))\,|m^s_{\lambda}\rangle, \end{aligned} \tag{2.32}$$

we obtain after integration with respect to the angular parameter ψ the following expression for the irreducible tensorial set (2.25);

$$\begin{aligned} (j_0\mathbf{j}[ms])^{\sigma}{}_{j\mu} = \rho_{\sigma}[j_0\mathbf{j}] \sum_{\kappa=-\min(\sigma,j)}^{\min(\sigma,j)} \int d\mu(\phi,\theta,\gamma) \\ \times D([j_0\mathbf{j}]\phi\theta\gamma)^{\dagger\sigma\kappa}{}_{j\mu}([ms]\phi,\theta,\gamma)_{\sigma\kappa}. \end{aligned} \tag{2.33}$$

The orthogonality and the completeness of the functions

$$\begin{aligned} D([j_0\mathbf{j}]\phi\theta\gamma)^{j'\mu'}{}_{j\mu} &\overset{\text{DEF}}{=} D([j']R(\phi,\theta,0))^{\mu'}{}_{\mu} \\ &\times D([j_0\mathbf{j}]B(\gamma))^{j'\mu}{}_{j\mu} \end{aligned} \tag{2.34}$$

are expressed by the relations

$$\begin{aligned} \sum_{\lambda=-s}^{s} \int d\mu(\phi,\theta,\gamma) D([j_0\mathbf{j}]\phi\theta\gamma)^{j\mu}{}_{s\lambda}\, D([j_0'\mathbf{j}']\phi\theta\gamma)^{*j'\mu'}{}_{s\lambda} \\ = (\rho_s[j_0\mathbf{j}])^{-1}\delta_{j_0 j_0'}\delta(i\mathbf{j} - i\mathbf{j}')\delta^{jj'}\delta^{\mu\mu'}, \end{aligned} \tag{2.35a}$$

$$d\mu(\phi,\theta,\gamma) = (d\phi/2\pi)(\sin\theta\, d\theta/2)[(\sinh\gamma)^2\, d\gamma/2], \tag{2.35b}$$

$$\rho_s[j_0\mathbf{j}] = 4(j_0^2 - \mathbf{j}^2)/[\pi(2s+1)], \tag{2.35c}$$

and

$$\begin{aligned} \sum_{j_0=-s}^{s} \int_0^{i\infty} \frac{1}{i}\, d\mathbf{j}\rho_s[j_0\mathbf{j}] \sum_{j'=|j_0|}^{\infty} \sum_{\mu'=-j'}^{j'} D([j_0\mathbf{j}]\phi\theta\gamma)^{j'\mu'}{}_{j\mu} \\ \times D([j_0\mathbf{j}]\phi'\theta'\gamma')^{*j'\mu'}{}_{j\lambda} \\ = \delta_{\mu\lambda}\delta[\mu(\phi,\theta,\gamma) - \mu(\phi',\theta',\gamma')], \end{aligned} \tag{2.36a}$$

$$\delta[\mu(\phi,\theta,\gamma)] = \{8\pi/[\sin\theta(\sinh\gamma)^2]\}\delta(\phi)\delta(\theta)\delta(\gamma). \tag{2.36b}$$

Based on this relation is the derivation of the Poincaré-multipole expansion for the spin density matrix

$$\rho([ms]p;\omega) = \sum_{\lambda,\lambda'=-s}^{s} |p^s_{\lambda};\omega\rangle\, a(p)^{\lambda}{}_{\lambda'}\langle p^{\lambda'}_{s};\omega|. \tag{2.37}$$

If we introduce the $[ISO(3,1)\uparrow SO(3,1)]$-Clebsch-Gordan coefficients

$$\begin{aligned} &\langle {}^{j\,\mu}_{j_0 j,\sigma}\,|\, p^s_{\lambda};-p^{\lambda'}_{s};\omega\rangle \\ &= \sum_{\nu=-\min(\sigma,j)}^{\min(\sigma,j)} \langle {}^{\lambda-\lambda'}_{\sigma}\,|\, {}^{s\lambda'}_{\lambda s}\rangle D^{\sigma}(R_{\omega 0})^{\nu}{}_{\lambda-\lambda'}\, D([j_0\mathbf{j}]\phi\theta\gamma)^{\sigma\mu}{}_{\sigma\nu}, \end{aligned} \tag{2.38}$$

Eq. (5.58) of Ref. 1, this Poincaré-multipole expansion can be expressed as

$$\begin{aligned} \rho([ms]p;\omega) = \sum_{\sigma=0}^{2s} \sum_{j_0=-\sigma}^{\sigma} \sum_{j=|j_0|}^{\infty} \sum_{\mu=-j}^{j} \int_0^{i\infty} \frac{1}{i}\, d\mathbf{j}(j_0\mathbf{j}[ms])^{\sigma}{}_{j\mu} \\ \times \sum_{\lambda,\lambda'=-s}^{s} a(p)^{\lambda'}{}_{\lambda} \langle {}^{j\,\mu}_{j_0 j,\sigma}\,|\, p^s_{\lambda'};-p^{\lambda}_{s};\omega\rangle. \end{aligned} \tag{2.39}$$

In order to establish the connection between the tensorial operator set (2.1) at zero 4-momentum transfer and the set of the $ISO(3,1)\uparrow SO(3,1)$-irreducible tensor operators (2.25), we utilize the matrix realizations (2.12) and (2.33). If $t=0$ and $v=(0,0,0)$ [that is, $\Omega(v)$ is the 4×4 unit matrix], Eq. (2.12) simplifies to

$$\begin{aligned} (t=0,\tau[ms])^{\nu-\nu'}{}_{\kappa} = \rho[\tau]\int d\lambda(\phi,\alpha) D([\tau]\phi,\alpha,0)^{\dagger\nu-\nu'}{}_{\kappa} \\ \times |(\phi,\alpha)^{[ms]}_{\nu}\rangle\langle(\phi,\alpha)^{\nu'}_{[ms]}|, \end{aligned} \tag{2.40a}$$

where

$$|(\phi, \alpha)^{[ms]}_{\nu}\rangle = |p(\alpha, \phi)^{s}_{\nu}; 3\rangle,$$

with

$$p^{\lambda}(\phi, \alpha) = m\Omega_3(\phi, \alpha, 0)_0{}^{\lambda}. \tag{2.40b}$$

Since

$$\Omega_3(\phi, \alpha, 0)_0{}^{\lambda} = \Omega_0(\phi, \theta = \pi/2, \gamma = \alpha)_0{}^{\lambda}, \tag{2.41}$$

the helicity rearrangement transformation (1.17) implies that

$$|(\phi, \alpha)^{[ms]}_{\nu}\rangle = \sum_{\lambda=-s}^{s} |(\phi, \pi/2, \alpha)^{[ms]}_{\lambda}\rangle\, d^{s}(-\pi/2)^{\lambda}{}_{\nu}, \tag{2.42a}$$

where

$$|(\phi, \pi/2, \alpha)^{[ms]}_{\lambda}\rangle = |p(\phi, \pi/2, \alpha)^{s}_{\lambda}; 0\rangle$$

with

$$p^{\lambda}(\phi, \pi/2, \alpha) = m\Omega_0(\phi, \pi/2, \alpha)_0{}^{\lambda}. \tag{2.42b}$$

By virtue of Eq. (2.42a), the dyadic product in the expression (2.40a) can be subject to the reduction (2.39). We thus establish the connection

$$\begin{aligned}(t = 0, \tau[ms])^{\nu-\nu'}{}_{\kappa} &= \rho[\tau] \sum_{\sigma=0}^{2s} \sum_{j_0=-\sigma}^{\sigma} \sum_{j=|j_0|}^{\infty} \sum_{\mu=-j}^{j} \int_0^{i\infty} \frac{1}{i}\, dj(j_0 j[ms])^{\sigma}{}_{j\mu} \\ &\times \sum_{\lambda,\lambda'=-s}^{s} \langle {}^{\lambda-\lambda'}_{\sigma} \,|\, {}^{s\lambda'}_{\lambda s}\rangle d^{s}\left(-\frac{\pi}{2}\right)^{\lambda}_{\nu} d^{s}\left(-\frac{\pi}{2}\right)^{\lambda'}_{\nu'} \\ &\times \int d\lambda(\phi, \alpha) D([\tau]\phi, \alpha, 0)^{\dagger\nu-\nu'}{}_{\kappa} \\ &\times D\left([j_0 j]\phi, \frac{\pi}{2}, \alpha\right)^{j\mu}_{\sigma,\lambda-\lambda'}\end{aligned} \tag{2.43}$$

Since

$$(v, t\tau[ms])^{\nu-\nu'}{}_{\kappa} = T(\Omega(v))(t\tau[ms])^{\nu-\nu'}{}_{\kappa}, \tag{2.44}$$

the transformation property

$$\begin{aligned}&T(\Omega(v))(j_0 j[ms])^{\sigma}{}_{j\mu} \\ &\quad = \sum_{j'=|j_0|}^{\infty} \sum_{\mu'=-j'}^{j'} (j_0 j[ms])^{\sigma}{}_{j'\mu'} D([j_0 j]\Omega(v))^{j'\mu'}{}_{j\mu}\end{aligned} \tag{2.45}$$

[Eq. (5.36) of Ref. 1] and the relation (2.43) provide the reduction of the tensor operators (2.1) at zero 4-momentum transfer into their Poincaré-irreducible components. After integrating with respect to the angular variable ϕ, we obtain

$$\begin{aligned}&(v, t = 0, \tau[ms])^{\nu-\nu'}{}_{\kappa} \\ &\quad = \rho[\tau] \sum_{j_0=-\kappa}^{\kappa} \sum_{\sigma=|j_0|}^{2s} \sum_{j=|j_0|}^{\infty} \sum_{j'=|j_0|}^{\infty} \sum_{\mu'=-j'}^{j'} \int_0^{i\infty} \frac{1}{i}\, dj(j_0 j[ms])^{\sigma}{}_{j'\mu'} D([j_0 j]\Omega(v))^{j'\mu'}{}_{j\kappa} \sum_{\lambda,\lambda'=-s}^{s} d^{s}\left(-\frac{\pi}{2}\right)^{\lambda}_{\nu} d^{s}\left(\frac{\pi}{2}\right)^{\nu'}_{\lambda'} \\ &\quad \times d^{j}\left(\frac{\pi}{2}\right)^{\kappa}_{(\lambda-\lambda')} \langle {}^{\lambda-\lambda'}_{\sigma} \,|\, {}^{s\lambda'}_{\lambda s}\rangle \int d\lambda(\alpha) D([\tau]0, \alpha, 0)^{\dagger\nu-\nu'}{}_{\kappa} D([j_0 j]B(\alpha))^{j,(\lambda-\lambda')}{}_{\sigma,(\lambda-\lambda')},\end{aligned}$$

where

$$d\lambda(\alpha) = \tfrac{1}{2} \sinh \alpha\, d\alpha,\ 0 \leq \alpha < \infty. \tag{2.46}$$

The integration on the boost variable α can be carried out after performing the K transformation of Sciarrino and Toller,[4,12,13] which provides an expansion of the $SO(3, 1)$ matrices $D([j_0 j]B(\alpha))$ in terms of the $SO(2, 1)$ matrices $D([\tau]0, \alpha, 0)$. In our notation this expansion is [see Eq. (4.27) of Ref. 4 or Eq. (19) of Ref. 12]

$$\begin{aligned}&D([j_0 j]B(\alpha))^{j\lambda}{}_{j'\lambda} \\ &\quad = \sum_{\mu=-j}^{j} \sum_{\mu'=-j'}^{j'} d^{j}\left(\frac{\pi}{2}\right)^{\lambda}_{\mu} d^{j'}\left(-\frac{\pi}{2}\right)^{\mu'}_{\lambda} \\ &\qquad \times \sum_{\tau=\pm} \left(\int_{-\infty}^{\infty} \rho[\sigma, \epsilon]\, d\sigma K^{j_0 j}_{\mu}(\sigma, r, j)^* \right. \\ &\qquad \times D([\sigma]0, \alpha, 0)^{\mu}{}_{\mu'} K^{j_0 j}_{\mu'}(\sigma, r, j') \\ &\qquad + \delta_{\operatorname{sgn}\mu, \operatorname{sgn}\mu'} \sum_{\eta=\operatorname{sgn}\mu}^{\min(|\mu|,|\mu'|)} \sum_{k=1+\epsilon} \rho[k] K^{j_0 j}_{\mu}(k^{\eta}, r, j)^* \\ &\qquad \left. \times D([k^{\eta}]0, \alpha, 0)^{\mu}{}_{\mu'} K^{j_0 j}_{\mu'}(k^{\eta}, r, j') \right),\end{aligned}$$

$$\operatorname{sgn}\mu = \mu/|\mu|. \tag{2.47}$$

The inverse of this expansion is [see Eq. (4.31) of Ref. 4]

$$\begin{aligned}&\sum_{j,j'=|j_0|}^{\infty} \sum_{\lambda=-j}^{j} K^{j_0 j}_{\mu}(\tau, r, j) d^{j}\left(\frac{\pi}{2}\right)^{\mu}_{\lambda} D([j_0 j]B(\alpha))^{j\lambda}{}_{j'\lambda} \\ &\qquad \times d^{j'}\left(-\frac{\pi}{2}\right)^{\lambda}_{\mu'} K^{j_0 j}_{\mu'}(\tau', r', j')^* \\ &\quad = \frac{1}{\rho[\tau]} \delta(\tau, \tau')\delta_{r,r'} D([\tau]0, \alpha, 0)^{\mu}{}_{\mu'},\end{aligned} \tag{2.48}$$

$$r = +, -;\ \delta(\tau, \tau') = \begin{cases} \delta(\sigma - \sigma'), & \text{if } \tau = -\tfrac{1}{2} + i\sigma, \\ & \tau' = -\tfrac{1}{2} + i\sigma', \\ \delta_{k,k'}, & \text{if } \tau = k^{\eta},\ \tau' = k'^{\eta} \\ 0, & \text{otherwise.} \end{cases}$$

Symmetry properties and explicit expressions in terms of hypergeometric functions for the K functions are derived in Refs. 4, 12, 13. We reproduce here the definition [Eq. (4.25) of Ref. 4 or Eq. (1) of Ref. 12].

$$\begin{aligned}K^{j_0 j}_{\mu}(\tau, \pm, j) &= (2j + 1)^{\frac{1}{2}}(-1)^{\mu\mp j_0} \int (\cosh \alpha)^{j-1} \\ &\quad \times d^{j}[\theta^{\pm}(\alpha)]^{j_0}{}_{\mu} D([\tau]0, \alpha, 0)^{\mu}{}_{\pm j_0}\, d\lambda(\alpha),\end{aligned} \tag{2.49a}$$

$$0 \leq \theta^+ < \pi/2, \quad \theta^+(\alpha) = 2\tan^{-1}\tanh\alpha/2,$$
$$\pi/2 < \theta^- \leq \pi, \quad \theta^-(\alpha) = 2\cot^{-1}\tanh\alpha/2. \quad (2.49b)$$

By substituting the expansion (2.47) for the $SO(3,1)$-matrix elements appearing in the decomposition (2.46) and by utilizing the orthogonality relation (2.8), we can evaluate the integral in (2.46):

$$\int d\lambda(\alpha) D([\tau]0,\alpha,0)^{\dagger\nu-\nu'}{}_{\kappa} D([j_0 j]B(\alpha))^{j,\lambda-\lambda'}{}_{\sigma,\lambda-\lambda'}$$
$$= d^j(\pi/2)^{\lambda-\lambda'}{}_{\kappa}\, d^j(-\pi/2)^{\nu-\nu'}{}_{\lambda-\lambda'} \times \sum_{r=+,-} K_{\mu}^{j_0 j}(\tau,r,j)^* K_{\nu-\nu'}^{j_0 j}(\tau,r,\mathcal{A}).$$

Hence,

$$(v,t=0,\tau[ms])^{\nu-\nu'}{}_{\kappa}$$
$$= \rho[\tau] \sum_{j_0=-\kappa}^{\kappa} \sum_{\sigma=|j_0|}^{2s} \sum_{j=|j_0|}^{\infty} F(\nu,\nu',\kappa,s)_{j\sigma} \times \left[\sum_{r=\pm} K_{\kappa}^{j_0 j}(\tau,r,j)^* K_{\nu-\nu'}^{j_0 j}(\tau,r,\mathcal{A})\right] \times \sum_{j'=|j_0|}^{\infty} \sum_{\mu'=-j'}^{j'} \int_0^{i\infty} \frac{1}{i} dj(j_0 j[ms])^{\sigma}{}_{j'\mu'} \times D([j_0 j]\Omega(v))^{j'\mu'}{}_{j\kappa}, \quad (2.50a)$$

where

$$F(\nu,\nu',\kappa,s)_{j\sigma} = \sum_{\lambda,\lambda'=-s}^{s} d^s(\pi/2)^{\nu}{}_{\lambda}\, d^s(\pi/2)^{\nu'}{}_{\lambda'} (-1)^{\kappa-\lambda+\lambda'} [d^j(\pi/2)^{\lambda-\lambda'}{}_{\kappa}]^2 \times d^{\sigma}(\pi/2)^{\lambda-\lambda'}{}_{\nu-\nu'} \langle {}^{\lambda-\lambda'}_{\sigma} \mid {}^{s\lambda'}_{\lambda s}\rangle. \quad (2.50b)$$

If $t = 0$, the relations (2.16) and (2.18) imply that the orbiting transformation $\Omega(v)$ can be restricted from the general parametrizations (2.11a) or (2.11b) to the one-parameter transformations

$$\Omega(v) = \Omega_0(0,\theta_v,0), \quad 0 \leq \theta_v \leq \pi, \quad (2.51a)$$

or

$$\Omega(v) = \Omega_3(0,0,\zeta_v), \quad -\infty < \zeta_v < \infty. \quad (2.51b)$$

The elements of the transformation matrix $D([j_0 j]\Omega(v))$ which appear in Eqs. (2.46) and (2.50a) may therefore be reduced to either rotation or boost functions. By virtue of the relations (2.30), the $SO(3,1)$-matrix realizations of the transformations (2.51a) and (2.51b) are

$$D([j_0 j]\Omega_0(0,\theta_v,0))^{j'\mu'}{}_{j\kappa} = d^{j'}(\theta_v)^{\mu'}{}_{\kappa}\, \delta^{j'}{}_{j} \quad (2.52a)$$

and

$$D([j_0 j]\Omega_3(0,0,\zeta_v))^{j'\mu'}{}_{j\kappa} = \begin{cases} D([j_0 j]B(\zeta_v))^{j'\kappa}{}_{j\kappa}\, \delta^{\mu'}{}_{\kappa}, & \text{if } \zeta_v > 0 \\ (-1)^{j'+\kappa}\delta^{\mu'}{}_{-\kappa}\, D([j_0 j]B(|\zeta_v|))^{j'\kappa}{}_{j\kappa}, & \text{if } \zeta_v < 0 \end{cases} \quad (2.52b)$$

For the derivation of the second equation (2.52b) we used the obvious relation

$$\Omega_3(0,0,-|\zeta_v|) = \Omega_0(0,\pi,0)\Omega_3(0,0,|\zeta_v|)$$

in conjunction with the property

$$d^{j'}(\pi)^{\mu'}{}_{\kappa} = (-1)^{j'+\kappa}\delta^{\mu'}{}_{-\kappa}.$$

3. THE CONNECTION BETWEEN POINCARÉ- AND LORENTZ-IRREDUCIBLE TENSOR OPERATORS

The momentum-helicity state vectors introduced in Sec. 1 transform irreducibly under the Poincaré group but not under the (homogeneous) Lorentz group. The $ISO(3,1)$-irreducible basis

$$\{|p_{\lambda}^s;\omega\rangle : p^2 = m^2, -s \leq \lambda \leq s\},$$
$$\langle p'^{\lambda'}_{s};\omega \mid p_{\lambda}^s;\omega\rangle = 2|p^0|\,\delta^3(\mathbf{p}'-\mathbf{p})\delta^{\lambda'}{}_{\lambda}, \quad (3.1)$$

and the $SO(3,1)$-irreducible basis

$$|{}^{j_0 j}_{j\mu}\rangle : j_0 = \begin{cases} 0, \pm 1, \pm 2, \cdots, \\ \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \cdots, \end{cases} \quad j = |j_0|, |j_0|+1, \cdots, \quad \mu = -j, -j+1, \cdots, j, \quad (3.2)$$

which transforms according to the unitary irreducible representations of the principal series (2.28), i.e.,

$$T(\Lambda)\,|{}^{j_0 j}_{j\mu}\rangle = \sum_{j'\mu'} |{}^{j_0 j}_{j'\mu'}\rangle\, D([j_0 j]\Lambda)^{j'\mu'}{}_{j\mu}, \quad (3.3)$$

are connected by means of the relation

$$|p_{\lambda}^s;\omega\rangle = \sum_{j_0,j,\mu} \int \frac{1}{i} dj\, |{}^{j_0 j}_{j\mu}\rangle\, Y_{j_0 j}^{j\mu}(p;\omega)_{s\lambda}, \quad (3.4)$$

where the transformation coefficients

$$Y_{j_0 j}^{j\mu}(p;\omega)_{s\lambda} = \langle {}^{j\mu}_{j_0 j} \mid p_{\lambda}^s;\omega\rangle,$$
$$Y_{j\mu}^{j_0 j}(p;\omega)^{s\lambda} = Y_{j_0 j}^{j\mu}(p;\omega)^*{}_{s\lambda} \quad (3.5)$$

are referred to as $SO(3,1)$ harmonics. The expansion (3.4) is obviously consistent with

$$\langle {}^{j'\mu'}_{j_0' j'} \mid {}^{j_0 j}_{j\mu}\rangle = \delta_{j_0' j_0}\delta(ij'-ij)\delta^{j'}{}_{j}\delta^{\mu'}{}_{\mu}. \quad (3.6)$$

The completeness relation

$$\sum_{j_0,j,\mu} \int \frac{1}{i} dj Y_{j\mu}^{j_0 j}(p';\omega)^{s\lambda'} Y_{j_0 j}^{j\mu}(p;\omega)_{s\lambda} = 2|p^0|\,\delta^3(\mathbf{p}'-\mathbf{p})\delta^{\lambda'}{}_{\lambda} \quad (3.7)$$

follows from the expansion (3.4) together with the orthogonality relations (3.1) and (3.6). The relation inverse to (3.4) is then

$$|{}^{j_0 j}_{j\mu}\rangle = \sum_{\lambda=-s}^{s} \int \frac{d^3\mathbf{p}}{2|p^0|}\, |p_{\lambda}^s;\omega\rangle\, Y_{j\mu}^{j_0 j}(p;\omega)^{s\lambda}, \quad (3.8)$$

and the orthogonality relation

$$\sum_{\lambda=-s}^{s}\int\frac{d^3\mathbf{p}}{2\,|p^0|}\,Y^{j'\mu'}_{j_0'j'}(p;\omega)_{s\lambda}Y^{j_0j}_{j\mu}(p;\omega)^{s\lambda} = \delta_{j_0'j_0}\delta(ij'-ij)\delta^{j'}{}_{j}\delta^{\mu'}{}_{\mu} \quad (3.9)$$

is an immediate consequence of (3.6) and (3.8). Since the basis vectors (3.1) are angular momentum eigenvectors, the equation

$$Y^{j\mu}_{j_0j}(p;\omega)_{s\lambda} = \langle{}^{j\mu}_{j_0j}|\,T(\Omega_\omega(p))\,|m^s_\lambda\rangle \quad (3.10)$$

entails that an orthogonality relation of the form

$$Y^{j\mu}_{j_0j}(m)_{s\lambda} = \langle{}^{j\mu}_{j_0j}\,|\,m^s_\lambda\rangle = K([ms]j_0j)\delta^{j}{}_{s}\delta^{\mu}{}_{\lambda} \quad (3.11)$$

must hold. The normalization constant $K([ms]j_0j)$ will be determined below. With the orbiting transformation (1.3) one derives from Eqs. (3.3), (3.10), and (3.11) the connection between the $SO(3,1)$-harmonics and the matrix elements (2.34),

$$\begin{aligned}Y^{j\mu}_{j_0j}(\phi\Theta\gamma)_{s\lambda} &= \langle{}^{j\mu}_{j_0j}|\,T(\Omega_0(\phi,\theta,\gamma))\,|m^s_\lambda\rangle_{j\mu}\\ &= K([ms]j_0j)D([j_0j]\phi\theta\gamma)^{j\mu}{}_{s\lambda}.\end{aligned} \quad (3.12)$$

If the last expression in (3.12) is substituted for the $SO(3,1)$ harmonics appearing in the orthogonality relation (3.9), the equations

$$d^3\mathbf{p}/(2\,|p^0|) = \tfrac{1}{2}p^2\sinh^2\gamma\,\sin\theta\,d\phi\,d\theta\,d\gamma$$

and

$$\sum_{\lambda=-s}^{s}\int d\mu(\phi,\theta,\gamma)D([j_0j]\phi\theta\gamma)^{j\mu}{}_{s\lambda}\,D([j_0'j']\phi\theta\gamma)^{*j'\mu'}{}_{s\lambda} = (\rho_s[j_0j])^{-1}\delta_{j_0j_0'}\delta(ij-ij')\delta^{jj'}\delta^{\mu\mu'},$$

imply that

$$\begin{aligned}K([ms]j_0j) &= [\rho_s[j_0j]/(4\pi m^2)]^{\frac{1}{2}}\\ &= \frac{1}{\pi m}\left(\frac{(j_0^2-j^2)}{(2s+1)}\right)^{\frac{1}{2}}.\end{aligned} \quad (3.13)$$

Therefore

$$\begin{aligned}&Y^{j\mu}_{j_0j}(\phi,\theta,\gamma)_{s\lambda}\\ &\quad= \frac{1}{\pi m}\left(\frac{(j_0^2-j^2)}{(2s+1)}\right)^{\frac{1}{2}}D([j_0j]\phi\theta\gamma)^{j\mu}{}_{s\lambda}.\end{aligned} \quad (3.14)$$

For the type of parametrization characterized by $\omega = 0$, the expansions (3.4) and (3.8) are therefore

$$|^{[ms]}_{\lambda}\phi\theta\gamma\rangle = \sum_{j_0=-|\lambda|}^{|\lambda|}\int_0^{i\infty}\frac{1}{i}\,dj\left(\frac{\rho_s[j_0j]}{4\pi m^2}\right)^{\frac{1}{2}}\sum_{j=|\lambda|}^{\infty}\sum_{\mu=-j}^{j}|^{j_0j}_{j\mu}\rangle \times D([j_0j]\phi\theta\gamma)^{j\mu}{}_{s\lambda} \quad (3.15)$$

and

$$|^{j_0j}_{j\mu}\rangle = (4\pi m^2\rho_s[j_0j])^{\frac{1}{2}}\sum_{\lambda=-s}^{s}\int d\mu(\phi\theta\gamma)\,|^{[ms]}_{\lambda}\phi\theta\gamma\rangle \times D([j_0j]\phi\theta\gamma)^{\dagger s\lambda}{}_{j\mu}, \quad (3.16)$$

where

$$|^{[ms]}_{\lambda}\phi\theta\gamma\rangle = |p^s_\lambda;0\rangle. \quad (3.17)$$

In the space spanned by the basis vectors (3.1), we now introduce as the linear superpositions

$$(\bar{j_0}\bar{j}\,{}^{j_0j}_{j_0'j'})_{\bar{j}\bar{\mu}} = \sum_{j\mu j'\mu'}|^{j_0'j'}_{j'\mu'}\rangle\langle{}^{j'\mu'}_{j_0'j'},\,{}^{j_0j}_{j\mu}\,|\,{}^{\bar{j}_0\bar{j}}_{\bar{j}\bar{\mu}}\rangle\langle{}^{j\mu}_{j_0j}| \quad (3.18)$$

the tensor operators transforming by the unitary irreducible $SO(3,1)$ representations of the principal series. In the expression (3.18), the $SO(3,1)$-Clebsch–Gordan coefficients are defined by means of the reduction[14]

$$\begin{aligned}&D([j_0'j']\Lambda)^{j'\mu'}{}_{s'\lambda'}\,D([j_0j]\Lambda)^{\dagger s\lambda}{}_{j\mu}\\ &\quad= \sum_{\bar{j}_0\bar{j}\bar{\mu}\bar{s}\bar{\lambda}}\frac{1}{i}\int d\bar{j}\rho[\bar{j}_0\bar{j}]\langle{}^{j'\mu'}_{j_0'j'},\,{}^{j_0j}_{j\mu}\,|\,{}^{\bar{j}_0\bar{j}}_{\bar{j}\bar{\mu}}\rangle\\ &\qquad\times D([\bar{j}_0\bar{j}]\Lambda)^{\bar{j}\bar{\mu}}{}_{\bar{s}\bar{\lambda}}\langle{}^{\bar{s}\bar{\lambda}}_{\bar{j}_0\bar{j}}\,|\,{}^{j_0'j'}_{s'\lambda'}\,{}^{s\lambda}_{j_0j}\rangle,\end{aligned} \quad (3.19)$$

which ensures the transformation property

$$T(\Lambda)(\bar{j_0}\bar{j}\,{}^{j_0j}_{j_0'j'})_{\bar{j}\bar{\mu}} = \sum_{\bar{j}'\bar{\mu}'}(\bar{j_0}\bar{j}\,{}^{j_0j}_{j_0'j'})_{\bar{j}'\bar{\mu}'}\,D([\bar{j}_0\bar{j}]\Lambda)^{\bar{j}'\bar{\mu}'}{}_{\bar{j}\bar{\mu}}. \quad (3.20)$$

To the decomposition (2.30) of a general $SO(3,1)$-matrix realization into rotation and boost matrices corresponds the factorization of a general $SO(3,1)$-Clebsch–Gordan coefficient into a reduced $SO(3,1)$- and a $SO(3)$-Clebsch–Gordan coefficient

$$\langle{}^{j'\mu',\;j_0j}_{j_0'j',\;j\mu}\,|\,{}^{\bar{j}}_{\bar{j}\bar{\mu}}\rangle = \langle{}^{j',\;j_0j}_{j_0'j',\;j}\,|\,{}^{\bar{j}_0\bar{j}}_{\bar{j}\bar{\mu}}\rangle\langle{}^{\mu'j}_{j'\mu}\,|\,{}^{\bar{j}}_{\bar{\mu}}\rangle. \quad (3.21)$$

The reduced $SO(3,1)$-Clebsch–Gordan coefficients are defined by means of the reduction for the boost matrices

$$\begin{aligned}&d_{\nu'}([j_0'j']B)^{j'}{}_{s}\,d_{\nu}([j_0j]B)^{\dagger s}{}_{j}\\ &\quad= \sum_{\bar{j}_0\bar{j}\bar{s}}\int\frac{1}{i}\,dj\rho[\bar{j}_0\bar{j}]\langle{}^{j'}_{j_0'j'},\,{}^{j_0j}_{j}\,|\,{}^{\bar{j}_0\bar{j}}_{\bar{j}}\rangle\\ &\qquad\times d_{\nu+\nu'}([\bar{j}_0\bar{j}]B)^{\bar{j}}{}_{\bar{s}}\langle{}^{\bar{s}}_{\bar{j}_0\bar{j}}\,|\,{}^{j_0'j'}_{s}\,{}^{s}_{j_0j}\rangle.\end{aligned} \quad (3.22)$$

The reduction formula (6.17) implies the completeness

$$\sum_{\bar{j}_0\bar{j}\bar{\mu}}\int d\bar{j}\rho[\bar{j}_0\bar{j}]\langle{}^{j'\mu'}_{j_0'j'},\,{}^{j_0j}_{j\mu}\,|\,{}^{\bar{j}_0\bar{j}}_{\bar{j}\bar{\mu}}\rangle\langle{}^{\bar{j}\bar{\mu}}_{\bar{j}_0\bar{j}}\,|\,{}^{j_0'j'}_{s'\lambda'}\,{}^{s\lambda}_{j_0j}\rangle = \delta^{j'}{}_{s'}\,\delta^{\mu'}{}_{\lambda'}\,\delta^{s}{}_{j}\,\delta^{\lambda}{}_{\mu}, \quad (3.23)$$

and consequently the orthogonality

$$\sum_{j'\mu'j\mu}\langle{}^{\bar{j}'\bar{\mu}'}_{\bar{j}_0'\bar{j}'}\,|\,{}^{j_0'j'}_{j'\mu'}\,{}^{j\mu}_{j_0j}\rangle\langle{}^{j'\mu'}_{j_0'j'}\,{}^{j_0j}_{j\mu}\,|\,{}^{\bar{j}_0\bar{j}}_{\bar{j}\bar{\mu}}\rangle = \frac{1}{\rho[\bar{j}_0\bar{j}]}\,\delta_{\bar{j}_0'\bar{j}_0}\delta(i\bar{j}'-i\bar{j})\delta^{\bar{j}'}{}_{\bar{j}}\,\delta^{\bar{\mu}'}{}_{\bar{\mu}}. \quad (3.24)$$

With this property, we derive from the reduction

formula (3.19) the result

$$\frac{1}{\rho[\bar{j}_0\bar{j}]}\,\delta_{\bar{j}_0\bar{j}_0'}\delta(i\bar{\jmath}-i\bar{\jmath}')D([\bar{j}_0\bar{j}]\Lambda)^{\bar{\jmath}\bar{\mu}}{}_{\bar{\jmath}'\bar{\mu}'}$$
$$=\sum_{\substack{j'\mu'j\mu\\ s'\lambda' s\lambda}}\langle{}^{\bar{\jmath}\bar{\mu}}_{\bar{j}_0\bar{\jmath}}\,|\,{}^{j_0'j'\ j\ \mu}_{j'\mu'\ j_0 j}\rangle D([j_0'j']\Lambda)^{j'\mu'}{}_{s'\lambda'}$$
$$\times D([j_0 j]\Lambda)^{\dagger s\lambda}{}_{j\mu}\langle{}^{j_0'j'\ s\ \lambda}_{s'\lambda'\ j_0 j}\,|\,{}^{\bar{j}_0'\bar{\jmath}'}_{\bar{\jmath}'\bar{\mu}'}\rangle. \quad (3.25)$$

By virtue of the completeness relation (3.23), the expansion (3.15), and its Hermitian adjoint, we arrive at the following decomposition into the $SO(3,1)$-irreducible tensor operators (3.18) of a momentum–helicity dyadic with the orbit parametrization $\omega = 0$:

$$|{}^{[ms]}_{\lambda}\phi\Theta\gamma\rangle\langle{}^{\lambda'}_{[ms]}\phi'\Theta'\gamma'|$$
$$=\frac{1}{4\pi m^2}\sum_{j_0=-|\lambda|}^{|\lambda|}\sum_{j_0'=-|\lambda'|}^{|\lambda'|}\int_0^{i\infty}\frac{1}{i}\,dj(\rho_s[j_0 j])^{\frac{1}{2}}$$
$$\times\int_0^{i\infty}\frac{1}{i}\,dj'(\rho_s[j_0'j'])^{\frac{1}{2}}$$
$$\times\sum_{j=|j_0|}^{\infty}\sum_{j'=|j_0'|}^{\infty}\sum_{\mu=-j}^{j}\sum_{\mu'=-j'}^{j'}D([j_0 j]\phi\Theta\gamma)^{j\mu}{}_{s\lambda}$$
$$\times D([j_0'j']\phi'\theta'\gamma')^{\dagger s\lambda'}{}_{j'\mu'}$$
$$\times\sum_{\bar{\jmath}_0=-|j'-j|}^{|j'-j|}\int_0^{i\infty}\frac{1}{i}\,d\bar{\jmath}\rho[\bar{j}_0\bar{\jmath}]$$
$$\times\sum_{\bar{\jmath}=|j'-j|}^{j'+j}\sum_{\bar{\mu}=-\bar{\jmath}}^{\bar{\jmath}}(\bar{j}_0\bar{\jmath}\,{}^{j_0'j'}_{j_0 j})_{\bar{\jmath}\bar{\mu}}\langle{}^{\bar{\jmath}\bar{\mu}}_{\bar{j}_0\bar{\jmath}}\,|\,{}^{j_0 j\ j'\mu'}_{j\ \mu\ j_0'j'}\rangle. \quad (3.26)$$

If $(\phi', \Theta', \gamma') = (\phi, \Theta, \gamma)$, this decomposition can be simplified by means of the reduction formula (3.19) and the orthogonality relation (3.24):

$$|{}^{[ms]}_{\lambda}\phi\Theta\gamma\rangle\langle{}^{\lambda'}_{[ms]}\phi\Theta\gamma|$$
$$=\frac{1}{4\pi m^2}\sum_{j_0=-|\lambda|}^{|\lambda|}\sum_{j_0'=-|\lambda'|}^{|\lambda'|}\int_0^{i\infty}\frac{1}{i}\,dj(\rho_s[j_0 j])^{\frac{1}{2}}$$
$$\times\int_0^{i\infty}\frac{1}{i}\,dj'(\rho_s[j_0'j'])^{\frac{1}{2}}$$
$$\times\sum_{\bar{\jmath}_0=-|\lambda-\lambda'|}^{|\lambda-\lambda'|}\int_0^{i\infty}\frac{1}{i}\,d\bar{\jmath}\rho[\bar{j}_0\bar{\jmath}]\sum_{\bar{\jmath}=|\bar{j}_0|}^{\infty}\sum_{\bar{\mu}=-\bar{\jmath}}^{\bar{\jmath}}(\bar{j}_0\bar{\jmath}\,{}^{j_0'j'}_{j_0 j})_{\bar{\jmath}\bar{\mu}}$$
$$\times\sum_{\bar{s}=|\lambda-\lambda'|}^{2s}D([\bar{j}_0\bar{\jmath}]\phi\Theta\gamma)^{\bar{\jmath}\bar{\mu}}{}_{\bar{s}\lambda}\langle{}^{\bar{s}\lambda}_{\bar{j}_0\bar{\jmath}}\,|\,{}^{j_0 j\ s\lambda'}_{\lambda\ j_0'j'}\rangle. \quad (3.27)$$

From this decomposition together with the orthogonality relation (2.35) for the D functions and the factorization formula (3.21) then follows the expansion of the $[ISO(3,1)\uparrow SO(3,1)]$-irreducible tensor operators (2.25) in terms of the $SO(3,1)$-irreducible tensor operators (3.18):

$$(\bar{j}_0\bar{\jmath}[ms])^{\sigma}{}_{\bar{\jmath}\bar{\mu}}=\frac{\rho_s[\bar{j}_0\bar{\jmath}]}{4\pi m^2}\sum_{j_0,j_0'=-s}^{s}\int_0^{i\infty}\frac{1}{i}\,dj(\rho[j_0 j])^{\frac{1}{2}}$$
$$\times\int_0^{i\infty}\frac{1}{i}\,dj'(\rho[j_0'j'])^{\frac{1}{2}}\langle{}^{\sigma}_{\bar{j}_0\bar{\jmath}}\,|\,{}^{j_0'j'\ s}_{s\ \ j_0 j}\rangle(\bar{j}_0\bar{\jmath}\,{}^{j_0 j}_{j_0'j'})_{\bar{\jmath}\bar{\mu}}. \quad (3.28)$$

The substitution of this expression into the reduction formula (2.50) establishes the connection between the tensorial set (2.1) at zero momentum transfer and the $SO(3,1)$-irreducible tensor operators (3.18). The decomposition (3.27) also leads to the multipole expansion of the spin density matrix

$$\rho([ms]p;\omega)=\sum_{\lambda,\lambda'=-s}^{s}|p^s_{\lambda'};\omega\rangle\,a(p)^{\lambda'}{}_{\lambda}\,\langle p^{\lambda}_{s};\omega| \quad (3.29)$$

in terms of the $SO(3,1)$-irreducible tensor operators (3.18):

$$\rho([ms]p;\omega)$$
$$=\frac{1}{4\pi m^2}\sum_{j_0=-2s}^{2s}\int_0^{i\infty}\frac{1}{i}\,d\bar{\jmath}\rho_s[\bar{j}_0\bar{\jmath}]$$
$$\times\sum_{\sigma=|\bar{j}_0|}^{2s}\sum_{\bar{\jmath}=|\bar{j}_0|}^{\infty}\sum_{\bar{\mu}=-\bar{\jmath}}^{\bar{\jmath}}\sum_{\lambda,\lambda'=-s}^{s}\langle{}^{\bar{\jmath}\bar{\mu}}_{\bar{j}_0\bar{\jmath},\sigma}\,|\,p^s_{\lambda'};-p^{\lambda}_{s};\omega\rangle a(p)^{\lambda'}{}_{\lambda}$$
$$\times\sum_{j_0,j_0'=-s}^{s}\int_0^{i\infty}\frac{1}{i}\,dj(\rho[j_0 j])^{\frac{1}{2}}$$
$$\times\int_0^{i\infty}\frac{1}{i}\,dj'(\rho[j_0'j'])^{\frac{1}{2}}\langle{}^{\sigma}_{\bar{j}_0\bar{\jmath}}\,|\,{}^{j_0'j'\ s}_{s\ \ j_0 j}\rangle(\bar{j}_0\bar{\jmath}\,{}^{j_0 j}_{j_0'j'})_{\bar{\jmath}\bar{\mu}}, \quad (3.30)$$

where the $[ISO(3,1)\uparrow SO(3,1)]$-Clebsch–Gordan coefficients defined by means of the Eq. (2.38) appear. In the derivation of (3.30) the reduction

$$D^s(R_{\omega 0})^{\mu}{}_{\lambda}\,D^s(R_{\omega 0})^{\dagger\lambda'}{}_{\mu'}=\sum_{\sigma=0}^{2s}\langle{}^{\mu\ s}_{s\,\mu'}\,|\,{}^{\sigma}_{\bar{\mu}}\rangle D^{\sigma}(R_{\omega 0})^{\bar{\mu}}{}_{\lambda}\,\langle{}^{\lambda}_{\sigma}\,|\,{}^{s\lambda'}_{\lambda\ s}\rangle$$

and the factorization (3.21) have been used. The Lorentz multipole expansion (3.30) may also be derived by substituting the relation (3.28) into the Poincaré-multipole expansion (2.39). The relation (3.26) provides the Lorentz-multipole expansion of the spin–momentum density operator (2.22),[15] if it is rewritten as [by means of the helicity rearrangement transformation (1.16), (1.19)]

$$\rho([ms]a)=\frac{m^4}{16\pi^2}\int d\mu(\phi,\Theta,\gamma)\int d\mu(\phi',\theta',\gamma')$$
$$\times\sum_{\lambda,\lambda'=-s}^{s}|{}^{[ms]}_{\lambda}\phi\theta\gamma\rangle$$
$$\times d^s[\Theta_{30}(\phi,\theta,\gamma)]^{\lambda}{}_{\nu}\,a(\phi,\theta,\gamma;\phi'\theta',\gamma')^{\nu}{}_{\nu'}$$
$$\times d^s[\Theta_{30}(\phi',\theta',\gamma')]^{\dagger\nu'}{}_{\lambda'}\langle{}^{\lambda'}_{[ms]}\phi'\theta'\gamma'|. \quad (3.31)$$

The connection between the $ISO(3,1)\uparrow SO(2,1)$-irreducible tensorial set (2.1) for arbitrary but nonvanishing (spacelike) 4-momentum transfer and the

$[ISO(3,1)\uparrow SO(3,1)]$-irreducible tensorial set (2.25) can be established through the intermediary of the $SO(3,1)$-irreducible tensor operators (3.18). The $SO(3,1)$-irreducible tensor operators (3.18) can be expanded in terms of the Poincaré-irreducible set (2.1) in accordance with the relation (3.16) and the helicity-rearrangement transformation (1.16). An expansion of the tensor operators (3.18) in terms of the $[ISO(3,1)\uparrow SO(3,1)]$-irreducible tensor operators is evidently impossible, which means that the decomposition (3.28) is not invertible. This can also be inferred from the relation (3.25). By substituting the expansion of the Lorentz-irreducible tensor operators (3.18) in terms of the Poincaré-irreducible tensor operators (2.1) into the decomposition (3.28), a relationship between the two classes of Poincaré-irreducible tensor operators (2.1) and (2.25) is obtained.

4. THE ASSOCIATIVE ALGEBRA OF THE POINCARÉ-IRREDUCIBLE TENSOR OPERATORS

We now derive a relativistic generalization of a relation given by Biedenharn[16] for the ordinary spin tensor operators. For the spin tensor operators defined by (2.26), this relation is [Eq. (2.32) of Ref. 17]

$$(m,s)_{\sigma\kappa}(m,s)_{\sigma'\kappa'} = [(2\sigma+1)(2\sigma'+1)]^{\frac{1}{2}} \times \sum_{\bar\sigma} (m,s)^{-}_{\bar\sigma\bar\kappa}\langle {}^{\bar\kappa}_{\bar\sigma} \mid {}^{\sigma\ \sigma'}_{\kappa\ \kappa'}\rangle (-1)^{2s-\bar\sigma}\begin{Bmatrix}\sigma & \sigma' & \bar\sigma\\ s & s & s\end{Bmatrix}, \quad (4.1)$$

where the $6j$-coefficients appear in the angular momentum recoupling relation

$$\langle {}^{\mu_1\ \mu_2}_{j_1\ j_2} \mid {}^{j_{12}}_{\mu_{12}}\rangle\langle {}^{\mu_{12}\ \mu_3}_{j_{12}\ j_3} \mid {}^{j}_{\mu}\rangle = \sum_{j_{23}} \langle {}^{\mu_2\ \mu_3}_{j_2\ j_3} \mid {}^{j_{23}}_{\mu_{23}}\rangle\langle {}^{\mu_1\ \mu_{23}}_{j_1\ j_{23}} \mid {}^{j}_{\mu}\rangle \times [(2j_{12}+1)(2j_{23}+1)]^{\frac{1}{2}}(-1)^{j_1+j_2+j_3+j}\begin{Bmatrix} j_1 & j_2 & j_{12}\\ j_3 & j & j_{23}\end{Bmatrix}. \quad (4.2)$$

For the operators (2.32) the relation corresponding to (4.1) is

$$([ms]\phi\theta\gamma)_{\sigma\kappa}([ms]\phi'\theta'\gamma')_{\sigma'\kappa'} = [2/(m^2(\sinh\gamma)^2\sin\theta)]\delta(\gamma-\gamma')\delta(\theta-\theta')\delta(\phi-\phi') \times [(2\sigma+1)(2\sigma'+1)]^{\frac{1}{2}} \times \sum_{\bar\sigma}([ms]\phi\theta\gamma)^{-}_{\bar\sigma\bar\kappa}\langle {}^{\bar\kappa}_{\bar\sigma} \mid {}^{\sigma\ \sigma'}_{\kappa\ \kappa'}\rangle (-1)^{2s-\bar\sigma}\begin{Bmatrix}\sigma & \sigma' & \bar\sigma\\ s & s & s\end{Bmatrix}. \quad (4.3)$$

This result, the relation (2.33), the reduction[14]

$$D([j_0\boldsymbol{j}]\Lambda)^{\dagger s\kappa}{}_{j\mu}\, D([j_0'\boldsymbol{j}']\Lambda)^{\dagger s'\kappa'}{}_{j'\mu'} = \sum_{\bar j_0\bar j\bar\mu\bar\sigma\bar\kappa}\int \frac{1}{i}\,d\bar{\boldsymbol{j}}\langle {}^{\sigma\ \kappa\ \ \sigma'\kappa'}_{j_0\boldsymbol{j}\ j_0'\boldsymbol{j}'} \mid {}^{\bar j_0\bar{\boldsymbol{j}}}_{\bar\sigma\bar\kappa}\rangle \times D([\bar j_0\bar{\boldsymbol{j}}]\Lambda)^{\dagger\bar\sigma\bar\kappa}{}_{\bar j\bar\mu}\langle {}^{\bar j\bar\mu}_{\bar j_0\bar{\boldsymbol{j}}} \mid {}^{j_0 j\ \ j_0'j'}_{j\ \mu\ \ j'\mu'}\rangle, \quad (4.4)$$

and the factorization

$$\langle {}^{\sigma\ \kappa\ \ \sigma'\kappa'}_{j_0\boldsymbol{j}\ j_0'\boldsymbol{j}'} \mid {}^{\bar j_0\bar{\boldsymbol{j}}}_{\bar\kappa}\rangle = \langle {}^{\sigma}_{j_0\boldsymbol{j}\ j_0'\boldsymbol{j}'} \mid {}^{\bar j_0\bar{\boldsymbol{j}}}\rangle\langle {}^{\kappa\kappa'}_{\sigma\ \sigma'} \mid {}^{\bar\sigma}_{\bar\kappa}\rangle \quad (4.5)$$

are the essential relations for the construction of the associative algebra determined by the matrix multiplication of $[ISO(3,1)\uparrow SO(3,1)]$-irreducible tensor operators. This algebra is characterized by the equation

$$(j_0\boldsymbol{j}[ms])^{\sigma}{}_{j\mu}\,(j_0'\boldsymbol{j}'[ms])^{\sigma'}{}_{j'\mu'} = \sum_{\bar\sigma=|\sigma-\sigma'|}^{\sigma+\sigma'}\ \sum_{\bar j=|j-j'|}^{j+j'}\ \sum_{\bar\mu=-\bar j}^{\bar j}\ \sum_{j_0=-\min(\bar\sigma,\bar j)}^{\min(\bar\sigma,\bar j)} \times \int_0^{i\infty}\frac{1}{i}\,d\bar{\boldsymbol{j}}\begin{pmatrix}[ms] & [ms] & \bar j_0\bar{\boldsymbol{j}}\\ j_0\boldsymbol{j} & j_0'\boldsymbol{j}' & [ms]\end{pmatrix}^{\bar\sigma\bar j\bar\mu}_{\sigma j\mu;\sigma' j'\mu'}(\bar j_0\bar{\boldsymbol{j}}[ms])_{\bar j\bar\mu}, \quad (4.6a)$$

with the structure constants

$$\begin{pmatrix}[ms] & [ms] & \bar j_0\bar{\boldsymbol{j}}\\ j_0\boldsymbol{j} & j_0'\boldsymbol{j}' & [ms]\end{pmatrix}^{\bar\sigma\bar j\bar\mu}_{\sigma j\mu;\sigma' j'\mu'} = \frac{[(2\sigma+1)(2\sigma'+1)]^{\frac{1}{2}}}{4\pi m^2}\,\rho_{\sigma}[j_0\boldsymbol{j}]\rho_{\sigma'}[j_0'\boldsymbol{j}'](\rho_{\bar\sigma}[\bar j_0\bar{\boldsymbol{j}}])^{-1} \times (-1)^{2s-\sigma}\begin{Bmatrix}\sigma & \sigma' & \bar\sigma\\ s & s & s\end{Bmatrix}\langle {}^{\sigma\ \ \sigma'}_{j_0\boldsymbol{j}\ j_0'\boldsymbol{j}'} \mid {}^{\bar\sigma}_{\bar j_0\bar{\boldsymbol{j}}}\rangle\langle {}^{\bar j\bar\mu}_{\bar j_0\bar{\boldsymbol{j}}} \mid {}^{j_0 j\ \ j_0'j'}_{j\ \mu\ \ j'\mu'}\rangle. \quad (4.6b)$$

With respect to ordinary operator multiplication (matrix multiplication), the set of the $[ISO(3,1)\uparrow SO(3,1)]$-irreducible tensor operators (2.25) is therefore closed. In contrast, the ordinary operator product of two $[ISO(3,1)\uparrow SO(2,1)]$-irreducible tensors (2.1) can be expressed as an (infinite) linear superposition of the tensor operators (2.1) at zero 4-momentum transfer ($Q=0$). In accordance with the decomposition (2.50), these tensor operators are not Poincaré-irreducible. Consequently, the Poincaré-irreducible tensorial set (2.1), $Q<0$, is not closed under ordinary operator multiplication. Equations (4.6) therefore constitute the relativistic generalization of the Biedenharn relation (4.1).

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Theorem on the Convergence Rate of Generalized Fourier Series*

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We prove a theorem on the convergence rate of generalized Fourier expansions. Our result is not restricted to any particular basis.

1. INTRODUCTION

We wish to consider the expansion of a state $|f\rangle$ in an orthonormal basis $|n\rangle$. In many particular problems, where the bases are classical orthogonal polynomials, the rate of convergence is well known.[1,2] However, few results are known for expansions in more complicated bases. Recently, new efforts in obtaining more general results have been very fruitful.[3] The theorem we present gives a bound on the rate of convergence which holds in general.

Section 2 contains the statement and proof of the theorem. This theorem shows how the rate of convergence depends on the properties of $|f\rangle$. The final section presents some brief examples.

2. CONVERGENCE RATE

Let $\Lambda_1, \Delta_2, \cdots, \Lambda_r$ be a set of operators with a corresponding complete orthonormal basis $|n\rangle$. The label n represents the complete set of labels needed to specify the state. These vectors are the eigenvectors of the Λ_i with eigenvalues $\lambda_i(n)$,

$$\Lambda_i |n\rangle = \lambda_i(n) |n\rangle. \tag{1}$$

For any state $|f\rangle$ in the space spanned by the basis we have

$$|f\rangle = \sum a(n) |n\rangle,$$

where the expansion coefficients are

$$a(n) = \langle n | f\rangle.$$

Theorem 1: If the quantities $(\Lambda_i)^{\sigma_i} |f\rangle$ are bounded, then the expansion coefficients are bounded:

$$|a(n)| \leq \|(\Lambda_i)^{\sigma_i} |f\rangle\| / |\lambda_i(n)^{\sigma_i}|$$

Proof: From the orthogonality of the basis states and (1) we have

$$\Lambda_i^+ |n\rangle = \lambda_i^*(n) |n\rangle. \tag{2}$$

Operate on $|f\rangle$ with the operator Λ_i as many times as the result is bounded in norm, that is, σ_i times. Then take the scaler product with $\langle m|$ and from (1) and (2) we have

$$\langle m | (\Lambda_i)^{\sigma_i} |f\rangle = \langle f | (\Lambda_i^+)^{\sigma_i} |m\rangle^* = \lambda_i(m)^{\sigma_i} a(m)$$

or dividing by $\lambda_i(m)^{\sigma_i}$

$$a(m) = \langle m | (\Lambda_i)^{\sigma_i} |f\rangle / \lambda_i(m)^{\sigma_i}.$$

Finally using the Schwartz inequality, we have

$$|a(m)| \leq \|(\Lambda_i)^{\sigma_i} |f\rangle\| / |\lambda_i(m)^{\sigma_i}|.$$

It is important to realize that the σ_i can all be very different and that the utility of this result depends on finding a Λ_i such that $\lambda_i(n)$ is an increasing function of n. In addition, we are not restricted to local differential operators or any particular representation. In many familiar cases Λ_i is a differential operator, and then the theorem connects the rate of decrease of $a(n)$ with the degree of differentiability of $\langle X_1, X_2, \cdots, X_r | f\rangle$.

3. EXAMPLES

Our first example is the classic Fourier series where we use the complex form

$$f(\Phi) = \sum_{m=-\infty}^{m=\infty} a(m) \frac{e^{im\Phi}}{(2\pi)^{\frac{1}{2}}}.$$

The appropriate operator is L_z, which corresponds to $-id/d\Phi$. In this case we have

$$|a(m)| \leq |m^\sigma|^{-1} \|(L_z)^\sigma |f\rangle\|$$

or

$$|a(m)| \leq |m^\sigma|^{-1} \left(\left(-i \frac{d}{d\Phi} \right)^\sigma f(\Phi), \left(-i \frac{d}{d\Phi} \right)^\sigma f(\Phi) \right)^{\frac{1}{2}}.$$

If $f(\Phi)$ is differentiable k times, we have $\sigma = k$. If we know that the $k+1$ derivative is of bounded variation, we have $\sigma = k+1$. This case is especially simple and often treated in the literature.[1,2,4]

The second example is that of the spherical harmonics

$$f(\theta, \phi) = \sum_l \sum_m a(l, m) Y_{lm}(\theta, \phi).$$

The operators here are very familiar ones, namely, L^2 and L_z:

$$L^2 |l, m\rangle = l(l+1) |l, m\rangle, \; L_z |l, m\rangle = m |l, m\rangle.$$

Thus we have

$$|a(l, m)| \leq [|l(l+1)|^{\sigma_1}]^{-1} \|(L^2)^{\sigma_1} |f\rangle\|$$

and

$$|a(l, m)| \leq (|m|^{\sigma_2})^{-1} \|(L_z)^{\sigma_2} |f\rangle\|,$$

or, combining these, we get

$$|a(l, m)| \leq [|l(l+1)|^{\sigma_1}]^{-1}(|m|^{\sigma_2})^{-1} \|(L^2)^{\sigma_1}(L_z)^{\sigma_2} |f\rangle\|,$$

where this last result only holds if the resulting norm is bounded. We are presently applying this result to the convergence properties of generalized spherical harmonic expansions applied to the three-body problem.

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Group-Theoretic Derivation of Crossing Sum Rules

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Crossing relations between amplitudes with definite isospin for $\pi\pi$ scattering are expressed in terms of the symmetric group S_3. The sum rules, involving s-channel partial wave amplitudes, are then derived without reference to the Balachandran and Nuyts expansion and are shown to be a direct consequence of the group-theoretic orthogonality relations. This results in closed expressions for all possible sum rules.

1. INTRODUCTION

In this paper we give an alternative derivation of the sum rules for the $\pi\pi$ partial wave amplitudes derived by Roskies[1] as a consequence of isospin invariance and crossing. By emphasizing the role played by the symmetric group S_3, we have avoided the use of the Balachandran and Nuyts expansion.[2] The approach is analogous to that used by Basdevant, Cohen-Tannoudji, and Morel[3] in deducing πK crossing sum rules, where the relevant group is S_2. (We are grateful to Professor A. Martin for drawing our attention to this work.)

The purpose of Sec. 2 is to summarize a few notions concerning the group S_3 and its representations. We calculate the projection operators for the irreducible representations and prove a simple orthogonality relation, which is the basis of the sum rules. We also introduce the isospin amplitudes and show how the crossing conditions imply very simple transformation properties for certain linear combinations of the amplitudes. The group theory for this section may be found in the book by Hamermesh.[4]

Section 3 is devoted to the explicit derivation of the $\pi\pi$ crossing sum rules from the group-theoretic properties already given. Since the sum rules so obtained correspond to integrals over definite orthogonal polynomials in two variables, we have been able to suppress the apparent arbitrariness in the results of Ref. 3 without having to go through the complicated derivations of Ref. 1. This indeed allows us to write closed expressions for all possible sum rules of arbitrary order, which are both necessary and sufficient to ensure the known crossing properties of the full scattering amplitude.

2. GROUP-THEORETIC PRELIMINARIES

The permutation group (S_3) on three objects (s, t, and u in the present case), which is isomorphic with the group of operations leaving an equilateral triangle invariant, has the following elements:

$$\begin{pmatrix} s\,t\,u \\ s\,t\,u \end{pmatrix} = E, \qquad \begin{pmatrix} s\,t\,u \\ t\,u\,s \end{pmatrix} = C = (stu),$$

$$\begin{pmatrix} s\,t\,u \\ u\,s\,t \end{pmatrix} = C^2 = (sut), \qquad \begin{pmatrix} s\,t\,u \\ s\,u\,t \end{pmatrix} = \sigma = (tu),$$

$$\begin{pmatrix} s\,t\,u \\ t\,s\,u \end{pmatrix} = \sigma C = (st), \qquad \begin{pmatrix} s\,t\,u \\ u\,t\,s \end{pmatrix} = \sigma C^2 = (su),$$

where the final column represents the elements written in cyclic notation.

In terms of the dihedral group D_3, the elements have the following interpretation: C is a rotation of $2\pi/3$ in the plane of the triangle and σ is a reflection in the line containing the center and the vertex s.

and

$$|a(l, m)| \leq (|m|^{\sigma_2})^{-1} \|(L_z)^{\sigma_2} |f\rangle\|,$$

or, combining these, we get

$$|a(l, m)| \leq [|l(l+1)|^{\sigma_1}]^{-1}(|m|^{\sigma_2})^{-1} \|(L^2)^{\sigma_1}(L_z)^{\sigma_2} |f\rangle\|,$$

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$$\begin{pmatrix} s\,t\,u \\ t\,s\,u \end{pmatrix} = \sigma C = (st), \qquad \begin{pmatrix} s\,t\,u \\ u\,t\,s \end{pmatrix} = \sigma C^2 = (su),$$

where the final column represents the elements written in cyclic notation.

In terms of the dihedral group D_3, the elements have the following interpretation: C is a rotation of $2\pi/3$ in the plane of the triangle and σ is a reflection in the line containing the center and the vertex s.

The most useful results from the multiplication table are the following:

$$\sigma^2 = E, \quad C^3 = E, \quad \sigma C = C^2\sigma, \quad \sigma C^2 = C\sigma.$$

There are only three inequivalent irreducible unitary representations of S_3:

(1) the symmetric representation

$$D^1(g) = 1 \ \forall \ g \in S_3,$$

(2) the alternating representation

$$D^2(g) = 1 \ \forall \ g \in A_3$$
$$= -1 \text{ for the remainder,}$$

[A_3 is the alternating subgroup of S_3 .]

(3) the two-dimensional representation D^3 which is chosen as follows ($\omega^3 = 1$, $\omega^2 + \omega + 1 = 0$):

$$D^3(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$D^3(\sigma) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$D^3(C) = \tfrac{1}{2}\begin{pmatrix} -1 & 1+2\omega \\ 1+2\omega & -1 \end{pmatrix},$$

$$D^3(\sigma C) = \tfrac{1}{2}\begin{pmatrix} -1 & 1+2\omega \\ -1-2\omega & 1 \end{pmatrix},$$

$$D^3(C^2) = \tfrac{1}{2}\begin{pmatrix} -1 & -1-2\omega \\ -1-2\omega & -1 \end{pmatrix},$$

$$D^3(\sigma C^2) = \tfrac{1}{2}\begin{pmatrix} -1 & -1-2\omega \\ 1+2\omega & 1 \end{pmatrix}.$$

As in Ref. 4, we define projection operators corresponding to these irreducible representations as follows:

$$\hat{P}_i^\mu = (n_\mu/|G|)\sum_{g\in G} D_{ii}^\mu(g^{-1})\hat{g},$$

where n_μ is the dimension of D^μ, $|G|$ is the order of the group (6 in the case where $G = S_3$), and $\hat{g}$ is the operator corresponding to $g \in G$. For $g \in S_3$, $\hat{g}$ acts on any function of s, t, and u: E.g., $\hat{C}f(s,t,u) = f(t,u,s)$.

In Appendix A we show that

$$\hat{P}_i^\mu \hat{P}_j^\nu = \delta_{\mu\nu}\delta_{ij}\hat{P}_i^\mu, \tag{2.1}$$

as is expected.

The projection operators for the various representations are given below.

1. Symmetric representation: Write

$$\hat{S} = \hat{P}_1^1, \quad n_1 = 1, \quad D_{11}^1(g^{-1}) = 1 \ \forall \ g \in S_3.$$
$$\hat{S} = \tfrac{1}{6}(\hat{E} + \hat{\sigma})(\hat{E} + \hat{C} + \hat{C}^2)$$
$$= \tfrac{1}{6}(\hat{E} + \hat{C} + \hat{C}^2)(\hat{E} + \hat{\sigma}).$$

2. Alternating representation: Write

$$\hat{A} = \hat{P}_1^2, \quad n_2 = 1, \quad D_{11}^2(g^{-1}) = 1 \ \forall \ g \in A_3,$$
$$= -1 \text{ for the remainder.}$$
$$\hat{A} = \tfrac{1}{6}(\hat{E} - \hat{\sigma})(\hat{E} + \hat{C} + \hat{C}^2)$$
$$= \tfrac{1}{6}(\hat{E} + \hat{C} + \hat{C}^2)(\hat{E} - \hat{\sigma}).$$

3. Two-dimensional representation:

$$\hat{M}_1 = \hat{P}_1^3, \quad \hat{M}_2 = \hat{P}_2^3, \quad n_3 = 2.$$
$$\hat{M}_1 = \tfrac{1}{6}(\hat{E} + \hat{\sigma})(2\hat{E} - \hat{C} - \hat{C}^2)$$
$$= \tfrac{1}{6}(2\hat{E} - \hat{C} - \hat{C}^2)(\hat{E} + \hat{\sigma}),$$
$$\hat{M}_2 = \tfrac{1}{6}(\hat{E} - \hat{\sigma})(2\hat{E} - \hat{C} - \hat{C}^2)$$
$$= \tfrac{1}{6}(2\hat{E} - \hat{C} - \hat{C}^2)(\hat{E} - \hat{\sigma}).$$

It is simple to show explicitly that (2.1) is satisfied. The following obvious relations are also useful:

$$\tfrac{1}{2}(\hat{E} + \hat{\sigma}) = \hat{S} + \hat{M}_1, \quad \tfrac{1}{2}(\hat{E} - \hat{\sigma}) = \hat{A} + \hat{M}_2,$$
$$\tfrac{1}{3}(\hat{E} + \hat{C} + \hat{C}^2) = \hat{S} + \hat{A},$$
$$\tfrac{1}{3}(2\hat{E} - \hat{C} - \hat{C}^2) = \hat{M}_1 + \hat{M}_2.$$

So we deduce $\hat{S} + \hat{A} + \hat{M}_1 + \hat{M}_2 = \hat{E}$, and we may write any function $f(s,t,u)$ in the form $f = \hat{S}f + \hat{A}f + \hat{M}_1 f + \hat{M}_2 f$. Now we define a bilinear form (f,f'):

$$(f,f') = \iiint_\Delta ds\, dt\, du\, \delta(s + t + u - 4\mu^2)$$
$$\times f(s,t,u)f'(s,t,u),$$

where Δ is the triangular region of the Mandelstam diagram; f and f' are arbitrary functions of s, t, and u; and the latter have their usual interpretation. μ is the mass of the pion. This bilinear form has the obvious but important property that

$$(\hat{g}f, \hat{g}f') = (f,f'), \tag{2.2}$$

where g is any member of S_3. We next prove a simple orthogonality property:

$$(\hat{P}_i^\mu f, \hat{P}_j^\nu f')$$
$$= (n_\mu/|S_3|)\sum_{g\in S_3} D_{ii}^\mu(g^{-1})(\hat{g}f, \hat{P}_j^\nu f') \quad \text{(bilinearity)}$$
$$= (n_\mu/|S_3|)\sum_{g\in S_3} D_{ii}^\mu(g^{-1})(f, \hat{g}^{-1}\hat{P}_j^\nu f') \quad \text{(from 2.2)}$$
$$= (n_\mu/|S_3|)\sum_{g_1\in S_3} \{D^\mu(g_1^{-1})\}_{ii}^{-1}(f, \hat{g}_1\hat{P}_j^\nu f').$$

However, $(D^\mu)_{ii}^{-1} = (D^\mu)_{ii}^*$ from unitarity and, for our representations, $(D^\mu)_{ii}^* = D_{ii}^\mu$; so, using the bilinearity property again, we have

$$(\hat{P}_i^\mu f, \hat{P}_j^\nu f') = (f, \hat{P}_i^\mu \hat{P}_j^\nu f')$$
$$= \delta_{ij}\delta_{\mu\nu}(f, \hat{P}_i^\mu f') \quad \text{from (2.1).}$$

This gives us twelve orthogonality relations, such as

$$\iint_\Delta ds\,dt\,(\hat{S}f)(\hat{A}f') = 0,$$

$$\iint_\Delta ds\,dt\,(\hat{A}f)(\hat{M}_1 f') = 0, \tag{2.3}$$

$$\iint_\Delta ds\,dt\,(M_1 f)(M_2 f') = 0,$$

etc.

We now turn to the $\pi\pi$ s-channel amplitude, as written by Chew and Mandelstam[5]:

$$T_{\alpha\beta,\gamma\delta}(s,t,u) = \delta_{\alpha\beta}\delta_{\gamma\delta}A(s,t,u) + \delta_{\alpha\gamma}\delta_{\beta\delta}B(s,t,u) + \delta_{\alpha\delta}\delta_{\beta\gamma}C(s,t,u),$$

where crossing implies

$$A(s,t,u) = A(s,u,t), \tag{2.4}$$

$$B(s,t,u) = A(t,s,u), \tag{2.5}$$

$$C(s,t,u) = A(u,t,s). \tag{2.6}$$

The isospin invariant amplitudes are

$$F^{(0)} = 3A + B + C, \tag{2.7}$$

$$F^{(1)} = B - C, \tag{2.8}$$

$$F^{(2)} = B + C. \tag{2.9}$$

Via the elements of S_3, (2.4)–(2.6) become

$$A = \hat{\sigma}A, \quad B = \hat{\sigma}\hat{C}A, \quad C = \hat{\sigma}\hat{C}^2A, \tag{2.10}$$

and (2.7)–(2.9) become

$$F^{(0)} = 3A + (\hat{C} + \hat{C}^2)A = 3A + F^{(2)},$$
$$F^{(1)} = (\hat{C}^2 - \hat{C})A, \quad F^{(2)} = (\hat{C} + \hat{C}^2)A,$$

where use has been made of (2.10).

We now have the following results immediately:

$$\hat{S}A = \tfrac{1}{3}(\hat{E} + \hat{C} + \hat{C}^2)A, \qquad \hat{A}A = 0,$$
$$\hat{M}_1A = \tfrac{1}{3}(2\hat{E} - \hat{C} - \hat{C}^2)A, \quad \hat{M}_2A = 0,$$

and, in consequence,

$$\left.\begin{aligned} \hat{S}F^{(2)} &= 2\hat{S}A \\ \hat{A}F^{(2)} &= 0 \\ \hat{M}_1F^{(2)} &= -\hat{M}_1A \\ \hat{M}_2F^{(2)} &= 0 \end{aligned}\right\} \Rightarrow F^{(2)} = (\hat{S} + \hat{M}_1)F^{(2)} = (2\hat{S} - \hat{M}_1)A, \tag{2.11}$$

$$\left.\begin{aligned} \hat{S}F^{(0)} &= 5\hat{S}A \\ \hat{A}F^{(0)} &= 0 \\ \hat{M}_1F^{(0)} &= 2\hat{M}_1A \\ \hat{M}_2F^{(0)} &= 0 \end{aligned}\right\} \Rightarrow F^{(0)} = (\hat{S} + \hat{M}_1)F^{(0)} = (5\hat{S} + 2\hat{M}_1)A, \tag{2.12}$$

$$\hat{S}F^{(1)} = \hat{A}F^{(1)} = \hat{M}_1F^{(0)} = 0, \quad \hat{M}_2F^{(1)} = F^{(1)}. \tag{2.13}$$

Then (2.11) and (2.13) imply

$$\hat{S}A = \tfrac{1}{9}(F^{(0)} + 2F^{(2)}), \tag{2.14}$$

$$\hat{M}_1A = \tfrac{1}{9}(2F^{(0)} - 5F^{(2)}). \tag{2.15}$$

Incidentally, we notice at once from these results that since $\hat{S}F^{(1)} = 0$ and $\hat{S}(F^{(0)} - 5F^{(2)}) = 0$ at the symmetry point $s = t = u = 4\mu^2/3$, $F^{(1)} = 0$ and $F^{(2)} = 2F^{(0)}/5$ at this point—a result noted by Basdevant *et al.*[3]

If we re-express (2.13), (2.14), and (2.15) in terms of A, B, and C, we have

$$(\hat{S} - \hat{E})(A + B + C) = 0, \tag{2.16}$$

$$(\hat{M}_1 - \hat{E})(2A - B - C) = 0, \tag{2.17}$$

$$(\hat{M}_2 - \hat{E})(B - C) = 0. \tag{2.18}$$

Clearly these conditions are necessary, but it is not difficult, though somewhat tedious, to show that they are not sufficient to ensure the crossing relations (2.4)–(2.6). In fact, there is another relation

$$(\hat{C}^2 - \hat{C})(2A - B - C) = 3(B - C); \tag{2.19}$$

in Appendix B it is shown that the relations (2.16)–(2.19) are indeed sufficient.

3. $\pi\pi$ SUM RULES DERIVED

Using the conditions imposed on the amplitudes A, B, and C by crossing symmetry, we have seen that we can form certain linear combinations of the isospin amplitudes that transform irreducibly under S_3. Our aim is to impose these crossing relations on the partial wave amplitudes, by using the orthogonality relations proved above [Eq. (2.3)].

Then, via Eqs. (2.16)–(2.18), the orthogonality relations immediately give

$$\iint_\Delta ds\,dt\,(F^{(0)} + 2F^{(2)}) \begin{bmatrix} \hat{A} \\ \hat{M}_1 \\ \hat{M}_2 \end{bmatrix} G(s,t,u) = 0, \tag{3.1a–c}$$

$$\iint_\Delta ds\,dt\,(2F^{(0)} - 5F^{(2)}) \begin{bmatrix} \hat{S} \\ \hat{A} \\ \hat{M}_2 \end{bmatrix} G(s,t,u) = 0, \tag{3.2a–c}$$

$$\iint_\Delta ds\,dt\,F^{(1)} \begin{bmatrix} \hat{S} \\ \hat{A} \\ \hat{M}_1 \end{bmatrix} G(s,t,u) = 0, \tag{3.3a–c}$$

where $G(s,t,u)$ is an arbitrary analytic function.

We next consider the remaining condition implied by crossing symmetry [Eq. (2.19)],

$$(\hat{C}^2 - \hat{C})(2A - B - C) = 3(B - C)$$

and

$$\hat{M}_2(\hat{C}^2 - \hat{C})(2A - B - C) = 3\hat{M}_2(B - C) = 3(B - C).$$

Then, for an arbitrary function $G(s, t, u)$,

$$\iiint_\Delta ds\, dt\, du\, \delta(s + t + u - 4\mu^2) \times [\tfrac{1}{9}(\hat{C} - \hat{C}^2)(2F^{(0)} - 5F^{(2)}) + F^{(1)}]G(s, t, u) = 0;$$

but we recall that the functions $(\hat{C} - \hat{C}^2)(2F^{(0)} - 5F^{(2)})$ and $F^{(1)}$ both transform irreducibly under $\hat{M}_2$, and we have already used the orthogonality properties of these functions with $\hat{S}G$, $\hat{A}G$, and $\hat{M}_1G$ in Eqs. (3.3) and (3.4). Therefore, the only new equation is

$$\iiint_\Delta ds\, dt\, du\, \delta(s + t + u - 4\mu^2) \times [\tfrac{1}{9}(\hat{C} - \hat{C}^2)(2F^{(0)} - 5F^{(2)}) + F^{(1)}]\hat{M}_2G(s, t, u) = 0.$$

As it stands this integral is still not useful, since the integrand vanishes identically. However, we can use the crossing symmetric form of the measure to obtain

$$\iiint_\Delta ds\, dt\, du\, \delta(s + t + u - 4\mu^2) \times \{\tfrac{1}{9}(2F^{(0)} - 5F^{(2)})\hat{M}_2[G(u, t, s) - G(t, s, u)] + F^{(1)}\hat{M}_2G(s, t, u)\} = 0. \quad (3.4)$$

The sum rules now follow by using the above relations to project out partial waves. We therefore define the s-channel I-spin partial waves

$$f_l^{(I)}(s) = \tfrac{1}{2}\int_{-1}^{1} dz_s\, F^{(I)}(s, t, u)P_l(z_s),$$

where

$$z_s = 1 + 2t/(s - 4\mu^2), \quad \text{with } \mu = \text{pion mass.}$$

We first look at Eqs. (3.1a), (3.1c), (3.2b), (3.2c), (3.3a), and (3.3c), and see that they are satisfied by the well-known requirements that

$$f_{2l+1}^{(0)}(s) = f_{2l+1}^{(2)}(s) = f_{2l}^{(1)}(s) = 0, \quad \text{for all } l, s.$$

[This is because $\hat{A}G(s, z_s)$ and $\hat{M}_2G(s, z_s)$ are antisymmetric under the interchange of t and u, and so can be functions of only odd powers of z_s, while $\hat{S}G$ and $\hat{M}_1G$ are functions of only even powers of z_s.]

This leaves us with the following four integrals:

$$\iint_\Delta ds\, dt\, (2F^{(0)} - 5F^{(2)})\hat{S}G(s, t, u) = 0, \quad (3.5)$$

$$\iint_\Delta ds\, dt\, F^{(1)}\hat{A}G(s, t, u) = 0, \quad (3.6)$$

$$\iint_\Delta ds\, dt\, (F^{(0)} + 2F^{(2)})\hat{M}_1G(s, t, u) = 0, \quad (3.7)$$

$$\iint_\Delta ds\, dt\, \{\tfrac{1}{9}(2F^{(0)} - 5F^{(2)})\hat{M}_2[G(u, t, s) - G(t, s, u)] + F^{(1)}\hat{M}_2G(s, t, u)\} = 0. \quad (3.8)$$

In the above integrals (3.5)–(3.8), we are free to choose any $G(s, t, u)$ which is an analytic function of its arguments. This analyticity requirement allows us to express G in powers of s, t, and u. We now first construct the most general crossing symmetric function $\hat{S}G$. To do this, it is useful to change to crossing symmetric variables[1]: $w = s + t + u = 4\mu^2$, $x = st + tu + us$, $y = stu$.

Then $\hat{S}G$ will be polynomial in w, x, y, so that we can write

$$\hat{S}G(s, t, u) = \sum_{m,n} \lambda_{mn}x^m y^n,$$

where λ_{mn} are arbitrary constants.

We see that the integral (3.5) vanishes for all crossing symmetric functions, and so vanishes for each value of (m, n) separately, regardless of λ_{mn}.

We consider next the integrals (3.6)–(3.8). As shown by Roskies,[1] we can write arbitrary $\hat{A}G$, $\hat{M}_1G$, and $\hat{M}_2G$ as follows:

$$\hat{A}G(s, t, u) = (s - t)(t - u)(u - s)g_1(s, t, u),$$
$$\hat{M}_1G(s, t, u) = (2s - t - u)g_2(s, t, u) + (2s^2 - t^2 - u^2)g_3(s, t, u),$$
$$\hat{M}_2G(s, t, u) = (t - u)g_4(s, t, u) + (t^2 - u^2)g_5(s, t, u),$$

where the g_i, $i = 1, \cdots, 5$, are arbitrary functions symmetric in their arguments, which we know we can write as

$$g_i(s, t, u) = \sum_{m,n} \lambda_{mn}^{(i)}x^m y^n.$$

Again we see that the integrals (3.6)–(3.8) will now vanish for each (m, n), regardless of the $\lambda_{mn}^{(i)}$. By writing the integrals in the form of the orthogonality relations, we see we have removed the necessity for introducing the infinite set of arbitrary constants $\lambda_{m,n}^{(i)}$. These correspond to the arbitrary constants that Roskies finds he has to eliminate before he can write each sum rule.

We now go on to write closed expressions for all the $\pi\pi$ sum rules. We take

$$\hat{A}G(s, t, u) = [(4\mu^2 - s)(3s - 4\mu^2)^2 z_s - (4\mu^2 - s)^3 z_s^3]x^m y^n, \quad (3.9)$$

$$\hat{M}_1G(s, t, u) = (3s - 4\mu^2)x^m y^n, \quad (3.10)$$

$$= [4s^2 - (4\mu^2 - s)^2 - (4\mu^2 - s)^2 z_s^2]x^m y^n, \quad (3.11)$$

$$\hat{M}_2G(s, t, u) = (4\mu^2 - s)z_s x^m y^n, \quad (3.12)$$

$$= (4\mu^2 - s)^2 z_s x^m y^n; \quad (3.13)$$

then

$$\hat{M}_2[G(u,t,s)-G(t,s,u)]$$
$$=(3s-4\mu^2)x^m y^n \tag{3.14}$$
$$=\tfrac{1}{2}[4s^2-(4\mu^2-s)^2-(4\mu^2-s)^2 z_s^2]x^m y^n, \tag{3.15}$$

respectively.

We next express $x^m y^n$ in terms of s and z as

$$x^m y^n=\frac{m!\,n!}{4^{m+n}}\sum_{j=0}^{m}\sum_{k=0}^{n}\times\frac{(-1)^{j+k}s^n(4\mu^2-s)^{j+m+2n}(3s+4\mu^2)^{m-j}}{j!\,k!\,(m-j)!\,(n-k)!}\cdot z^{2(j+k)},$$

and we substitute this form into Eqs. (3.9)–(3.15) in turn, and putting these into their respective orthogonality relations [Eqs. (3.5)–(3.8)] gives us, on performing the z_s integration, the required closed expressions, which we simplify by first defining the two terms a^i_{jkl} and ξ^i_{jkl}:

$$a^0_{jkl}=\frac{4^l(4l+1)(j+k+l)!(2j+2k)!}{(j+k-l)!(2j+2k+2l+1)!},$$
$$a^1_{jkl}=\frac{4^l(4l+3)(j+k+l+1)!(2j+2k+2)!}{(j+k+1)(j+k-l)!(2j+2k+2l+3)!},$$
$$a^2_{jkl}=\frac{4^l(4l+1)(j+k+l+1)!(2j+2k+2)!}{(j+k-l+1)!(2j+2k+2l+3)!},$$
$$a^3_{jkl}=\frac{4^l(4l+3)(j+k+l+2)!(2j+2k+4)!}{(j+k+2)(j+k-l+1)!(2j+2k+2l+5)!},$$

and

$$\xi^i_{jkl}=\frac{(-1)^{j+k}a^i_{jkl}}{j!\,k!\,(m-j)!\,(n-k)!}.$$

We now write the closed forms for all the crossing sum rules with the following notational simplification:

$$\sum\!\!\int\equiv\sum_{j=0}^{m}\sum_{k=0}^{n}\int_0^{4\mu^2}ds;$$

we then have, from Eqs. (3.5)–(3.8)

$$\sum\!\!\int s^n(4\mu^2-s)^{j+m+2n+1}(3s+4\mu^2)^{m-j}\times\sum_{l=0}^{j+k}\xi^0_{jkl}[2f^{(0)}_{2l}(s)-5f^{(2)}_{2l}(s)]=0, \tag{3.16}$$

$$\sum\!\!\int s^n(4\mu^2-s)^{j+m+2n+2}(3s+4\mu^2)^{m-j}\times\Big((3s-4\mu^2)^2\sum_{l=0}^{j+k}\xi^1_{jkl}f^{(1)}_{2l+1}(s)-(4\mu^2-s)^2\sum_{l=0}^{j+k+1}\xi^3_{jkl}f^{(1)}_{2l+1}(s)\Big)=0, \tag{3.17}$$

$$\sum\!\!\int s^n(4\mu^2-s)^{j+m+2n+1}(3s+4\mu^2)^{m-j}(3s-4\mu^2)\times\sum_{l=0}^{j+k}\xi^0_{jkl}[f^{(0)}_{2l}(s)+2f^{(2)}_{2l}(s)]=0, \tag{3.18}$$

$$\sum\!\!\int s^n(4\mu^2-s)^{j+m+2n+1}(3s+4\mu^2)^{m-j}\times\Big([4s^2-(4\mu^2-s)^2]\sum_{l=0}^{j+k}\xi^0_{jkl}[f^{(0)}_{2l}(s)+2f^{(2)}_{2l}(s)]-(4\mu^2-s)^2\sum_{l=0}^{j+k+1}\xi^2_{jkl}[f^{(0)}_{2l}(s)+2f^{(2)}_{2l}(s)]\Big)=0, \tag{3.19}$$

$$\sum\!\!\int s^n(4\mu^2-s)^{j+m+2n+1}(3s+4\mu^2)^{m-j}\times\Big((3s-4\mu^2)\sum_{l=0}^{j+k}\xi^0_{jkl}[2f^{(0)}_{2l}(s)-5f^{(2)}_{2l}(s)]+9(4\mu^2-s)\sum_{l=0}^{j+k}\xi^1_{jkl}f^{(1)}_{2l+1}(s)\Big)=0, \tag{3.20}$$

$$\sum\!\!\int s^n(4\mu^2-s)^{j+m+2n+1}(3s+4\mu^2)^{m-j}\times\Big([4s^2-(4\mu^2-s)^2]\sum_{l=0}^{j+k}\xi^0_{jkl}[2f^{(0)}_{2l}(s)-5f^{(2)}_{2l}(s)]-(4\mu^2-s)^2\sum_{l=0}^{j+k+1}\xi^2_{jkl}[2f^{(0)}_{2l}(s)-5f^{(2)}_{2l}(s)]+18(4\mu^2-s)^2\sum_{l=0}^{j+k}\xi^1_{jkl}f^{(1)}_{2l+1}(s)\Big)=0, \tag{3.21}$$

with $m, n = 0, 1, 2, \cdots, \infty$.

We shall now use these closed expressions to obtain the crossing conditions on the lowest $\pi\pi$ partial waves.

(i) We consider Eq. (3.16) with $m=n=0$; then we have immediately that

$$\int_0^{4\mu^2}ds\,[(4\mu^2-s)(2f^{(0)}_0(s)-5f^{(2)}_0(s)]=0. \tag{3.22}$$

(ii) We now turn to Eq. (3.17) with $m=n=0$, which gives

$$\int_0^{4\mu^2}ds\,(4\mu^2-s)(21s^2-48\mu^2 s+16\mu^4)f^{(1)}_1(s)=\int_0^{4\mu^2}ds\,(4\mu^2-s)^4 f^{(1)}_3(s). \tag{3.23}$$

(iii) We take Eq. (3.18) in its simplest form, i.e., with $m=n=0$; then

$$\int_0^{4\mu^2}ds\,(4\mu^2-s)(3s-4\mu^2)[f^{(0)}_0(s)+2f^{(2)}_0(s)]=0. \tag{3.24}$$

(iv) We next consider Eq. (3.20) with $m=n=0$; then

$$\int_0^{4\mu^2}ds\,(4\mu^2-s)(3s-4\mu^2)[2f^{(0)}_0(s)-5f^{(2)}_0(s)]=-9\int_0^{4\mu^2}ds\,(4\mu^2-s)^2 f^{(1)}_1(s). \tag{3.25}$$

There are two more sum rules which just involve s and p waves, which can be obtained as follows:

(v) We consider Eq. (3.21) in its simplest form

$(m = n = 0)$, which gives us

$$\int_0^{4\mu^2} ds\,(4\mu^2 - s) \times \{(4s^2 + 16\mu^2 s - 32\mu^4)[2f_0^{(0)}(s) - 5f_0^{(2)}(s)] - (4\mu^2 - s)^2[2f_2^{(0)}(s) - 5f_2^{(2)}(s)] + 27(4\mu^2 - s)^2 f_1^{(1)}(s)\} = 0. \quad (3.26)$$

To eliminate the d-wave term, we consider Eq. (3.16) with $m = 1$, $n = 0$:

$$\int_0^{4\mu^2} ds\,(4\mu^2 - s)^2\{(5s + 4\mu^2)[2f_0^{(0)}(s) - 5f_0^{(2)}(s)] - (4\mu^2 - s)[2f_2^{(0)}(s) - 5f_2^{(2)}(s)]\} = 0. \quad (3.27)$$

We subtract this from Eq. (3.26) to give us

$$\int_0^{4\mu^2} ds\,(4\mu^2 - s)s^2[2f_0^{(0)}(s) - 5f_0^{(2)}(s)] = -3\int_0^{4\mu^2} ds\,(4\mu^2 - s)^3 f_1^{(1)}(s). \quad (3.28)$$

(vi) To obtain the last sum rule involving just s and p waves, we first consider Eq. (3.20) with $m = 1$, $n = 0$. This relates the s and d waves of $(2F^{(0)} - 5F^{(2)})$ to the p and f waves of $F^{(1)}$. To eliminate the $f_3^{(1)}$ term, we use Eq. (3.23) and, to eliminate the $(2f_2^{(0)} - 5f_2^{(2)})$ term, we need to use Eq. (3.16) with $m = 0$, $n = 1$ and $m = 1$, $n = 0$. We then finally obtain

$$\int_0^{4\mu^2} ds\, s^2(4\mu^2 - s)^2[2f_0^{(0)}(s) - 5f_0^{(2)}(s)] = -3\int_0^{4\mu^2} ds\, s(4\mu^2 - s)^2(8\mu^2 - 3s)f_1^{(1)}(s). \quad (3.29)$$

We conclude by noting that we can reverse the general procedure given above, so that we can write a set of orthogonality relations involving $(2F^{(0)} - 5F^{(2)})$, $F^{(1)}$, and $(F^{(0)} + 2F^{(2)})$, with arbitrary functions having particular transformation properties under S_3. The arbitrariness of these latter functions is sufficient to ensure that the above combinations of isospin amplitudes have the correct transformation properties. Equation (3.8) may also be used to derive the condition (2.19) on the amplitudes. It is shown in Appendix B that from these properties the crossing relations on A, B, and C can be regained. This guarantees that the integral constraints (3.16)–(3.21) that we have found on the partial wave amplitudes are sufficient to ensure the known crossing properties of the full scattering amplitude.

APPENDIX A

Proof of the relation $\hat{P}_i^\mu \hat{P}_j^\nu = \delta_{ij}\delta_{\mu\nu}\hat{P}_i^\mu$ [Eq. (2.1)]:

$$\begin{aligned}\hat{P}_i^\mu \hat{P}_j^\nu &= (n_\mu n_\nu/|G|^2) \sum_{g_1, g_2 \in G} D_{ii}^\mu(g_1^{-1}) D_{jj}^\nu(g_2^{-1})\hat{g}_1\hat{g}_2 \\ &= (n_\mu n_\nu/|G|^2) \sum_{g_1, g_3 \in G} D_{ii}^\mu(g_1^{-1}) D_{jj}^\nu(g_3^{-1}g_1)\hat{g}_3, \quad g_3 = g_1 g_2, \\ &= (n_\mu n_\nu/|G|^2) \sum_{g_1, g_3 \in G} \sum_{k=1}^{n_\nu} D_{ii}^\mu(g_1^{-1}) D_{jk}^\nu(g_3^{-1}) D_{kj}^\nu(g_1)\hat{g}_3 \\ &= (n_\mu n_\nu/|G|^2) \sum_{g_3 \in G} \sum_{k=1}^{n_\nu} D_{jk}^\nu(g_3^{-1})\delta_{ij}\delta_{ik}\delta_{\mu\nu}(|G|/n_\nu)\hat{g}_3,\end{aligned}$$

where use has been made of the orthogonality theorem for group representations; so finally we have

$$\begin{aligned}\hat{P}_i^\mu \hat{P}_j^\nu &= \delta_{ij}\delta_{\mu\nu}(n_\nu/|G|) \sum_{g \in G} D_{ii}^\mu(g^{-1})\hat{g} \\ &= \delta_{ij}\delta_{\mu\nu}\hat{P}_i^\mu.\end{aligned}$$

APPENDIX B

Here we demonstrate that the relations (2.16)–(2.19) are sufficient to ensure the crossing relations (2.4)–(2.6). We recall

$$(\hat{S} - \hat{E})(A + B + C) = 0, \quad (2.16)$$

$$(\hat{M}_1 - \hat{E})(2A - B - C) = 0, \quad (2.17)$$

$$(\hat{M}_2 - \hat{E})(B - C) = 0, \quad (2.18)$$

$$(\hat{C}^2 - \hat{C})(2A - B - C) = 3(B - C). \quad (2.19)$$

From (2.16)–(2.18) alone it is possible to deduce the symmetry property of A; but there are a number of possibilities for B and C, and (2.19) is necessary to eliminate all but the correct solution, (2.5) and (2.6).

From (2.16) we have

$$(\hat{E} - \hat{\sigma})(A + B + C) = 0, \quad (B1)$$

$$(2\hat{E} - \hat{C} - \hat{C}^2)(A + B + C) = 0. \quad (B2)$$

From (2.17),

$$(\hat{E} - \hat{\sigma})(2A - B - C) = 0, \quad (B3)$$

$$(\hat{E} + \hat{C} + \hat{C}^2)(2A - B - C) = 0. \quad (B4)$$

From (2.18),

$$(\hat{E} + \hat{\sigma})(B - C) = 0, \quad (B5)$$

$$(\hat{E} + \hat{C} + \hat{C}^2)(B - C) = 0. \quad (B6)$$

$$\text{(B1) \& (B3)} \Rightarrow (\hat{E} - \hat{\sigma})A = 0, \quad (\hat{E} - \hat{\sigma})(B + C) = 0, \quad (B7)$$

i.e., $\hat{\sigma}A = A$ [Eq. (2.4)].

$$\text{(B5) \& (B7)} \Rightarrow \hat{\sigma}B = C \quad (\text{and } \hat{\sigma}C = B). \quad (B8)$$

$$\text{(B4) \& (B6)} \Rightarrow (\hat{E} + \hat{C} + \hat{C}^2)(A - B) = 0, \quad (\hat{E} + \hat{C} + \hat{C}^2)(A - C) = 0,$$

or

$$(\hat{C} + \hat{C}^2)B = (\hat{E} + \hat{C} + \hat{C}^2)A - B,$$
$$(\hat{C} + \hat{C}^2)C = (\hat{E} + \hat{C} + \hat{C}^2)A - C.$$

These together with (B2) give

$$B + C = (\hat{C}^2 + \hat{C})A, \quad \text{(B9)}$$
$$\text{(B9) \& (2.19)} \Rightarrow B - C = (\hat{C}^2 - \hat{C})A,$$

and so

$$B = \hat{C}^2 A \quad (\text{and } C = \hat{C}A). \quad \text{(B10)}$$

With the help of (2.4), we can replace (B8) and (B10) by

$$B = \hat{\sigma}\hat{C}A \quad (2.10)$$

and

$$C = \hat{\sigma}\hat{C}^2 A. \quad (2.10)$$

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Remarks on the Existence of Solutions of the Two-Particle Lippmann–Schwinger Equation

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(Received 21 January 1971)

We prove the following: The kernel K_l of the partial wave Lippmann–Schwinger (LS) equation for the lth partial wave with complex energy having positive- or negative-definite imaginary part belongs to the Hilbert–Schmidt (L^2) class if the potential V is spherically symmetric and such that

(A) $$\lim_{r\to 0} r^{\delta}V(r) = 0, \quad -\infty < \delta < \tfrac{3}{2}, \quad V(r)_{r\to\infty} = O(r^{-\eta}), \quad \eta > \tfrac{1}{2},$$

(B) for $V(r) = g/r^{\alpha}$, $1 < \alpha < \tfrac{3}{2}$, the kernel K of the full Lippmann–Schwinger equation satisfies

$$\text{Tr}\,\{(K^{\dagger})^m K^m\} < \infty, \quad \text{if} \quad \alpha > (2m+1)/2m, \quad m = 2, 3, \cdots.$$

For $\tfrac{1}{2} < \alpha \leq 1$, Tr $\{(K^{\dagger})^m K^m\}$ is not absolutely convergent for any finite m, even though, for each partial wave, K_l belongs to L^2 class. An appendix deals with obtaining expressions for the T matrix in terms of eigensolutions of the mth iterated kernel when it belongs to L^2 class.

I. INTRODUCTION

A sufficient condition for the existence of unique solutions for the Lippmann–Schwinger (LS) integral equation

$$\Psi^{(+)} = \Psi_0 + G_0^{+}(E)V\Psi^{(+)} \quad (1)$$

can be obtained by proving that the kernel $K = G_0^{+}V$ belongs to the Hilbert–Schmidt class (L^2)[1,2]:

$$\text{Tr}\,\{K^{\dagger}K\} < \infty. \quad (2)$$

In Eq. (1) $\Psi^{(+)}$ is the scattering state evolved from the "in state" Ψ_0 due to the interaction V. Ψ_0 is an eigenstate of the free Hamiltonian H_0 and

$$G_0^{+}(E) = (E - H_0 + i\epsilon)^{-1}, \quad (3)$$

$\epsilon > 0$ and E is real. $\epsilon < 0$ corresponds to $\psi^{(-)}$ and it can be studied using an exactly similar procedure described in this paper. The sufficient conditions on V obtained in the literature[2] to establish Eq. (2) is

$$\int d^3r\, |V(r)|^2 < \infty \quad (4)$$

for $\epsilon > 0$. For $\epsilon = 0$, a modified kernel $K_S = V^{\frac{1}{2}}G_0^{+}V^{\frac{1}{2}}$ belongs to L^2 class if

$$\int d^3r\, V|(r)| < \infty, \quad (5a)$$

$$\int d^3r\, |V(\mathbf{r} - \mathbf{r}')|\, r'^{-2} < M < \infty, \quad (5b)$$

or

$$(\hat{C} + \hat{C}^2)B = (\hat{E} + \hat{C} + \hat{C}^2)A - B,$$
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These together with (B2) give

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$$\int d^3r\, |V(\mathbf{r} - \mathbf{r}')|\, r'^{-2} < M < \infty, \quad (5b)$$

where M is a constant independent of r. Weinberg[3,4] has shown that, for spherically symmetric potentials, the partial wave LS equation belongs to L^2 if

$$\int_0^{C<\infty} r^2\,dr\,|V(r)|^2 < \infty, \tag{6a}$$

$$\int_{C'>0}^{\infty} dr\,|V(r)|^2 < \infty, \tag{6b}$$

and this includes the Coulomb potential. However, according to Titchmarsh,[5] the solutions of the radial Schrödinger equation corresponding to continuous spectrum exist if the potential $V(r) \to 0$ as $r \to \infty$. Clearly, Eqs. (4) and (5a)–(6b) do not cover all potentials having this behavior.

The existence of the unique solutions for the full three-dimensional LS equation can be proved if one can show that any finite power of the kernel K belongs to L^2. This incorporates a larger class of V than suggested by (5a)–(6b). This is proved in the next section. This extension is possible if, instead of the representation for G_0^+ used by Weinberg,[3,4] one uses the spherical wave expansion and the conditions on the existence of solutions of the iterated equations. Weinberg[3] used a different criterion, namely,

$$\mathrm{Tr}\,\{(K^\dagger K)^2\}$$

for examining the Coulomb problem. See Note Added in Proof in Ref. 3. In fact, we found that indeed $\mathrm{Tr}\,(K^\dagger K)^2 < \infty$ for the Coulomb problem whereas $\mathrm{Tr}\,\{K^{\dagger 2}K^2\}$ is not. This is the same as

$$\mathrm{Tr}\,\{(K^\dagger)^2K^2\}$$

only if K is a normal operator.

II. STATEMENT OF THE THEOREM AND ITS PROOF

Theorem: The kernel K_l of the partial wave Lippmann–Schwinger equation for the lth partial wave with a complex energy, with arbitrarily small nonzero imaginary part, belongs to the Hilbert–Schmidt class (L^2) for a spherically symmetric potential $V(r)$ such that

(A) $\lim_{r\to 0} r^\delta V(r) = 0, \quad \delta < \frac{3}{2},$

$V(r)|_{r\to\infty} = O(r^{-\eta}), \quad \eta > \frac{1}{2},$

(B) for $V(r) = g/r^\alpha, \quad 1 < \alpha < \frac{3}{2},$

$\mathrm{Tr}\,\{(K^\dagger)^m K^m\} < \infty$

if

$$\alpha > (2m+1)/2m, \quad m = 2, 3, \cdots.$$

Here K is the kernel of the full LS equation.

Proof: First we evaluate the $\mathrm{Tr}\,(K^\dagger K)$, assuming $\epsilon > 0$:

$$\mathrm{Tr}\,(K^\dagger K) = \int d^3r \langle \mathbf{r}|\, K^\dagger K\,|\mathbf{r}\rangle$$

$$= \int d^3r\, d^3r_1 \langle \mathbf{r}|\, K^\dagger\,|\mathbf{r}_1\rangle\langle \mathbf{r}_1|\, K\,|\mathbf{r}\rangle. \tag{7}$$

Now

$$\langle \mathbf{r}_1|\, K\,|\mathbf{r}\rangle = \langle \mathbf{r}_1|\, G_0^+\,|\mathbf{r}\rangle V(\mathbf{r}) \tag{8}$$

if V is a local potential. Similarly,

$$\langle \mathbf{r}|\, K^\dagger\,|\mathbf{r}_1\rangle = \langle \mathbf{r}_1|\, K\,|\mathbf{r}\rangle^* = V(\mathbf{r})\langle \mathbf{r}|\, G_0^-\,|\mathbf{r}_1\rangle. \tag{9}$$

We now use

$$\langle \mathbf{r}_1|\, G_0^+\,|\mathbf{r}\rangle = \int \frac{d^3k}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r})}}{\Delta_k^+} \tag{10}$$

and

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}(\hat{k}) Y_{lm}^*(\hat{r}) \tag{11}$$

with $\Delta_k^\pm = (E - k^2/2\mu \pm i\epsilon)$, μ being the reduced mass, to obtain

$$\langle \mathbf{r}_1|\, K\,|\mathbf{r}\rangle = \sum_{lm} \frac{2}{\pi} \int_0^\infty \frac{k^2\,dk}{\Delta_k^+} j_l(kr_1) Y_{lm}(\hat{r}_1) j_l(kr) Y_{lm}^*(\hat{r}) V(r). \tag{12}$$

The various symbols here have their usual significance (cf. Ref. 2). This form is different from the one used by Weinberg.[3] We then obtain

$$\mathrm{Tr}\,\{K^\dagger K\} = \sum_{l=0}^\infty (2l+1)\,\mathrm{Tr}\,(K^\dagger K)_l$$

$$= \sum_{l=0}^\infty (2l+1)\left(\frac{2}{\pi}\right)^2 \int_0^\infty r^2\,dr \int_0^\infty \frac{k^2\,dk}{|\Delta_k^+|^2} j_l^2(kr) V^2(r). \tag{13}$$

In Eq. (13), the k integration is convergent for $0 < r < \infty$ if $|\epsilon| > 0$, and, similarly, the r integration is convergent for every $0 < k < \infty$. Now let us consider the double integral in (13):

$$I = \int_0^\infty r^2 V^2(r)\,dr \int_0^\infty \frac{k^2\,dk}{|\Delta_k^+|^2} j_l^2(kr).$$

The k integration can be carried out explicitly. Thus

$$I_k = \int_0^\infty \frac{k^2\,dk}{|\Delta_k^+|^2} j_l^2(kr)$$

$$= \frac{1}{2\epsilon}\,\mathrm{Im} \int_{-\infty}^\infty \frac{k^2\,dk\, j_l^2(kr)}{(E - k^2/2m - i\epsilon)}$$

$$= \frac{m}{2\epsilon}\,\mathrm{Im} \left(\int_{-\infty}^\infty \frac{k^2\,dk\, j_l(kr) h_l^{(1)}(kr)}{(k - k_+)(k_- - k)} + \int_{-\infty}^\infty \frac{k^2\,dk\, j_l(kr) h_l^{(2)}(kr)}{(k - k_-)(k_+ - k)} \right),$$

$$k_+ = -k_- = -|2m(E - i\epsilon)|^{\frac{1}{2}}(\cos\theta_0 - i\sin\theta_0),$$

$$\theta_0 = \tan^{-1}\left(\frac{\epsilon}{E}\right).$$

$h_l^{(1)}$ and $h_l^{(2)}$ are the usual spherical Hankel functions. The integrals can be evaluated by contour integration:

$$I_k = -(m\pi/2\epsilon)\,\mathrm{Im}\,[ik_+ j_l(k_+r)h_l^{(1)}(k_+r) - ik_- j_l(k_-r)h_l^{(2)}(k_-r)].$$

Therefore,

$$I = -\frac{m\pi}{2\epsilon}\left(\mathrm{Im}\int_0^\infty ik_+ j_l(k_+r)V^2(r)h_l^{(1)}(k_+r)r^2\,dr - \mathrm{Im}\int_0^\infty ik_- j_l(k_-r)V^2(r)h_l^{(2)}(k_-r)r^2\,dr\right).$$

Both integrals in the above expression for I will exist provided that

$$\lim_{r\to 0} r^\delta V(r) = 0, \qquad \delta < \tfrac{3}{2},$$

and

$$V(r)_{r\to\infty} = O(r^{-\eta}), \quad \eta > \tfrac{1}{2}.$$

It may be pointed out that under these conditions the interchange of orders of integrations is justified. Using Ref. 6, the Tonelli–Hobson theorem, employing the other order of integrations in (13) gives us the same conditions as above, as they indeed must. This proves part A of the theorem. If the sum in (13) diverges, then we know that K does not belong to L^2. Let us consider the potential

$$V(r) = g/r^\alpha. \tag{14}$$

Then

$$\langle k_1 l|\, V^2(r)\,|k_2 l\rangle = \int_0^\infty r^2\,dr\, j_l(k_1r)V^2(r)j_l(k_2r) = \frac{\pi g^2}{2^{\lambda'+1}}\,\frac{(k_1k_2)^{\mu-\frac{1}{2}}\Gamma(\mu+\frac{1}{2}(1-\lambda'))}{(k_1+k_2)^{2\mu-\lambda'+1}\Gamma(\mu+1)\Gamma(\frac{1}{2}(1+\lambda'))} \tag{15}$$

$$\times\, {}_2F_1\left(\mu+\tfrac{1}{2}(1-\lambda'),\mu+\tfrac{1}{2};2\mu+1;\frac{4k_1k_2}{(k_1+k_2)^2}\right), \tag{16}$$

where

$$2\mu+1 > \mathrm{Re}\,\lambda' > -1, \quad k_1>0, \quad k_2>0, \tag{17}$$

and

$$\mu = l+\tfrac{1}{2}, \quad \lambda' = 2\alpha - 1, \tag{18}$$

for $k_1 = k_2 > 0, 2\mu+1 > \mathrm{Re}\,\lambda' > 0$. These formula are obtained from Ref. 7. This gives, after some algebra, the asymptotic behavior in l,

$$|\langle lk|\, V^2(r)\,|lk\rangle| = O(k^{\lambda'-2}\mu^{-\lambda'}), \tag{19}$$

and $k^{\lambda'-2}$ determines the k dependence entirely. Equation (19) together with the ratio test shows that, for $1<\alpha<\frac{3}{2}$, the series (13) for Tr $(K^\dagger K)$ is not absolutely convergent. Thus we find that Tr $(K^\dagger K)$ is divergent for $V(r) = g/r^\alpha$ in agreement with Eq. (4). One also notices that the k dependence of (16) does not make the k integration divergent.

Now let us consider the Tr $\{(K^\dagger)^2K^2\}$, Tr $\{(K^\dagger)^3K^3\}$, etc., to determine whether they are finite. This will determine if the iterated kernels belong to the L^2 class. It is straightforward to obtain the following representations for spherically symmetric potentials:

$$\langle \mathbf{r}|\, K^2\,|\mathbf{r}'\rangle = \sum_{lm}\left(\frac{2}{\pi}\right)^2\int_0^\infty \frac{k_1^2\,dk_1}{\Delta_{k_1}^+}\int_0^\infty \frac{k_2^2\,dk_2}{\Delta_{k_2}^+} \times j_l(k_1r)Y_{lm}(\hat r)\langle k_1 l|\, V\,|k_2 l\rangle j_l(k_2r')Y_{lm}^*(\hat r')V(r'), \tag{20}$$

$$\langle \mathbf{r}|\, K^3\,|\mathbf{r}^\dagger\rangle = \sum_{lm}\left(\frac{2}{\pi}\right)^3\int_0^\infty \frac{k_1^2\,dk_1}{\Delta_{k_1}^+}\int_0^\infty \frac{k_2^2\,dk_2}{\Delta_{k_2}^+}\int_0^\infty \frac{k_3^2\,dk_3}{\Delta_{k_3}^+} j_l(k_1r)Y_{lm}(\hat r) \times \langle k_1 l|\, V\,|k_2 l\rangle\langle k_2 l|\, V\,|k_3 l\rangle j_l(k_3r')Y_{lm}^*(\hat r')V(r'), \tag{21}$$

$$\langle \mathbf{r}|\,(K^\dagger)^2\,|\mathbf{r}'\rangle = \sum_{lm}\left(\frac{2}{\pi}\right)^2\int_0^\infty \frac{k_1^2\,dk_1}{\Delta_{k_1}^-}\int_0^\infty \frac{k_2^2\,dk_2}{\Delta_{k_2}^-} \times V(r)j_{l_1}(k_1r)Y_{lm}^*(\hat r)\langle k_1 l|\, V\,|k_2 l\rangle j_l(k_2r')Y_{lm}(\hat r'), \tag{22}$$

$$\langle \mathbf{r}|\,(K^\dagger)^3\,|\mathbf{r}'\rangle = \sum_{lm}\left(\frac{2}{\pi}\right)^3\int_0^\infty \frac{k_1^2\,dk_1}{\Delta_{k_1}^-}\int_0^\infty \frac{k_2^2\,dk_2}{\Delta_{k_2}^-}\int_0^\infty \frac{k_3^2\,dk_3}{\Delta_{k_3}^-} \times V(r)j_l(k_1r)Y_{lm}^*(\hat r)\langle k_1 l|\, V\,|k_2 l\rangle \times \langle k_2 l|\, V\,|k_3 l\rangle j_l(k_3r')Y_{lm}(\hat r'). \tag{23}$$

Generalizations to $\langle \mathbf{r}|\, K^m\,|\mathbf{r}'\rangle$, $\langle \mathbf{r}|\,(K^\dagger)^m\,|\mathbf{r}'\rangle$ are straight forward. Now we obtain

$$\mathrm{Tr}\,\{(K^\dagger)^2K^2\} = \sum_{l=0}^\infty\left(\frac{2}{\pi}\right)^4(2l+1)\int_0^\infty \frac{k_1'\,dk_1'}{\Delta_{k_1'}^-}\int_0^\infty \frac{k_2^2\,dk_2}{|\Delta_{k_2}^+|^2}\int_0^\infty \frac{k_1^2\,dk_1}{\Delta_{k_1}^+} \times \langle k_1' l|\, V\,|k_2 l\rangle\langle k_2 l|\, V\,|k_1 l\rangle\langle k_1 l|\, V^2\,|k_1' l\rangle. \tag{24}$$

In general, it can be shown that

$$\mathrm{Tr}\,\{(K^\dagger)^mK^m\} = \sum_{l=0}^\infty\left(\frac{2}{\pi}\right)^{2m}(2l+1)\int_0^\infty \frac{k_1'^2\,dk_1'}{\Delta_{k_1'}^-}\cdots\int_0^\infty \frac{k_{m-1}'^2}{\Delta_{k'_{m-1}}^-}\,dk_{m-1}' \times\int_0^\infty \frac{k_m^2\,dk_m}{|\Delta_{k_m}^+|^2}\int_0^\infty \frac{k_{m-1}^2\,dk_{m-1}}{\Delta_{k_{m-1}}^+}\cdots\int_0^\infty \frac{k_1^2\,dk_1}{\Delta_{k_1}^+} \times \langle k_1' l|\, V\,|k_2' l\rangle\langle k_2' l|\, V\,|k_3' l\rangle\cdots \times \langle k_{m-1}' l|\, V\,|k_m l\rangle\langle k_m l|\, V\,|k_{m-1} l\rangle\cdots \times \langle k_2 l|\, V\,|k_1 l\rangle\langle k_1 l|\, V^2\,|k_1' l\rangle. \tag{25}$$

In all these we have freely used the Tonelli–Hobson theorem[6] to interchange the orders of integration and to investigate the absolute convergence of the traces. Now we shall show explicitly that each term in the l series in Eq. (24) exists and is finite for $1<\alpha<\frac{3}{2}$,

and establish its l dependence to study the convergence of the sum. First we establish a bound for $\langle k_1 l|\, V(r)\, |k_2 l\rangle$ given by (16) with g^2 replaced by g and λ' by λ. For this purpose we shall use the representation[8]

$$F(a, b; c; z) = \frac{2^{c-b}\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \times \int_0^\infty \frac{(\sinh t)^{2a-2c+1}(\cosh t - 1)^{b+c-a-1}}{[(1+z) + (1-z)\cosh t]^a}\, dt, \qquad \operatorname{Re} c > \operatorname{Re} b > 0.$$

In our case

$$a = \mu + \tfrac{1}{2}(1-\lambda), \quad b = \mu + \tfrac{1}{2}, \quad c = 2\mu + 1, \qquad z = 4k_1k_2/(k_1+k_2)^2.$$

To study $\langle k_1 l\,|V_2|\, k_2 l\rangle$, λ is to be replaced by λ'. In the above integral, the numerator behaves like $e^{-\lambda t}/2$ for $t \to \infty$, and, since $\lambda > 0$, this goes to zero exponentially in t. Similarly, one sees that $(\sinh t)^{2a-2c+1}$ $(\cosh t - 1)^{b+c-a-1}$ is regular at $t = 0$ for $1 < \alpha < \frac{3}{2}$ and $l = 0, 1, \cdots$. We also note that $a > 0$ and $(1+z) + (1-z)\cosh t \geq 2$. Therefore, we write

$$|F(a, b; c; z)| \leq \frac{2^{c-b-a}}{\Gamma(b)\Gamma(c-b)} \times \int_0^\infty (\sinh t)^{2a-2c+1}(\cosh t - 1)^{b+c-a-1}\, dt.$$

But

$$\int_0^\infty (\sinh t)^{2a-2c+1}(\cosh t - 1)^{b+c-a-1}\, dt = \int_0^\infty (\sinh t)^{-\lambda}(\cosh t - 1)^{\lambda/2}\left(\frac{\cosh t - 1}{\sinh t}\right)^{2\mu} dt \leq \int_0^\infty (\sinh t)^{-\lambda}(\cosh t - 1)^{\lambda/2}\, dt = c_1(\lambda).$$

In the above we have used the fact that

$$(\cosh t - 1)/\sinh t \leq 1, \text{ for } 0 \leq t \leq \infty, \text{ and } \mu > 0.$$

$c_1(\lambda)$ is independent of μ (and hence l). Therefore,

$$|F(a, b; c; z)| \leq c_1(\lambda) 2^{c-b-a}\Gamma(c)/\Gamma(b)\Gamma(c-b).$$

This gives immediately the bound

$$|\langle k_1 l|\, V\, |k_2 l\rangle| \leq \pi g \frac{\Gamma(\mu + \frac{1}{2}(1-\lambda))}{\Gamma(\mu+1)} \frac{\Gamma(2\mu+1)}{\Gamma(\frac{1}{2}(1+\lambda))} \times \frac{c_1(\lambda)(k_1+k_2)^{\lambda-2}}{[\Gamma(\mu+\frac{1}{2})]^2 2^{\frac{1}{2}\lambda+1}}\left(\frac{k_1k_2}{(k_1+k_2)^2}\right)^{\mu-\frac{1}{2}}.$$

These bounds are generally valid for $l = 0, 1, \cdots, 1 < \alpha < \frac{3}{2}$ and k_1, k_2 real and positive.

Evidently from the above,

$$|\langle k_1 l|\, V\, |k_2 l\rangle| \leq \frac{\pi g \Gamma(\mu + \frac{1}{2}(1-\lambda))\Gamma(2\mu+1)c_1(\lambda)(k_1+k_2)^{\lambda-2}}{\Gamma(\mu+1)\Gamma(\frac{1}{2}(1+\lambda))[\Gamma(\mu+\frac{1}{2})]^2 2^{\frac{1}{2}\lambda+1}}.$$

These bounds are generally valid for $l = 0, 1, 2, \cdots$, $1 < \alpha < \frac{3}{2}$ and k_1, k_2 real and positive. Now let us consider the absolute convergence of the multiple integral in (24), for the case where $m = 2$:

$$I_2 = \int_0^\infty \frac{k_1'^2\, dk_1'}{\Delta^-_{k_1'}} \int_0^\infty \frac{k_2^2\, dk_2}{|\Delta^+_{k_2}|^2} \int_0^\infty \frac{k_1^2\, dk_1}{\Delta^+_{k_1}} \times \langle k_1' l|\, V\, |k_2 l\rangle\langle k_2 l|\, V\, |k_1 l\rangle\langle k_1 l|\, V^2\, |k_1' l\rangle < \langle c_2^2(g, \lambda, \mu) c_2(g^2, \lambda', \mu)$$
$$\times \int_0^\infty \frac{k_1'^2\, dk_1'}{|\Delta^-_{k_1'}|\, k_1'^{\frac{9}{2}-2\alpha}} \int_0^\infty \frac{k_2^2\, dk_2}{|\Delta^+_{k_2}|^2} \times \int_0^\infty \frac{k_1^2\, dk_1}{|\Delta^+_{k_1}|\, k_1^{\frac{9}{2}-2\alpha}} < \infty, \quad \text{for } 1 < \alpha < \tfrac{3}{2}.$$

In obtaining the above we have used the inequality $(k_1 + k_1')^2 > k_1 k_1'$. In the k_2 integral we note the additional k_2 dependence due to $|\Delta^+_{k_2}|^{-2}$. So, we use the inequalities $k_1 + k_2 \geq k_1$ and $k_1' + k_2 \geq k_1'$. $c_2(g, \lambda, \mu)$ is given by

$$c_2(g, \lambda, \mu) = \frac{\pi g \Gamma(\mu + \frac{1}{2}(1-\lambda))\Gamma(2\mu+1)c_1(\lambda)}{\Gamma(\mu+1)\Gamma(\frac{1}{2}(1+\lambda))[\Gamma(\mu+\frac{1}{2})]^2 2^{\frac{1}{2}\lambda+1}}.$$

This result shows that, for $1 < \alpha < \frac{3}{2}$, $\operatorname{Tr}\{(K^\dagger)^2 K^2\}_l < \infty$. The result $\operatorname{Tr}\{(K^\dagger)^m K^m\}_l < \infty$ can be proved in a similar way. The integrals in the k variables are absolutely convergent.

By using asymptotic expansion of the gamma functions, the following asymptotic behavior in l valid for real and positive k_1 and k_2 can be obtained from the above analysis:

$$|\langle k_1 l|\, V\, |k_2 l\rangle|_{l\to\infty} = O\left[\mu^{-\frac{1}{2}\lambda}\left(\frac{4k_1k_2}{(k_1+k_2)^2}\right)^{\mu-\frac{1}{2}} \frac{1}{(k_1+k_2)^{2-\lambda}}\right]. \quad (26)$$

One notices that the $\langle k_1 l|\, V\, |k_2 l\rangle$ matrix element falls off exponentially in l as $l \to \infty$ if $k_1 \neq k_2$. When $k_1 = k_2$, we use the asymptotic behavior in l established earlier in Eq. (19). The uniform convergence in l and absolute convergence in k variables enable us to estimate the convergence of the l sum by just considering the most divergent part of the multiple k integrals as a function of l. The most divergent part for the l series occurs when $k_1 = \cdots = k_m = k_1' = \cdots = k_{m-1}'$. Corresponding to this, the l series is convergent if

$$\alpha > (2m+1)/2m.$$

This follows from a simple ratio test. By the same arguments, for $\frac{1}{2} < \alpha \leq 1$, $\operatorname{Tr}\{K^m(K^\dagger)^m\}$ is not absolutely convergent for any m. In the Appendix, we construct a method of solution in terms of the eigensolution of the mth iterated kernel, when the mth iterated kernel belongs to L^2 class.

III. DISCUSSION

The above analysis has some important consequences. For the full three-dimensional LS equation, the kernel is compact only if $V(r)$ satisfies (4); this means $V(r)$ falls faster than $r^{-\frac{3}{2}}$ at infinity. One can improve over this by iterating the full three-dimensional LS equation; however, for the Coulomb problem one has to iterate the LS equation an infinite number of times to obtain a modified LS equation with compact kernel. This means that one will not be able to incorporate the potential $V(r) = g/r^{\alpha}$, $\frac{1}{2} < \alpha \leq 1$, in the full LS formalism, using the arguments given here. This point is more transparent when one recalls the asymptotic wavefunction for the Coulomb problem. One finds that this asymptotic wavefunction contains contributions from all powers of g.

We must point out that our method differs from the method used by Weinberg in two respects. One, we employ the representation (1) without integrating over k and the formula (11) to express it only in terms of spherical Bessel functions. Weinberg used an integrated form of (1), which in (10) led him to a combination of spherical Bessel and Hankel functions. Second, Weinberg[3] employs Tr $\{(K^{\dagger}K)^2\}$ to discuss the Coulomb problem. (See the Note Added in Proof to Ref. 3.) It may be noted that we employ the conventional condition on the L^2 structure of the iterated kernels unlike Weinberg. Also, since K is not a normal operator [cf. Eqs. (8) and (9)], Tr $\{(K^{\dagger})^m K^m\}$ is not equal to Tr $\{(K^{\dagger}K)^m\}$. Another feature of our approach is the appearance of the matrix elements of both $V(r)$ and $V^2(r)$ between spherical waves. We may note that the usual condition (4) obtains if we employ the relation

$$1 = 4\pi \sum_{l=0}^{\infty} (2l+1) j_l^2(kr)$$

and a bound on the k integration for $\epsilon \neq 0$. The above arguments are all valid for $\epsilon < 0$ since the traces are all even in ϵ.

For the Coulomb potential $[V(r) = ze^2/r]$, we can explicitly compute Tr $(K^{\dagger}K)_l$:

$$\text{Tr}\,(K^{\dagger}K)_l = \frac{z^2e^4\mu}{(2l+1)\,|\epsilon|}\left[1 + \frac{2}{\pi}\tan^{-1}\left(\frac{E}{|\epsilon|}\right)\right]$$

Clearly, then, the partial wave LS equation has solutions for $\epsilon \neq 0$, while the full problem requires infinite number of iterations. Note also that, for $E < 0$, the limit $\epsilon \to 0$ exists while the full trace still diverges. The analysis of majorizing the Born series and Fredholm determinant requires Tr $\{K^m\} < \infty$ for some $m > 1$. See, for instance, Newton's book.[2] Our representation for K enables us to study Tr $\{K^m\}$ quite easily using the procedure developed in this paper, and the result of such an analysis may be summarized in the form of another theorem.

Theorem: The trace of the kernel K_l of the partial wave LS equation is finite for the lth partial wave with complex energy having nonzero but, however, small imaginary part if the potential V is spherically symmetric and such that

(A′) $$\lim_{r\to 0} r^{\delta}V(r) = 0, \qquad -\infty < \delta < 2,$$
$$V(r) \underset{r\to\infty}{=} O(r^{-\beta}), \qquad \beta > 1,$$

(B′) For $V(r) = g/r^{\alpha}$, $1 < \alpha < 2$, the kernel of the full LS equation satisfies

$$|\text{Tr}\,K^m| < \infty \text{ if } \alpha > 1 + 2/m, \quad m = 2, 3, \cdots.$$

For $\alpha \leq 1$, $|\text{Tr}\,K^m|$ may not be bounded for any m as before, even though for each partial wave $|\text{Tr}\,K_l|$ exists. This is because the resulting l series is not absolutely convergent.

It should be remarked that α now goes up to 2 instead of $\frac{3}{2}$ obtained from the earlier discussion. Another point to be noted is that, for $\alpha \geq 2$, the k integration carried out after r integration diverges while evaluating $|\text{Tr}\,\{K^m\}|$. It is important to stress that all the conditions stated and proved here are only sufficient.

For a discussion of the significance of this theorem and an application of this to the three-body problem, one may refer to a forthcoming monograph.[9]

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APPENDIX

In this appendix we develop a generalized theory of Sturmian functions when some power of the kernel of the LS equation belongs to the Hilbert–Schmidt class. The conventional theory for example presented by Kharchenko *et al.*[10] (see also Ref. 8) is for the Hilbert–Schmidt kernels and is a special case of the formalism presented here. Also, from our theorem in the text, the original Sturmian theory, supposedly valid for short-range potentials behaving like r^s near $r = 0$ with $s > -2$, can now be generalized to cases where $s > -\frac{3}{2}$, decreasing at infinity as $r^{-\alpha}$ with $1 < \alpha < \frac{3}{2}$. The following procedure gives a method for constructing formal separable type expressions for the T matrix and the Green's function.[11]

The equation satisfied by T when it is iterated p

times may be written symbolically as

$$T = V^{(p)} + (K)^q T. \tag{A1}$$

Let us introduce the notation

$$V^{(p)} = \mathfrak{V}^{(1)} + \mathfrak{V}^{(2)} + \cdots + \mathfrak{V}^{(p)}, \tag{A2}$$

$$K^{(p)} = (K)^p = \mathfrak{V}^{(p)} G_0, \tag{A3}$$

with

$$\mathfrak{V}^{(p)} = (K)^{p-1} V, p = 1, 2, \cdots. \tag{A4}$$

The generalized Sturmians are defined as the eigenfunctions of the iterated kernel:

$$\int \mathfrak{V}^{(p)}(kqz)\left(z - \frac{q^2}{2m}\right)^{-1} \mathfrak{S}_n^{(p)}(qz)\, d^3q = \eta_n^{(p)}(z)\mathfrak{S}_n^{(p)}(kz). \tag{A5}$$

Here n is a quantum number, discrete or continuous as the case may be, and $\eta_n^{(p)}(z)$ is the eigenvalue, z is a complex number, and m is the reduced mass. The orthonormality and completeness of $\{\mathfrak{S}_n^{(p)}(kz)\}$ are

$$\int \mathfrak{S}_{n'}^{(p)}(kz)\mathfrak{S}_n^{(p)}(kz)\left(\frac{k^2}{2m} - z\right)^{-1} d^3k = \delta_{nn'}, \tag{A6}$$

$$\sum_n \mathfrak{S}_n^{(p)}(kz)\mathfrak{S}_n^{(p)}(k'z) = \left(\frac{k^2}{2m} - z\right)\delta^{(3)}(\mathbf{k} - \mathbf{k}'). \tag{A7}$$

[If n is continuous, the sum is replaced by an integral in (A7) and by a delta function in the right side of (A6).] It is easy to verify then that

$$\mathfrak{V}^{(p)}(kk'z) = -\sum_n \eta_n^{(p)}\mathfrak{S}_n^{(p)}(kz)\mathfrak{S}_n^{(p)}(k'z), \tag{A8}$$

$$V^{(p)}(kk'z) = \sum_{n,n'} c_{nn'}^{(p)}(z)\mathfrak{S}_n^{(p)}(kz)\mathfrak{S}_{n'}^{(p)}(k'z), \tag{A9}$$

with

$$\begin{aligned} c_{n,n'}^{(p)}(z) &= \int d^3k \int d^3k' \mathfrak{S}_n^{(p)}(kz)\left(z - \frac{k^2}{2m}\right)^{-1} V^{(p)}(kk'z) \\ &\quad \times \mathfrak{S}_{n'}^{(p)}(k'z)\left(z - \frac{k'^2}{2m}\right)^{-1} \\ &\equiv -\delta_{nn'}\eta_n^{(p)}(z) + \tilde{c}_{n,n'}^{(p)}(z). \end{aligned} \tag{A10}$$

Then it can be shown quite easily that

$$T(k, k'; z) = -\sum_n \frac{\eta_n^{(p)}(z)}{1 - \eta_n^{(p)}(z)} \mathfrak{S}_n^{(p)}(kz)\mathfrak{S}_n^{(p)}(k'z) + \sum_{n,n'} \frac{\tilde{c}_{nn'}^{(p)}(z)}{1 - \eta_n^{(p)}(z)} \mathfrak{S}_n^{(p)}(kz)\mathfrak{S}_{n'}^{(p)}(k'z), \tag{A11}$$

$$G(k, k'; z) = \left(z - \frac{k^2}{2m}\right)^{-1}\left(-\sum_n \frac{\mathfrak{S}_n^{(p)}(kz)\mathfrak{S}_n^{(p)}(k'z)}{1 - \eta_n^{(p)}(z)} + \sum_{nn'} \frac{\tilde{c}_{nn'}^{(p)}(z)}{1 - \eta_n^{(p)}(z)} \mathfrak{S}_n^{(p)}(kz)\mathfrak{S}_{n'}^{(p)}(k'z)\right)\left(z - \frac{k'^2}{2m}\right)^{-1} \tag{A12}$$

For $p = 1$, these reduce to the corresponding well-known Sturmian representations for T and G. An application of these to Faddeev equations proceeds in the usual way. It may be remarked that, for the Coulomb problem, explicit solutions $\{\mathfrak{S}_n(kz)\}$ exist in the literature.[9]

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$$\int\int |f(s,t)|\, ds\, dt, \quad \int ds \int |f(s,t)|\, dt, \quad \int dt \int |f(s,t)|\, ds$$

exists, then the integrals

$$\int\int f(s,t)\, ds\, dt, \quad \int ds \int f(s,t)\, dt, \quad \int dt \int f(s,t)\, ds$$

all exist and are equal to one another.
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[11] Note that the quantities $\mathfrak{S}_n^{(p)}$, T, and G depend on momentum *vectors*; for convenience we have omitted the vector notations in the arguments of these quantities.

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Evaluation of Certain Statistical Averages in the Hamiltonian Form

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A compact method is presented for the evaluation of certain statistical averages involving a quadratic Hamiltonian generator.

I. INTRODUCTION

Given a Hamiltonian operator

$$H = H^0 + V, \tag{1}$$

where H^0 is the unperturbed component and V is the perturbation, one is frequently called upon to evaluate a stastical average of the form

$$\langle V^{M'} \rangle = \mathrm{Tr}\, e^{-\beta H^0} V(t_1) \cdots V(t_{M'}) / \mathrm{Tr}\, e^{-\beta H^0} \tag{2}$$

in the interaction representation, where

$$V(t) = e^{iH^0 t} V e^{-iH^0 t}.$$

It is the purpose of this paper to formulate a theory to evaluate averages of the form (2) for an electron–boson system, comprised of a single electron interacting with a boson-producing environment, having the Hamiltonian operator H defined by

$$H^0 = \sum_n \left[\epsilon(n) + \sum_s H_s^0(n) \right] a^\dagger(n) a(n),$$
$$V = \sum_s V_s, \quad [H_s^0(n), H_{s'}^0(n')] = 0, \tag{3}$$

where

$$H_s^0(n) = \sum_{i(s)} \omega_{i(s)} (b_{i(s)}^\dagger b_{i(s)} + \tfrac{1}{2}) + \sum_{i(s)} V_{i(s)}(n)(b_{i(s)} + b_{i(s)}^\dagger) + \sum_{i(s),j(s)} V'_{i(s),j(s)}(n)(b_{i(s)} + b_{i(s)}^\dagger)(b_{j(s)} + b_{j(s)}^\dagger),$$

$$V_s = \sum_{i(s),m,n;m\neq n} V_{i(s)}(m,n)(b_{i(s)} + b_{i(s)}^\dagger) a^\dagger(m) a(n) + \sum_{i(s),j(s),m,n;m\neq n} V'_{i(s),j(s)}(m,n)(b_{i(s)} + b_{i(s)}^\dagger) \times (b_{j(s)} + b_{j(s)}^\dagger) a^\dagger(m) a(n). \tag{4}$$

In expressions (3) and (4), the operators $a^\dagger(n)$, $a(n)$ represent electron creation and annihilation operators for the electronic state n; the operators $b_{i(s)}^\dagger$, $b_{i(s)}$ represent boson creation and annihilation operators satisfying

$$[b_{i(s)}, b_{j(s)}^\dagger] = \delta_{i(s),j(s)},$$
$$[b_{i(s)}, b_{j(s)}] = [b_{i(s)}^\dagger, b_{j(s)}^\dagger] = 0 \tag{5}$$

for the boson mode $i(s)$, which is a member of a set s of boson modes coupled by the interaction coefficients $V'_{i(s),j(s)}(n)$ and $V'_{i(s),j(s)}(m,n)$; the elements $\epsilon_{(n)}$, $\omega_{i(s)}$, $V_{i(s)}(n)$, $V'_{i(s),j(s)}(n)$, $V_{i(s)}(m,n)$, and $V'_{i(s),j(s)}(m,n)$ are the appropriate energy quantities taken in this case to be real numbers. By taking a single electron we have deliberately made the electronic contribution to our theory as simple as possible while retaining the property that V, and only V, will shift the electronic state. By dividing the total set of boson modes of number $\bar{N}$ into uncoupled subsets s of number N_s, we have provided for the possibility of factorization over s in an expression such as (2). Thus, H includes linear and quadratic terms in the boson coordinates, while anharmonicity and other cubic effects are neglected. Inserting (4) into (3) into (1) into (2), one is forced to calculate—once the electron operators are removed—a variety of multiple-time boson functions of the form

$$K(\{\alpha\}, \{m\}, 0, M) = \Pi_s K_s(\{\alpha\}, \{m\}, 0, M),$$
$$K_s(\{\alpha\}, \{m\}, 0, M) = \mathrm{Tr}_s[f_s(\alpha_1, m_1) x_{i_1(s)}(0) \cdots f_s(\alpha_M, m_M) x_{i_M(s)}(0)], \tag{6}$$

where

$$f_s(\alpha, m) = \exp[\alpha H_s^0(m)], \quad x_{2N+1}(0) = 1,$$
$$x_{i(s)}(0) = b_{i(s)} \quad \text{if} \quad [1 \leq i(s) \leq N_s],$$
$$x_{i(s)}(0) = b_{i(s)}^\dagger \quad \text{if} \quad [N_s + 1 \leq i(s) \leq 2N_s],$$

and α_p may be of the form 0, $-\beta + i(t_1 - t_{M'})$, $i(t_{q+1} - t_q)$, etc. Because of the factorization over s, we can in essence concentrate on the formulation of $K_s(\{\alpha\}, \{m\}, 0, M)$ and in so doing drop the subscript over s for practical purposes. The key to our solution of (6) will be to adopt the procedure of [1] choosing a particular $x_{i(s)}(0)$, [2] moving it to the right (within the trace over boson states in s) through commutation, [3] using the cyclic property of the trace to return it from the last to the first position, and finally [4] moving it to the right again through commutation to its original position. In so doing we generate a solution to (6) in terms of functions of lower order in b or $b^\dagger$. The solution of the lowest-order function

generated by this procedure then completes the problem. For purposes of bookkeeping, a representation

$$H_s^0(n) = \sum_{i(s)} \omega_{i(s)}(n)[b_{i(s)}^\dagger(n)b_{i(s)}(n) + \tfrac{1}{2}] \qquad (7)$$

would be greatly preferred over that given by (4) and, to facilitate the process of commutation, the operators $b_i^\dagger(n)$, $b_j(n)$—dropping the subscript s—should have the same c-numbers as $b_i^\dagger$, b_j. Thus, we have defined the first hurdle that we must cross in the development of the theory, that hurdle being the construction of a transformation $\mathbf{T}$ that will operate on $\mathbf{x}(0)$—with elements $x_i(0)$—converting $H_s^0(n)$, as defined in (4), to (7) while preserving the commutation properties on the b's. Following the solution of $K(\{\alpha\}, \{m\}, 0, M)$, we shall work a simple example in order to illustrate the theory.

II. A CANONICAL TRANSFORMATION

Let $\mathbf{x}(m)$, denoted by the index (m), be a member of a set S of vectors in a $(2N + 1)$-dimensional operator space[1] such that the components of $\mathbf{x}(m)$, in vector notation

$$x_1(m) \cdots x_{2N+1}(m),$$

are operators having the commutation property

$$[x_i(m), x_j(m)] = c_{ij}(m, m) = c_{ij}, \qquad (8)$$

where $c_{ij}(m, m)$ is a c-number and a constant over the set S. Since we shall use the components of $\mathbf{x}(m)$ in place of $[b(m), b^\dagger(m)]$, they must obey the special relations

$$x_{i+N}(m) = x_i^\dagger(m) \quad \text{for} \quad 1 \leq i \leq N, \quad x_{2N+1}(m) = 1,$$
$$[x_i(m), x_{i+N}(m)] = 1 \quad \text{for} \quad 1 \leq i \leq N,$$
$$[x_i(m), x_j(m)] = 0 \quad \text{otherwise}, \qquad (9)$$

thereby placing certain conditions on c_{ij} as defined in (8). Expression (8) may be rewritten in the form

$$\mathbf{x}(m)x_i(m) = x_i(m)\mathbf{x}(m) + \mathbf{c}^i, \quad (\mathbf{c}^i)_j \equiv c_j^i = c_{ji}, \qquad (10)$$

$\mathbf{c}^i$ having the components c_{ji} for all j. Let $\omega(m)$ be a vector in S whose coefficients $\omega_i(m)$ are real undetermined parameters, and define the quadratic Hamiltonian operator

$$2H^0(m) = \sum_{i=1}^{N} [\omega_i(m)x_{i+N}(m)x_i(m) + \omega_{i+N}(m)x_i(m)x_{i+N}(m)] + \omega_{2N+1}(m), \qquad (11)$$

analogous to (7). Expressing (11) in tensor notation[2] as

$$H^0(m) = \mathbf{x}^\dagger(m)\mathbf{H}^D(m)\mathbf{x}(m), \quad H_{ij}^D(m) = \tfrac{1}{2}\omega_i(m)\delta_{ij}, \qquad (12)$$

we introduce the transformation

$$\mathbf{x}(0) = \mathbf{T}(n)\mathbf{x}(n), \quad \mathbf{x}(n) = \mathbf{T}^{-1}(n)\mathbf{x}(0),$$
$$\mathbf{T}(n) = \mathbf{T}(0, n) \qquad (13)$$

from a reference vector $\mathbf{x}(0)$ [see (6)] in S to the vector $\mathbf{x}(n)$. In terms of $\mathbf{x}(0)$ the Hamiltonian $H^0(m)$ can be written as

$$H^0(m) = \mathbf{x}^\dagger(0)\mathbf{H}(m)\mathbf{x}(0), \qquad (14)$$

where $\mathbf{H}(m)$—whose components may be correlated to physical input—serves as the reference tensor defining $H^0(m)$. Inserting (13) into (14) and employing (12), we give the tensor $\mathbf{H}(m)$ in the diagonal form $\mathbf{H}^D(m)$ by the relation

$$\mathbf{H}^D(m) = \mathbf{T}^\dagger(m)\mathbf{H}(m)\mathbf{T}(m). \qquad (15)$$

We further require that the transformation $\mathbf{T}(n)$ not be reducible in the sense that for any given partition of the modes N,

$$N = N_1 + N_2,$$

the Hamiltonian $H^0(m)$, as defined through a given $H_s^0(n)$ in (4), cannot be decomposed relative to N, or

$$\mathbf{x}^\dagger(0)\mathbf{H}(m)\mathbf{x}(0) \neq H^0(m)]_{N_1} + H^0(m)]_{N_2}. \qquad (16)$$

Introduce now a general transformation within S given by

$$\mathbf{x}(m) = \mathbf{T}(m, n)\mathbf{x}(n), \quad \mathbf{T}(m, n) = \mathbf{T}^{-1}(m)\mathbf{T}(n)$$

or

$$x_i(m) = \sum_j T_{ij}(m, n)x_j(n), \quad T_{ij}(m, m) = \delta_{ij}, \qquad (17)$$

with an inverse defined through the relations

$$\sum_j T_{ij}(m, n)T_{jk}(n, m) = \delta_{ik}, \quad \mathbf{T}^{-1}(m, n) = \mathbf{T}(n, m),$$

and subject to the restrictions

$$T_{2N+1,j}(n, m) = 0 \quad \text{if} \quad j \neq 2N + 1,$$
$$T_{2N+1,2N+1}(n, m) = 1, \qquad (18)$$

consistent with conditions (9). The transformation $\mathbf{T}(m, n)$ is said to be canonical within S in the sense that expression (8) requires that

$$\sum_{kk'} T_{ik}(m, n)c_{kk'}\tilde{T}_{k'j}(m, n) = c_{ij}, \quad \tilde{T}_{ij}(m, n) = T_{ji}(m, n). \qquad (19)$$

That an identical expression holds also for $\mathbf{T}(n)$ follows from its definition in (13). Applying (17) to (10), we obtain

$$\mathbf{x}(m)x_i(n) = x_i(n)\mathbf{x}(m) + \mathbf{c}^i(n, m),$$
$$c_k^i(n, m) = \sum_j T_{ij}(n, m)c_k^j, \qquad (20)$$

the latter simplifying, upon using (9), to

$$c_k^i(n, m) = T_{i,k+N}(n, m), \qquad 1 \leq k \leq N,$$
$$c_k^i(n, m) = -T_{i,k-N}(n, m), \quad N + 1 \leq k \leq 2N. \quad (21)$$

If we break down the $(2N + 1)^2$ structure of our tensors into four N^2 tensors, two N-dimensional column and two N-dimensional row vectors, plus a scalar term (A1), we find from the Appendix that it is possible to further simplify the theory. In particular, using (A2)–(A4), we obtain

$$\omega_i(n) = \omega_{i+N}(n), \quad T_{ij}(n) = T_{i+N,j+N}(n),$$
$$T_{i,j+N}(n) = T_{i+N,j}(n), \quad 1 \leq (i, j) \leq N. \quad (22)$$

Also, since we confine ourselves to the consideration of a real $\mathbf{H}(n)$, it is possible to reduce relations (A5) to a more compact form by defining

$$2T_{ij}(n) = [S_{ij}(n) + S_{ji}^{-1}(n)],$$
$$2T_{i,j+N}(n) = [S_{ij}(n) - S_{ji}^{-1}(n)], \quad (23)$$

such that, for $1 \leq i \leq N$,

$$2\sum_{k,k'=1}^{N} S_{ki}(n)[H_{kk'}(n) + H_{k,k'+N}(n)]S_{k'j}(n) = \omega_i(n)\delta_{ij}, \quad j \geq i, \quad (24)$$
$$\sum_{k=1}^{N} S_{ik}(n)\omega_k(n)S_{jk}(n) = 2[H_{ij}(n) - H_{i,j+N}(n)], \quad j \geq i.$$

Expressions (24) represent $N(N + 1)$ equations in $N(N + 1)$ real unknowns, and combine to form the eigenvalue representation

$$\sum_{k=1}^{N}\{[H_{ik}(n) - H_{i,k+N}(n)][H_{ik}(n) + H_{i,k+N}(n)] - [\tfrac{1}{2}\omega_j(n)]^2\delta_{ik}\}S_{kj}(n) = 0, \quad (25)$$

which in turn defines a characteristic or secular equation for $[\omega_i(n)]^2$, $1 \leq i \leq N$. The multiplicative constants for the eigenvectors and the signs on $\omega_i(n)$ are then determined by substituting back into the N expressions defining $\omega_i(n)$ in (24) and using the fact that $\mathbf{S}(n)$ must be real. Also, using (24) along with the first part of (A6), we obtain

$$T_{i,2N+1}(n) = -2\sum_{k,k'=1}^{N} S_{ik}(n)\omega_k^{-1}(n)S_{k'k}(n)H_{k',2N+1}(n), \quad (26)$$

for $1 \leq i \leq N$. Taking the inverse of $\mathbf{T}(m)$ and substituting it along with $\mathbf{T}(n)$ into the definition of $\mathbf{T}(m, n)$ in (17), we find that $\mathbf{T}(m, n)$ has the structure of $\mathbf{T}$—that is, expression (A3)—except that now

$$2T_{ij}(m, n) = \sum_{k=1}^{N}[S_{ik}^{-1}(m)S_{kj}(n) + S_{ki}(m)S_{jk}^{-1}(n)],$$
$$2T_{i,j+N}(m, n) = \sum_{k=1}^{N}[S_{ik}^{-1}(m)S_{kj}(n) - S_{ki}(m)S_{jk}^{-1}(n)],$$
$$T_{i,2N+1}(m, n) = \sum_{k=1}^{N}S_{ik}^{-1}(m)[T_{k,2N+1}(n) - T_{k,2N+1}(m)],$$
$$1 \leq (i, j) \leq N. \quad (27)$$

Finally, using (A7) and (A8), we can write

$$\omega_{2N+1}(n) = 2 \cdot \det\,[H^0(n)]/\det\,[H^r(n)], \quad (28)$$

which completes our development of $\mathbf{T}$ and $\mathbf{H}^D$, this development being based on the proposition that one can define or represent $\mathbf{H}(n)$ in the form given by (A2).

III. STATISTICS

Construct now a function

$$f(\alpha, m) = \exp\,[\alpha H^0(m)] \quad (29)$$

in terms of $H^0(m)$ and the parameter α, such that

$$x_i(m)f(\alpha, m) = \lambda_i(\alpha, m)f(\alpha, m)x_i(m)$$

or in vector notation

$$\mathbf{x}(m)f(\alpha, m) = \mathbf{\Lambda}(\alpha; m, m)f(\alpha, m)\mathbf{x}(m), \quad (30)$$

where

$$\Lambda_{ij}(\alpha; m, m) = \lambda_i(\alpha, m)\delta_{ij}.$$

Inserting (9) into (11), we easily see that

$$\lambda_i(\alpha, m) = \exp\,[\alpha\omega_i(m)], \quad 1 \leq i \leq N,$$
$$\lambda_i(\alpha, m) = \exp\,[-\alpha\omega_{i-N}(m)], \quad N + 1 \leq i \leq 2N,$$
$$\lambda_i(\alpha, m) = 1, \quad i = 2N + 1, \quad (31)$$

where from (22)

$$\omega_i(m) = \tfrac{1}{2}\omega_i(m) + \tfrac{1}{2}\omega_{i+N}(m), \quad 1 \leq i \leq N.$$

By inserting (11) into (29) and using (9), it is also evident that

$$\frac{\partial f}{\partial \alpha}(\alpha, m) = \left(\sum_{i=1}^{N}[\omega_i(m)x_{i+N}(m)x_i(m) + \tfrac{1}{2}\omega_i(m)] + \tfrac{1}{2}\omega_{2N+1}(m)\right)f(\alpha, m). \quad (32)$$

Applying (17) to (30), we obtain

$$x_i(n)f(\alpha, m) = \sum_j \Lambda_{ij}(\alpha; m, n)f(\alpha, n)x_j(n)$$

or

$$\mathbf{x}(n)f(\alpha, m) = \mathbf{\Lambda}(\alpha; m, n)f(\alpha, m)\mathbf{x}(n), \quad (33)$$

where

$$\Lambda_{ij}(\alpha; m, n) = \sum_k T_{ik}(n, m)\lambda_k(\alpha, m)T_{kj}(m, n). \quad (34)$$

Using $x_i(n)$ and $f(\alpha, m)$, we now construct the statistical function [a generalization of (6)]

$$K(\{\alpha\}, \{m\}, \{n\}, M) = \mathrm{Tr}\,[f(\alpha_1, m_1)x_{i_1}(n_1)\cdots f(\alpha_M, m_M)x_{i_M}(n_M)]$$

over a complete set of states of the system, with a replacement of $x_{i_p}(n_p)$ at the p position by an arbitrary quantity Q indicated by

$$\begin{aligned}K(\{\alpha\}, \{m\}, \{n\}, M{:}p, Q) &= \mathrm{Tr}\,[f(\alpha_1, m_1)x_{i_1}(n_1)\cdots f(\alpha_{p-1}, m_{p-1})x_{i_{p-1}}(n_{p-1})\\ &\quad\times f(\alpha_p, m_p)Qf(\alpha_{p+1}, m_{p+1})x_{i_{p+1}}(n_{p+1})\\ &\quad\times\cdots\times f(\alpha_M, m_M)x_{i_M}(n_M)],\end{aligned}$$

a double replacement of $x_{i_p}(n_p)$ and $x_{i_q}(n_q)$ at the p and q positions by Q and Q' respectively by

$$K(\{\alpha\}, \{m\}, \{n\}, M{:}p, Q; q, Q'),$$

etc. We then move $\mathbf{x}(n_p)$ to the right in

$$K(\{\alpha\}, \{m\}, \{n\}, M{:}p, \mathbf{x}(n_p)),$$

using expressions (20) and (33) and the cyclic property of the trace until $\mathbf{x}(n_p)$ is returned to its original position. The expression generated by this procedure is

$$\begin{aligned}K(\{\alpha\},\{m\},\{n\},M{:}\,p,\mathbf{x}(n_p)) &= \mathbf{\Lambda}(\{\alpha\},\{m\};n_p,p,M)K(\{\alpha\},\{m\},\{n\},M{:}\,p,\mathbf{x}(n_p))\\ &\quad+\sum_{q=1}^{M-1}\mathbf{\Lambda}(\{\alpha\},\{m\};n_p,p,q)\mathbf{c}^{i_{p+q}}(n_{p+q},n_p)\\ &\quad\times K(\{\alpha\},\{m\},\{n\},M;p,1;p+q,1),\end{aligned}$$

$$\mathbf{\Lambda}(\{\alpha\},\{m\};n_p,p,q) = \mathbf{\Lambda}(\alpha_{p+1};m_{p+1},n_p)\cdots\mathbf{\Lambda}(\alpha_{p+q};m_{p+q},n_p), \quad (35)$$

and, from the cyclic nature of the trace,

$$p+q\equiv p+q-M, \quad \text{if} \quad M<p+q\le 2M,$$
$$p+q\equiv p+q+M, \quad \text{if} \quad -M<p+q\le 0.$$

It is easy to verify via (34) and (35) in conjunction with (18) and (31) that

$$\Lambda_{2N+1,j}(\{\alpha\},\{m\};n_p,p,q)=0 \quad \text{if} \quad j\neq 2N+1,$$
$$\Lambda_{2N+1,2N+1}(\{\alpha\},\{m\};n_p,p,q)=1, \quad (36)$$

and via (9), (10), (18), and (20) that

$$c^i_{2N+1}(n,m)=c^{2N+1}_i(n,m)=0 \quad \text{for all } i. \quad (37)$$

Define a tensor $\mathbf{Y}(\{\alpha\},\{m\};n_p,p,q)$, such that

$$Y_{i,2N+1}(\{\alpha\},\{m\};n_p,p,q) = \Lambda_{i,2N+1}(\{\alpha\},\{m\};n_p,p,q),$$
$$Y_{ij}(\{\alpha\},\{m\};n_p,p,q)=0 \quad \text{if} \quad j\neq 2N+1. \quad (38)$$

Then, upon expressing

$$\mathbf{\Lambda}(\{\alpha\},\{m\};n_p,p,q) = 1+\mathbf{Y}(\{\alpha\},\{m\};n_p,p,q)-\mathbf{X}(\{\alpha\},\{m\};n_p,p,q) \quad (39)$$

to define an $\mathbf{X}$, we obtain, using (35) and multiplying on the left by $\mathbf{X}^{-1}$,

$$\begin{aligned}K(\{\alpha\},\{m\},\{n\},M{:}\,p,\mathbf{x}(n_p)) &= \mathbf{X}^{-1}(\{\alpha\},\{m\};n_p,p,M)\mathbf{Y}(\{\alpha\},\{m\};n_p,p,M)\\ &\quad\times K(\{\alpha\},\{m\},\{n\},M{:}\,p,\mathbf{x}(n_p))\\ &\quad+\sum_{q=1}^{M-1}\mathbf{X}^{-1}(\{\alpha\},\{m\};n_p,p,M)\\ &\quad\times[1-\mathbf{X}(\{\alpha\},\{m\};n_p,p,q)]\mathbf{c}^{i_{p+q}}(n_{p+q},n_p)\\ &\quad\times K(\{\alpha\},\{m\},\{n\},M{:}\,p,1;p+q,1), \quad (40)\end{aligned}$$

where expressions (37) and (38) indicate that there is no contribution to (40) from

$$\mathbf{Y}(\{\alpha\},\{m\};n_p,p,q)\mathbf{c}^{i_{p+q}}(n_{p+q},n_p).$$

Finally, taking the i_pth component of (40) and using (9), we arrive at

$$\begin{aligned}K(\{\alpha\},\{m\},\{n\},M) &= Z_{i_p,2N+1}(\{\alpha\},\{m\};n_p,p,M)\\ &\quad\times K(\{\alpha\},\{m\},\{n\},M{:}\,p,1)\\ &\quad+\sum_{q=1}^{M-1}\mathbf{z}_{i_p}(\{\alpha\},\{m\},p,q,M{:}\,i_{p+q},n_{p+q},n_p)\\ &\quad\times K(\{\alpha\},\{m\},\{n\},M{:}\,p,1;p+q,1), \quad (41)\end{aligned}$$

where

$$\begin{aligned}\mathbf{Z}(\{\alpha\},\{m\};n_p,p,M) &= \mathbf{X}^{-1}(\{\alpha\},\{m\};n_p,p,M)\mathbf{Y}(\{\alpha\},\{m\};n_p,p,M),\\ \mathbf{z}(\{\alpha\},\{m\},p,q,M{:}\,i_{p+q},n_{p+q},n_p) &= \mathbf{X}^{-1}(\{\alpha\},\{m\};n_p,p,M)\\ &\quad\times[1-\mathbf{X}(\{\alpha\},\{m\};n_p,p,q)]\mathbf{c}^{i_{p+q}}(n_{p+q},n_p). \quad (42)\end{aligned}$$

From the definition of $\mathbf{X}$ in (39), we see, upon employing (36) and (38), that

$$X_{i,2N+1}(\{\alpha\},\{m\};n_p,p,q) = X_{2N+1,i}(\{\alpha\},\{m\};n_p,p,q)=0 \quad \text{if} \quad i\neq 2N+1,$$
$$X_{2N+1,2N+1}(\{\alpha\},\{m\};n_p,p,q)=1, \quad (43)$$

with similar expressions for $\mathbf{X}^{-1}$. Thus, for $i_p = 2N+1$, it is apparent upon inspecting (42) and (43) that relation (41) becomes an identity, while, for $i_p\neq 2N+1$, relation (41) expresses $K(\{\alpha\},\{m\},\{n\},M)$ in terms of functions of lower order in the operator x_i, $i\neq 2N+1$. When $i_{p+q}=2N+1$, use of (37) and (42) tells us that these contributions to the right-hand side of relation (41) will vanish. Continued use of (41)

will finally express any $K(\{\alpha\}, \{m\}, \{n\}, M)$ in terms of the function

$$K(\{\alpha\}, \{m\}, M) = \mathrm{Tr}\,[f(\alpha_1, m_1)\cdots f(\alpha_M, m_M)]. \tag{44}$$

In order to determine $K(\{\alpha\}, \{m\}, M)$, for a given M, we first utilize (32) along with (30) and (44) to obtain

$$\begin{aligned}\frac{\partial K}{\partial \alpha_p}(\{\alpha\}, \{m\}, M) &= \sum_{i_p=1}^{N} \omega_{i_p}(m_p)\lambda_{i_p}(\alpha_p, m_p) \\ &\times \mathrm{Tr}\,[f(\alpha_1, m_1)\cdots f(\alpha_{p-1}, m_{p-1})x_{i_p+N}(m_p) \\ &\times f(\alpha_p, m_p)x_{i_p}(m_p)f(\alpha_{p+1}, m_{p+1})\cdots f(\alpha_M, m_M)] \\ &+ \frac{1}{2}\left[\sum_{i=1}^{N}\omega_{i+N}(m_p) + \omega_{2N+1}(m_p)\right]K(\{\alpha\}, \{m\}, M).\end{aligned} \tag{45}$$

Under the restrictions that

$$\begin{aligned} n_p = n_{p-1} = m_p, \quad i_{p-1} = i_p + N, \\ i_{p+q} = 2N + 1 \quad \text{if} \quad q \neq (0, M-1),\end{aligned}$$

we twice insert (41) into the right-hand side of expression (45) and arrive at the differential equation

$$\begin{aligned}\frac{\partial K}{\partial \alpha_p}(\{\alpha\}, \{m\}, M) &= \sum_{i_p=1}^{N}\omega_{i_p}(m_p)\lambda_{i_p}(\alpha_p, m_p)[Z_{i_p,2N+1}(\{\alpha\}, \{m\}; m_p, p, M) \\ &\times Z_{i_p+N,2N+1}(\{\alpha\}, \{m\}; m_p, p-1, M) \\ &+ z_{i_p}(\{\alpha\}, \{m\}, p, M-1, M: i_p + N, m_p, m_p)] \\ &\times K(\{\alpha\}, \{m\}, M) + R_N(m_p)K(\{\alpha\}, \{m\}, M),\end{aligned} \tag{46}$$

where

$$R_N(m) = \frac{1}{2}\left[\sum_{i=1}^{N}\omega_i(m) + \omega_{2N+1}(m)\right].$$

Equation (46) has the solution

$$\begin{aligned}K(\{\alpha\}, \{m\}, M) &= K^p(\{\alpha\}, \{m\}, M)\exp\,[\alpha_p R_N(m_p) \\ &+ F(\{\alpha\}, \{m\}, M) + F'(\{\alpha\}, \{m\}, M)],\end{aligned}$$

$$\begin{aligned}F(\{\alpha\}, \{m\}, M) &= \int_0^{\alpha_p} d\alpha_p \sum_{i_p=1}^{N}\omega_{i_p}(m_p)\lambda_{i_p}(\alpha_p, m_p) \\ &\times Z_{i_p,2N+1}(\{\alpha\}, \{m\}; m_p, p, M) \\ &\times Z_{i_p+N,2N+1}(\{\alpha\}, \{m\}; m_p, p-1, M),\end{aligned} \tag{47}$$

$$\begin{aligned}F'(\{\alpha\}, \{m\}, M) &= \int_0^{\alpha_p} d\alpha_p \sum_{i_p=1}^{N}\omega_{i_p}(m_p)\lambda_{i_p}(\alpha_p, m_p) \\ &\times z_{i_p}(\{\alpha\}, \{m\}, p, M-1, M: i_p + N, m_p, m_p),\end{aligned}$$

where $K^p(\{\alpha\}, \{m\}, M)$ is $K(\{\alpha\}, \{m\}, M)$ at $\alpha_p = 0$. For $p = M$,

$$K^p(\{\alpha\}, \{m\}, M) = K(\{\alpha\}, \{m\}, M-1), \tag{48}$$

and expression (47) has the effect of reducing the sequence over which $K(\{\alpha\}, \{m\}, M)$ runs by one. Repeated use of (47) for $p = M$ reduces a given $K(\alpha), \{m\}, M)$ to $K(\{\alpha\}, \{m\}, 0)$, that is Tr 1. However, the zero limit of the integral in $K(\{\alpha\}, \{m\}, 1)$ will cancel $K(\{\alpha\}, \{m\}, 0)$ which eliminates this obstacle. In order to clarify the situation, we introduce the permutation operator P, such that

$$\begin{aligned} P\alpha_q = \alpha_{q-1}, \quad Pm_q = m_{q-1}, \quad \text{if} \quad q > 1, \\ P\alpha_q = Pm_q = \epsilon \to 0, \quad \text{if} \quad q = 1,\end{aligned}$$

where α_q and m_q are members of $\{\alpha\}$ and $\{m\}$, respectively. Also, if $\{\alpha\}'$ and $\{m\}'$ are contained in $\{\alpha\}$ and $\{m\}$, respectively, then, for an arbitrary function $A(\{\alpha\}', \{m\}')$,

$$PA(\{\alpha\}', \{m\}') = A(P\{\alpha\}', P\{m\}').$$

However, and of utmost importance, if P operates on an isolated member of a product and this member is consequently found to be directly (or inversely) proportional to ϵ as $\epsilon \to 0$, then the ϵ factor is retained until the full product can be assembled and simplified or until further operation with P provides a means for cancellation. For example,

$$\begin{aligned}P^2(1) &= P^2[(\alpha_1 + \alpha_2)/(\alpha_1 + \alpha_2)] \\ &= P^2(\alpha_1 + \alpha_2)/P^2(\alpha_1 + \alpha_2) \\ &= P(\alpha_1)/P(\alpha_1) = \epsilon(1/\epsilon) = 1, \quad \text{not } 0(1/0), \\ P^2[\alpha_1/(\alpha_1 + \alpha_2)] &= P(\epsilon/\alpha_1) = \epsilon/\epsilon = 1.\end{aligned}$$

Thus,

$$\begin{aligned} PK(\{\alpha\}, \{m\}, p) = K(\{\alpha\}, \{m\}, p-1), \quad \text{if} \quad p \geq 1, \\ PK(\{\alpha\}, m, 0) = K(\{\alpha\}, m, 0),\end{aligned}$$

and, upon combining these conditions with expressions (47) and (48), we obtain

$$\begin{aligned}K(\{\alpha\}, \{m\}, M) &= K(\{\alpha\}, m, 0)\exp\left(\sum_{p=1}^{M}\{\alpha_p R_N(m_p) \right. \\ &\left. + P^{p-1}[F(\{\alpha\}, \{m\}, M) + F'(\{\alpha\}, \{m\}, M)]\}\right),\end{aligned} \tag{49}$$

where

$$P^M[F(\{\alpha\}, \{m\}, M) + F'(\{\alpha\}, \{m\}, M)] = 0.$$

However, operating on (49) with P^{M-q} produces

$$\begin{aligned}K(\{\alpha\}, \{m\}, q) &= K(\{\alpha\}, m, 0)\exp\left(\sum_{p=1}^{q}\{\alpha_p R_N(m_p) \right. \\ &\left. + P^{M-p}[F(\{\alpha\}, \{m\}, M) + F'(\{\alpha\}, \{m\}, M)]\}\right),\end{aligned} \tag{50}$$

which informs us upon consulting (29), (32), and (44) that

$$\log K(\{\alpha\}, m, 0) = -\lim_{\alpha_1 \to -\infty} P^{M-1}[F(\{\alpha\}, \{m\}, M) + F'(\{\alpha\}, \{m\}, M)], \tag{51}$$

upon setting $K(\{\alpha\}, \{m\}, 1) = 1$ and using (50) for $q = 1$.

We have thus formed the basis for a solution to $K(\{\alpha\}, \{m\}, M)$, although there is no guarantee that the integrals contained in (47) can be performed analytically. Also, we have completed our primary goal, that is, to develop a theory for the evaluation of $K(\{\alpha\}, \{m\}, 0, M)$, by means of $K(\{\alpha\}, \{m\}, n, M)$.

IV. THE DEBYE-WALLER FORM

Recently, we[3] presented a method of evaluating a general time-dependent thermal average $\langle A(q, p; \{t\})\rangle$ of the form

$$\langle A(q, p; \{t\})\rangle = \prod_i \langle A_i(q, p; \{t\})\rangle,$$

$$\langle e^{\theta}\rangle \equiv \operatorname{Tr} e^{-\beta H} e^{\theta} / \operatorname{Tr} e^{-\beta H}, \quad \beta = 1/k_B T,$$

$$A_i(q, p; \{t\}) = \exp[\theta_i(q, t_q)] \exp[\theta_i(q+1, t_{q+1})] \cdots \exp[\theta_i(p, t_p)],$$

$$p \geq q \text{ integers},$$

$$\theta_i(q, t) = e^{iHt}\theta_i(q)e^{-iHt}, \qquad \theta_i(q) = c_i(q)a_i + d_i(q)a_i^{\dagger}, \qquad H = \sum_i \omega_i(a_i^{\dagger}a_i + \tfrac{1}{2}), \tag{52}$$

subject to the commutation relations

$$[\theta_i(q), \theta_i(q')] = 0, \quad [a_i, a_j^{\dagger}] = \delta_{ij}, \quad [a_i, a_j] = 0, \text{ etc.}$$

The solution was expressed as

$$\langle A_i(1, p; \{t\})\rangle = \exp\left(\tfrac{1}{2}\sum_{q=1}^{p}\sum_{q'=1}^{p} c_i(q)d_i(q') \times [N_i g_i^{-}(t_q, t_{q'}) + (N_i + 1)g_i^{+}(t_q, t_{q'})]\right) \tag{53}$$

in terms of

$$N_i = (e^{\beta\omega_i} - 1)^{-1}$$

and an ordered function

$$g_i^{\pm}(t_q, t_{q'}) = \exp[\pm i\omega_i(t_q - t_{q'})], \quad q > q'; \qquad = 1, \quad q = q'; \qquad = \exp[\pm i\omega_i(t_{q'} - t_q)], \quad q < q'.$$

Relations for constructing expressions for averages involving products of A, a, and $a^{\dagger}$ were also given. Expressions (52) represent an extended Debye–Waller form as they emphasize the transformation operator θ rather than the Hamiltonian operator H. However, assuming $\theta_i(q)$ is anti-Hermitian such that

$$\theta_i(q) = \theta_i'(n_q) + \theta_i'^{\dagger}(m_q), \quad 0 = \theta_i'(n_q) + \theta_i'^{\dagger}(n_q)$$

and

$$m_q = n_{q+1}, \quad m_p = n_1,$$

it follows that

$$\langle A(q, p; \{t\})\rangle = \operatorname{Tr}\exp[-\beta H(n_q)]\exp[iH(n_q)(t_q - t_p)] \times \exp[iH(n_{q+1})(t_{q+1} - t_q)] \times \cdots \times \exp[iH(n_p)(t_p - t_{p-1})] / \operatorname{Tr}\exp(-\beta H), \tag{54}$$

where[4]

$$H(n) = \sum_{i=1}^{N} \exp[-\theta_i'(n)]H_i \exp[\theta_i'(n)], \quad H = \sum_{i=1}^{N} H_i,$$

and one returns to a more direct Hamiltonian formulation for the thermal average. Expression (54) is in fact just a special case of the more general statistical form defined by (6). We shall now consider a special example to illustrate the theory outlined in Secs. II and III.

V. A NONTRIVIAL EXAMPLE

It is not the purpose of this paper to rederive expression (53) using the new formalism, although this can easily be done upon taking $N = 1$ and letting

$$\langle A_i(1, p; \{t\})\rangle \to K(\{\alpha\}, \{m\}, p)/K(\{\alpha\}, \{m\}, 1),$$

where

$$(-\beta + it_1 - it_p) \to \alpha_1, \qquad i(t_2 - t_1) \to \alpha_2, \cdots, i(t_p - t_{p-1}) \to \alpha_p, \qquad \exp[-\theta_i'(n)]\omega_i(a_i^{\dagger}a_i + \tfrac{1}{2})\exp[\theta_i'(n)] \to H^0(n), \text{ etc.} \tag{55}$$

We leave this verification—as an exercise for the reader— to be undertaken with the aid of a previous work.[3] We wish rather to consider an example which will not only clarify and illustrate the theory but will also represent a situation not encompassed by (52). Let us take the example of a phonon mode interacting with an electron in the state n. The Hamiltonian for the system (ignoring phonon subscripts) can be written

$$H'(n) = \epsilon(n) + \omega(b^{\dagger}b + \tfrac{1}{2}) + V(n)(b + b^{\dagger}) + V'(n)(b + b^{\dagger})(b + b^{\dagger}), \tag{56}$$

in terms of the electron energy $\epsilon(n)$, the phonon energy $\omega(\omega > 0)$, and the phonon creation and annihilation operators $b^{\dagger}$ and b. As this Hamiltonian includes a general electron–phonon interaction $V'(n)[|V'(n)| < \omega/4]$ quadratic in the phonon coordinate, it cannot be correlated to the Debye–Waller form through, for example, expression (54).

We shall develop the form for the spectral-absorption function[5] between the electronic states $\epsilon(2) > \epsilon(1)$,

$$K_{12}(\bar{\omega}, H') = \frac{1}{2\pi\rho_1}\int_{-\infty}^{\infty} ds \exp(i\bar{\omega}s)K_{12}(s, H'),$$
$$K_{12}(s, H') = \mathrm{Tr}\, e^{-\beta H'(1)}e^{iH'(1)s}e^{-iH'(2)s}/\sum_n \mathrm{Tr}\, e^{-\beta H'(n)}, \tag{57}$$

where ρ_1 is the density of the ground electronic state and $\bar{\omega}$ is the photon energy, by calculating $K_{12}(s, H')$ using the theory of Sec. III.

We begin by considering the case

$$N = 1, \quad \alpha_1 = (-\beta + is), \quad \alpha_2 = -is, \quad m_1 = 1, \quad m_2 = 2, \quad b = x_1(0), \quad b^\dagger = x_2(0) \tag{58}$$

such that

$$K_{12}(s, H') = \frac{\exp[-\beta\epsilon(1) - i\omega_{12}s]K(\{\alpha\}, \{m\}, 2)}{\sum_n e^{-\beta\epsilon(n)}\mathrm{Tr}\, K(-\beta, n, 1)}, \tag{59}$$

with

$$H'(n) = H^0(n) + \epsilon(n), \quad \omega_{12} = \epsilon(2) - \epsilon(1).$$

Having established $H^0(n)$ in (56) and assuming all its coefficients to be real numbers, we can equate it to (14) and arrive at a matrix representation

$$\begin{bmatrix} \frac{1}{2}\omega + V'(n) & V'(n) & \frac{1}{2}V(n) \\ V'(n) & \frac{1}{2}\omega + V'(n) & \frac{1}{2}V(n) \\ \frac{1}{2}V(n) & \frac{1}{2}V(n) & 0 \end{bmatrix} \tag{60}$$

for $\mathbf{H}(n)$ consistent with (A2). Dropping the subscript i over phonon modes, we obtain

$$\omega(n) = \omega_1(n) = \{\omega[\omega + 4V'(n)]\}^{\frac{1}{2}},$$
$$\exp[-\phi(n)] = \pm S_{11}(n) = [\omega/\omega(n)]^{\frac{1}{2}}, \tag{61}$$

upon inserting the elements of (60) into expressions (25) and (24). Employing relations (26) and (27), we conclude that $\mathbf{T}(m, n)$ can be represented as

$$\begin{bmatrix} \cosh[\phi(m) - \phi(n)] & \sinh[\phi(m) - \phi(n)] & T_3(m, n) \\ \sinh[\phi(m) - \phi(n)] & \cosh[\phi(m) - \phi(n)] & T_3(m, n) \\ 0 & 0 & 1 \end{bmatrix},$$

where

$$T_3(m, n) = T_{1,3}(m, n) = \pm[\omega \cdot \omega(m)]^{\frac{1}{2}}[V(m)/\omega^2(m) - V(n)/\omega^2(n)]. \tag{62}$$

Upon substituting the elements of $\mathbf{T}(m, n)$ into expression (34) and using (31), (A4), and (61), the elements of $\mathbf{\Lambda}(\alpha; m, n)$ become

$$\begin{aligned}
\Lambda_{11}(\alpha; m,n) &= \Lambda_{22}(-\alpha; m, n) \\
&= \cosh[\alpha\omega(m)] + \cosh 2[\phi(m) - \phi(n)] \\
&\quad \times \sinh[\alpha\omega(m)], \\
\Lambda_{12}(\alpha; m, n) &= \Lambda_{21}(-\alpha; m, n) \\
&= \sinh[\alpha\omega(m)]\sinh 2[\phi(m) - \phi(n)], \\
\Lambda_{13}(\alpha; m, n) &= \Lambda_{23}(-\alpha; m, n) \\
&= \langle e^{[\phi(m)-\phi(n)]}\sinh[\alpha\omega(m)] - e^{-[\phi(m)-\phi(n)]} \\
&\quad \times \{1 - \cosh[\alpha\omega(m)]\}\rangle T_3(m, n), \\
\Lambda_{31}(\alpha; m, n) &= \Lambda_{32}(\alpha; m, n) = 0, \quad \Lambda_{33}(\alpha; m, n) = 1.
\end{aligned} \tag{63}$$

Returning to expressions (47), (58), and (59), we find that we can calculate $K(\{\alpha\}, \{m\}, 2)$, where $M = 2$, by setting $p = 2$ and considering

$$\begin{aligned}
\mathbf{\Lambda}(\{\alpha\}, \{m\}; 2, 2, 2) &= \mathbf{\Lambda}(\alpha_1; 1, 2)\mathbf{\Lambda}(\alpha_2; 2, 2), \\
\mathbf{\Lambda}(\{\alpha\}, \{m\}; 2, 1, 2) &= \mathbf{\Lambda}(\alpha_2; 2, 2)\mathbf{\Lambda}(\alpha_1; 1, 2), \\
\mathbf{\Lambda}(\{\alpha\}, \{m\}; 2, 2, 1) &= \mathbf{\Lambda}(\alpha_1; 1, 2),
\end{aligned} \tag{64}$$

upon employing (35). Inserting the elements (63) into (64) and utilizing (31), (17), (21), (38), (39), (42), (A4), (61), and (62), we obtain

$$\begin{aligned}
&F(\{\alpha\}, \{m\}, 2) \\
&\quad = \omega(1)\omega(2)[A(1)/\omega^2(1) - A(2)/\omega^2(2)]^2/ \\
&\quad\quad \{\omega(1)\coth[\tfrac{1}{2}\alpha_1\omega(1)] + \omega(2)\coth[\tfrac{1}{2}\alpha_2\omega(2)]\},
\end{aligned} \tag{65}$$

where

$$A(m) = (2\omega)^{\frac{1}{2}}V(m),$$

and

$$\begin{aligned}
F'(\{\alpha\}, \{m\}, 2) = \log[e^{-\frac{1}{2}\alpha_2\omega(2)}(\{\cosh[\alpha_1\omega(1)] - 1\} \\
\times \{\cosh[\alpha_2\omega(2)]\cosh[\alpha_1\omega(1)] - 1 \\
+ \tfrac{1}{2}[\omega(1)/\omega(2) + \omega(2)/\omega(1)] \\
\times \sinh[\alpha_2\omega(2)]\sinh[\alpha_1\omega(1)]\}^{-1})^{\frac{1}{2}}].
\end{aligned} \tag{66}$$

Also, using (A7) and (60), along with the definition in (46), we have

$$R_1(m) = \tfrac{1}{2}[\omega(m) - A^2(m)/\omega^2(m)].$$

Inserting (65) and (66) into (51) and applying P, we now arrive at

$$K(\{\alpha\}, \{m\}, 0) = -\lim_{\alpha_1 \to -\infty} e^{\frac{1}{2}\alpha_1\omega(1)}\sinh[\tfrac{1}{2}\alpha_1\omega(1)]/[\tfrac{1}{2}\epsilon\omega(\epsilon)] = \epsilon^{-1}\omega^{-1}(\epsilon).$$

Proceeding in the same manner with (49), we obtain

$$\begin{aligned}
K(\{\alpha\}, \{m\}, 2) &= \tfrac{1}{2}\exp\{-\tfrac{1}{2}[\alpha_1 A^2(1)/\omega^2(1) + \alpha_2 A^2(2)/\omega^2(2)]\} \\
&\quad \times F''(\{\alpha\}, \{m\}, 2)e^{F'(\{\alpha\},\{m\},2)},
\end{aligned} \tag{67}$$

where

$$F''(\{\alpha\},\{m\},2) = 2^{\frac{1}{2}}\{\cosh[\alpha_2\omega(2)]\cosh[\alpha_1\omega(1)] - 1 + \tfrac{1}{2}[\omega(1)/\omega(2) + \omega(2)/\omega(1)] \times \sinh[\alpha_2\omega(2)]\sinh[\alpha_1\omega(1)]\}^{-\frac{1}{2}},$$

and with (50) (for $q = 1$) we obtain

$$K(\{\alpha\},\{m\},1) = 2^{-\frac{1}{2}}\exp\{-\tfrac{1}{2}[\alpha_1 A^2(1)/\omega^2(1)]\} \times \{\cosh[\alpha_1\omega(1)] - 1\}^{-\frac{1}{2}}. \quad (68)$$

Replacing $m_1 = 1$ in (68) by m and setting $\alpha_1 = -\beta$, we find that the denominator in expression (59) cannot be factored between the electron and phonon coordinates and the electron density ρ must be written as

$$\rho_n = \frac{\exp[-\beta\bar{\epsilon}(n)]\sinh^{-1}[\frac{1}{2}\beta\omega(n)]}{\sum_m \exp[-\beta\bar{\epsilon}(m)]\sinh^{-1}[\frac{1}{2}\beta\omega(m)]}, \quad (69)$$

where

$$\bar{\epsilon}(m) = \epsilon(m) - \tfrac{1}{2}A^2(m)/\omega^2(m).$$

One can now express, for $\alpha_1 = (-\beta + is)$ and $\alpha_2 = -is$,

$$K_{12}(s,H')/\rho_1 = \exp(i\bar{\omega}_{12}s)\sinh[\tfrac{1}{2}\beta\omega(1)] \times F''(\{\alpha\},\{m\},2)e^{F'(\{\alpha\},\{m\},2)}, \quad (70)$$
$$\bar{\omega}_{12} = \bar{\epsilon}(2) - \bar{\epsilon}(1)$$

upon substituting (67) back into (59), and we are in agreement with O'Rourke[6] regarding the expression for the spectral-absorption function. The single phonon mode used in this example can be replaced by a set of uncoupled phonon modes simply by taking a product of $K_{12}(s,H')/\rho_1$ over phonon modes [see (6)] before forming its transform. In the case of ρ_n the product is formed over phonon modes for each term in both the numerator and the denominator of relation (69).

Let us briefly mention a few more applications to the theory. The spectral absorption function $K_{12}(\bar{\omega},H')$ defined in (57) and developed in this section could be utilized by approximate methods discussed previously by Howgate[5] to calculate a nonradiative electron transition rate for a Hamiltonian of the form (1), upon ignoring coupling between different phonon modes:

$$V'_{ij}(n) = V'_{ij}(m,n) = 0, \quad \text{if} \quad i \neq j.$$

A more rigorous approach would be to calculate the nonradiative electron transition rate from a thermal average of the form $\langle V^2\rangle$ [see (2)] via (57) in conjunction with the reduction formula (41). In order to include coupling between different phonon modes, the transform for the spectral absorption function $K_{12}(\bar{\omega},H')$—utilizing H^0—could, for example, be calculated for the case of two coupled phonon modes

$$V'_{12}(n) = V'_{21}(n) \neq 0$$

by going to $N = 2$, $M = 2$, and the appropriate Hamiltonian matrix $\mathbf{H}(n)$ defined through (A2) by

$$H^{11}(n) = \begin{bmatrix} \frac{1}{2}\omega + V'_{11}(n) & V'_{12}(n) \\ V'_{12}(n) & \frac{1}{2}\omega + V'_{22}(n) \end{bmatrix},$$

$$H^{12}(n) = \begin{bmatrix} V'_{11}(n) & V'_{12}(n) \\ V'_{12}(n) & V'_{22}(n) \end{bmatrix},$$

$$H^3(n) = \begin{bmatrix} \frac{1}{2}V_1(n) \\ \frac{1}{2}V_2(n) \end{bmatrix}, \quad H^C(n) = 0.$$

Further illustrations for the theory are abundant.

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APPENDIX

In order to clarify the $(2N + 1)^2$ structure of the tensors defined in this paper, we shall choose—for an arbitrary tensor $\mathbf{Z}(n)$—the matrix representation

$$\begin{bmatrix} Z^{11}(n) & Z^{12}(n) & Z^3(n) \\ Z^{21}(n) & Z^{22}(n) & Z^4(n) \\ \tilde{Z}^5(n) & \tilde{Z}^6(n) & Z^C(n) \end{bmatrix}, \quad (A1)$$

where $Z^{11}(n)$, $Z^{12}(n)$, $Z^{21}(n)$, and $Z^{22}(n)$ are $N \times N$ matrices, $Z^3(n)$, $Z^4(n)$, $Z^5(n)$, and $Z^6(n)$ are N-dimensional column vectors, and $Z^C(n)$ is the element $Z_{2N+1,2N+1}(n)$. In terms of the representation (A1) we shall require that our input Hamiltonian $\mathbf{H}(n)$ can be put into the Hermitian form

$$\begin{bmatrix} H^{11}(n) & H^{12}(n) & H^3(n) \\ [H^{12}(n)]^* & [H^{11}(n)]^* & [H^3(n)]^* \\ [\tilde{H}^3(n)]^* & \tilde{H}^3(n) & H^C(n) \end{bmatrix}, \quad (A2)$$

where

$$H^{11}(n) = [H^{11}(n)]^\dagger, \quad H^{12}(n) = \tilde{H}^{12}(n).$$

This requirement eliminates any arbitrariness from the definition of $\mathbf{H}(n)$. From requirements (9) and its definition in (13), the transformation $\mathbf{T}(n)$ must satisfy the representation

$$\begin{bmatrix} T^{11}(n) & T^{12}(n) & T^3(n) \\ [T^{12}(n)]^* & [T^{11}(n)]^* & [T^3(n)]^* \\ 0 & 0 & 1 \end{bmatrix}. \quad (A3)$$

Thus, according to relations (15), (12), (19), (8), and (9), $\mathbf{H}^{D}(n)$ must have the form

$$\begin{bmatrix} H^{D,11}(n) & 0 & 0 \\ 0 & H^{D,11}(n) & 0 \\ 0 & 0 & H^{D,C}(n) \end{bmatrix}, \qquad \text{(A4)}$$

such that via (12)

$$\omega_i(n) = \omega_{i+N}(n), \quad 1 \leq i \leq N,$$

and $\mathbf{T}(n)$ can be determined from the set of $N(2N-1)$ complex and $2N$ real coupled equations for the $2N^2$ complex elements of $T^{11}(n)$ and $T^{12}(n)$ and the N real elements of $H^{D,11}(n)$. We can express these equations, using (15) and (19), in the form

$$\begin{aligned}
\omega_i(n)\delta_{ij} = 2 \sum_{k,k'=1}^{N} & [T^{*}_{ki}(n)H_{kk'}(n)T_{k'j}(n) \\
& + T_{k,i+N}(n)H^{*}_{k',k+N}(n)T_{k'j}(n) \\
& + T^{*}_{ki}(n)H_{k,k'+N}(n)T^{*}_{k',j+N}(n) \\
& + T_{k,i+N}(n)H^{*}_{kk'}(n)T^{*}_{k',j+N}(n)], \quad j \geq i,
\end{aligned}$$

$$\begin{aligned}
0 = \sum_{k,k'=1}^{N} & [T^{*}_{ki}(n)H_{kk'}(n)T_{k',j+N}(n) \\
& + T_{k,i+N}(n)H^{*}_{k',k+N}(n)T_{k',j+N}(n) \\
& + T^{*}_{ki}(n)H_{k,k'+N}(n)T^{*}_{k'j}(n) \\
& + T_{k,i+N}(n)H^{*}_{kk'}(n)T^{*}_{k'j}(n)], \quad j \geq i,
\end{aligned}$$

$$\delta_{ij} = \sum_{k=1}^{N} [T_{ik}(n)T^{*}_{jk}(n) - T_{i,k+N}(n)T^{*}_{j,k+N}(n)], \quad j \geq i,$$

$$0 = \sum_{k=1}^{N} [T_{ik}(n)T_{j,k+N}(n) - T_{i,k+N}(n)T_{jk}(n)], \quad j > i. \qquad \text{(A5)}$$

The N complex elements of $T^{3}(n)$, and $H^{D,C}(n)$ are then determined from the relations

$$\begin{aligned}
0 = \sum_{k,k'=1}^{N} & [T^{*}_{ki}(n)H_{kk'}(n)T_{k',2N+1}(n) \\
& + T_{k,i+N}(n)H^{*}_{k',k+N}(n)T_{k',2N+1}(n) \\
& + T^{*}_{ki}(n)H_{k,k'+N}(n)T^{*}_{k',2N+1}(n) \\
& + T_{k,i+N}(n)H^{*}_{kk'}(n)T^{*}_{k',2N+1}(n)] \\
& + \sum_{k=1}^{N} [T^{*}_{ki}(n)H_{k,2N+1}(n) + T_{k,i+N}(n)H^{*}_{k,2N+1}(n)],
\end{aligned}$$

$$\begin{aligned}
\omega_{2N+1}(n) = {} & 2H_{2N+1,2N+1}(n) \\
& + 4\,\mathrm{Re} \sum_{k=1}^{N} [T^{*}_{k,2N+1}(n)H_{k,2N+1}(n) \\
& + H^{*}_{k,2N+1}(n)T_{k,2N+1}(n)] \\
& + 4\,\mathrm{Re} \sum_{k,k'=1}^{N} [T^{*}_{k,2N+1}(n)H_{kk'}(n)T_{k',2N+1}(n) \\
& + T_{k,2N+1}(n)H^{*}_{k,k'+N}(n)T_{k',2N+1}(n)], \qquad \text{(A6)}
\end{aligned}$$

where Re denotes the real part. In both (A5) and (A6) indices i and j are confined to the values 1–N. This completes the primary development of $\mathbf{T}(n)$ and $\mathbf{H}^{D}(n)$ although two supplementary relations involving the elements of $\mathbf{H}^{D}(n)$ can be derived for the sake of convenience. These relations

$$\begin{aligned}
\prod_{i=1}^{N} \omega_i(n) &= 2^N \{\det [H^r(n)]\}^{\frac{1}{2}}, \\
\tfrac{1}{2}\omega_{2N+1}(n) &= \det [H(n)]/\det [H^r(n)], \qquad \text{(A7)}
\end{aligned}$$

where det is the determinant of the matrix representation of $\mathbf{H}^{r}(n)$ and $\mathbf{H}(n)$ and

$$H^{r}_{ij}(n) \equiv H_{ij}(n) \quad \text{if} \quad i \neq 2N+1, \quad j \neq 2N+1, \qquad \text{(A8)}$$

are contained in the general description provided by (A5) and (A6). They can be arrived at by employing expressions (9) and (19) to show that

$$\det [T(n)] = \det [\tilde{T}(n)] = \pm 1,$$

using (A5) to show that the diagonalization (15) applies equally well in the $(2N)^2$ subspace (r) defined in (A8) and equating determinants between the Hamiltonian in its diagonal and in its nondiagonal form. Requirement (16) implies that one cannot equate determinants in a subspace of dimension less than $(2N)^2$. If we confine ourselves to the consideration of a real $\mathbf{H}(n)$, then it is possible to reduce relations (A5) to a more compact form as illustrated in the text.

[1] We use the term operator space here instead of the term vector space because vectors and tensors—as used in this paper—are defined primarily for purposes of notation.

[2] A second-rank tensor is denoted by a boldface upper case letter; a vector is denoted by a boldface lower case letter.

[3] D. W. Howgate, J. Math. Phys. **10**, 604 (1969).

[4] The details of this transformation are clarified upon consulting Ref. 3.

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Unit Adjoint Tensor Operators in $SO(n)$

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Unit adjoint tensor operators in $SO(n)$ have been obtained, and the eigenvalues of the invariants connected with them evaluated. These adjoint tensor operators are keys to the solution of the multiplicity problem of the Wigner coefficients of $SO(n)$. These adjoint tensor operators are used in the calculation of the Wigner coefficients of $SO(5)$ in the direct product of the 10-dimensional representation with an arbitrary representation. The results agree with Hecht [K. T. Hecht, Nucl. Phys. **63**, 177 (1965)].

INTRODUCTION

Recently Louck and Biedenharn[1] have obtained unit adjoint tensor operators for $SU(n)$. Once these operators are known, it is not difficult to extend the results to all tensor operators of $SU(n)$. Since the matrix elements of these tensor operators are related through the Wigner–Eckart theorem to the Clebsch–Gordan coefficients of $SU(n)$, we can say that the Clebsch–Gordan coefficients of $SU(n)$, together with its multiplicity problem, are now within reach of a solution.

We wish to show that similar sets of unit adjoint tensor operators of $SO(n)$ can be obtained. To achieve this purpose, one must be able to solve the following problems. (1) One must obtain a set of l independent invariants, where l is the rank of the group. In our case, the groups are $SO(2l+1)$ and $SO(2l)$. (2) One must obtain l sets of mutually orthogonal adjoint tensor operators, each set transforming like the infinitesimal generators of $SO(n)$. (3) In order to be able to evaluate explicitly these adjoint tensor operators, one must obtain the eigenvalues of the invariants formed from these operators. These three topics will be considered in the following three sections.

I. INVARIANTS OF THE ORTHOGONAL GROUP

It is important to realize from the start that the invariants are closely connected with the adjoint tensor operators. This can be seen from the example of $SU(n)$. In $SU(n)$ we have at least two different sets of invariants, one obtained by Biedenharn[2] and another by Gel'fand[3] and Racah[4] and formulated by Gruber and O'Raifeartaigh.[5]

Biedenharn's invariants are

$$G_n = [i_1 i_2 j_1][j_1 i_3 j_2][j_2 i_4 j_3]\cdots[j_{n-2} i_{n-1} i_n] X_{i_1} X_{i_2} \cdots X_{i_n}, \tag{1}$$

where $[ijk]$ are the symmetrically coupled constants given in Eq. (16) of Biedenharn's paper and the X_i are the generators. In Eq. (1) and all subsequent equations in this paper, the summation sign from 1 to n is always implied over repeated indices.

The Gel'fand invariants are

$$I_n = E_{i_1 i_2} E_{i_2 i_3} \cdots E_{i_n i_1}, \tag{2}$$

where E_{ij} is a matrix with one at the ith row and jth column, but zero elsewhere.

If we use Biedenharn's invariants, G_2 and G_3 say, in $SU(3)$, we obtain the mutually orthogonal adjoint tensor operators

$$X_A, \quad A = 1, 2, \cdots, 8, \tag{3}$$

and

$$G_3 X_A - G_2 X_A^{(2)}, \tag{4}$$

where the $X_A^{(2)}$ are the symmetrically coupled generators.

However, if one uses the Gel'fand invariants $I_2 = E_{ij}E_{ji}$ and $I_3 = E_{ij}E_{jk}E_{ki}$, one obtains the mutually orthogonal adjoint tensor operators

$$E_{ij}, \quad i, j = 1, 2, 3, \quad E_{ii} = 0, \tag{5}$$

and

$$I_3 E_{ij} - I_2 E_{ik} E_{kj}. \tag{6}$$

Throughout expressions (3), (4), (5), and (6), we have neglected normalization, which can be easily restored. Since E_{ij} and X_A are linearly related [see Eqs. (9)–(12)], they can be used interchangeably; so one can see that (3) and (5) are equivalent. It is, however, more important to note that (4) and (6) are also equivalent, leading to the conclusion that the adjoint tensor operators are independent of the form of the invariants used. We shall give the proof below as to why (4) and (6) are equivalent.

In expressions (3) and (4) we write the eight generators of $SU(3)$ as $H_1, H_2, E_1, E_{-1}, E_2, E_{-2}, E_3,$

and E_{-3}. Then

$$G_2 = H_1^2 + H_2^2 + (2/3^{\frac{1}{2}})H_1 + 2E_{-i}E_i, \tag{7}$$

$$\begin{aligned} G_3 = {} & \tfrac{1}{3}H_2(1 + H_2 + 3^{\frac{1}{2}}H_1)(1 - H_2 + 3^{\frac{1}{2}}H_1) \\ & + (1 - H_2 + 3^{\frac{1}{2}}H_1)E_{-2}E_2 \\ & + (1 + 2H_2)E_{-1}E_1 - (1 + H_2 + 3^{\frac{1}{2}}H_1)E_3E_{-3} \\ & + 6^{\frac{1}{2}}(E_{-1}E_{-3}E_2 + E_{-2}E_3E_1). \end{aligned} \tag{8}$$

But H_1, H_2, and E_i are related to E_{ij} as follows:

$$H_1 = (1/2\sqrt{3})(2E_{11} + E_{22}), \tag{9}$$

$$H_2 = -\tfrac{1}{2}E_{22}, \tag{10}$$

$$E_{33} = -E_{11} - E_{22}, \tag{11}$$

$$E_1 = 6^{-\frac{1}{2}}E_{13}, \quad E_2 = 6^{-\frac{1}{2}}E_{12}, \quad E_3 = 6^{-\frac{1}{2}}E_{32}. \tag{12}$$

It is then straightforward to see that

$$I_2 = 6G_2, \tag{13}$$

$$I_3 = 18G_3 + 9G_2 = (18X_A^{(2)} + 9X_A)X_{-A}. \tag{14}$$

From Eqs. (13) and (14) one can construct an adjoint tensor operator, in the same way as (6), which is orthogonal to X_A, i.e.,

$$I_3X_A - G_2(18X_A^{(2)} + 9X_A) = 18G_3X_A - 18G_2X_A^{(2)}. \tag{15}$$

After normalization, expression (15) is exactly the same as (4). Thus we have shown that the adjoint tensor operators are unique, i.e., independent of the form of the invariants used.

In the case of the orthogonal group, as far as we know, there are also two different sets of invariants, one found by Racah[4] and formulated explicitly by Gruber and O'Raifeartaigh[5] and another by Louck.[6]

Louck's invariants are, for $SO(n)$,

$$I_{2k}(L) = \left(\sum_{i_s=1}^{n}(-1)^P J_{i_1i_2}J_{i_3i_4}\cdots J_{i_{k-1}i_k}\right)^2, \tag{16}$$

where $(-1)^P$ is either $+1$ or -1, depending on whether the permutation

$$\begin{pmatrix} 123 & \cdots & k \\ i_1 i_2 i_3 & \cdots & i_k \end{pmatrix}$$

is even or odd.

Racah's invariants are

$$I_{2k}(R) = J_{i_1i_2}J_{i_2i_3}J_{i_3i_4}\cdots J_{i_ki_1}. \tag{17}$$

For $SO(2k)$, the invariants I_{2k} expressed by both (16) and (17) do not distinguish between positive and negative values of $m_{2k,k}$. However, they are still invariants, and we can continue to use them for our purposes.

As we have seen from the example of $SU(n)$, the adjoint tensor operators can be extracted from the respective invariants and are, moreover, independent of the form of the invariants used. For $SO(n)$ it is much easier to extract the adjoint tensor operators (see Sec. II) from Racah's invariants (17) than from Louck's invariants (16). This is done in the next section. In Sec. III, we calculate the eigenvalues that result from these tensor operators. The eigenvalues of Louck's invariants have been calculated by Louck using trace formulas and recurrence relations. They are useful sometimes as a check on the eigenvalues of Racah's invariants.

II. ADJOINT TENSOR OPERATORS IN $SO(n)$

The main result of this section depends on the following theorem.

Theorem 1: In $SO(n)$, the operator

$$V_{ij}(2q+1) \equiv J_{ii_1}J_{i_1i_2}\cdots J_{i_{2q}j} - J_{ji_1}J_{i_1i_2}\cdots J_{i_{2q}i} \tag{18}$$

transforms as J_{ij}. In other words, $V_{ij}(2q+1)$ satisfies the commutation relation

$$[J_{ab}, V_{ij}] = i(\delta_{ai}V_{bj} + \delta_{aj}V_{ib} + \delta_{bi}V_{ja} + \delta_{bj}V_{ai}). \tag{19}$$

Proof: Although Eq. (19) can eventually be obtained by repeated application of the commutation relations between the generators J_{ij}, i.e.,

$$[J_{ab}, J_{ij}] = i(\delta_{ai}J_{bj} + \delta_{aj}J_{ib} + \delta_{bi}J_{ja} + \delta_{bj}J_{ai}), \tag{20}$$

we shall break down the proof into three cases so as to simplify the massive notation which results from large q.

Case 1: $a \neq i$, $b \neq j$: It is quite easy to see that in this case

$$[J_{ab}, V_{ij}] = 0. \tag{21}$$

Actually,

$$[J_{ab}, J_{ii_1}J_{i_1i_2}\cdots J_{i_pj}] = 0 \quad \text{for any } p. \tag{22}$$

Case 2: $a = i$, $b \neq j$: In this case we shall show that

$$[J_{ab}, J_{ai_1}J_{i_1i_2}\cdots J_{i_pj}] = iJ_{bi}J_{i_1i_2}\cdots J_{i_pj} \tag{23}$$

for any p. Let us take first a simple case where $p = 2$. Then

$$\begin{aligned} [J_{ab}, J_{ai_1}J_{i_1i_2}J_{i_2j}] &= i[J_{bi_1}J_{i_1i_2}J_{i_2j}\,(i_1 \neq a) + J_{ba}J_{ai_2}J_{i_2j}] \\ &= iJ_{bi_1}J_{i_1i_2}J_{i_2j}. \end{aligned} \tag{24}$$

Similarly, one can see that (23) is true. From (23), one easily proves that

$$[J_{ab}, V_{aj}] = iV_{bj}. \tag{25}$$

The other cases where $a = j$, $b \neq i$, or $a \neq i$, $b = j$, or $a \neq j$, $b = i$ can be treated in exactly the same way.

Case 3: $a = i$, $b = j$: In this case we find

$$[J_{ab}, J_{ai_1}J_{i_1i_2}\cdots J_{i_pb}] = i(J_{bi_1}J_{i_1i_2}\cdots J_{i_pb} - J_{ai_1}J_{i_1i_2}\cdots J_{i_pa}). \quad (26)$$

Using (26), we see that

$$[J_{ab}, V_{ab}] = 0. \quad (27)$$

Therefore, Eq. (19) is proved, and the $V_{ij}(2q+1)$ are the vector operators in $SO(n)$ similar to $V_{ij}(q) = E_{ii_1}E_{i_1i_2}\cdots E_{i_{q-1}j}$ in the case of $SU(n)$.

Next we define the invariants $I(p, q)$ in terms of the vector operators:

$$I(p, q) \equiv V_{ij}(2p-1)V_{ji}(2q-1). \quad (28)$$

Since $V_{ij}(1) = 2J_{ij}$, we see that the invariants defined in (17) are

$$4I_{2k}(R) = I(1, 2k-1). \quad (29)$$

In general, it should be noted that $I(p, q) \neq I(1, p+q-1)$. However, one can reduce $I(p, q)$ in the following way:

$$I(p, q) = I(1, p+q-1) + a_1I(1, p+q-3) + a_2I(1, p+q-5) + \cdots + a_nI(1, 1), \quad (30)$$

where the a_i are some numbers. Therefore, to obtain $I(p, q)$, it is sufficient to evaluate only $I(1, 2k-1)$ or $I_{2k}(R)$.

With the vector operators and the invariants defined, we now use the Schmidt orthogonalization procedure to obtain the unit adjoint tensor operators $X_{ij}(q)$ as follows:

$$X_{ij}(q) \equiv N_q^{-\frac{1}{2}} \det \begin{bmatrix} I(1,1) & I(1,3) & \cdots & I(1,2q-1) \\ I(3,1) & I(3,3) & \cdots & I(3,2q-1) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I(2q-3,1) & I(2q-3,3) & \cdots & I(2q-3,2q-1) \\ V_{ij}(1) & V_{ij}(3) & \cdots & V_{ij}(2q-1) \end{bmatrix}, \quad (31)$$

$$N_q = (\det Y_{q-1})(\det Y_q), \quad (32)$$

$$Y_0 = 1, \quad (33)$$

$$Y_q = \begin{bmatrix} I(1,1) & I(1,3) & \cdots & I(1,2q-1) \\ I(3,1) & I(3,3) & \cdots & I(3,2q-1) \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ I(2q-1,1) & I(2q-1,3) & \cdots & I(2q-1,2q-1) \end{bmatrix}. \quad (34)$$

The orthogonality relation now takes the form

$$X_{ij}(p)X_{ji}(q) = \delta_{p,q}. \quad (35)$$

III. EIGENVALUES OF THE INVARIANTS OF $SO(n)$

Since the invariants $I(p, q)$ can be expressed as linear combinations of $I(1, 2r-1) = 4I_{2r}(R)$, we only need to evaluate the latter. There are at least two ways one can proceed. The first one is to utilize the known eigenvalues of Louck's invariants $I_{2r}(L)$ and express $I(R)$ in terms of $I(L)$. Thus, for example, for $SO(5)$,

$$I_4(L) = (m_{51}+1)(m_{51}+2)m_{52}(m_{52}+1), \quad (36)$$

$$I_4(R) = 2I_2^2 + 6I_2 - 4I_4(L), \quad (37)$$

$$I_2 = \tfrac{1}{2}J_{ij}J_{ij} = m_{51}^2 + m_{52}^2 + 3m_{51} + m_{52}, \quad (38)$$

$$\therefore \quad I_4(R) = 2(m_{51}^4 + m_{52}^4 + 6m_{51}^3 + 2m_{52}^3 + 12m_{51}^2 + 9m_{51} - m_{52}). \quad (39)$$

However, it would be desirable to obtain a general formula relating $I_{2r}(R)$ to $I_{2r}(L)$.

The second method is to express $I_{2r}(R)$ in $SO(n)$ in terms of $I_{2r}(R)$ in $SO(n-1)$, and continue the process until one reaches $SO(2)$, where everything is known. We shall use this method to obtain the invariant $I_4(R)$ for $SO(n)$.

From now on we use the notation defined in a previous paper,[7] and let the invariant I_4 act on the highest weight. In that case, the generator $J_{2p,2p-1} = H_p$ has the eigenvalue m_{np}. Then one can express I_{2r} in terms of A_p^q, B_p^q, C_p^q, D_p^q, E_{2k+1}^p, and F_{2k+1}^p defined in Ref. 7 and commute the raising generators over. As a result, one only needs to evaluate $V_{2p,2p-1}(2r-1)$.

For example, in $SO(n)$,

$$I_4 = \tfrac{1}{2}J_{ij}(J_{jk}J_{ks}J_{si} - J_{ik}J_{ks}J_{sj}) = -(3 + J_{21})V_{21}(3) - (1 + J_{43})V_{43}(3). \quad (39')$$

We thus need to obtain recurrence relations between $V^{(n)}_{2p,2p-1}(2r-1)$ and $V^{(n-1)}_{2p,2p-1}(2r-1)$. For the fourth-order invariants I_4, the recurrence relations are summarized in the following equations:

$$V^{(2n+1)}_{2p,2p-1}(3) = -2H_p^2 + 2\sum_{i=p+1}^{n} H_i - 2(2n-p-1)H_p + V^{(2n)}_{2p,2p-1}(3), \quad p \le n, \quad (40)$$

$$V^{(2n)}_{2p,2p-1}(3) = -2H_p^2 - 2(2n-p-2)H_p + 2\sum_{i=p+1}^{n-1} H_i + 2H_n^2 + V^{(2n-1)}_{2p,2p-1}, \quad p < n, \quad (41)$$

$$V^{(2n-1)}_{2p,2p-1}(3) = -2(2n-p-3)H_p - 2H_p + \sum_{i=p+1}^{n-1} 2H_i + V^{(2n-2)}_{2p,2p-1}(3), \quad p < n, \quad (42)$$

$$V^{(2n)}_{2n,2n-1}(3) = V^{(2n-1)}_{2n,2n-1}(3) - 2H_n^3 - 2H_n\sum_{i=1}^{n-1} H_i, \quad (43)$$

$$V^{(2n-1)}_{2n,2n-1}(3) = V^{(2n-2)}_{2n,2n-1}(3) - 2H_n\sum_{i=1}^{n-1} H_i, \quad (44)$$

$$V^{(2n)}_{2p,2p-1}(3) = V^{(2n-1)}_{2p,2p-1}(3) + 2H_nH_p - 2nH_p, \quad p > n, \quad (45)$$

$$V^{(2n-1)}_{2p,2p-1}(3) = V^{(2n-2)}_{2p,2p-1}(3) - 2H_p - (2n-4)H_p, \quad p > n, \quad (46)$$

$$V^{(2)}_{2p,2p-1}(3) = 2H_1H_p - 2H_p, \quad p > 1, \quad (47)$$

$$V^{(2)}_{2,1}(3) = -2H_1^3. \quad (48)$$

Using these recurrence relations, we obtain

$$I_4^{(3)} = 2m_{31}^2(m_{31}+1)^2, \quad (49)$$

$$I_4^{(4)} = 2(m_{41}^4 + m_{42}^4 + 4m_{41}^3 + 5m_{41}^2 - m_{42}^2 + 2m_{41}), \quad (50)$$

$$I_4^{(5)} = 2(m_{51}^4 + m_{52}^4 + 6m_{51}^3 + 2m_{52}^3 + 12m_{52}^2 + 9m_{51} - m_{52}), \quad (51)$$

$$I_4^{(6)} = 2(m_{61}^4 + 8m_{61}^3 + 22m_{61}^2 + 24m_{61} + m_{62}^4 + 4m_{62}^3 + 4m_{62}^2 + m_{63}^4 - 2m_{63}^2), \quad (52)$$

$$I_4^{(7)} = 2(m_{71}^4 + m_{72}^4 + m_{73}^4 + 10m_{71}^3 + 35m_{71}^2 + 50m_{71} + 6m_{72}^3 + 11m_{72}^2 + 6m_{72} + 2m_{73}^3 - m_{73}^2 - 2m_{73}). \quad (53)$$

One can also obtain these results from $I^{(n)}_{2k}(L)$ by the following relations:

$$I^{(n)}_{2k}(R) = -4I^{(n)}_{2k}(L) + 2I_2^2 + (n-2)(n-3)I_2, \quad n \ge 4, \quad (54)$$

where

$$I_2 = \tfrac{1}{2}J_{ij}J_{ij}. \quad (55)$$

In principle, these two methods can be extended to the case of $I^{(n)}_{2k}(R)$ for any k and any n. However, so far we have not been able to obtain the eigenvalue of $I^{(n)}_{2k}(R)$ in closed form.

IV. WIGNER COEFFICIENTS OF $SO(5)$

We have used the adjoint tensor operators obtained above to calculate the Wigner coefficients of $SO(5)$ in the direct product of the 10-dimensional representation with an arbitrary representation. The results agree with Hecht's.[8] Out of 10 terms, four (56, 57, 59, and 60) are exactly the same as in Table 4a of Hecht's paper, and the other six terms are obtained in a different but slightly simpler form. The last four (62, 63, 64, and 65) can be shown to be algebraically equal to Hecht's. The third (58) and sixth (61) terms are very complicated, containing, according to Hecht's expression, approximately 400 terms when expanded. We have substituted numerical values and found that they agree in all cases. We use the same notation below as Hecht:

Doubled-barred Wigner coefficients of $SO(5)$:

$$\langle (J_m\Lambda_m)J_1\Lambda_1; (10)J_2\Lambda_2 \,\|\, (J_m\Lambda_m)J\Lambda\rangle_2$$

$$m = J_m + \Lambda_m - J - \Lambda, \quad n = J_m - \Lambda_m - J + \Lambda, \quad G_m = J_m(J_m+2) + \Lambda_m(\Lambda_m+1),$$

$$Y = 2\Lambda_m(2\Lambda_m+2)(2J_m+1)(2J_m+3)(J_m-\Lambda_m)(J_m-\Lambda_m+1)(J_m+\Lambda_m+1)(J_m+\Lambda_m+2),$$

$$\langle (J_m\Lambda_m)J\,\Lambda+1; (10)01 \,\|\, (J_m\Lambda_m)J\Lambda\rangle_2 = \left(\frac{m(n+1)(2\Lambda_m+2+n)(2J_m+1-n)(2J_m-2\Lambda_m-n)(2\Lambda_m+1-m)(2J_m+2-m)}{2(2\Lambda+1)(2\Lambda+2)Y} \times (2J_m+2\Lambda_m+3-m)G_m\right)^{\frac{1}{2}}, \quad (56)$$

$$\langle (J_m\Lambda_m)J\,\Lambda-1; (10)01 \,\|\, (J_m\Lambda_m)J\Lambda\rangle_2 = -\left(\frac{n(m+1)(2\Lambda_m+1+n)(2J_m+2-n)(2J_m-2\Lambda_m+1-n)(2\Lambda_m-m)(2J_m+1-m)}{2(2\Lambda)(2\Lambda+1)Y} \times (2J_m+2\Lambda_m+2-m)G_m\right)^{\frac{1}{2}}, \quad (57)$$

$$\langle (J_m\Lambda_m)J\Lambda;(10)01 \parallel (J_m\Lambda_m)J\Lambda\rangle_2$$
$$= -2\left(\frac{\Lambda(\Lambda+1)G_m}{Y}\right)^{\frac{1}{2}}\left(\frac{(J_m-\Lambda_m+J-\Lambda+1)(J_m+\Lambda_m+J-\Lambda+2)(J_m+\Lambda_m-J+\Lambda+1)}{2\Lambda(2\Lambda+2)}\right.$$
$$\times (J_m-\Lambda_m-J+\Lambda)+\frac{(\Lambda-J)(J_m^2+\Lambda_m^2+2J_m+\Lambda_m-J^2-\Lambda^2-2J-\Lambda)}{(\Lambda+1)}+(\Lambda-J)$$
$$\left.-(J+\Lambda)(J-\Lambda)-\frac{(J_m+\Lambda_m+1)(J_m+\Lambda_m+2)(J_m-\Lambda_m)(J_m-\Lambda_m+1)}{G_m}\right), \tag{58}$$

$$\langle (J_m\Lambda_m)J+1\,\Lambda;(10)10 \parallel (J_m\Lambda_m)J\Lambda\rangle_2$$
$$= \left(\frac{nm(2\Lambda_m+1+n)(2J_m+2-n)(2J_m-2\Lambda_m+1-n)(2J_m+2-m)(2\Lambda_m+1-m)}{2(2J+1)(2J+2)Y}\right.$$
$$\left.\times (2J_m+2\Lambda_m+3-m)G_m\right)^{\frac{1}{2}}, \tag{59}$$

$$\langle (J_m\Lambda_m)J-1\,\Lambda;(10)10 \parallel (J_m\Lambda_m)J\Lambda\rangle_2$$
$$= -\left(\frac{(m+1)(n+1)(2\Lambda_m+2+n)(2J_m+1-n)(2J_m-2\Lambda_m-n)(2J_m+1-m)}{2(2J)(2J+1)Y}\right.$$
$$\left.\times (2\Lambda_m-m)(2J_m+2\Lambda_m+2-m)G_m\right)^{\frac{1}{2}}, \tag{60}$$

$$\langle (J_m\Lambda_m)J\,\Lambda;(10)10 \parallel (J_m\Lambda_m)J\Lambda\rangle_2$$
$$= -2\left(\frac{J(J+1)G_m}{Y}\right)^{\frac{1}{2}}\left(\frac{(J_m-\Lambda_m+\Lambda-J+1)(J_m+\Lambda_m+\Lambda-J+2)(J_m+\Lambda_m-\Lambda+J+1)}{2J(2J+2)}\right.$$
$$\times (J_m-\Lambda_m-\Lambda+J)+\frac{(J-\Lambda)(J_m^2+\Lambda_m^2+2J_m+\Lambda_m-\Lambda^2-J^2-2\Lambda-J)}{(J+1)}+(J-\Lambda)$$
$$\left.-(J+\Lambda)(\Lambda-J)-\frac{(J_m+\Lambda_m+1)(J_m+\Lambda_m+2)(J_m-\Lambda_m)(J_m-\Lambda_m+1)}{G_m}\right), \tag{61}$$

$$\langle (J_m\Lambda_m)J+\tfrac{1}{2}\,\Lambda+\tfrac{1}{2};(10)\tfrac{1}{2}\tfrac{1}{2} \parallel (J_m\Lambda_m)J\Lambda\rangle_2$$
$$= -\left(\frac{m(2J_m+2\Lambda_m+3-m)(2J_m+2-m)(2\Lambda_m+1-m)}{(2J+1)(2\Lambda+1)YG_m}\right)^{\frac{1}{2}}$$
$$\times [(J_m+\Lambda_m+1)(J_m+\Lambda_m+2)(J_m-\Lambda_m)(J_m-\Lambda_m+1)-(J-\Lambda)^2G_m], \tag{62}$$

$$\langle (J_m\Lambda_m)J-\tfrac{1}{2}\,\Lambda-\tfrac{1}{2};(10)\tfrac{1}{2}\tfrac{1}{2} \parallel (J_m\Lambda_m)J\Lambda\rangle_2$$
$$= \left(\frac{(m+1)(2J_m+2\Lambda_m+2-m)(2J_m+1-m)(2\Lambda_m-m)}{(2J+1)(2\Lambda+1)YG_m}\right)^{\frac{1}{2}}$$
$$\times [(J_m+\Lambda_m+1)(J_m+\Lambda_m+2)(J_m-\Lambda_m)(J_m-\Lambda_m+1)-(J-\Lambda)^2G_m], \tag{63}$$

$$\langle (J_m\Lambda_m)J+\tfrac{1}{2}\,\Lambda-\tfrac{1}{2};(10)\tfrac{1}{2}\tfrac{1}{2} \parallel (J_m\Lambda_m)J\Lambda\rangle_2$$
$$= \left(\frac{n(2\Lambda_m+1+n)(2J_m+2-n)(2J_m-2\Lambda_m+1-n)}{(2J+1)(2\Lambda+1)YG_m}\right)^{\frac{1}{2}}$$
$$\times [(J_m+\Lambda_m+1)(J_m+\Lambda_m+2)(J_m-\Lambda_m)(J_m-\Lambda_m+1)-(J+\Lambda+1)^2G_m], \tag{64}$$

$$\langle (J_m\Lambda_m)J-\tfrac{1}{2}\,\Lambda+\tfrac{1}{2};(10)\tfrac{1}{2}\tfrac{1}{2} \parallel (J_m\Lambda_m)J\Lambda\rangle_2$$
$$= \left(\frac{(n+1)(2\Lambda_m+2+n)(2J_m+1-n)(2J_m-2\Lambda_m-n)}{(2J+1)(2\Lambda+1)YG_m}\right)^{\frac{1}{2}}$$
$$\times [(J_m+\Lambda_m+1)(J_m+\Lambda_m+2)(J_m-\Lambda_m)(J_m-\Lambda_m+1)-(J+\Lambda+1)^2G_m]. \tag{65}$$

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 8 AUGUST 1971

Space–Time of the de Broglie Wave Field

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A geometrical characterization is given of the space–time with a metric satisfying the equations of the de Broglie wave field. To do this, we exploit a formal analogy with a "perfect fluid" whose energy and pressure depend on the components of the metric field and its derivatives. To determine the properties of the space–time, we use the Ricci principal directions.

I. INTRODUCTION

Following the lines of thought inaugurated by Eddington,[1] we can say that in the finiteness of space we have the clue to atomicity. The argument runs as follows: Atomicity is merely the oldest, best known and still most important expression of the inherent discontinuities in nature. Generally speaking, the latter are accounted for in wave mechanics by means of a close analogy with the discontinuous sets of proper modes of vibrating systems. However, only a finite system possesses discontinuous proper modes. So, if the space were infinite, it would be hard to explain atomicity along these lines because its proper vibrations would form a continuous sequence.

Perhaps Schrödinger was the first[2] who believed that the ψ waves are to be identified with waves representing disturbances of the metric field of space–time. But then, of course, the components of the metric field cannot be a solution of Einstein's equations because of the inherent dualism of field and source of field (energy momentum tensor). This dualism for ψ waves is hardly acceptable, and, as a matter of fact, the Schrödinger, Klein–Gordon, or Dirac equations do not contain any term describing the source of the ψ-field.

We assume that matter waves are described by a metric field which satisfies the field equations of the de Broglie wave field.[3,4] These equations are similar to the Einstein equations but do not contain any terms which we could call sources. Let us note that from the field equations it follows that the second derivatives of the metric field have essential discontinuities on the characteristic 3-surfaces. These characteristic 3-surfaces represent a history of a two-wave surface of a wave which has a phase velocity identical with the phase velocity of an ordinary de Broglie wave. The wave with the phase velocity of a de Broglie wave is propagated in a 3-space (usually called chronometrical 3-space[5]) everywhere perpendicular to the lines x^4.[3] In a synchronous coordinate system (say the system comoving with the particle) the characteristic 3-surfaces and chronometrical 3-space coincide.

The field equations impose conditions which are to be satisfied by space–time. In order to characterize the space–time, we use the notion of principal direction introduced by Ricci.[6] The method we use is the same as in Ref. 7. We exploit the fact that the field equations have on the right-hand side a tensor formally identical with the energy–momentum tensor of a "perfect fluid." However, the proper density r and the pressure p of this "fluid" are functions of the metric field and its first and second derivatives. The pressure–density equation $r = p$ holds. It then follows from the conservation equations, which are a consequence of the field equations, that there is a property of space–time represented by a function which is conserved during the evolution of the space–time. This conserved scalar function is called the index function[8] (in analogy with the refractive index of a transparent medium) and it is a function of the components of the metric field and its first and second derivatives. The

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The field equations impose conditions which are to be satisfied by space–time. In order to characterize the space–time, we use the notion of principal direction introduced by Ricci.[6] The method we use is the same as in Ref. 7. We exploit the fact that the field equations have on the right-hand side a tensor formally identical with the energy–momentum tensor of a "perfect fluid." However, the proper density r and the pressure p of this "fluid" are functions of the metric field and its first and second derivatives. The pressure–density equation $r = p$ holds. It then follows from the conservation equations, which are a consequence of the field equations, that there is a property of space–time represented by a function which is conserved during the evolution of the space–time. This conserved scalar function is called the index function[8] (in analogy with the refractive index of a transparent medium) and it is a function of the components of the metric field and its first and second derivatives. The

stream lines satisfy the variational principle, formally identical with Fermat's optical principle, where, however, the refraction index of a transparent medium is replaced by the index function. If Ricci's principal directions are indeterminate, the space–time cannot be considered as a space–time of a "perfect fluid."

II. IDENTIFICATION WITH PERFECT FLUID

We can write the field equations[3,4] in the form

$$R_{ab} - \tfrac{1}{2}Rg_{ab} - \frac{\mathcal{K}^2}{h^2}\,g_{ab} = -\left(R + 4\frac{\mathcal{K}^2}{h^2}\right)(\tfrac{1}{2}g_{ab} - \dot{x}_a\dot{x}_b), \quad (1)$$

where $\mathcal{K}$ is the rest mass, h is Planck's constant, and $\dot{x}^a$ are the components of the unit 4-vector normal to the 3-wave surface of the de Broglie wave. The left-hand side of (1) is a well-known tensor whose covariant divergence vanishes, and we have from (1) four conservation equations

$$g^{kb}\left[\left(R + 4\frac{\mathcal{K}^2}{h^2}\right)(\tfrac{1}{2}g_{ab} - \dot{x}_a\dot{x}_b)\right]_{|k} = 0. \quad (2)$$

The normal vector $\dot{x}^a$ has unit magnitude, and we can rewrite (2) as

$$\dot{x}^a_{|a} = -\frac{1}{2}\left(R + 4\frac{\mathcal{K}^2}{h^2}\right)\frac{\partial R}{\partial x^a}\,\dot{x}^a. \quad (3)$$

Equation (3) implies that

$$\frac{\partial}{\partial x^a}(-g)^{\frac{1}{2}}\left(R + 4\frac{\mathcal{K}^2}{h^2}\right)^{\frac{1}{2}}\dot{x}^a = 0 \quad (4)$$

or

$$((R + 4\mathcal{K}^2/h^2)^{\frac{1}{2}}\dot{x}^a)_{|a} = 0. \quad (5)$$

Whenever a relation in the form of Eq. (5) holds, there exists a conserved integral. Consequently, in our case the value of the integral

$$\oint (R + 4\mathcal{K}^2/h^2)^{\frac{1}{2}}\dot{x}^4(-g)^{\frac{1}{2}}\,dx^1\,dx^2\,dx^3$$

is a constant, independent of time. The energy tensor of a "perfect fluid" has the form

$$T^{ab} = (r + p)\dot{x}^a\dot{x}^b - pg^{ab}, \quad (6)$$

where r is the proper energy density and p is the pressure. On comparing (6) with the right-hand side of (1), we have

$$r + p = R + 4\mathcal{K}^2/h^2, \quad p = \tfrac{1}{2}(R + 4\mathcal{K}^2/h^2). \quad (7)$$

Combining (7), we obtain

$$r = \tfrac{1}{2}(R + 4\mathcal{K}^2/h^2). \quad (8)$$

On account of the foregoing identification, the tensor on the right-hand side of (1) represents a "perfect fluid" for which $r = p$ is true. From (7) and (8) we see that r and p are functions of the components of the metric field and its first and second derivatives. The index function[8] σ may be written in the form

$$\sigma = \exp\int\frac{dr}{r + p},$$

and characterizes the space–time property which is conserved during the evolution of space–time. From the foregoing equation, using the pressure density relation $r = p$, we obtain

$$\sigma = (2)^{-\frac{1}{2}}(R + 4\mathcal{K}^2/h^2)^{\frac{1}{2}}.$$

The stream lines of our "perfect fluid" satisfy the variational principle[8]

$$\delta\int(R + 4\mathcal{K}^2/h^2)^{\frac{1}{2}}\,ds = 0.$$

This variational principle is formally identical with Fermat's optical principle in a transparent medium of refractive index σ. But the problem of determining the stream lines is not the same as that of finding the rays in a given medium, even after allowing for the fact that we are dealing with a curved manifold of four dimensions with an indefinite metric form. In the optical problem the refractive index is supposed to be known, whereas in our problem σ is not known: For its determination the field equations must be solved, since σ depends on the components of the metric field and its first and second derivatives. If we write

$$\overline{ds}^2 = (R + 4\mathcal{K}^2/h^2)\,ds^2,$$

the variational principle has form

$$\delta\int\overline{ds} = 0$$

and the streamlines are geodesics of a metric $\overline{ds}^2$ conformal to the metric ds^2 of the space–time.[9]

III. GEOMETRIC CHARACTERIZATION OF SPACE–TIME

The contravariant components λ^i_k of the Ricci[7] principal directions are solutions of the homogenous systems

$$(R_{ij} + \rho_k g_{ij})\lambda^i_k = 0 \quad (9)$$

(no summation over k), where ρ_k is any root of the determinant

$$D\|R_{ij} + \rho_k g_{ij}\| = 0 \quad (10)$$

of the matrix of system (9). When the roots of (10)

are simple, the principal directions are uniquely determined by (9), and any two of these directions at a point are orthogonal. When a root of (10) is multiple, say of order s, and the elementary divisors are simple, the directions corresponding to this root are linearly expressible in terms of s mutually orthogonal directions, which are orthogonal also to the directions corresponding to any other root. Hence, when all the elementary divisors are simple, an orthogonal n-tuple of principal directions can be found. Equation (9) may be replaced by

$$R_{ij} = -\sum_{k=1}^{4} \rho_k \lambda_{ki} \lambda_{kj}, \tag{11}$$

where $\lambda_{kj} = g_{ij}\lambda_k^i$. Hence, substituting R_{ab} from (1) into (9), we obtain

$$[-\mathcal{H}^2/h^2 g_{ab} + (R + 4\mathcal{H}^2/h^2)\dot{x}_a\dot{x}_b + \rho_k g_{ab}]\lambda_k^a = 0. \tag{12}$$

Now, if we assume that $\dot{x}^a = \lambda_1^a$, and since $\dot{x}^a$ is unitary, we have that $g_{ab}\lambda_1^a\lambda_1^b = 1$ and from (12) we get

$$(R + 3\mathcal{H}^2/h^2 + \rho_1)\dot{x}_a = 0. \tag{13}$$

Hence,

$$\rho_1 = -(R + 3\mathcal{H}^2/h^2). \tag{14}$$

Now if λ_l^i are components of any vector orthogonal to $\dot{x}^a$, then from (12) we get

$$\rho_l = \mathcal{H}^2/h^2. \tag{15}$$

Since every vector orthogonal to $\dot{x}^a$ satisfies this condition it follows that ρ_l is a triple root of (12) and the elementary divisors are simple. Hence we see that the unit 4-vector $\dot{x}^a$ normal to the 3-wave surface is the principal direction determined by the simple root ρ_1 given by (14). The triple root ρ_l is always constant, as follows from Eq. (15). For the scalar curvature of space–time, from Eqs. (14) and (15) we obtain

$$R = -(\rho_1 + 3\rho_l)_1, \tag{16}$$

and ρ_1 and ρ_l are the mean curvatures in the directions $\dot{x}^a$ and λ_l^i, respectively. When ρ_1 and ρ_l are equal, we have from (14) and (15)

$$R + 4\mathcal{H}^2/h^2 = 0. \tag{17}$$

The principal directions are indeterminate and thus space–time cannot be identified with the one manifold of "perfect fluid" noted above. Under condition (17), Eqs. (1) reduce to the special form

$$R_{ab} - \tfrac{1}{4}Rg_{ab} = 0$$

and the conservation law (2) is fulfilled identically.[9]

IV. SYNCHRONOUS COORDINATE SYSTEM

The unitary 4-vector $g_{a4}(g_{44})^{-\frac{1}{2}}$ is tangent to the lines x^4 and represents the normal 4-vector of the 3-space (usually called[5] chronometrical 3-space) which is everywhere perpendicular to the lines x^4. If we assume that

$$\dot{x}_a = g_{a4}(g_{44})^{-\frac{1}{2}}, \tag{18}$$

the chronometrical 3-space is identical, at least locally, with the 3-wave surface of the de Broglie wave. Equations (18) are the coordinate conditions specifying a synchronous coordinate system.

Substituting (18) into (1), we get for the components of the Ricci tensor

$$R_{ab} = (g_{a4}g_{b4}/g_{44})(R + 3\mathcal{H}^2/h^2) - (\mathcal{H}^2/h^2) \times (g_{ab} - g_{a4}g_{b4}/g_{44}). \tag{19}$$

The conservation law (4), with the help of (18), gives

$$\frac{\partial}{\partial x^4}\sqrt{\gamma}\,(R + 4\mathcal{H}^2/h^2)^{\frac{1}{2}} = 0, \tag{20}$$

where $\gamma = \det \|\gamma_{\alpha\beta}\|$ and $\gamma_{\alpha\beta} = g_{\alpha\beta} - g_{\alpha 4}g_{\beta 4}/g_{44}$, $\alpha, \beta = 1, 2, 3$. After integration we get from (20), for the scalar curvature R,

$$R = -4\mathcal{H}^2/h^2 + F^2(x^\alpha)/\gamma, \tag{21}$$

where $F(x^\alpha)$ is a function of the variables x^1, x^2, x^3. Substituting from (19) into (9), we obtain

$$[(g_{a4}g_{b4}/g_{44})(R + 3\mathcal{H}^2/h^2) - \mathcal{H}^2/h^2\gamma_{ab} - g_{ab}\rho_k]\lambda_k^a = 0 \tag{22}$$

(no summation over k), which for the single root ρ_1 and values λ_1^a given by

$$\lambda_1^a = \delta_4^a/(g_{44})^{\frac{1}{2}}$$

becomes

$$g_{b4}/(g_{44})^{\frac{1}{2}}(R + 3\mathcal{H}^2/h^2 - \rho_1) = 0. \tag{23}$$

Hence, the simple root

$$\rho_1 = -(R + 3\mathcal{H}^2/h^2), \tag{24}$$

and, using (21), we can write

$$\rho_1 = \mathcal{H}^2/h^2 - F^2(x^\alpha)/\gamma. \tag{25}$$

In order that the elementary divisors corresponding to the triple root ρ_l be simple, it is necessary and sufficient that (9) for ρ_l be satisfied by the values (1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0) for the covariant components of λ_k^i. If we write (9) in the form

$$(R_b^a + \rho_l\delta_b^a)\lambda_a = 0, \tag{26}$$

the conditions are

$$R_j^\alpha + \rho_l \delta_j^\alpha = 0, \quad \alpha = 1, 2, 3, \quad j = 1, 2, 3, 4, \quad (27)$$

and thus from (27) and (19) we have

$$\rho_l = \mathcal{H}^2/h^2. \quad (28)$$

We see that ρ_1 and ρ_l are equal only when in (21) the function $F(x^\alpha) = 0$. When $F(x^\alpha) = 0$, the field equations (1) in the synchronous coordinate system are equivalent to the generally covariant equations[9]

$$R_{ab} - \tfrac{1}{4} R g_{ab} = 0, \quad R + 4\mathcal{H}^2/h^2 = 0.$$

In combining (21) with (7) one sees immediately that the total energy density e of the "perfect fluid" in the synchronous coordinate system is given by

$$e = r + p = F^2(x^\alpha)/\gamma. \quad (29)$$

Thus e is a function of the components of the metric field $g_{\alpha\beta}$, $\alpha, \beta = 1, 2, 3$, and does not depend on the first and second derivatives. The same is true for the proper material density r and pressure p.

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Kinematic Dynamo Theory: The Dyson Equation and the Large-Scale Field; the Bethe–Salpeter Equation and the Fluctuation Intensity

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(Received 16 February 1971)

An exact statistical set of kinematic dynamo equations is given representing turbulent generation of both a large-scale magnetic field and a small-scale turbulent field. These equations do not rely on approximately solving the fluctuation equations and using the results in the ordered field equations as do most treatments of statistical kinematic dynamos. Instead they treat both the fluctuation equations and the ordered field equation exactly. The results obtained indicate several points. First: The fluctuation intensity equation has the character of the Bethe–Salpeter equation. Depending on whether one uses the long-slow or the short-sudden approximation there may, or may not, be an upper limit on the velocity turbulence in order that the energy density stored in the magnetic field fluctuations remain finite. No such restriction is found using approximate kinematic dynamo equations. Second: The normal modes of the large-scale field (which obeys a Dyson equation) may, or may not, be mirrored in the singular eigenmodes of the fluctuation intensity equation. Third: the structure of the exact statistical kinematic dynamo equations is very different from the structure of the approximate kinematic dynamo equations—particularly in the equation describing the fluctuation intensity. We have done this problem in order to demonstrate that the exact solution of at least one problem in statistical kinematic dynamo theory introduces new and interesting phenomena which are not brought to light in approximate treatments of the same phenomena.

I. INTRODUCTION

In other papers[1–8] the basic properties of kinematic dynamos driven by turbulent velocity fields have been outlined. In particular we have demonstrated how the normal modes of the large-scale magnetic field are influenced by bulk convection, large-scale shearing and the turbulent Lorentz force. We have also estimated the influence of both large-scale boundaries and fluctuations in resistivity on the dynamo equations.

In all the above analyses (with the exception of Ref. 4) two basic assumptions were made. The first (which is inherent to kinematic dynamo theory) is that both the large-scale velocity and the turbulent velocity can be freely specified. That is, they are not changed by any induced magnetic activity but do induce magnetic activity. The second basic assumption is that, in handling the fluctuating (or random) part of the turbulent dynamo equations, truncation of fluctuations at the two-point, two-time level of their correlation functions is a reasonable assumption.[9]

The purpose of the present paper is to obtain

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The purpose of the present paper is to obtain

equations describing both the large-scale magnetic field and its fluctuations in terms of the velocity fluctuations without making the conventional truncation of turbulent correlations at the two-point level. Instead, we assume the velocity field is of such a nature that all correlation functions entering the equations below are *reducible* to the two-point level. Note that this is by no means the same as *truncating* the fluctuations at the two-point level.

We show that the equation describing the intensity of the random component of the magnetic field is a generalized Bethe–Salpeter equation of tensor form in sixteen variables. The equation describing the large-scale field is an extension of the Dyson equation of vector form involving eight variables.

II. FLUCTUATION INTENSITY AND THE BETHE–SALPETER EQUATION

Consider an infinite medium of constant resisivity η. Then, when bulk motions are absent and the only fluid velocity is the random turbulence $\delta\mathbf{v}$ (the notation and derivation of the kinematic dynamo equations used herein is described more fully in Papers I and II), we have

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)A_i = \epsilon_{ijk}\langle\delta v_j \delta B_k\rangle, \tag{1}$$

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)\delta A_i = \epsilon_{ijk}(\delta v_j B_k + \delta v_j \delta B_k - \langle\delta v_j \delta B_k\rangle), \tag{2}$$

where

$$\delta B_i = \epsilon_{ijk}\frac{\partial \delta A_k}{\partial x_j}, \quad B_i = \epsilon_{ijk}\frac{\partial A_k}{\partial x_j}.$$

Let $\mathbf{G}(\mathbf{x}, \mathbf{x}', t, t')$ satisfy

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)\mathbf{G} - \nabla \times (\delta\mathbf{v} \times \mathbf{G} - \langle\delta\mathbf{v} \times \mathbf{G}\rangle) = [\nabla \times (\delta\mathbf{v} \times \mathbf{B})]'\delta(\mathbf{x} - \mathbf{x}')\delta(t - t'), \tag{3}$$

and let $G_0(\mathbf{x}, \mathbf{x}', t, t')$ satisfy

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)G_0 = \delta(\mathbf{x} - \mathbf{x}')\delta(t - t'). \tag{4}$$

In Eq. (3) the term $[\nabla \times (\delta\mathbf{v} \times \mathbf{B})]'_i$ is an abbreviation for

$$\epsilon_{ijk}\frac{\partial}{\partial x'_j}[\epsilon_{klm}\delta v_l(\mathbf{x}', t')B_m(\mathbf{x}', t')].$$

From Eq. (3) it follows that

$$\delta\mathbf{B}(\mathbf{x}, t) = \int d^3\mathbf{x}'\, dt'\mathbf{G}(\mathbf{x}, \mathbf{x}', t, t'). \tag{5}$$

Use of Eq. (4) enables Eq. (3) to be cast in the integral form

$$\begin{aligned}\mathbf{G}(\mathbf{x}, \mathbf{x}', t, t') = {} & [\nabla \times (\delta\mathbf{v} \times \mathbf{B})]'G_0(\mathbf{x}, \mathbf{x}', t, t') \\ & + \int d^3\mathbf{x}''\, dt''G_0(\mathbf{x}, \mathbf{x}'', t, t'')\nabla_{\mathbf{x}''} \\ & \times \{\delta\mathbf{v}(\mathbf{x}'', t'') \times \mathbf{G}(\mathbf{x}'', \mathbf{x}', t'', t') \\ & - \langle\delta\mathbf{v}(\mathbf{x}'', t'') \times \mathbf{G}(\mathbf{x}'', \mathbf{x}', t'', t')\rangle\}. \end{aligned} \tag{6}$$

Consider now the ensemble average quantity

$$\begin{aligned}\langle G_a(\mathbf{x}, \mathbf{x}', t, t')G_b(\tilde{\mathbf{x}}, \mathbf{x}'', \tilde{t}, t'')\rangle = {} & G_0(\mathbf{x}, \mathbf{x}', t, t')G_0(\tilde{\mathbf{x}}, \mathbf{x}'', \tilde{t}, t'') \\ & \times \left\langle \left\{ \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}\frac{\partial}{\partial x'_j}[\delta v_l(\mathbf{x}', t')B_m(\mathbf{x}', t')]\frac{\partial}{\partial x''_\alpha}[\delta v_\mu(\mathbf{x}'', t'')B_\nu(\mathbf{x}'', t'')] \right\rangle \right. \\ & + \int d^3\boldsymbol{\zeta}\, d\sigma\, d^3\boldsymbol{\eta}\, dn\epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu} \\ & \times \frac{\partial G_0}{\partial \zeta_j}(\mathbf{x}, \boldsymbol{\zeta}, t, \sigma)\cdot\frac{\partial G_0}{\partial \eta_\alpha}(\tilde{\mathbf{x}}, \boldsymbol{\eta}, \tilde{t}, n)\left\langle \{\delta v_l(\boldsymbol{\zeta}, \sigma)G_m(\boldsymbol{\zeta}, \mathbf{x}', \sigma, t') - \langle\delta v_l(\boldsymbol{\zeta}, \sigma)G_m(\boldsymbol{\zeta}, \mathbf{x}', \sigma, t')\rangle\}\right. \\ & \left.\left. \times \{\delta v_\mu(\boldsymbol{\eta}, n)G_\nu(\boldsymbol{\eta}, \mathbf{x}'', n, t'') - \langle\delta v_\mu(\boldsymbol{\eta}, n)G_\nu(\boldsymbol{\eta}, \mathbf{x}'', n, t'')\rangle\}\right\rangle\right\rangle. \end{aligned} \tag{7}$$

The reason for considering the quantity $\langle G_a G_b\rangle$ is clear. Take

$$\langle\delta B_i(\mathbf{x}, t)\delta B_j(\mathbf{x}', t')\rangle \equiv \int d^3\mathbf{r}\, d\tau\, d^3\mathbf{x}''\, dt''\langle G_i(\mathbf{x}, \mathbf{x}'', t, t'')G_j(\mathbf{x}', \mathbf{r}, t', \tau)\rangle. \tag{8}$$

Equation (8) (with $i = j, \mathbf{x} = \mathbf{x}', t = t'$) represents the average energy density stored in the fluctuating magnetic field.

To solve Eq. (7) for $\langle G_a G_b\rangle$, we need to know the statistical properties of $\delta\mathbf{v}$.

In order to make progress with Eq. (7) and at the same time preserve the essential physics of the fluctuation intensity equation, we assume for the remainder that the statistical properties of $\delta\mathbf{v}$ are such that all ensemble averages of the random variables entering Eq. (7) are reducible to the two-point, two-time level. We realize that this is by no means the most general form of velocity turbulence. However, it will suffice to illustrate the basic physical behavior of the equations associated with the fluctuation intensity and it will serve to keep the mathematical complexities to a minimum.

Under this assumption, Eq. (7) reduces to

$$\langle G_a(\mathbf{x}, \mathbf{x}', t, t')G_b(\tilde{\mathbf{x}}, \mathbf{x}'', \tilde{t}, t'')\rangle = G_0(\mathbf{x}, \mathbf{x}', t, t')G_0(\tilde{\mathbf{x}}, \mathbf{x}'', \tilde{t}, t'')\epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}$$
$$\times \left\langle \frac{\partial}{\partial x_j'}[\delta v_l(\mathbf{x}', t')B_m(\mathbf{x}', t')]\frac{\partial}{\partial x_\alpha''}[\delta v_\mu(\mathbf{x}'', t'')B_\nu(\mathbf{x}'', t'')]\right\rangle + \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}$$
$$\times \int d^3\zeta\, d\sigma\, d^3\eta\, dn \frac{\partial G_0}{\partial \zeta_j}(\mathbf{x}, \zeta, t, \sigma)\frac{\partial G_0}{\partial \eta_\alpha}(\tilde{\mathbf{x}}, \eta, \tilde{t}, n)\{\langle \delta v_l(\zeta, \sigma)\delta v_\mu(\eta, n)\rangle \langle G_m(\zeta, \mathbf{x}', \sigma, t')G_\nu(\eta, \mathbf{x}'', n, t'')\rangle$$
$$+ \langle \delta v_l(\zeta, \sigma)G_\nu(\eta, \mathbf{x}'', n, t'')\rangle \langle \delta v_\mu(\eta, n)G_m(\zeta, \mathbf{x}', \sigma, t')\rangle\}. \tag{9}$$

The last two terms on the right-hand side of Eq. (9) can be reduced further by taking Eq. (6), multiplying by $\delta\mathbf{v}(\mathbf{x}', t')$, ensemble-averaging the result, and using the statement that all correlations are reducible to the two-point, two-time level. Upon so doing we obtain Eq. (9) in the form

$$\langle G_a(\mathbf{x}, \mathbf{x}', t, t')G_b(\tilde{\mathbf{x}}, \mathbf{x}'', \tilde{t}, t'')\rangle = G_0(\mathbf{x}, \mathbf{x}', t, t')G_0(\tilde{\mathbf{x}}, \mathbf{x}'', \tilde{t}, t'')\epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}$$
$$\times \left\langle \frac{\partial}{\partial x_j'}[\delta v_l(\mathbf{x}', t')B_m(\mathbf{x}', t')]\frac{\partial}{\partial x_\alpha''}[\delta v_\mu(\mathbf{x}'', t'')B_\nu(\mathbf{x}'', t'')]\right\rangle + \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}\epsilon_{mpq}\epsilon_{vrs}\epsilon_{qef}\epsilon_{sgh}$$
$$\times \int d^3\zeta\, d^3\eta\, d\sigma\, dn \frac{\partial G_0}{\partial \zeta_j}(\mathbf{x}, \zeta, t, \sigma)\cdot\frac{\partial G_0}{\partial \eta_\alpha}(\tilde{\mathbf{x}}, \eta, \tilde{t}, \sigma)\frac{\partial G_0}{\partial x_p'}(\zeta, \mathbf{x}', \sigma, t')\cdot\frac{\partial G_0}{\partial x_r''}(\eta, \mathbf{x}'', n, t'')$$
$$\times B_h(\mathbf{x}'', t'')B_f(\mathbf{x}', t')\langle \delta v_l(\zeta, \sigma)\delta v_g(\mathbf{x}'', t'')\rangle \langle \delta v_\mu(\eta, n)\delta v_i(\mathbf{x}', t')\rangle + \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}$$
$$\times \int d^3\zeta\, d^3\eta\, d\sigma\, dn \frac{\partial G_0}{\partial \zeta_j}(\mathbf{x}, \zeta, t, \sigma)\frac{\partial G_0}{\partial \eta_\alpha}(\tilde{\mathbf{x}}, \eta, \tilde{t}, n)\cdot\langle \delta v_l(\zeta, \sigma)\delta v_\mu(\eta, n)\rangle$$
$$\times \langle G_m(\zeta, \mathbf{x}', \sigma, t')G_\nu(\eta, \mathbf{x}'', n, t'')\rangle. \tag{10}$$

We recognize Eq. (10) as a tensor Bethe–Salpeter equation for $\langle G_aG_b\rangle$ in 16 variables, viz., $(\mathbf{x}, t)$, $(\mathbf{x}', t')$, $(\mathbf{x}'', t'')$, $(\tilde{\mathbf{x}}, \tilde{t})$.

As remarked earlier, we are interested in the fluctuation intensity $\langle \delta\mathbf{B}\cdot\delta\mathbf{B}\rangle$.

If we write $\langle G_aG_b\rangle$ as a Fourier transform,

$$\langle G_a(\mathbf{x}, \mathbf{x}', t, t')G_b(\tilde{\mathbf{x}}, \mathbf{x}'', \tilde{t}, t'')\rangle$$
$$\equiv \int R_{ab}(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2; \mathbf{k}_3, \omega_3; \mathbf{k}_4, \omega_4)$$
$$\times \exp[i(\mathbf{k}_1\cdot\mathbf{x} + \mathbf{k}_2\cdot\mathbf{x}' + \mathbf{k}_3\cdot\tilde{\mathbf{x}} + \mathbf{k}_4\cdot\mathbf{x}''$$
$$- \omega_1 t - \omega_2 t' - \omega_3\tilde{t} - \omega_4 t'')]\prod_{i=1}^{4} d^3\mathbf{k}_i\, d\omega_i, \tag{11}$$

then, from Eqs. (8) and (11),

$$\langle \delta B_a(\mathbf{x}, t)\delta B_b(\mathbf{x}, t)\rangle$$
$$= (2\pi)^8 \int R_{ab}(\mathbf{k}_1, \omega_i; 0, 0; \mathbf{k}_3, \omega_3; 0, 0)$$
$$\times \exp\{i[(\mathbf{k}_1 + \mathbf{k}_3)\cdot\mathbf{x} - t(\omega_1 + \omega_3)]\}$$
$$\times d^3\mathbf{k}_1\, d^3\mathbf{k}_3\, d\omega_1\, d\omega_3$$
$$\equiv \int P_{ab}(\mathbf{k}, \omega)\exp[i(\mathbf{k}\cdot\mathbf{x} - \omega t)]\, d^3\mathbf{k}\, d\omega. \tag{12}$$

If we now define the spectral intensity $P(\mathbf{k}, \omega)$ as

$$P(\mathbf{k}, \omega) = P_{aa}(\mathbf{k}, \omega), \tag{13}$$

it follows from Eq. (12) that

$$P(\mathbf{k}, \omega) = (2\pi)^8 \int d^3\mathbf{k}_1\, d\omega_1$$
$$\times R_{aa}(\mathbf{k}_1, \omega_1; 0, 0; \mathbf{k} - \mathbf{k}_1, \omega - \omega_1; 0, 0). \tag{14}$$

It is fortunate that, for power computations, we require only the trace of the generalized Bethe–Salpeter equation with eight of the variables set to zero. The combination of these two simplifications (apparently due to serendipity) is just sufficient to enable us to solve the problem at hand. So our main interest in the generalized Bethe–Salpeter equation [Eq. (10)] is to obtain an expression for

$$R_{aa}(\mathbf{k}_1, \omega_1, \alpha, 0; \mathbf{k} - \mathbf{k}_1, \omega - \omega_1; 0, 0).$$

We Fourier-transform Eq. (10) in the 16 variables, as in Eq. (11), to obtain, after some elementary, but

extremely tedious, integrations, that

$$
\begin{aligned}
R_{ab}(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2; \mathbf{k}_3, \omega_3; \mathbf{k}_4, \omega_4) = {} & -k_{1j}k_{3\alpha}\epsilon_{ajk}\epsilon_{b\alpha\beta}\epsilon_{klm}\epsilon_{\beta\mu\nu}\int d^3\mathbf{K}\, d\Omega \Pi_{l\mu}(\mathbf{k}_1 - \mathbf{K}, \omega_1 - \Omega) \\
& \times R_{m\nu}(\mathbf{K}, \Omega; \mathbf{k}_2, \omega_2; \mathbf{k}_3 + \mathbf{k}_1 - \mathbf{K}, \omega_3 + \omega_1 - \Omega; \mathbf{k}_4, \omega_4) \\
& - (2\pi)^{-8}(k_{4\alpha} + k_{3\alpha})(k_{2j} + k_{1j})(\eta k_1^2 - i\omega_1)^{-1}(\eta k_3^2 - i\omega_3)^{-1} \\
& \times \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}\int d^3\mathbf{K}\, d\Omega B_m(\mathbf{K}, \Omega) \\
& \times B_\nu(\mathbf{k}_1 + \mathbf{k}_1 + \mathbf{k}_3 + \mathbf{k}_4 - \mathbf{K}, \omega_1 + \omega_2 + \omega_3 + \omega_4 - \Omega) \\
& \times \Pi_{l\mu}(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{K}, \omega_1 + \omega_2 - \Omega) \\
& + (2\pi)^{-8}k_{1j}k_{3\alpha}\epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}\epsilon_{mpq}\epsilon_{qef}\epsilon_{vrs}\epsilon_{sgh} \\
& \times (\eta k_1^2 - i\omega_1)^{-1}(\eta k_3^2 - i\omega_3)^{-1}\int d^3\mathbf{K}\, d\Omega\, d^3\mathbf{k}\, d\omega k_p(K_r - k_{4r} - k_{1r} + k_r) \\
& \times (\eta k^2 - i\omega)^{-1}[\eta\,|\mathbf{K} - \mathbf{k}_4 - \mathbf{k}_1 + \mathbf{k}|^2 - i(\omega_4 + \omega_1 - \Omega - \omega)]^{-1} \\
& \times B_h(\mathbf{K}, \Omega)B_f(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4 - \mathbf{K}, \omega_1 + \omega_2 + \omega_3 + \omega_4 - \Omega) \\
& \times \Pi_{lg}(\mathbf{k}_1 - \mathbf{k}, \omega_1 - \omega) \\
& \times \Pi_{\mu e}(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{K} - \mathbf{k}, \omega_1 + \omega_2 + \omega_3 - \Omega - \omega), \qquad (15)
\end{aligned}
$$

where we have assumed homogeneity and stationariness of the two-point, two-time velocity fluctuations, and have therefore written

$$\langle \delta v_i(\mathbf{x}, t)\delta v_j(\mathbf{x}', t')\rangle = \Pi_{ij}(\mathbf{x} - \mathbf{x}', t - t'), \qquad (16a)$$

with

$$\Pi_{ij}(\mathbf{r}, \tau) = \int d^3\mathbf{k}\, d\omega \Pi_{ij}(\mathbf{k}, \omega) \exp\,[i(\mathbf{k}\cdot\mathbf{r} - \omega\tau)] \qquad (16b)$$

Furthermore, we have written the large-scale field

$$\mathbf{B}(\mathbf{x}, t) = \int d^3\mathbf{k}\, d\omega \mathbf{B}(\mathbf{k}, \omega) \exp\,[i(\mathbf{k}\cdot\mathbf{x} - \omega t)].$$

Now, for power computations, as remarked earlier, we are interested in $\mathbf{k}_2 = \omega_2 = \mathbf{k}_4 = \omega_4 = 0$ in Eq. (15). For brevity we write

$$R_{ab}(\mathbf{k}_1, \omega_1; 0, 0; \mathbf{k}_3, \omega_3; 0, 0) \equiv R_{ab}(\mathbf{k}_1, \omega_1; \mathbf{k}_3, \omega_3), \qquad (17)$$

with the understanding that the "2" and "4" variables are set to zero and the ordering of the remaining "1" and "3" variables in the abbreviated representation (17) is always in the order "1" followed by "3". Then Eq. (15) becomes

$$
\begin{aligned}
& R_{ab}(\mathbf{k}_1, \omega_1; \boldsymbol{\varkappa} - \mathbf{k}_1, \varpi - \omega_1) + k_{1j}(\kappa_\alpha - k_{1\alpha})(\eta k_1^2 - i\omega_1)^{-1} \\
& \quad \times [\eta\,|\boldsymbol{\varkappa} - \mathbf{k}_1|^2 - i(\varpi - \omega_1)]^{-1}\epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}\int d^3\mathbf{K}\, d\Omega \Pi_{l\mu}(\mathbf{k}_1 - \mathbf{K}, \omega_1 - \Omega)R_{m\nu}(\mathbf{K}, \Omega; \boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega) \\
& = -(2\pi)^{-8}k_{1j}(\kappa_\alpha - k_{1\alpha})(\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\boldsymbol{\varkappa} - \mathbf{k}_1|^2 - i(\varpi - \omega_1)]^{-1} \\
& \quad \times \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}\int d^3\mathbf{K}\, d\Omega\Big\{B_m(\mathbf{K}, \Omega)B_\nu(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega) \\
& \quad \times \Pi_{l\mu}(\mathbf{k}_1 - \mathbf{K}, \omega_1 - \Omega) - \epsilon_{mpq}\epsilon_{qef}\epsilon_{vrs}\epsilon_{sgh}\int d^3\mathbf{k}\, d\omega B_h(\mathbf{K}, \Omega) \\
& \quad \times B_f(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega)k_p(K_r + k_r - k_{1r})(\eta k^2 - i\omega)^{-1}[\eta\,|\mathbf{K} + \mathbf{k} - \mathbf{k}_1|^2 - i(\omega_1 - \Omega - \omega)]^{-1} \\
& \quad \times \Pi_{lg}(\mathbf{k}_1 - \mathbf{k}, \omega_1 - \omega)\Pi_{\mu l}(\boldsymbol{\varkappa} - \mathbf{k} - \mathbf{K}, \varpi - \Omega - \omega)\Big\}. \qquad (18)
\end{aligned}
$$

We shall refer to Eq. (18) as the reduced Bethe–Salpeter tensor equation since it involves only the eight variables $\mathbf{k}$, $\mathbf{k}_1$, ϖ, ω_1, whereas the generalized Bethe–Salpeter equation [Eq. (15)] involved 16 variables.

For arbitrary two-point, two-time spatially homogeneous and stationary turbulent velocity correlation dyadics, we have been unable to solve Eq. (18) in general. However, there are two approximations that have been extensively used in the literature in discussing

kinematic dynamo activity. They are the "short-sudden" approximation[2] and the "long-slow" approximation.[7]

In terms of $\Pi_{l\mu}(\mathbf{k}, \omega)$, the "short-sudden" approximation is written

$$\Pi_{l\mu}(\mathbf{k}, \omega) = D_{l\mu}, \tag{19}$$

where $D_{l\mu}$ is a constant tensor independent of $\mathbf{k}$ and ω. This corresponds to assuming that $\Pi_{l\mu}(\mathbf{r}, \tau) \propto \delta(\mathbf{r})\delta(\tau)$, i.e., on the space and time scales over which $\Pi_{l\mu}(\mathbf{r}, \tau)$ changes appreciably the large-scale field $\mathbf{B}(\mathbf{r}, \tau)$ does not change substantially, and, conversely, over the space and time scales over which $\mathbf{B}(\mathbf{r}, \tau)$ changes substantially, the velocity turbulence changes infinitely rapidly as through Eq. (19) (or its Fourier transform).

In terms of $\Pi_{l\mu}(\mathbf{k}, \omega)$, the "long-slow" approximation is written

$$\Pi_{l\mu}(\mathbf{k}, \omega) = A_{l\mu}\delta(\mathbf{k})\delta(\omega), \tag{20}$$

where $A_{l\mu}$ is a constant tensor independent of $\mathbf{k}$ and ω. In this limit the velocity turbulence $\Pi_{l\mu}(\mathbf{r}, t)$ does not change appreciably over the space and time scales of the variations in the large-scale field. (For a more detailed exposition of the crucial differences between the "short-sudden" approximation and the "long-slow" approximation see Ref. 1.) It is clear that either the "short-sudden" approximation to the velocity turbulence or the "long-slow" approximation drastically simplifies the reduced Bethe–Salpeter equation (18).

We point out here that the reduced Bethe–Salpeter tensor equation (18) has associated with it all the usual singularities and divergencies of the "standard" Bethe–Salpeter occurring in quantum field theory (see, e.g., Ref. 10). These divergencies and singularities are usually split into two classes.

Class I: Consider Eq. (18) when the Fourier modes of the large-scale field are zero, i.e., $B_i(\mathbf{k}, \omega) = 0$. Then Eq. (18) is a homogeneous equation in R_{ab} and possesses a solution if and only if a dispersion relation is satisfied. (The precise form of the dispersion relation depends on detailed statements of the two-point, two-time turbulent velocity correlation dyadic.) In quantum mechanics [Ref. 10, Vol. 1, Sec. 9(c)], the corresponding dispersion statement determines the allowed bound states of the system at hand.

Class II: Consider Eq. (18) when $B_i(k, \omega) \not\equiv 0$. Then a particular solution for R_{ab} can, in principle, be found. This normally has a resonance structure leading to absolutely divergent integrals and corresponds to a scattering type of problem in quantum theory. In quantum field theory the divergence is removed by "mass renormalization" (Ref. 10, Vol. 1, Sec. 25). In the present context the analog of "mass renormalization" is (i) the statement of infinitesimal velocity turbulence occurring at an infinite rate using the "short-sudden" approximation, i.e., the $D_{l\mu}$ of Eq. (19) will turn out to be infinitesimal in order that a finite solution for the power spectrum obtain (but see Ref. 3 for a detailed statement of this normalization of the velocity turbulence), and (ii) in the "long-slow" approximation the analog is finite velocity turbulence occurring at an infinitesimal rate, i.e., the $A_{l\mu}$ of Eq. (20) will be finite, its precise level depending on the structure assumed for $B_i(\mathbf{k}, \omega)$ and on boundary and/or initial value statements of $\langle \delta B_i \delta B_j \rangle$.

Consider Eq. (18) first under the "long-slow" approximation and then under the "short-sudden" approximation.

III. FLUCTUATIONS IN THE LONG-SLOW LIMIT

With $\Pi_{l\mu} = A_{l\mu}\delta(\mathbf{k})\delta(\omega)$, where $A_{l\mu}$ is a constant tensor independent of $\mathbf{k}$ and ω, Eq. (18) reduces to

$$\begin{aligned} R_{ab}(\mathbf{k}_1, \omega_1; \boldsymbol{\varkappa} - \mathbf{k}_1, \varpi - \omega_1) = {} & -k_{1j}(\kappa_\alpha - k_{1\alpha})(\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\boldsymbol{\varkappa} - \mathbf{k}_1|^2 - i(\varpi - \omega_1)]^{-1}\epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta} \\ & \times \epsilon_{\beta\mu\nu}A_{l\mu}R_{m\nu}(\mathbf{k}_1, \omega_1; \boldsymbol{\varkappa} - \mathbf{k}_1, \varpi - \omega_1) \\ & -(2\pi)^{-8}k_{1j}(\kappa_\alpha - k_{1\alpha})(\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\boldsymbol{\varkappa} - \mathbf{k}_1|^2 - i(\varpi - \omega_1)]^{-1} \\ & \times \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}\{A_{l\mu}B_m(\mathbf{k}_1, \omega_1)B_\nu(\boldsymbol{\varkappa} - \mathbf{k}_1, \varpi - \omega_1) \\ & -(\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\boldsymbol{\varkappa} - \mathbf{k}_1|^2 - i(\varpi - \omega_1)]^{-1}\epsilon_{mpq}\epsilon_{vrs}\epsilon_{qef}\epsilon_{sgh}A_{lg}A_{\mu e} \\ & \times k_{1p}(\kappa_r - k_{1r})B_h(\boldsymbol{\varkappa} - \mathbf{k}_1, \varpi - \omega_1)B_f(\mathbf{k}_1, \omega_1)\}, \end{aligned} \tag{21}$$

which is an algebraic equation for R_{ab} rather than an integral equation as is the reduced Bethe–Salpeter tensor equation (18).

Equation (21) can be written

$$\begin{aligned} & R_{ab}(\mathbf{k}_1, \omega_1, \boldsymbol{\varkappa} - \mathbf{k}_1, \varpi - \omega_1)\{1 + (\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\boldsymbol{\varkappa} - \mathbf{k}_1|^2 - i(\varpi - \omega_1)]^{-1}A_{j\alpha}k_{1j}(\kappa_\alpha - k_{1\alpha})\} \\ & \quad = -(2\pi)^{-8}B_a(\mathbf{k}_1, \omega_1)B_b(\boldsymbol{\varkappa} - \mathbf{k}_1, \varpi - \omega_1)(\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\boldsymbol{\varkappa} - \mathbf{k}_1|^2 - i(\varpi - \omega_1)]^{-1} \\ & \qquad \times \{A_{j\alpha}k_j(\kappa_\alpha - k_\alpha) - k_jA_{j\alpha}(\kappa_\alpha - k_\alpha)k_e(\kappa_\mu - k_\mu)A_{\mu e}(\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\boldsymbol{\varkappa} - \mathbf{k}_1|^2 - i(\varpi - \omega_1)]^{-1}\}. \end{aligned} \tag{22}$$

The general solution to Eq. (22) gives

$$P_{ab}(\mathbf{x}, \varpi) = -\int d^3\mathbf{k}\, d\omega\{B_a(\mathbf{k}, \omega)B_b(\mathbf{x}-\mathbf{k}, \varpi-\omega)k_j(\kappa_\alpha - k_\alpha)A_{j\alpha}$$
$$\times (\eta k^2 - i\omega)^{-1}[\eta\,|\mathbf{x}-\mathbf{k}|^2 - i(\varpi-\omega)]^{-1}[(\eta k^2 - i\omega)[\eta\,|\mathbf{x}-\mathbf{k}|^2 - i(\varpi-\omega)] + A_{j\alpha}k_j(\kappa_\alpha - k_\alpha)]$$
$$\times [(\eta k^2 - i\omega)[\eta\,|\mathbf{x}-\mathbf{k}|^2 - i(\varpi-\omega)] - k_e(\kappa_\mu - k_\mu)A_{\mu e}]^{*-1}$$
$$+ \lambda_{ab}(\mathbf{k}, \mathbf{x}, \varpi, \omega)\delta[(\eta k^2 - i\omega)[\eta\,|\mathbf{x}-\mathbf{k}|^2 - i(\varpi-\omega)] + A_{j\alpha}k_j(\kappa_\alpha - k_\alpha)]\}, \tag{23}$$

where we have written for brevity $Px^{-1} \equiv x^{*-1}$. Also λ_{ab} is a tensor, as yet unknown. Suppose, for illustrative purposes only, that $A_{j\alpha} = A\delta_{j\alpha}$, where A is real and positive. Then Eq. (23) becomes

$$P_{ab}(\mathbf{x}, \omega) = -A\int d^3\mathbf{k}\, d\omega\{B_a(k, \omega)B_b(\mathbf{x}-\mathbf{k}, \varpi-\omega)(\mathbf{k}\cdot\mathbf{x} - k^2)$$
$$\times (\eta k^2 - i\omega)^{-1}[\eta\,|\mathbf{x}-\mathbf{k}|^2 - i(\varpi-\omega)]^{-1}[(\eta k^2 - i\omega)[\eta\,|\mathbf{x}-\mathbf{k}|^2 - i(-\varpi\omega)] - A(\mathbf{k}\cdot\mathbf{x} - k^2)]$$
$$\times [(\eta k^2 - i\omega)[\eta\,|\mathbf{x}-\mathbf{k}|^2 - i(\varpi-\omega)] + A(\mathbf{k}\cdot\mathbf{x} - k^2)]^{*-1}$$
$$+ \lambda_{ab}(\mathbf{k}, \mathbf{x}, \varpi, \omega)\delta[(\eta k^2 - i\omega)[\eta\,|\mathbf{x}-\mathbf{k}|^2 - i(\varpi-\omega)] + A(\mathbf{k}\cdot\mathbf{x} - k^2)]\}. \tag{24}$$

By inspection of Eq. (24), it is clear that we require more information before we can obtain $P_{ab}(\mathbf{x}, \varpi)$. First we require the behavior of $B_a(\mathbf{k}, \omega)$. This depends on boundary and/or initial conditions together with source terms. So, until some specific problem is under consideration, no general statement about $B_a(\mathbf{k}, \omega)$ can be made (except, of course, for the usual divergence condition $k_aB_a = 0$).

Second we require the functional form of

$$\lambda_{ab}(\mathbf{k}, \mathbf{x}, \varpi, \omega).$$

As has been shown elsewhere[11–13] knowledge of λ_{ab} depends on initial value and/or boundary value statements for the fluctuating quantities. For example, we could demand that $\langle\delta B_a(\mathbf{x}, 0)\delta B_b(\mathbf{x}, 0)\rangle = 0$, which would then relate λ_{ab} to integrals over the large-scale field **B**.

We see then that the singular eigenfunction approach to $P_{ab}(\mathbf{x}, \varpi)$ leads automatically to a well-posed problem in which the singularities (i.e., the normal modes of the homogeneous problem) act to "absorb" the divergencies of the particular solution (represented by the principle value integral over the large-scale field). The arbitrary tensor λ_{ab} is to be found in standard manner by consideration of initial value and boundary value conditions.

Before we can consider Eq. (24) in any detail, it is clear that we need the behavior of $B_a(\mathbf{k}, \omega)$ in order to evaluate the integral over $\mathbf{k}$, ω occurring in Eq. (24). We defer any discussion of this until Sec. V.

Consider now the "short-sudden" approximation.

IV. FLUCTUATIONS IN THE SHORT-SUDDEN APPROXIMATION

With $\Pi_{l\mu}(\mathbf{k}, \omega) = D_{l\mu}$, where $D_{l\mu}$ is a constant tensor independent of $\mathbf{k}$ and ω, Eq. (18) reduces to

$$R_{ab}(\mathbf{k}_1, \omega_1; \mathbf{x}-\mathbf{k}_1, \varpi-\omega_1) = -(2\pi)^{-8}k_{1j}(\kappa_\alpha - k_{1\alpha})(\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\mathbf{x}-\mathbf{k}_1|^2 - i(\varpi-\omega_1)]^{-1}$$
$$\times D_{l\mu}\epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}P_{m\nu}(\mathbf{x}, \varpi)$$
$$- (2\pi)^{-8}k_{1j}(\kappa_\alpha - k_{1\alpha})(\eta k_1^2 - i\omega_1)^{-1}[\eta\,|\mathbf{x}-\mathbf{k}_1|^2 - i(\varpi-\omega_1)]^{-1}$$
$$\times \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu\nu}\int d^3\mathbf{K}\, d\Omega\Big\{B_m(\mathbf{x}, \Omega)B_\nu(\mathbf{x}-\mathbf{K}, \varpi-\Omega)D_{l\mu}$$
$$- \epsilon_{mpq}\epsilon_{vrs}\epsilon_{qef}\epsilon_{sgh}D_{lg}D_{\mu e}B_h(\mathbf{K}, \Omega)B_f(\mathbf{x}-\mathbf{K}, \varpi-\Omega)$$
$$\times \int d^3\mathbf{k}\, d\omega k_p(K_r + k_r - k_{1r})(\eta k^2 - i\omega)^{-1}[\eta\,|\mathbf{K}+\mathbf{k}-\mathbf{k}_1|^2 - i(\omega_1 - \Omega - \omega)]^{-1}\Big\}, \tag{25}$$

where

$$P_{m\nu}(\mathbf{x}, \varpi) = (2\pi)^8\int R_{m\nu}(\mathbf{k}, \omega; \mathbf{x}-\mathbf{k}, \varpi-\omega)\, d^3\mathbf{k}\, d\omega. \tag{26}$$

Note the crucial difference in the reduced Bethe–Salpeter equation for the long-slow and short-sudden approximations. In the former, Eq. (18) reduces to an algebraic equation for R_{ab} [cf., Eqs. (21) and (22)], while in the latter the reduction leads to an integral equation for R_{ab} [cf., Eq. (26)].

Further, as Parker[2,3] has remarked, in the short-sudden approximation one has infinitesimal turbulence occurring at an infinite rate. The mathematical expression of this physical statement has been considered elsewhere in considerable detail[1-4] under a wide variety of circumstances. In the present context the statement of infinitesimal turbulence occurring at an infinite rate requires $D_{l\mu}$ to be infinitesimal, as we now demonstrate directly.

Consider the integral

$$I_{pr} = \int d^3\mathbf{k}\, d\omega k_p(K_r + k_r - k_{1r})(\eta k^2 - i\omega)^{-1} \times [\eta\,|\mathbf{K} + \mathbf{k} - \mathbf{k}_1|^2 - i(\omega_1 - \Omega - \omega)]^{-1}, \quad (27)$$

which occurs in the last term on the right-hand side of Eq. (26). Upon performing the integral over ω, we have

$$I_{pr} = 2\pi \int d^3\mathbf{k} k_p(K_r + k_r - k_{1r}) \times [\eta\,|\mathbf{K} + \mathbf{k} - \mathbf{k}_1|^2 - i(\omega_1 - \Omega) + \eta k^2]^{-1}. \quad (28)$$

With $\boldsymbol{\zeta} = \mathbf{k} + \frac{1}{2}(\mathbf{K} - \mathbf{k}_1)$ Eq. (28) becomes

$$I_{pr} = 2\pi \int d^3\boldsymbol{\zeta}[\zeta_p - \tfrac{1}{2}(K_p - k_{1p})][\zeta_r + \tfrac{1}{2}(K_r - k_{1r})] \times [2\eta\zeta^2 + \tfrac{1}{2}\eta\,|\mathbf{K} - \mathbf{k}_1|^2 - i(\omega_1 - \Omega)]^{-1}. \quad (29)$$

Upon performing the angular part of the $\boldsymbol{\zeta}$ integral in Eq. (29), we have

$$I_{pr} = 8\pi^2 \int_0^\infty \zeta^2\, d\zeta \times [\tfrac{1}{3}\zeta^2\delta_{pr} - \tfrac{1}{4}(K_p - k_{1p})(K_r - k_{1r})] \times [2\eta\zeta^2 + \tfrac{1}{2}\eta\,|\mathbf{K} - \mathbf{k}_1|^2 - i(\omega_1 - \Omega)]^{-1}. \quad (30)$$

And the integral over ζ in Eq. (30) diverges as $\zeta \to \infty$. In order to circumvent this divergence, we follow Parker's physical statement; its mathematical expression is to write $D_{l\mu} = \mathfrak{D}_{l\mu}[\int_0^\infty \zeta^2\, d\zeta]^{-1}$, and regard $\mathfrak{D}_{l\mu}$ as finite so that $D_{l\mu}$ is infinitesimal (alternatively we can run all divergent integrals up to some large wavenumber, say k_*, define $D_{l\mu} = \mathfrak{D}_{l\mu} 3k_*^{-3}$, and let $k_* \to \infty$ *after* performing all computations with $\mathfrak{D}_{l\mu}$ held finite so that $D_{l\mu}$ is infinitesimal).

Then write

$$D_{l\mu} I_{pr} = \Delta_{l\mu}\delta_{pr}, \quad (31)$$

or, equivalently, $\Delta_{l\mu} = \mathfrak{D}_{l\mu} 4\pi^2/3\eta$.

Upon integrating Eq. (25) over $d^3\mathbf{k}_1\, d\omega_1$ and using Eq. (31), we obtain

$$P_{mv}(\boldsymbol{\varkappa}, \varpi)[\delta_{ma}\delta_{vb} - \Delta_{l\mu}\delta_{aj}\epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu v}] = \epsilon_{ajk}\epsilon_{klm}\epsilon_{b\alpha\beta}\epsilon_{\beta\mu v}\delta_{j\alpha}\int d^3\mathbf{K}\, d\Omega \times \{\Delta_{l\mu}B_m(\mathbf{K}, \Omega)B_v(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega) - \delta_{pr}\epsilon_{mpq}\epsilon_{vrs}\epsilon_{qef}\epsilon_{sgh}\Delta_{lg}\Delta_{\mu e}B_h(\mathbf{K}, \Omega)B_f(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega)\}. \quad (32)$$

In order to compare and contrast the fluctuation spectra in the long-slow approximation with the short-sudden results we take, for illustrative purposes only, $\Delta_{ij} = \Delta\delta_{ij}$. Then Eq. (32) can be solved for $P_{ab}(\boldsymbol{\varkappa}, \varpi)$, since it is only algebraic, yielding

$$P_{ab}(\boldsymbol{\varkappa}, \varpi)(1 - \Delta^2) = \Delta \int d^3\mathbf{K}\, d\Omega \Big\{\delta_{ab}(1 - \Delta)B_m(\mathbf{K}, \Omega)B_m(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega) \times \left[1 + \frac{\Delta(3 + \Delta)}{(1 - 2\Delta)}\right] + \Delta B_a(\mathbf{K}, \Omega)B_b(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega) - \Delta^2 B_a(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega)B_b(\mathbf{K}, \Omega)\Big\}. \quad (33)$$

And then

$$P(\boldsymbol{\varkappa}, \varpi) \equiv P_{aa}(\boldsymbol{\varkappa}, \varpi) = \frac{\Delta(3 + \Delta)}{(1 - 2\Delta)} \times \int d^3\mathbf{K}\, d\Omega B_m(\mathbf{K}, \Omega)B_m(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega). \quad (34)$$

But we have

$$\mathfrak{E} \equiv \mathbf{B}(\mathbf{x}, t) \cdot \mathbf{B}(\mathbf{x}, t) = \int d^3\mathbf{K}\, d\Omega B_m(\mathbf{K}, \Omega)B_m(\boldsymbol{\varkappa} - \mathbf{K}, \varpi - \Omega) \times \exp[i(\boldsymbol{\varkappa} \cdot \mathbf{x} - \varpi t)]\, d^3\boldsymbol{\varkappa}\, d\varpi. \quad (35)$$

So, from Eqs. (13), (34), and (35) we have

$$\delta\mathfrak{E} \equiv \langle \delta\mathbf{B}(\mathbf{x}, t) \cdot \delta\mathbf{B}(\mathbf{x}, t)\rangle = \Delta(3 + \Delta)(1 - 2\Delta)^{-1}\mathfrak{E}. \quad (36)$$

The ratio of energy density stored in magnetic fluctuations to that stored in the large-scale field is

$$\delta\mathfrak{E}/\mathfrak{E} = \Delta(3 + \Delta)/(1 - 2\Delta). \quad (37)$$

From Eq. (37) it is clear that, in order to keep the energy density stored in the fluctuations at a finite level, we require $2\Delta < 1$.

But, *prime facie*, there is no mathematical, or

physical, reason, either explicit or implicit, why the "strength" of the velocity turbulence should be restricted to less than some fixed level (except, of course, for the *a posteriori* reason that energy density is positive and finite).

In order to account for this apparent dichotomy, we note that, although we have replaced the two-point, two-time velocity fluctuations by δ-function correlations in $(\mathbf{x}, t)$ space for mathematical convenience, in reality they will extend over finite domains in both space and time. This complicates the analysis of Eq. (18) *vide* Eq. (25). In particular, instead of an equation whose structure is the same as the left-hand side of Eq. (32), we would arrive at an equation whose structure has $\mathbf{k}$ and ω dependence in its left-hand side, as does, for example, Eq. (22).

That is to say, in physical reality we would arrive at an expression of the form $[1 - 2\Delta f(\varkappa, \varpi)]$ instead of $(1 - 2\Delta)$. This would give rise to singular eigen modes in much the same manner as were obtained in the long-slow approximation (Sec III, q.v.).

An alternative way to look at this point of view is to note that neither Eq. (33) nor Eq. (34) admits of any freedom in choice of boundary conditions for $\langle \delta B_a \delta B_b \rangle$. Once the boundary conditions on the large-scale field are specified, according to Eq. (33) the fluctuation field intensity is uniquely specified. This apparently contradicts the original Eqs. (1) and (2) which allow for boundary value and/or initial value statements on *both* $\mathbf{B}$ and $\delta\mathbf{B}$.

But under the strong statement of the "short-sudden" approximation (see Ref. 1, Footnote 3) the fluctuations are not convected, sheared, nor diffused during their lifetime. And under this statement it is clear that we are restricting our consideration of Eq. (2) to the particular solution. So there is no contradiction with the original equation.

To sum up: (1) Under the *mathematical* assumption of δ-function velocity correlations, the *physics* of the problem requires $\Delta < \frac{1}{2}$. [This corresponds to the strong statement of the short-sudden approximation (Ref. 1, Footnote 3).] (2) Under the *physical* assumption of finite (but very small) range velocity correlations the *mathematics* of the problem requires the addition of the singular van Kampen modes as also occurred in Sec. III in order to allow for boundary and/or initial value statements on $P_{ab}(\mathbf{q}, t)$. [This corresponds to the weak statement of the short-sudden approximation (Ref. 1, Footnote 3).]

Under the present conditions we are working in the strong statement of the short-sudden approximation and then $\Delta < \frac{1}{2}$ for physical reasons.

The solution of the reduced Bethe–Salpeter tensor equation for the fluctuations involves the large-scale field. And while it is possible to determine the "structure" of the fluctuations in terms of integrals over the large-scale field (and in the case of the short-sudden approximation it is possible to compute the relative energy density stored in fluctuations to that stored in the large-scale field), it is clear that we require the behavior of the large-scale field in order to obtain *absolute* levels of fluctuation intensity rather than *relative* levels [cf. Eq. (37)].

So we now consider the large-scale field.

V. THE LARGE-SCALE FIELD AND THE DYSON EQUATION

From Eq. (1) we have

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)\mathbf{B} - \nabla \times \langle \delta\mathbf{v}(\mathbf{x}, t) \times \delta\mathbf{B}(\mathbf{x}, t)\rangle = \nabla \times \mathbf{S}(\mathbf{x}, t). \quad (38)$$

We have written the right-hand side of Eq. (38) as $\nabla \times \mathbf{S}$ instead of zero, so that *all* boundary value and initial value statements on $\mathbf{B}$ are to be considered as incorporated in $\mathbf{S}$.

Using the Green's function for $\delta\mathbf{B}$, together with the statement that the statistical properties of $\delta\mathbf{v}$ are such that all correlations entering Eq. (38) are reducible to the two-point, two-time level, we obtain Eq. (38) in the form

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)B_i + \epsilon_{ijk}\epsilon_{kab}\epsilon_{blm}\epsilon_{m\mu\nu}\frac{\partial}{\partial x_j}\int d^3\mathbf{x}'\,dt'\langle \delta v_a(\mathbf{x}, t)\delta v_\mu(\mathbf{x}', t')\rangle \frac{\partial G_0}{\partial x_l'}(\mathbf{x}, \mathbf{x}', t, t')B_\nu(\mathbf{x}', t') = \epsilon_{ijk}\frac{\partial S_k}{\partial x_j}(\mathbf{x}, t). \quad (39)$$

With

$$B_i(\mathbf{x}, t) = \int \mathfrak{G}_i(\mathbf{x}, \mathbf{x}', t, t')\,d^3\mathbf{x}'\,dt', \quad (40)$$

we have the propagator equation for the large-scale field as

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)\mathfrak{G}_i(\mathbf{x}, \mathbf{x}', t, t') + \epsilon_{ijk}\epsilon_{kab}\epsilon_{blm}\epsilon_{m\mu\nu}\frac{\partial}{\partial x_j}\int d^3\mathbf{x}''\,dt\;\Pi_{a\mu}(\mathbf{x} - \mathbf{x}', t - t')\frac{\partial G_0}{\partial x_l''}(\mathbf{x}, \mathbf{x}'', t, t'')\mathfrak{G}_\nu(\mathbf{x}'', \mathbf{x}', t'', t') = \epsilon_{ijk}\frac{\partial S_k}{\partial x_j'}(\mathbf{x}', t')\delta(\mathbf{x} - \mathbf{x}')\delta(t - t'), \quad (41)$$

where we have used Eq. (16a) to rewrite the two-point, two-time velocity correlation. We recognize Eq. (41) as the vector form of Dyson's equation.

Upon Fourier-transforming Eq. (39) in both space and time, we obtain, after some elementary but tedious integrations,

$$(\eta k^2 - i\omega)B_i(\mathbf{k}, \omega) + \epsilon_{ijk}\epsilon_{kab}\epsilon_{blm}\epsilon_{m\mu\nu}\int d^3\mathbf{k}'\, d\omega' \Pi_{a\mu}(\mathbf{k} - \mathbf{k}', \omega - \omega')k'_l k_j(\eta k'^2 - i\omega')^{-1}B_\nu(\mathbf{k}, \omega) = \epsilon_{ijk}k_j S_k(\mathbf{k}, \omega), \tag{42}$$

where, since $k_i B_i = 0$, we have written the Fourier transform of the source term at right angles to $\mathbf{k}$.

Consider now the structure of the solution to Eq. (42) under both the "long-slow" and the "short-sudden" approximations for $\Pi_{a\mu}$.

A. The Large-Scale Field in the Long-Slow Approximation

Here, as before, we set

$$\Pi_{a\mu}(\mathbf{k}, \omega) = A\delta_{a\mu}\delta(\mathbf{k})\delta(\omega), \tag{43}$$

when Eq. (41) becomes

$$B_i(\mathbf{k}, \omega)[(\eta k^2 - i\omega) + k^2 A(\eta k^2 - i\omega)^{-1}] = \epsilon_{ijk}k_j S_k(\mathbf{k}, \omega), \tag{44}$$

with

$$B_i(\mathbf{k}, \omega) = \epsilon_{ijk}k_j g_k(k, \omega)[(\eta k^2 - i\omega)^2 + k^2 A]^{-1}, \tag{45}$$

where we have absorbed a factor $(\eta k^2 - i\omega)$ into S_k and have therefore written $g_k = (\eta k^2 - i\omega)S_k$.

Note that the dispersion relation for the large-scale field [given by setting the coefficient of B_i to zero in Eq. (44)] is *not* the same as the dispersion relation for the fluctuation intensity [given by the zeros of the δ function in Eq. (24)] indicating that a single normal mode of the large-scale field does not act as a source of a single mode for the fluctuation magnetic field. Instead it generates a band of $\mathbf{k}$ and ω values giving rise, therefore, to nonlinear mode–mode coupling terms in the fluctuation field.

In particular, note that, for the large-scale field, those normal modes with $\eta k < A^{\frac{1}{2}}$ are regenerative while those with $\eta k > A^{\frac{1}{2}}$ are degenerative. The correspondence to be made with the fluctuation intensity is to note that at $\boldsymbol{\varkappa} = 0 = \varpi$ the δ function in Eq. (24) contributes to $P_{ab}(0, 0)$ for $\eta k > A^{\frac{1}{2}}$ and does not contribute for $\eta k < A^{\frac{1}{2}}$, thereby representing the "break" between regeneration and degeneration of the normal modes of the large-scale field. For real values of $\boldsymbol{\varkappa}$ and ϖ differing from zero in Eq. (24), the δ function contributes when both

$$\omega\,|\boldsymbol{\varkappa} - \mathbf{k}|^2 = -k^2(\varpi - \omega) \tag{46a}$$

and

$$\eta^2 k^2\,|\boldsymbol{\varkappa} - \mathbf{k}|^2 + \omega(\varpi - \omega) = A(k^2 - \mathbf{k}\cdot\boldsymbol{\varkappa}) \tag{46b}$$

are satisfied.

There is no obvious direct representation of the "break" between regeneration and degeneration of the large-scale field normal modes under these more general conditions ($\boldsymbol{\varkappa} \neq 0 \neq \varpi$) due to the nonlinear [in $(\mathbf{k}, \omega)$ space] coupling of modes.

Further, in order to evaluate the integral occurring in Eq. (24), we need initial value and/or boundary value statements about *both* $B_i(\mathbf{x}, t)$ and $P_{ab}(\mathbf{x}, t)$ in order to (i) use Eq. (44) in the principle value integral in Eq. (24) and (ii) obtain an explicit representation of $\lambda_{ab}(\boldsymbol{\varkappa}, \varpi)$. Such statements clearly depend on the particular problem at hand. In the present analysis, in which we are concerned with the basic structure of the equations describing kinematic dynamo action, we reluctantly forego discussion of any such particular systems and/or situations.

Consider now the opposite extreme.

B. The Large-Scale Field in the Short-Sudden Approximation

Here we set

$$\Pi_{a\mu}(\mathbf{k}, \omega) = D\delta_{a\mu}, \tag{47}$$

and remember that, from Sec. IV, we require D to be infinitesimal in order that the fluctuation field energy density be finite. Then Eq. (42) becomes

$$B_i(\mathbf{k}, \omega)(\eta k^2 - i\omega) = \epsilon_{ijk}k_j S_k(\mathbf{k}, \omega), \tag{48}$$

since the velocity fluctuations do not contribute to the large-scale field in this approximation as can be seen directly by inspection of Eq. (42) using Eq. (47).

So, unless the boundary and/or initial value conditions are such as to be proportional to $B_i(\mathbf{k}, \omega)$ and hence lead to the possibility of regenerative states, under the short-sudden approximation, with no large-scale sheared velocity field present, the physical situation described by Eq. (48) corresponds to decay of the large-scale field. Once again note that the dispersion relation for the large-scale field ($\eta k^2 - i\omega = 0$) is not the same as the dispersion relation for the fluctuation intensity, which, in the present *mathematical* statement of δ-function approximations to the two-point, two-time turbulent velocity correlations is $1 - 2\Delta = 0$. But the *physical* constraints ensure that this is never satisfied, since the finite energy density [Eq. (27)] requires $\Delta < \frac{1}{2}$.

VI. DISCUSSION AND CONCLUSION

In the present paper we have discussed the basic equations describing kinematic dynamo theory in a

stationary, unsheared medium beyond the level of first-order smoothing theory. In particular, under the single assumption that the statistical properties of the velocity turbulence were such that all correlations entering Eqs. (7) and (38) were reducible to the two-point, two-time level, we obtained both the tensor Bethe–Salpeter equation (in 16 variables) and the vector Dyson equation (in eight variables) describing *exactly* the Maxwell stress tensor of the random component of the magnetic field and the *exact* behavior of the large-scale ensemble average field, respectively.

These equations were investigated further under the assumption that the two-point, two-time velocity tensor correlation was both stationary and homogeneous.

We found that, under the "long-slow" approximation, the behavior of the normal modes of the large-scale field changed from regenerative for small wavenumbers ($\eta k < A^{\frac{1}{2}}$) to degenerative at large wavenumbers ($\eta k > A^{\frac{1}{2}}$). This structure appeared in the equation describing the fluctuation intensity [Eq. (24)] through both the δ function [whose tensor coefficient represents initial value and/or boundary value statements on $P_{ab}(\mathbf{x}, t)$] and the principle value integral. It was most readily apparent at $\varkappa = 0 = \varpi$ when the δ function contributed to $P_{ab}(0, 0)$ for $\eta k > A^{\frac{1}{2}}$, but did not contribute for $\eta k < A^{\frac{1}{2}}$.

Under the "short-sudden" approximation we demonstrated that the *mathematical* approximation of δ functions for the velocity turbulence gave rise to a *physical* restriction that the intensity of the turbulence (in suitable units) must obey $2\Delta < 1$ in order to preserve physical sense. We also argued that a more physical approximation to the velocity turbulence viz., finite space and time scales for the correlation of one fluid velocity element with another, would have led us back to an equation involving singular eigenfunctions as obtained in the long-slow approximation. This regression is necessary on physical grounds in order to include initial and/or boundary value effects in the fluctuation equation [Eq. (2)]. These would otherwise be overlooked in a mathematical δ-function statement of the strong form of the "short-sudden" approximation.

We also demonstrated that the large-scale magnetic field has, in general, a different characteristic behavior than the fluctuation intensity—as represented through the dispersion relation for the large-scale field on the one hand and the zeros of the δ functions representing the singular eigenfunction statement on the other.

In particular: (i) The change over from regeneration to degeneration of the normal modes of the large-scale field in the long-slow approximation is incorporated in the fluctuation intensity equation. However, there is not a transparent correspondence between the two except when $\varkappa = 0 = \varpi$ in the fluctuation intensity equation; (ii) the degeneration of all the normal modes of the large-scale field (barring regeneration due to boundary conditions) in the short-sudden approximation is not reflected in the fluctuation intensity equation except through the selection rule $2\Delta < 1$. And this latter arises because of the mathematical δ-function statement of the "short-sudden" approximation.

We should, perhaps, point out that the statistical properties of the velocity turbulence used in the present paper are by no means the most general form of turbulence available. They do have the advantage that the fluctuation intensity equation and the mean field equation can be simply studied with the minimum amount of mathematics concomitant with physical understanding.

We would, of course, be interested in seeing more detailed developments of the properties of fluctuating, and ordered, magnetic fields than has been given here. Our development was intended to illustrate some of the basic properties of kinematic dynamos when the equations describing such dynamos are handled *exactly* rather than approximately as is the convention. The results contained in this paper should be viewed in that light. Different statistical descriptions of the velocity turbulence than those incorporated here will undoubtedly change the detailed structure of the fluctuation intensity equation and the ordered field equation. But the basic mathematical and physical properties (viz., the "singularities" of both the Bethe–Salpeter equation and of the normal modes of the Dyson equation) of exact kinematic dynamo theory will remain essentially as described herein.

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Korteweg–de Vries Equation and Generalizations. IV. The Korteweg–de Vries Equation as a Hamiltonian System

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It is shown that if a function of x and t satisfies the Korteweg–de Vries equation and is periodic in x, then its Fourier components satisfy a Hamiltonian system of ordinary differential equations. The associated Poisson bracket is a bilinear antisymmetric operator on functionals. On a suitably restricted space of functionals, this operator satisfies the Jacobi identity. It is shown that any two of the integral invariants discussed in Paper II of this series have a zero Poisson bracket.

I. A VARIATIONAL PRINCIPLE AND ITS HAMILTONIAN FORMULATION

The Korteweg–de Vries equation

$$u_t = uu_x + u_{xxx} \tag{1}$$

(subscripts denoting partial differentiations) can be derived from the variational principle

$$\delta \int L\, dt = 0,$$

where

$$L \equiv \int (\tfrac{1}{2}\phi_x\phi_t - \tfrac{1}{6}\phi_x^3 + \tfrac{1}{2}\phi_{xx}^2)\, dx \tag{2}$$

and ϕ is a potential for u; that is,

$$u = \phi_x.$$

(It is understood here that $\delta\phi$ has compact support.) This type of variational principle has been discussed by Whitham[1] in connection with a general class of systems of partial differential equations, of which the Korteweg–de Vries equation is the simplest nontrivial example.

We shall assume throughout that $u(x)$ is periodic with period 2π and has continuous derivatives of all orders. Thus u can be represented by means of its Fourier coefficients u_n, which are complex constants such that

$$u(x) = \sum_{n=-\infty}^{\infty} u_n e^{inx}. \tag{3}$$

If the functional F and function f are defined by

$$F\{u\} \equiv \int_0^{2\pi} f(u, u_x)\, dx \equiv \int_0^{2\pi} (\tfrac{1}{6}u^3 - \tfrac{1}{2}u_x^2)\, dx, \tag{4}$$

then (2) yields the Korteweg–de Vries equation in the form

$$u_t = \frac{\partial}{\partial x}\left(\frac{\delta F}{\delta u}\right). \tag{5}$$

Here $\delta F/\delta u$ means the functional derivative of F with respect to u. In general, if F is a functional and $u(x,\alpha)$ is its argument function, depending on a parameter α as well as on the variable x, then the functional derivative $\delta F/\delta u$ is defined by

$$\frac{d}{d\alpha} F\{u\} = \int_0^{2\pi} \frac{\delta F}{\delta u}\frac{\partial u}{\partial \alpha}\, dx. \tag{6}$$

Now the functional $F\{u\}$ may be regarded as a *function* of the variables u_n. Its partial derivative with respect to u_k is given by (6) and (3), as follows:

$$\frac{\partial F}{\partial u_k} = \int_0^{2\pi} \frac{\delta F}{\delta u} e^{ikx}\, dx. \tag{7}$$

Hence, we have the formula

$$\frac{\delta F}{\delta u} = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \frac{\partial F}{\partial u_{-n}} e^{inx}. \tag{8}$$

Putting this into (5), we obtain the differential equations satisfied by the Fourier components u_n, as follows:

$$\frac{du_n}{dt} = \frac{i}{2\pi} n \frac{\partial F}{\partial u_{-n}}. \tag{9}$$

Now (9) is essentially a Hamiltonian system. The analogy becomes exact if one defines (for $n > 0$)

$$q_n \equiv u_n/n, \quad p_n \equiv u_{-n}, \quad H \equiv (i/2\pi)F. \tag{10}$$

Then (9) becomes

$$\frac{dq_n}{dt} = \frac{\partial H}{\partial p_n}, \quad \frac{dp_n}{dt} = -\frac{\partial H}{\partial q_n}. \tag{11}$$

In terms of the variables q_n and p_n one can define the *Poisson bracket* of two functionals, F and G, as follows:

$$(F, G) \equiv \frac{i}{2\pi}\sum_{n=1}^{\infty}\left(\frac{\partial F}{\partial q_n}\frac{\partial G}{\partial p_n} - \frac{\partial F}{\partial p_n}\frac{\partial G}{\partial q_n}\right), \tag{12}$$

which, by (10), is the same as

$$\begin{aligned}(F, G) &= \frac{i}{2\pi}\sum_{n=1}^{\infty}\left(n\frac{\partial F}{\partial u_n}\frac{\partial G}{\partial u_{-n}} - n\frac{\partial F}{\partial u_{-n}}\frac{\partial G}{\partial u_n}\right)\\ &= \frac{i}{2\pi}\sum_{n=-\infty}^{\infty} n\frac{\partial F}{\partial u_n}\frac{\partial G}{\partial u_{-n}}.\end{aligned} \tag{13}$$

Using (8), we see that the Poisson bracket also is

$$(F, G) = \int_0^{2\pi} \frac{\delta F}{\delta u} \frac{\partial}{\partial x} \frac{\delta G}{\delta u}\, dx. \tag{14}$$

From now on it will be assumed that the functionals with which we shall deal are representable as integrals, as follows:

$$F\{u\} = \int_0^{2\pi} f(x, u, u_x, u_{xx}, \cdots)\, dx, \tag{15}$$

where f is an infinitely often differentiable function of x, u, and a finite number of derivatives of u and where f is defined for all values of its arguments. Then, if F and G are two such functionals, so is the Poisson bracket (F, G) defined by (14), since we have the familiar Euler expressions for the functional derivatives. Indeed,

$$\frac{\delta F}{\delta u} = y_0 f,$$

where the operator y_0 is defined by

$$y_0 \equiv \frac{\partial}{\partial u} - \frac{\partial}{\partial x}\frac{\partial}{\partial u_x} + \frac{\partial^2}{\partial x^2}\frac{\partial}{\partial u_{xx}} \cdots. \tag{16}$$

The Jacobi identity can now be verified. This is

$$((F, G), H) + ((G, H), F) + ((H, F), G) = 0. \tag{17}$$

If it were legitimate to make free use of (13), it would be very easy to verify (17). The difficulty, of course, is that one is not sure of the convergence of the infinite series one uses in this calculation. However, this difficulty can be avoided: Let g and h be the functions related to G and H as f is to F in (15). Suppose that f, g, and h are polynomials in the variables u, u_x, etc. Suppose that the argument function is

$$u^N(x) = \sum_{n=-N}^{N} u_n e^{inx}.$$

Then it is easily seen that if $|k|$ is large enough (how large depends on N and also on the polynomials f, g, and h) we have

$$\frac{\partial F}{\partial u_k} = 0, \quad \frac{\partial G}{\partial u_k} = 0, \quad \frac{\partial H}{\partial u_k} = 0.$$

In this case, in (13) and (17) we have only finite sums and we conclude rigorously that (17) is correct. Now let u^N tend to u by making N tend to infinity. Each term of (17) will tend to the correct limiting value [expressed by (14) and (16)]. We thus have removed the restriction that u be a trigonometric polynomial. Now we remove the restriction of f, g, and h to polynomials, by another limiting process. In the terms of (17), only a finite number of partial derivatives of f, g, and h occur, and one can find a sequence of polynomials f^N, g^N, and h^N which tend uniformly to f, g, and h and a finite set of whose derivatives tend uniformly to the corresponding derivatives of f, g, and h. This completes the proof of Jacobi's identity (17). Thus, the operator (14) and the space of functionals (15) define an infinite-dimensional Lie algebra.

II. INTEGRAL INVARIANTS

It was shown in Ref. 2 that the Korteweg–de Vries equation (1) possesses an infinite sequence of conservation laws—equations in the form

$$\frac{\partial T_n}{\partial t} + \frac{\partial X_n}{\partial x} = 0, \quad n = 1, 2, 3, \cdots, \tag{18}$$

where T_n, the conserved density, and $-X^n$, the flux of T_n, are polynomials in u, u_x, u_{xx}, etc. The polynomials T_n and X_n are of uniform ranks, n and $n + 1$ (see Ref. 2).

In this section we shall consider the functionals

$$F_n\{u\} = \int_0^{2\pi} T_n\, dx,$$

where u is assumed periodic. If u depends on t as well as on x and satisfies the Korteweg–de Vries equation (1), then the functionals F_n are constant in time and may be called integral invariants. It happens that F_3 is the Hamiltonian functional which yields the Korteweg–de Vries equation in the form (5). The fact that F_3 is an integral invariant then can be seen as follows:

$$\frac{\partial F_3}{\partial t} = \int_0^{2\pi} \left(\frac{\delta F_3}{\delta u}\right)\frac{\partial u}{\partial t}\, dx$$
$$= \int_0^{2\pi} \left(\frac{\delta F_3}{\delta u}\right)\frac{\partial}{\partial x}\left(\frac{\delta F_3}{\delta u}\right) dx = 0. \tag{19}$$

The statement that F_n is an integral invariant for the Korteweg–de Vries equation is equivalent to the formula

$$0 = \frac{\partial F_n}{\partial t} = \int_0^{2\pi} \left(\frac{\delta F_n}{\delta u}\right)\frac{\partial}{\partial x}\left(\frac{\delta F_3}{\delta u}\right) dx = (F_n, F_3); \tag{20}$$

that is, the Poisson bracket (F_n, F_3) vanishes. We will now show that in general

$$(F_m, F_n) = 0 \tag{21}$$

for all m and n.

The first step is to show the following theorem.

Theorem: A conserved density of uniform rank yields a nonzero integral invariant if and only if the rank is an integer.

Proof: If the function u be expressed in terms of its Fourier series, then an integral invariant with conserved density of rank r is of the following form:

$$F = \sum_{l_1+l_2+\cdots+l_k=0} A^{(m)}(l_1, l_2, \cdots, l_k)u_l, u_{l_2}, \cdots, u_{l_k} + \sum_{l_1+l_2+\cdots+l_{k+1}=0} A^{(m-2)}(l_1, l_2, \cdots, l_{k+1}) \times u_{l_1} \cdots u_{l_{k+1}} + \cdots. \quad (22)$$

Here $A^{(m)}$ is a homogeneous polynomial of degree $m = 2r - 2k$ and $A^{(m-2)}$ a polynomial of degree $2r - 2(k + 1)$, etc. Clearly we may assume that these polynomials are symmetric.

Now, if F is to be invariant, we have, by (9),

$$\sum_{n=-\infty}^{\infty} n \frac{\partial F_3}{\partial u_{-n}} \frac{\partial F}{\partial u_n} = 0. \quad (23)$$

Here F_3 is given by (4), or

$$F_3 = 2\pi \sum_{n=1}^{\infty} \tfrac{1}{2} n^2 u_n u_{-n} + \tfrac{1}{6} \sum_{l_1+l_2+l_3=0} u_{l_1}, u_{l_2}, u_{l_3}. \quad (24)$$

If now (23) is evaluated with the aid of (22) and (24), a series of terms results. The terms containing exactly k different wave numbers $l_1, l_2, \cdots, l_k$ arise from the first term of (22) and the first term of (24). This must be zero. The coefficient must be zero after being made symmetric. This yields the following:

$$(l_1^3 + l_2^3 + \cdots + l_k^3)A^{(m)}(l_1, \cdots, l_k) = S_3 A = 0, \quad (25)$$

provided

$$l_1 + \cdots + l_k = 0 = S_1. \quad (26)$$

Now it can be shown that (1) if $k = 2$ and m is odd, then $S_1 = 0$ implies $A = 0$ and (2) if $k > 2$ and $S_1 = 0$ implies $S_3 A = 0$, then $S_1 = 0$ implies $A = 0$. The first part follows if we observe that, for $S_1 = 0$, interchanging l_1, l_2 is the same as reversing the sign of each, and the interchange leaves A fixed because A is symmetric; and reversing the signs changes the sign of A because A has odd degree m; hence, $A = 0$. Part (2) can be proved by noting that A can be written as a polynomial in $S_1, S_2, \cdots, S_k$, where

$$S_i = l_1^i + l_2^i + \cdots + l_k^i.$$

If we set $S_1 = 0$, then A becomes a polynomial in $S_2, S_3, \cdots, S_k$. Here, the $S_2, S_3, \cdots, S_k$ may have arbitrary values, and hence $S_3 A = 0$ must be an identity. It then follows that $A = 0$.

Thus we have shown that there is no integral invariant whose conserved density is of nonintegral rank but zero; for if r is not an integer, the integer $m = 2r - 2k$ must be odd.

Now we can prove the following theorem.

Theorem: The Poisson bracket of any two integral invariants of the Korteweg–de Vries equation is zero.

The proof uses Jacobi's identity. In fact, we have

$$((F_m, F_n), F_3) + ((F_n, F_3), F_m) + ((F_3, F_m), F_n) = 0,$$

and the last two terms will be zero if F_m and F_n are integral invariants. Hence, we see that

$$(F_m, F_n)$$

will be an integral invariant; but the rank of the density of (F_m, F_n) is seen by (14) to be

$$m - 1 + n - 1 + \tfrac{1}{2},$$

which is not an integer. Hence, it follows that

$$(F_m, F_n) = 0. \quad (27)$$

Now, if we regard

$$(H, F_m)$$

as defining an operator on the space of functionals H akin to a directional derivative, then (27) shows that the operators defined by F_m and F_n commute. One obtains an especially interesting formula in this way by choosing for H the functional which assigns to the function $u(x)$ its value at $x = x_0$. This functional does not belong to the class for which we have proved Jacobi's identity. However, the result is valid. We may state it as follows: Let the functions g_m (of x, u, u_x, u_{xx}, etc.) be defined by

$$g_m = \frac{\partial}{\partial x}\left(\frac{\delta F_m}{\delta u}\right) = \frac{\partial}{\partial x} y_0 f_m.$$

Then the following commutation law follows from (27):

$$\left(g_m \frac{\partial}{\partial u} + g_m' \frac{\partial}{\partial u_x} + g_m'' \frac{\partial}{\partial u_{xx}} + \cdots\right) g_n = \left(g_n \frac{\partial}{\partial u} + g_n' \frac{\partial}{\partial u_x} + g_n'' \frac{\partial}{\partial u_{xx}} + \cdots\right) g_m. \quad (28)$$

Here,

$$g_m' = \frac{\partial}{\partial x} g_m, \quad g_m'' = \frac{\partial^2}{\partial x^2} g_m, \quad \text{etc.}$$

To show this, we proceed as follows: The left-hand side of (28) would be the value of $\partial g_n/\partial \alpha$ if $u(x, \alpha)$ were to depend on α in such a way that

$$\frac{\partial u}{\partial \alpha} = g_m. \quad (29)$$

Going to the Fourier representation, we see that (29) is

$$\frac{\partial u_k}{\partial \alpha} = \frac{ik}{2\pi} \frac{\partial F_m}{\partial u_{-k}}.$$

Thus, (28) is the following:

$$\sum \frac{ik}{2\pi} \frac{\partial F_m}{\partial u_{-k}} \frac{\partial}{\partial u_k} \left(\sum \frac{ik}{2\pi} \frac{\partial F_n}{\partial u_{-k}} e^{ikx} \right)$$

and the right-hand side is

$$\sum \frac{ik}{2\pi} \frac{\partial F_n}{\partial u_{-k}} \frac{\partial}{\partial u_k} \left(\sum \frac{ik}{2\pi} \frac{\partial F_m}{\partial u_{-k}} e^{ikx} \right).$$

The difference between the two sides is now

$$\sum \frac{ik}{2\pi} e^{ikx} \frac{\partial}{\partial u_{-k}} \left(\sum \frac{ik}{2\pi} \frac{\partial F_m}{\partial u_{-k}} \frac{\partial F_n}{\partial u_k} \right) = \sum \frac{ik}{2\pi} e^{ikx} \frac{\partial}{\partial u_{-k}} (F_n, F_m) = 0,$$

which proves the statement—at least when the above series terminate. As before, this can be extended to the general class of functionals to which F_m and F_n belong.

III. CANONICAL TRANSFORMATIONS

We shall now show formally how one can define a canonical transformation which transforms a solution u of an equation of the type

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \frac{\delta F}{\delta u} \tag{30}$$

into a solution u' of an equation

$$\frac{\partial u'}{\partial t} = \frac{\partial}{\partial x} \frac{\delta F}{\delta u'}, \tag{31}$$

where F is numerically equal to F but depends in a different way on u'.

In fact, one obtains such a transformation in terms of a generating functional Ψ, if one can solve the following for u':

$$u' = u + \frac{\partial}{\partial x} \frac{\delta}{\delta \tilde{u}} \Psi(\tilde{u}), \tag{32}$$

where $\tilde{u}$ is defined by

$$\tilde{u} = \tfrac{1}{2}(u + u'). \tag{33}$$

To see this, let us define ϕ, ϕ' as two potential functions such that

$$\frac{\partial \phi}{\partial x} = u, \quad \frac{\partial \phi'}{\partial x} = u'.$$

(Now ϕ and ϕ' are not periodic, in general.) We go back to the variational principle (2). We see that (32) can be written in the following two ways:

$$\phi_x = \phi'_x - \frac{\partial}{\partial x} \frac{\delta}{\delta \tilde{u}} \Psi, \tag{34}$$

$$\phi'_x = \phi_x + \frac{\partial}{\partial x} \frac{\delta}{\delta \tilde{u}} \Psi. \tag{35}$$

Let us multiply (34) and (35) by ϕ_t, ϕ'_t and subtract, and integrate with respect to x; we obtain

$$\int (\phi_x \phi_t - \phi'_x \phi'_t)\, dx = \int (\phi'_x \phi_t - \phi_x \phi'_t)\, dx - \int (\phi_t + \phi'_t) \frac{\partial}{\partial x} \frac{\delta \Psi}{\delta \tilde{u}}\, dx,$$

or

$$\int (\phi_x \phi_t - \phi'_x \phi'_t)\, dx = \int \left(\frac{\partial}{\partial x} (\phi' \phi_t) - \frac{\partial}{\partial t} (\phi' \phi_x) \right) dx + \int \frac{\partial}{\partial x} \left((\phi_t + \phi'_t) \frac{\delta \Psi}{\delta \tilde{u}} \right) dx + 2 \int \tilde{u}_t \frac{\delta \Psi}{\delta \tilde{u}}\, dx,$$

and, integrating with respect to t,

$$\iint (\phi_x \phi_t - \phi'_x \phi'_t)\, dx\, dt = \iint dx\, dt \frac{\partial}{\partial x} \left[\phi' \phi_t + (\phi_t + \phi'_t) \frac{\delta \Psi}{\delta \tilde{u}} \right] + \iint dx\, dt \frac{\partial}{\partial t} (-\phi' \phi_x) - 2 \int \frac{d\Psi}{dt}\, dt.$$

It follows now that

$$\delta \iint (\phi_x \phi_t - \phi'_x \phi'_t)\, dx\, dt = 0$$

(if $\delta\phi$ has compact support), and hence

$$\delta \left(\iint \phi_x \phi_t\, dx\, dt - 2 \int F\, dt \right) = \delta \left(\iint \phi'_x \phi'_t\, dx\, dt - 2 \int F\, dt \right) \tag{36}$$

if F is any functional of ϕ_x. Now (30) implies the vanishing of the variation on the left of (36), which in turn implies vanishing of the right of (36), which implies (31).

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Fredholm Methods in the Three-Body Problem. I*

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It is shown that, for three particles interacting via potentials that are bounded and decrease at least as fast as $r^{-\frac{7}{2}}$, the Green's function of the Schrödinger equation at physical energies can be calculated by the classical Fredholm methods for $\mathfrak{L}^2$ kernels.

1. INTRODUCTION

The central question in the quantum mechanical three-body problem is the construction of the Green's function

$$(E - H_0 - V_1 - V_2 - V_3)^{-1} = G_{123}(E) \quad (1.1)$$

in the center-of-mass system, if V_1, V_2, and V_3 are the potentials between particles 2 and 3, 1 and 3, and 1 and 2, respectively, and H_0 is the kinetic energy operator. The technique of Ref. 1 to remove the disconnected-diagram difficulties consists of writing

$$G_{123} = (\mathbb{1} - U_1 - U_2 - U_3)^{-1}G_0, \quad (1.2)$$

where

$$G_0(E) = (E - H_0)^{-1} \quad (1.3)$$

is the free Green's function and

$$U_i = G_0V_i. \quad (1.4)$$

Then

$$\begin{aligned}(\mathbb{1} - U_1 - U_2)^{-1} &= \mathcal{R}_1\mathcal{R}(\mathcal{C}_2\mathcal{C}_1)\mathcal{R}_2 = \mathcal{R}_2\mathcal{R}(\mathcal{C}_1\mathcal{C}_2)\mathcal{R}_1 \\ &= \mathbb{1} + \mathcal{R}_1\mathcal{R}(\mathcal{C}_2\mathcal{C}_1)\mathcal{C}_2 + \mathcal{R}_2\mathcal{R}(\mathcal{C}_1\mathcal{C}_2)\mathcal{C}_1, \quad (1.5)\end{aligned}$$

where

$$\mathcal{R}_i = \mathcal{R}(U_i) = (\mathbb{1} - U_i)^{-1},$$
$$\mathcal{C}_i = \mathcal{C}(U_i) = U_i(\mathbb{1} - U_i)^{-1} = \mathcal{R}_i - \mathbb{1},$$

and we get

$$\begin{aligned}&(\mathbb{1} - U_1 - U_2 - U_3)^{-1} \\ &= [\mathbb{1} - (\mathbb{1} - U_1 - U_2)^{-1}U_3]^{-1}(\mathbb{1} - U_1 - U_2)^{-1} \\ &= \mathcal{R}_3\bar{\mathcal{R}}_3\mathcal{R}_2\mathcal{R}(\mathcal{C}_1\mathcal{C}_2)\mathcal{R}_1 \\ &= (\mathbb{1} - U_1 - U_2)^{-1} \\ &\quad + (\mathbb{1} - U_1 - U_2)^{-1}\mathcal{C}_3\bar{\mathcal{R}}_3(\mathbb{1} - U_1 - U_2)^{-1} \quad (1.6)\end{aligned}$$

with the abbreviation

$$\bar{\mathcal{R}}_3 = [\mathbb{1} - \mathcal{R}_2\mathcal{R}(\mathcal{C}_1\mathcal{C}_2)\mathcal{C}_1\mathcal{C}_3 - \mathcal{R}_1\mathcal{R}(\mathcal{C}_2\mathcal{C}_1)\mathcal{C}_2\mathcal{C}_3]^{-1}. \quad (1.7)$$

In a more familiar notation these equations read

$$\begin{aligned}G_{12} \equiv (E - H_0 - V_1 - V_2)^{-1} &= (\mathbb{1} - U_1 - U_2)^{-1}G_0 \\ &= (\mathbb{1} + G_0T_1)(\mathbb{1} - G_0T_2G_0T_1)^{-1}G_2 \\ &= (\mathbb{1} + G_0T_2)(\mathbb{1} - G_0T_1G_0T_2)^{-1}G_1, \quad (1.8)\end{aligned}$$

$$G_{123} = (\mathbb{1} + G_0T_3)G\bar{\mathcal{R}}_{12} = G_{12} + G_{12}T_3\bar{\mathcal{R}}_3G_{12}, \quad (1.9)$$

$$\begin{aligned}\bar{\mathcal{R}}_3 = [\mathbb{1} &- (\mathbb{1} + G_0T_2)(\mathbb{1} - G_0T_1G_0T_2)^{-1}G_0T_1G_0T_3 \\ &- (\mathbb{1} + G_0T_1)(\mathbb{1} - G_0T_2G_0T_1)^{-1}G_0T_2G_0T_3]^{-1}, \quad (1.10)\end{aligned}$$

where

$$G_i = (E - H_0 - V_i)^{-1} \quad (1.11)$$

and

$$T_i = V_i + V_iG_iV_i \quad (1.12)$$

are the two-particle Green's function and T operators (on the three-particle Hilbert space), so that

$$G_0T_i = G_iV_i. \quad (1.13)$$

Thus the three-body Green's function G_{123} is expressed entirely in terms of two-body Green's functions and resolvents of "connected" operators.

While the manipulations leading to (1.6) result in "connectedness," the actual calculation of the necessary resolvents, or of the S-matrix elements for physical processes, requires the knowledge of more restricted mathematical properties of all the constituents of (1.6), and particularly at real positive energies. It is the purpose of the present paper to prove that, for a very large class of potentials [specified in (3.5)], the resolvents required in (1.6) or (1.9) may be calculated by classical Fredholm methods for $\mathfrak{L}^2$-integral kernels. This conclusion goes beyond the powerful results of Faddeev,[2] who showed that the fifth iterate of his kernel[3] is completely continuous in a suitable Banach space. It also transcends the results of Rubin, Sugar, and Tiktopoulos,[4] who showed that, for a superposition of Yukawa potentials, the Fredholm determinant of the Faddeev kernel exists.

The starting point of this paper is an attempt to show that an operator such as

$$G_0T_1G_0T_2 = G_1V_1G_2V_2$$

is in the Hilbert–Schmidt class (hereafter called HS). This, however, is asking too much. One reason why for real positive energies it is not in HS is the same as that for which the operator[5] g_0V on the two-particle Hilbert space (in the center-of-mass system) is not in

HS. The remedy there is to factorize[6]

$$V = uv, \quad |u| = v, \tag{1.14}$$

and to form vg_0u, which is in HS.

Generalizing this trick, we consider

$$\Omega_{12} = v_2G_1V_1G_2u_2 \equiv v_2\Gamma_{12}u_2 \tag{1.15}$$

so that

$$(\mathbb{1} - G_0T_1G_0T_2)^{-1} = \mathbb{1} + \Gamma_{12}u_2(\mathbb{1} - \Omega_{12})^{-1}v_2. \tag{1.16}$$

We find that for the class of potentials specified in (3.5) the kernel of Ω_{12} is indeed in $\mathfrak{L}^2$, provided that the (1, 3) system has no bound states (i.e., g_2 has no poles). If there are such bound states, then the argument becomes more complicated. It is as follows.

We split up G_2 into two parts,

$$G_2 = G_2' + G_2'', \tag{1.17}$$

where

$$G_2' = G_2(\mathbb{1} - P_2), \quad G_2'' = G_2P_2, \tag{1.17'}$$

and P_2 is the orthogonal projection onto the subspace spanned by the (1, 3) bound states. Concomitantly, Ω_{12} is split up

$$\Omega_{12} = \Omega_{12}' + \Omega_{12}''. \tag{1.18}$$

In Sec. 5 the kernel of Ω_{12}' is shown to be in $\mathfrak{L}^2$, and Ω_{12}'' can be written as the product

$$\Omega_{12}'' = \bar{\Omega}_{12}\tilde{\Omega}_2, \tag{1.19}$$

where

$$\bar{\Omega}_{12} = v_2G_1V_1P_2S_2,$$
$$\tilde{\Omega}_2 = S_2^{-1}P_2G_2u_2, \tag{1.19'}$$

and S_2 is explicitly given in (6.5). It is shown in Sec. 6 that the kernels of the operators $\bar{\Omega}_{12}$, $\tilde{\Omega}_2\Omega_{12}'$, and $\tilde{\Omega}_2\bar{\Omega}_{12}$ are in $\mathfrak{L}^2$. A lemma stated and proved in Appendix F therefore shows that the Fredholm theory for $\mathfrak{L}^2$ kernels is applicable to the construction of $(\mathbb{1} - \Omega_{12})^{-1}$ and hence, by (1.16), to that of $(\mathbb{1} - G_0T_1G_0T_2)^{-1}$.

The next step then is the construction of the resolvent $\bar{\mathcal{R}}_3$ given in (1.10). Using (1.12), we write

$$G_{123} = G_{12} + G_{12}(\mathbb{1} + V_3G_3)V_3\bar{\mathcal{R}}_3G_{12}$$
$$= G_{12} + G_{12}(\mathbb{1} + V_3G_3)v_3\tilde{\mathcal{R}}_3u_3G_{12} \tag{1.20}$$

and get

$$\tilde{\mathcal{R}}_3 = (\mathbb{1} - \Omega_3)^{-1}, \tag{1.21}$$

where

$$\Omega_3 = \Omega_{13} + \Omega_{23} + (v_3G_1u_1 + v_3\Gamma_{21}u_1)(\mathbb{1} - \Omega_{21})^{-1} \times (v_1\Gamma_{23}u_3) + (v_3G_2u_2 + v_3\Gamma_{12}u_2) \times (\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}u_3). \tag{1.22}$$

The bound states of the (1, 2) system (i.e., the poles of g_3) again cause special difficulties. We split up G_3 as in (1.17), and, correspondingly,

$$\Omega_3 = \Omega_3' + \Omega_3'', \quad \Gamma_{i3} = \Gamma_{i3}' + \Gamma_{i3}''. \tag{1.23}$$

The various terms of Ω_3' will be shown in Sec. 7 to be in HS, and Ω_3'' can be written as the product

$$\Omega_3'' = \bar{\Omega}_3\tilde{\Omega}_3, \tag{1.24}$$

where

$$\bar{\Omega}_3 = v_3G_1V_1P_3S_3 + v_3G_2V_2P_3S_3 + (v_3G_1u_1 + v_3\Gamma_{21}u_1)(\mathbb{1} - \Omega_{21})^{-1}v_1G_2V_2P_3S_3 + (v_3G_2u_2 + v_3\Gamma_{12}u_2)(\mathbb{1} - \Omega_{12})^{-1}v_2G_1V_1P_3S_3. \tag{1.25}$$

It will be shown in Sec. 7 that $\bar{\Omega}_3$, $\tilde{\Omega}_3\bar{\Omega}_3$, and $\bar{\Omega}_3\Omega_3'$ are in HS. Hence the lemma of Appendix F is again applicable and shows that Fredholm theory can be applied to the construction of $\tilde{\mathcal{R}}_3$.

There remains the possibility that $(\mathbb{1} - \Omega_{12})^{-1}$ fails to exist. This would mean that the three-particle system in which particles 1 and 2 do not interact with one another (but both interact with particle 3) has a bound state. At an energy at which there is such a bound state, the calculation of the full Green's function by means of (1.20) breaks down. It should be noted, though, that if this should occur at a given energy value, then it is only necessary to use one of the equivalent expressions

$$G_{123} = G_{13} + G_{13}(\mathbb{1} + V_2G_2)v_2\tilde{\mathcal{R}}_2u_2G_{13} \tag{1.20'}$$
$$= G_{23} + G_{23}(\mathbb{1} + V_1G_1)v_1\tilde{\mathcal{R}}_1u_1G_{13}, \tag{1.20''}$$

with

$$\tilde{\mathcal{R}}_1 = (\mathbb{1} - \Omega_1)^{-1}, \quad \tilde{\mathcal{R}}_2 = (\mathbb{1} - \Omega_2)^{-1},$$

$$\Omega_1 = \Omega_{21} + \Omega_{31} + v_1G_2u_2(\mathbb{1} - \Omega_{32})^{-1}v_2(\Gamma_{321} + \Gamma_{31})u_1 + v_1G_3u_3(\mathbb{1} - \Omega_{23})^{-1}v_3(\Gamma_{231} + \Gamma_{21})u_1, \tag{1.21'}$$

$$\Omega_2 = \Omega_{12} + \Omega_{32} + v_2G_1u_1(\mathbb{1} - \Omega_{31})^{-1}v_1(\Gamma_{312} + \Gamma_{32})u_2 + v_2G_3u_3(\mathbb{1} - \Omega_{13})^{-1}v_3(\Gamma_{132} + \Gamma_{12})u_2. \tag{1.21''}$$

The same kind of argument used in Appendix F can then be used to show that, even if Ω_{12}, Ω_{13}, and Ω_{23} all have the eigenvalue 1 at the same energy, G_{123} does not have a singularity.[7] The fact, however, remains that in such a case the present calculational methods break down.

As far as the Fredholm determinant of the three-particle system is concerned, (1.9) shows that the denominator factor that appears is given by

$$d_{123} \equiv \det(\mathbb{1} - \Omega_3), \tag{1.26}$$

where

$$d_{21} = d_{12} = \det(\mathbb{1} - \Omega_{12}). \tag{1.27}$$

The determinants

$$d_i = \det(\mathbb{1} - G_0 V_i) \tag{1.28}$$

do not exist and hence neither does $\det(\mathbb{1} - \sum U_i)$. Equivalent factorizations are given by

$$d_{231} = d_{23} \det(\mathbb{1} - \Omega_1) \tag{1.26'}$$
$$d_{132} = d_{13} \det(\mathbb{1} - \Omega_2), \tag{1.26''}$$
$$d_{32} = d_{23} = \det(\mathbb{1} - \Omega_{23}), \tag{1.27'}$$
$$d_{31} = d_{13} = \det(\mathbb{1} - \Omega_{13}). \tag{1.27''}$$

The result of this paper is that if the potentials satisfy (3.5), then each factor in these expressions is well defined as a Fredholm determinant of an $\mathfrak{L}^2$ kernel. If, at the energy considered, there is a bound state of the system without interaction between particles 1 and 2, then d_{12} vanishes and $\det(\mathbb{1} - \Omega_3)$ is infinite. In that case (1.26) is useless and (1.26') or (1.26'') should be used.[8]

We now turn to the detailed proofs. Section 2 deals with some kinematic preliminaries, and Sec. 3 examines the full two-particle Green's function $G(E)$ in some detail. Section 4 is preparatory for the study of Ω_{12}' in Sec. 5. Section 6 contains the investigation of Ω_{12}'', and Sec. 7, that of Ω_3. There are six appendices. In Appendix A we explicitly construct the Green's function G_0 and give bounds for it. Appendix B contains a simple evaluation of a product of two Green's functions. Appendices C, D, and E contain some auxiliary estimates of multiple integrals. In Appendix F we state and prove a lemma mentioned earlier.

2. KINEMATICS

We consider a system of three particles in its center-of-mass coordinate frame. Let the position vectors of the three particles be $\mathbf{R}_1$, $\mathbf{R}_2$, and $\mathbf{R}_3$ and their masses m_1, m_2, and m_3. There are then three customary sets of coordinates that are convenient to use. We shall label them $\mathbf{r}_i$ and $\boldsymbol{\rho}_i$, $i = 1, 2, 3$, so that $\mathbf{r}_1$ is a vector pointing from the third particle to the second:

$$\mathbf{r}_1 = (\mathbf{R}_2 - \mathbf{R}_3)(2\mu_1)^{\frac{1}{2}} \tag{2.1}$$

and $\boldsymbol{\rho}_1$ is a vector pointing from the center of mass of particles 2 and 3 to the position of particle 1:

$$\boldsymbol{\rho}_1 = [\mathbf{R}_1 - (m_2\mathbf{R}_2 + m_3\mathbf{R}_3)/(m_2 + m_3)](2\bar{\mu}_1)^{\frac{1}{2}}, \tag{2.1'}$$
$$\mu_1 = m_2 m_3/(m_2 + m_3), \quad \bar{\mu}_1 = (m_1/M)(m_2 + m_3),$$
$$M = m_1 + m_2 + m_3. \tag{2.2}$$

The other two sets, $\mathbf{r}_2$, $\boldsymbol{\rho}_2$ and $\mathbf{r}_3$, $\boldsymbol{\rho}_3$, are obtained by cyclic permutation of labels.

The conjugate momenta are

$$\mathbf{k}_i = \frac{1}{2}\frac{d\boldsymbol{\rho}_i}{dt}, \quad \mathbf{q}_i = \frac{1}{2}\frac{d\mathbf{r}_i}{dt}$$

or, in terms of the individual particle momenta $\mathbf{p}_i$,[9]

$$\mathbf{k}_1 = [2Mm_1(m_2 + m_3]^{-\frac{1}{2}}[(m_2 + m_3)\mathbf{p}_1 - m_1(\mathbf{p}_2 + \mathbf{p}_3)],$$
$$\mathbf{q}_1 = [2m_2m_3(m_2 + m_3)]^{-\frac{1}{2}}(m_3\mathbf{p}_2 - m_2\mathbf{p}_3). \tag{2.3}$$

In terms of these variables the kinetic energy operator in the center-of mass system is given by

$$H_0 = k_i^2 + q_i^2 = -\nabla_{\rho_i}^2 - \nabla_{r_i}^2. \tag{2.4}$$

The transition from the set $\mathbf{r}_i$, $\boldsymbol{\rho}_i$ to the set $\mathbf{r}_j$, $\boldsymbol{\rho}_j$ is made by

$$\mathbf{r}_2 = -[(\mu_1\mu_2)^{\frac{1}{2}}/m_3]\mathbf{r}_1 - (\mu_2/\bar{\mu}_1)^{\frac{1}{2}}\boldsymbol{\rho}_1,$$
$$\boldsymbol{\rho}_2 = (\mu_1/\bar{\mu}_2)^{\frac{1}{2}}\mathbf{r}_1 - [(\mu_1\mu_2)^{\frac{1}{2}}/m_3]\boldsymbol{\rho}_1 \tag{2.5}$$

and cyclic permutations. The Jacobian of this transformation is equal to 1:

$$\frac{\partial(\mathbf{r}_i, \boldsymbol{\rho}_i)}{\partial(\mathbf{r}_j, \boldsymbol{\rho}_j)} = 1.$$

The Hilbert space $\mathcal{H}$ of the three particles in their center-of-mass system can be thought of as the set of square-integrable functions of the six variables $\mathbf{r}_1$, $\boldsymbol{\rho}_1$ or, equivalently, of $\mathbf{r}_2$, $\boldsymbol{\rho}_2$ or of $\mathbf{r}_3$, $\boldsymbol{\rho}_3$. This space $\mathfrak{L}^2(R^6)$ is the direct product of two Hilbert spaces, which we may refer to as the r_i-space $\mathcal{H}_r^{(i)}$, and the ρ_i-space $\mathcal{H}_\rho^{(i)}$:

$$\mathcal{H} = \mathcal{H}_r^{(i)} \otimes \mathcal{H}_\rho^{(i)}, \quad i = 1, 2, 3.$$

It is also the direct integral of the Hilbert spaces $\mathcal{H}_r^{(i)}(k_i)$ in each of which the value of the $\mathbf{k}_i$ momentum is fixed. It is useful to view $\mathcal{H}$ from either one of these perspectives.

3. THE TWO-PARTICLE GREEN'S FUNCTION

Our first task is to study the Green's function $G(E)$ of the system when only one pair of particles interacts, say 1 and 2, whereas the third is free. We assume that the pair interaction is described by a local potential $V(\mathbf{R}_2 - \mathbf{R}_1)$, and we use the coordinates $\mathbf{r}_3$ and $\boldsymbol{\rho}_3$, which we shall, in this section, call simply $\mathbf{r}$ and $\boldsymbol{\rho}$. We wish to isolate in $G(E)$ the effects of possible bound states of the (1, 2) system.

Let us, to start with, work in the one-particle Hilbert space $\mathcal{H}_r = \mathfrak{L}^2(R^3)$. We split up the (real) potential in the form

$$V(\mathbf{r}) = u(\mathbf{r})v(\mathbf{r}), \quad v(\mathbf{r}) = |V(\mathbf{r})|^{\frac{1}{2}}. \tag{3.1}$$

The one-particle free Green's operator will be denoted

by $g_0(E)$; its integral kernel is given by

$$g_0(E; \mathbf{r}, \mathbf{r}') = -\exp(iE^{\frac{1}{2}}|\mathbf{r}-\mathbf{r}'|)/4\pi|\mathbf{r}-\mathbf{r}'|. \quad (3.2)$$

Let $k(E)$ be the operator whose kernel is[6]

$$k(E; \mathbf{r}, \mathbf{r}') = v(\mathbf{r})g_0(E; \mathbf{r}, \mathbf{r}')u(\mathbf{r}'). \quad (3.3)$$

It is well known that $k(E)$ is an analytic operator-valued function, regular everywhere in the open cut E plane. [This follows from the fact that $g_0(E)$ is the resolvent of the self-adjoint operator extension of

$$h_0^{(r)} = -\nabla^2 \quad (3.4)$$

whose spectrum is the positive real axis.]

We shall, throughout this paper, assume that the potential V satisfies the inequality

$$|V(r)| \leq M(r_0 + r)^{-\frac{7}{2}} \quad (3.5)$$

for some $r_0 < \infty$, $M < \infty$. This is certainly stronger than necessary for some purposes and probably stronger than needed for all. We have not tried to press this condition very hard.

It follows from (3.5) that

$$\int (d\mathbf{r})\,|V(\mathbf{r})| < \infty$$

and that there exists a constant M' such that for all $\mathbf{r}$

$$\int (d\mathbf{r}')\,|\mathbf{r}-\mathbf{r}'|^{-2}\,|V(\mathbf{r}')| < M'.$$

Under these conditions the operator $k(E)$ is in HS for every value of E in the cut plane, including values on the positive real axis.[10,11] Furthermore, there exists a positive constant $C < \infty$ such that

$$\|k(E)\|_2^2 \equiv \operatorname{tr} k(E)k^\dagger(E) \leq C \quad (3.6)$$

for all E. What is more,[12,13] as $|E| \to \infty$ with $0 < \arg E < 2\pi$,

$$\|k(E)\|_2 \to 0. \quad (3.7)$$

These facts imply the following statements about the operator

$$m(E) = [\mathbb{1} - k(E)]^{-1}, \quad (3.8)$$

in terms of which the t operator is given by

$$t(E) = vm(E)u. \quad (3.9)$$

The operator $m(E)$ is an analytic function of E regular in the open cut plane, except for those values E_n of E at which $k(E_n)$ has the eigenvalue 1. These are the bound states of the two-particle system.[14] We know that each $E_n \leq 0$ and that, under assumption (3.5) on the potential, their number N is finite.[15] Since, even for $E > 0$, $m(E)$ is the resolvent of a completely continuous operator, also its boundary values on the positive real axis are bounded operators. Equation (3.7) implies that for $0 < \arg E < 2\pi$, as $|E| \to \infty$,

$$\|m(E) - \mathbb{1}\| \to 0. \quad (3.10)$$

Let us write $g(E)$ for the resolvent operator of $h = h_0 + V$, i.e.,

$$g(E) = (E - h_0 - V)^{-1}. \quad (3.11)$$

It has the spectral decomposition

$$g(E) = \sum_1^N \frac{P_n}{E - E_n} + g'(E), \quad (3.12)$$

where P_n is the orthogonal projection onto the (finite-dimensional) eigenspace of h at E_n and $g'(E)$ is an analytic function regular everywhere in the open cut plane.

The operator $m(E)$ is related to $g(E)$ by the identity

$$m(E) = \mathbb{1} + vg(E)u \quad (3.13)$$

and consequently

$$m(E) = \sum_1^N \frac{vP_nu}{E - E_n} + m'(E), \quad (3.14)$$

$$m'(E) = \mathbb{1} + vg'(E)u. \quad (3.15)$$

For E not on the positive real axis, $m'(E)$ is a bounded operator, since $g'(E)$ is. For every $E \neq E_n$, $n = 1, 2, \cdots, N$, in the cut plane, including on the positive real axis, $m(E)$ is a bounded operator,[16] and so is the first term on the right of (3.14). Consequently, *the boundary values of $m'(E)$ on the positive real axis are bounded operators.* What is more, since the first term on the right-hand side of (3.14) approaches zero in the norm as $|E| \to \infty$, it follows from (3.10) that, as $|E| \to \infty$ for $0 < \arg E < 2\pi$,

$$\|m'(E) - \mathbb{1}\| \to 0. \quad (3.16)$$

We therefore conclude that for every finite real number A there exists a positive constant $C < \infty$ such that, for all E in $\operatorname{Re} E \leq A$,

$$\|m'(E)\| \leq C. \quad (3.17)$$

That is to say, the operator $m'(E)$ is *uniformly* bounded in every such region.

We now pass to the full Hilbert space $\mathcal{H}$. Let $G_0(E)$ be the free Green's operator, i.e., the resolvent of H_0 given by (2.4):

$$G_0(E) = (E - H_0)^{-1}. \quad (3.18)$$

It is a convolution operator on each of the Hilbert spaces $\mathcal{H}_r$ and $\mathcal{H}_p$ (that is, it conserves both of the momenta $\mathbf{k}$ and $\mathbf{q}$). The operator

$$K(E) = vG_0(E)u \quad (3.19)$$

(in which it must be remembered that both u and v are, on $\mathcal{H}_\rho$, multiples of the unity) is a convolution on $\mathcal{H}_\rho$ but not on $\mathcal{H}_r$. If we subject $\mathcal{H}_\rho$ to Fourier transformation (thus forming $\mathcal{H}_k$), i.e., go to the momentum representation, then K becomes a multiplicative operator there. Its kernel on $\mathcal{H}_k \otimes \mathcal{H}_r$ [or on $\mathcal{H}_r(k)$] then is

$$K(E; \mathbf{k}, \mathbf{r}, \mathbf{r}') = v(\mathbf{r})g_0(E - k^2; \mathbf{r}, \mathbf{r}')u(\mathbf{r}') = k(E - k^2; \mathbf{r}, \mathbf{r}'). \tag{3.20}$$

We now form

$$M(E) = [\mathbb{1} - K(E)]^{-1}. \tag{3.21}$$

Its kernel on $\mathcal{H}_k \otimes \mathcal{H}_r$ or on $\mathcal{H}_r(k)$ is given by $m(E - k^2; \mathbf{r}, \mathbf{r}')$, and on $\mathcal{H}_\rho \otimes \mathcal{H}_r$ the kernel of $M(E)$ is

$$M(E; \mathbf{r}, \boldsymbol{\rho}; \mathbf{r}', \boldsymbol{\rho}') = (2\pi)^{-3}\int (d\mathbf{k})e^{i\mathbf{k}\cdot(\boldsymbol{\rho}-\boldsymbol{\rho}')}m(E - k^2; \mathbf{r}, \mathbf{r}'). \tag{3.22}$$

Inserting (3.14) in this, we obtain

$$M(E) = \sum_1^N vP_n^{(r)}ug_0^{(\rho)}(E - E_n) + M'(E) = \sum_1^N vG(E)P_n^{(r)}u + M'(E), \tag{3.23}$$

where

$$G(E) = (E - H_0 - V)^{-1} \tag{3.24}$$

and we have used the fact that, because $P_n^{(r)}$ is the projection onto the eigenspace of $h^{(r)}$ at E_n, we have

$$G(E)P_n^{(r)} = g_0^{(\rho)}(E - E_n)P_n^{(r)}. \tag{3.25}$$

The superscripts r and ρ here indicate operators acting on $\mathcal{H}_r$ or $\mathcal{H}_\rho$ only (i.e., multiples of unity on the other space). The (multiplicative) operators u and v are understood to act on $\mathcal{H}_r$ only. Our results for $m(E)$ imply that for every value of E, including on the positive real axis, *$M'(E)$ is a bounded operator.*[17] This conclusion follows from the fact that, for every E, $m'(E - k^2)$ is a bounded operator on $\mathcal{H}_r(k)$ with a norm that is uniformly bounded for all $\mathbf{k}$. Thus on an element $\Psi(\mathbf{k}, \mathbf{r})$ of $\mathcal{H}_k \otimes \mathcal{H}_r$,

$$\|M'(E)\Psi\|^2 = \int (d\mathbf{k})\int (d\mathbf{r}')\left|\int (d\mathbf{r})m'(E - k^2; \mathbf{r}', \mathbf{r})\Psi(\mathbf{k}, \mathbf{r})\right|^2 \leq C\int (d\mathbf{k})\int (d\mathbf{r})\,|\Psi(\mathbf{k}, \mathbf{r})|^2$$

and M' is bounded.

We now consider the operator

$$G(E)u = G_0(E)[\mathbb{1} - VG_0(E)]^{-1}u = G_0(E)uM(E). \tag{3.26}$$

Insertion of (3.23) gives

$$\begin{aligned} G(E)u &= \sum_1^N G_0(E)VG(E)P_n^{(r)}u + G_0(E)uM'(E) \\ &= \sum_1^N G(E)P_n^{(r)}u - G_0(E)\sum_1^N P_n^{(r)}u \\ &\quad + G_0(E)uM'(E) \\ &= \sum_1^N P_n^{(r)}ug_0^{(\rho)}(E - E_n) - G_0(E) \\ &\quad \times \sum_1^N P_n^{(r)}u + G_0(E)uM'(E) \end{aligned} \tag{3.27}$$

because

$$G(E) = G_0(E) + G_0(E)VG(E). \tag{3.28}$$

We shall write (3.27) in the form

$$G(E)u = L(E) + G'(E)u, \tag{3.27'}$$

where $L(E) = G''(E)u$ in the notation of (1.17) or

$$L(E) = \sum_1^N P_n^{(r)}ug_0^{(\rho)}(E - E_n) \tag{3.29}$$

is the part of Gu that carries the most important effects of the bound states in the interacting two-particle systems, and

$$G'(E)u = -G_0(E)Pu + G_0(E)uM'(E) \tag{3.30}$$

with

$$P = \sum_1^N P_n^{(r)}. \tag{3.31}$$

P is the orthogonal projection onto the space spanned by the (normalizable) eigenstates of $h^{(r)}$ in $\mathcal{H}_r$. If these (normalized) eigenstates are $\varphi_n(\mathbf{r})$, then the kernel of P is given by

$$P(\mathbf{r}, \mathbf{r}') = \sum_1^N \varphi_n(\mathbf{r})\varphi_n^*(\mathbf{r}'). \tag{3.32}$$

4. THE OPERATOR $\mathfrak{G}(E)$

The next step is to study the operator

$$\mathfrak{G}(E) = G(E)VG_0(E) = G_0(E)T(E)G_0(E) \tag{4.1}$$

if $T(E)$ is the two-particle T operator on the full Hilbert space. We are interested in the structure of this operator for complex values of E and as E approaches the real axis from above.

For E not on the real axis, we may write

$$\mathfrak{G}(E) = \frac{1}{2\pi i}\int_C dz\, g_0^{(\rho)}(E - z)g^{(r)}(z)Vg_0^{(r)}(z), \tag{4.2}$$

where the contour C runs from ∞ to $-\infty$ above the spectrum of h and below the spectrum of $E - h_0$. This formula is easily proved by adding to C a semicircle at infinity in the upper half-plane and then

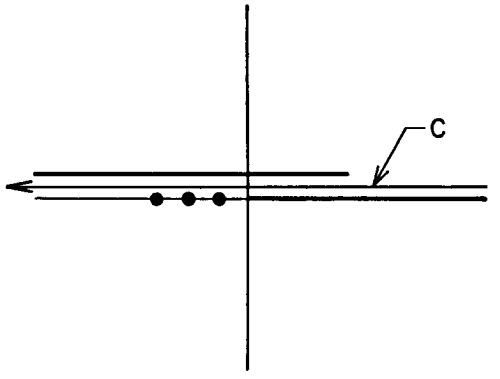

FIG. 1. The contour C used in the integral (4.2). The lower heavy line is the continuous spectrum of h, the dots, its point spectrum, and the upper heavy line, the spectrum of $E - h_0$ when Im $E > 0$.

distorting the contour to wrap around the spectrum of $E - h_0$ (see Fig. 1).

Let us now add to C in (4.2) a semicircle in the lower half-plane, and contract the contour to wrap around the spectrum of h, which may be partly discrete and partly continuous. That gives

$$\mathcal{G}(E) = \sum_{n=1}^{N} g_0^{(\rho)}(E - E_n)P_n^{(r)}Vg_0^{(r)}(E_n) + \frac{1}{2\pi i}\left(\int_0^{\infty - i\epsilon} - \int_0^{\infty + i\epsilon}\right) dz g_0^{(\rho)}(E - z) \times g^{(r)}(z)Vg_0^{(r)}(z).$$

The first sum on the right-hand side comes from the point spectrum of h on $\mathcal{K}_r$. Because $P_n^{(r)}$ is the projection onto the eigenspace of h at E_n, it follows that

$$P_n^{(r)}Vg_0^{(r)}(E_n) = P_n^{(r)} \tag{4.3}$$

and hence

$$\mathcal{G}(E) = \sum_{n=1}^{N} g_0^{(\rho)}(E - E_n)P_n^{(r)} + \frac{1}{2\pi i}\int_0^{\infty} dz g_0^{(\rho)}(E - z) \times [g^{(r)-}(z)Vg_0^{(r)-}(z) - g^{(r)+}(z)Vg_0^{(r)+}(z)] \tag{4.4}$$

in the conventional notation of Green's functions, i.e., with

$$g_0^{(r)\pm}(z) = \lim_{\epsilon \to 0+} (z - h_0^{(r)} \pm i\epsilon)^{-1}.$$

The three terms on the right-hand side of (4.4) will have to be considered separately:

$$\mathcal{G}(E) = A + I_- - I_+, \tag{4.4'}$$

$$A = \sum_{n=1}^{N} g_0^{(\rho)}(E - E_n)P_n^{(r)},$$

$$I_\pm = \frac{1}{2\pi i}\int_0^{\infty} dz g_0^{(\rho)}(E - z)g^{(r)\pm}(z)Vg_0^{(r)\pm}(z). \tag{4.5}$$

We first consider I_+. The arguments for I_- will be entirely analogous.

In the notation of (3.8) we have

$$g^{(r)+}(z)V = g_0^{(r)+}(z)[\mathbb{1} - Vg_0^{(r)+}(z)]^{-1}V = g_0^{(r)+}(z)um^+(z)v, \tag{4.6}$$

where

$$m^+(z) = \lim_{\epsilon \to 0+} m(z + i\epsilon)$$

is a bounded operator for all $z > 0$. The operator-valued function $m(z)$ is analytic and regular for Im $z > 0$, and $m^+(z)$ is its boundary value as Im $z \to 0+$. We denote its kernel by $m(z; \mathbf{r}, \mathbf{r}')$. In view of (4.6) and (3.2), the integral kernel of the operator I_+ is given by

$$I_+(\boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}') = \frac{a}{|\boldsymbol{\rho} - \boldsymbol{\rho}'|}\int \frac{(d\mathbf{r}'')(d\mathbf{r}''')u(\mathbf{r}'')v(\mathbf{r}''')}{|\mathbf{r} - \mathbf{r}'''|\,|\mathbf{r}' - \mathbf{r}'''|} \times J(\mathbf{r}, \mathbf{r}', \mathbf{r}'', \mathbf{r}'''; \boldsymbol{\rho}, \boldsymbol{\rho}'), \tag{4.7}$$

where

$$a = i\pi^{-4}2^{-7}$$

and

$$J = \int_0^{\infty} dz m^+(z; \mathbf{r}'', \mathbf{r}''') \exp\,[i(E - z)^{\frac{1}{2}}R' + iz^{\frac{1}{2}}R] \tag{4.8}$$

with

$$R' = |\boldsymbol{\rho} - \boldsymbol{\rho}'|,$$
$$R = |\mathbf{r} - \mathbf{r}''| + |\mathbf{r}' - \mathbf{r}'''|. \tag{4.9}$$

For real E, in order for $(E - z)^{\frac{1}{2}}$ to become positive imaginary when $E < z$, the integral here goes *below* the point $z = E$, as shown in Fig. 2. Note that the integrals in (4.7) are strongly damped by u and v and the integral in (4.8), by the exponential. So the required interchange in the order of integrations is allowed.

Our aim is to inquire if I_+ is in $\mathfrak{L}^2$. Thus we must study the convergence of the integral

$$i_+ = \int (d\mathbf{r})(d\mathbf{r}')(d\boldsymbol{\rho})(d\boldsymbol{\rho}')\,|I_+(\boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}')|^2. \tag{4.10}$$

The operator $m(z)$ may be split into three terms:

$$m(z) = \mathbb{1} + vg_0(z)u + vm''(z)u, \tag{4.11}$$

where

$$m''(z) = g(z)Vg_0(z) = g_0(z)Vg(z) = g_0(z)Vg_0(z) + g_0(z)Vg(z)Vg_0(z). \tag{4.12}$$

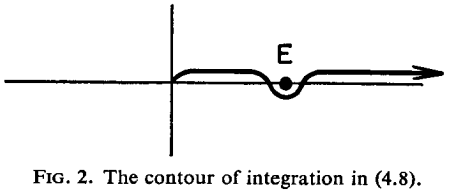

FIG. 2. The contour of integration in (4.8).

It is easy to see that, in contrast to the first two terms on the right of (4.11), the kernel $m''(z; \mathbf{r}'', \mathbf{r}''')$ is, for fixed z, a uniformly bounded function of $\mathbf{r}''$ and $\mathbf{r}'''$. It is also an analytic function of z (for fixed $\mathbf{r}''$ and $\mathbf{r}'''$) regular in the cut z plane (except at the point eigenvalues of h) and uniformly bounded for all complex z outside small circles around the bound states of h and for all real $\mathbf{r}''$ and $\mathbf{r}'''$.

The contributions to J that correspond to the three terms in (4.11) are

$$J_1 = \delta(\mathbf{r}'' - \mathbf{r}''')j_1,$$

$$j_1 = \int_0^\infty dz \exp\,[-(z - E)^{\frac{1}{2}}R' + iz^{\frac{1}{2}}R]$$

$$= 2\int_0^\infty dt\, t \exp\,[itR - (t^2 - E)^{\frac{1}{2}}R'], \quad (4.13)$$

$$J_2 = -\frac{1}{2\pi}\frac{v(\mathbf{r}'')u(\mathbf{r}''')}{|\mathbf{r}'' - \mathbf{r}'''|} \times \int_0^\infty dt\, t \exp\,[itR'' - (t^2 - E)^{\frac{1}{2}}R'], \quad (4.14)$$

$$R'' = |\mathbf{r} - \mathbf{r}''| + |\mathbf{r}' - \mathbf{r}'''| + |\mathbf{r}'' - \mathbf{r}'''|,$$

$$J_3 = 2v(\mathbf{r})u(\mathbf{r}''') \times \int_0^\infty dt\, tm''(t^2; \mathbf{r}'', \mathbf{r}''') \exp\,[itR - (t^2 - E)^{\frac{1}{2}}R']. \quad (4.15)$$

All the t integrals here run *below* the cut for $t < E^{\frac{1}{2}}$.

Let us add to and subtract from (4.13) an integral from 0 to $E^{\frac{1}{2}}$ running *above* the cut:

$$j_1 = 2\int_0^\infty dt\, t \exp\,[iRt - (t^2 - E)^{\frac{1}{2}}R'] + 4i\int_0^{E^{\frac{1}{2}}} dt\, te^{iRt} \sin\,[R'(t^2 - E)^{\frac{1}{2}}], \quad (4.16)$$

where the first integral now runs *above* $t = E^{\frac{1}{2}}$. We add a circular arc at infinity and distort the contour to run at an angle $\theta = \tan^{-1} R/R'$ with the real axis: $t = ue^{i\theta}$, $dt = due^{i\theta}$. Then for large $|t|$

$$\mathrm{Re}\,[iRt - (t^2 - E)^{\frac{1}{2}}R'] \simeq -u\bar{R},$$

where $\bar{R}^2 = R^2 + R'^2$, and the magnitude of the first integral in (4.16) is bounded by $C\bar{R}^{-2}$. The modulus of the second integral being bounded, we conclude that for each E there exist positive constants[18] C and R_0 such that for all $R \geq 0$ and $R' \geq 0$

$$|j_1| \leq C(\bar{R}^{-2} + R_0^{-2}). \quad (4.17)$$

The same argument applied to (4.14) shows that

$$|J_2| \leq [Cv(\mathbf{r}'')v(\mathbf{r}''')/|\mathbf{r}'' - \mathbf{r}'''|](\bar{R}'^{-2} + R_0^{-2}), \quad (4.18)$$

where $\bar{R}'^2 = R'^2 + R''^2$. Because of the remark below (4.13), the same argument may be used also for (4.15), and we get

$$|J_3| \leq Cv(\mathbf{r}'')v(\mathbf{r}''')(\bar{R}^{-2} + R_0^{-2}). \quad (4.19)$$

We want to find the asymptotic behavior of J for large values of R. Again we first consider j_1 of (4.13). Since the contour can be made to run above the real axis everywhere except in the neighborhood of $t = E^{\frac{1}{2}}$ (see Fig. 2), it is clear that, as $R \to \infty$, the leading contributions must come from the pieces of the integral near $t = 0$ and near $t = E^{\frac{1}{2}}$. It is easy to see that the contribution from $t \simeq 0$ goes at least as R^{-2}, uniformly in R'. In order to calculate the contribution from $t \simeq E^{\frac{1}{2}}$, we consider separately the two terms

$$j_{11} = 2i\int_0^\infty dt\, t \sin\,(tR) \exp\,[-(t^2 - E)^{\frac{1}{2}}R'], \quad (4.20)$$

$$j_{12} = 2\int_0^\infty dt\, t \cos\,(tR) \exp\,[-(t^2 - E)^{\frac{1}{2}}R']. \quad (4.21)$$

The value of the first integral is[19]

$$j_{11} = -\pi ERR'\bar{R}^{-2}H_2^{(1)}(E^{\frac{1}{2}}\bar{R}), \quad (4.22)$$

where $H_2^{(1)}$ is the Hankel function of the first kind of order two and again $\bar{R}^2 = R^2 + R'^2$. The asymptotic behavior of (4.22), as $R \to \infty$, is given by[20]

$$j_{11} \simeq -i(2\pi)^{\frac{1}{2}}E^{\frac{3}{4}}R'\bar{R}^{-\frac{3}{2}}e^{-\frac{1}{4}i\pi}e^{iE^{\frac{1}{2}}\bar{R}}. \quad (4.23)$$

Since we know that the asymptotically dominant part of (4.21) comes from $t \simeq E^{\frac{1}{2}}$ (or from $t \simeq 0$, which we have already evaluated) we may replace the factor t by $E^{\frac{1}{2}}$ and get[21]

$$j_{12} \simeq 2E^{\frac{1}{2}}\int_0^\infty dt \cos\,(tR) \exp\,[-(t^2 - E)^{\frac{1}{2}}R'] = i\pi ER'\bar{R}^{-1}H_1^{(1)}(E^{\frac{1}{2}}\bar{R}) \simeq (2\pi)^{\frac{1}{2}}E^{\frac{3}{4}}R'\bar{R}^{-\frac{3}{2}}e^{-i\frac{1}{4}\pi}e^{iE^{\frac{1}{2}}\bar{R}}. \quad (4.24)$$

Therefore,

$$j_1 \simeq -2i\pi^{\frac{1}{2}}E^{\frac{3}{4}}R'\bar{R}^{-\frac{3}{2}}e^{iE^{\frac{1}{2}}\bar{R}}. \quad (4.25)$$

The same arguments lead to the asymptotic values of (4.14) and (4.15) as $R \to \infty$

$$J_2 \simeq \tfrac{1}{2}i\pi^{-\frac{1}{2}}\frac{v(\mathbf{r}'')u(\mathbf{r}''')}{|\mathbf{r}'' - \mathbf{r}'''|}E^{\frac{3}{4}}R'\bar{R}'^{-\frac{3}{2}}e^{iE^{\frac{1}{2}}\bar{R}'}, \quad (4.26)$$

$$J_3 \simeq -v(\mathbf{r}'')u(\mathbf{r}''')m''(E; \mathbf{r}'', \mathbf{r}''')2i\pi^{\frac{1}{2}}E^{\frac{3}{4}}R'\bar{R}^{-\frac{3}{2}}e^{iE^{\frac{1}{2}}\bar{R}}. \quad (4.27)$$

These results, together with (4.17)–(4.19), allow us to conclude that for each fixed E there exist constants

C and R_0 such that, for all $\mathbf{r}$, $\mathbf{r}'$, $\mathbf{r}''$, $\mathbf{r}'''$, $\boldsymbol{\rho}$, and $\boldsymbol{\rho}'$,

$$|j_1| \leq C(R'\bar{R}^{-\frac{3}{2}} + R_0^{\frac{3}{2}}\bar{R}^{-2}), \tag{4.28a}$$

$$|J_2| \leq C\frac{v(\mathbf{r}'')v(\mathbf{r}''')}{|\mathbf{r}'' - \mathbf{r}'''|}(R'\bar{R}'^{-\frac{3}{2}} + R_0^{\frac{3}{2}}\bar{R}'^{-2}), \tag{4.28b}$$

$$|J_3| \leq Cv(\mathbf{r}'')v(\mathbf{r}''')(R'\bar{R}^{-\frac{3}{2}} + R_0^{\frac{3}{2}}\bar{R}^{-2}). \tag{4.28c}$$

Insertion of these inequalities and of (3.5) in (4.7) leads to three integrals estimated in Appendix C, in (C3), (C5), and (C7):

$$\begin{aligned}
&|I_+(\boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}')| \\
&\leq C\Bigg\{\frac{1}{|\mathbf{r} - \mathbf{r}'|^{\frac{3}{4}}}\frac{1}{(r_0 + r)^{\frac{11}{8}}(r_0 + r')^{\frac{11}{8}}} \\
&\quad \times \left(1 + \frac{R_0^{\frac{3}{2}}}{|\boldsymbol{\rho} - \boldsymbol{\rho}'|\,|\mathbf{r} - \mathbf{r}'|^{\frac{1}{2}}}\right) \\
&\quad + \left[\frac{1}{|\mathbf{r} - \mathbf{r}'|}\frac{1}{(r_0 + r)^{\frac{3}{4}}(r_0 + r')^{\frac{3}{4}}}\left(\frac{1}{r_0 + r} + \frac{1}{r_0 + r'}\right)\right. \\
&\quad \left. + \frac{1}{(r_0 + r)^{\frac{7}{4}}(r_0 + r')^{\frac{7}{4}}}\right] \\
&\quad \times \left(1 + \frac{R_0^{\frac{3}{2}}}{|\boldsymbol{\rho} - \boldsymbol{\rho}'|\,(r_0 + r)^{\frac{1}{4}}(r_0 + r')^{\frac{1}{4}}}\right)\Bigg\}.
\end{aligned} \tag{4.29}$$

It is also shown in Appendix C that the resulting $\mathbf{r}$ and $\mathbf{r}'$ integrals in (4.10) converge. On the other hand, the $\boldsymbol{\rho}$ and $\boldsymbol{\rho}'$ integrals in (4.10) require damping factors. If $f(\boldsymbol{\rho})$ and $g(\boldsymbol{\rho})$ are such that $|f|^2$ and $|g|^2$ satisfy (3.5), then the argument at the end of Appendix C shows that $f(\boldsymbol{\rho})g(\boldsymbol{\rho}')I_+(\boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}')$ is in $\mathfrak{L}^2$.

The method for I_- is the same, but somewhat simpler. The analog of (4.8) contains m^- instead of m^+ and $-iz^{\frac{1}{2}}R$ in place of $iz^{\frac{1}{2}}R$. We may therefore run the z contour everywhere just below the real axis instead of as in Fig. 2. As a result, the asymptotic behavior of I_- as a function of R is negligible compared to that of I_+. (It does not pick up the dominant contribution of I_+ from $z \simeq E$.) Consequently, I_- obeys (4.29) *a fortiori*.

We now turn to the first term in (4.4), i.e., A of (4.5). Its kernel is

$$A(\boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}') = \sum_{n=1}^{N} g_0(E - E_n; \boldsymbol{\rho}, \boldsymbol{\rho}')\varphi_n(\mathbf{r})\varphi_n^*(\mathbf{r}'), \tag{4.30}$$

where $\varphi_n(\mathbf{r})$ is the normalized eigenfunction of h at E_n and g_0 is given by (3.2). Hence

$$\begin{aligned}
\int(d\mathbf{r})(d\mathbf{r}')\,|A(\boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}')|^2 &= \sum_{1}^{N}|g_0(E - E_n; \boldsymbol{\rho}, \boldsymbol{\rho}')|^2 \\
&\leq C\,|\boldsymbol{\rho} - \boldsymbol{\rho}'|^{-2}.
\end{aligned} \tag{4.31}$$

Since it follows from (C1) that

$$\int(d\boldsymbol{\rho})(d\boldsymbol{\rho}')\,|f(\boldsymbol{\rho})|^2\,|g(\boldsymbol{\rho}')|^2\,|\boldsymbol{\rho} - \boldsymbol{\rho}'|^{-2} < \infty$$

if $|f|^2$ and $|g|^2$ obey (3.5), we conclude that $f(\boldsymbol{\rho})g(\boldsymbol{\rho}')A(\boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}')$ is in $\mathfrak{L}^2$.

Thus our conclusion is that if $|f(\boldsymbol{\rho})|^2$ and $|g(\boldsymbol{\rho})|^2$ satisfy (3.5), then the operator $\mathcal{G}(E)$ of (4.1) whose kernel is $\mathcal{G}(E; \boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}')$ is such that

$$f(\boldsymbol{\rho})g(\boldsymbol{\rho}')\mathcal{G}(E; \boldsymbol{\rho}, \mathbf{r}; \boldsymbol{\rho}', \mathbf{r}')$$

is, for all E, including real $E > 0$, in $\mathfrak{L}^2$.

5. THE OPERATOR Ω_{12}'

Let us now consider the operator

$$B_{12}(E) = v_2G_1(E)V_1G_0(E)u_2 = v_2\mathcal{G}_1(E)u_2 \tag{5.1}$$

whose central part $\mathcal{G}_1$ is of the structure (4.1), except that it is explicitly labeled, so that $\mathbf{r}$ in it means $\mathbf{r}_1$ and $\boldsymbol{\rho}$ means $\boldsymbol{\rho}_1$. By the same token $V_2 = v_2u_2$ means $V_2(\mathbf{r}_2)$, with $\mathbf{r}_2$ expressed in terms of $\mathbf{r}_1$ and $\boldsymbol{\rho}_1$ by (2.5). Since $\mathcal{G}_1$ is in $\mathfrak{L}^2$ as far as $\mathbf{r}_1$ is concerned, the factors v_2 and u_2 serve the same purpose as f and g in our considerations of Sec. 4, provided that V_2 obeys (3.5). We therefore conclude that B_{12} *is a Hilbert–Schmidt operator*.

The same argument applies to the operator

$$B_{312} = v_3G_1(E)V_1G_0(E)u_2. \tag{5.2}$$

It too is in HS.

The next step is to examine the operator

$$\Omega_{12}(E) = v_2G_1(E)V_1G_2(E)u_2. \tag{5.3}$$

We use the decomposition (3.7′) for G_2u_2, so that

$$\Omega_{12} = \Omega_{12}' + \Omega_{12}'', \tag{5.4}$$

where, according to (3.30) and (4.1),

$$\Omega_{12}' = v_2G_1V_1G_2'u_2 = v_2\mathcal{G}_1u_2M_2' - v_2\mathcal{G}_1P_2u_2, \tag{5.5}$$

$$\Omega_{12}'' = v_2G_1V_1L_2. \tag{5.6}$$

The first term on the right-hand side of (5.5) is equal to $B_{12}M_2'$. Since B_{12} is in HS and M_2' is bounded, this product is in HS. The second term of (5.5) is an operator whose kernel is (as a function of $\boldsymbol{\rho}_1$, $\mathbf{r}_1$, $\boldsymbol{\rho}_2'$, $\mathbf{r}_2'$)

$$\sum_{n=1}^{N} v_2(\mathbf{r}_2)\int(d\mathbf{r}_2')\mathcal{G}_1(E; \boldsymbol{\rho}_1, \mathbf{r}_1, \boldsymbol{\rho}_1', \mathbf{r}_1')\varphi_n(\mathbf{r}_2')\varphi_n^*(\mathbf{r}_2'')u_2(\mathbf{r}_2''),$$

where $\mathbf{r}_2$ must be expressed in terms of $\mathbf{r}_1$ and $\boldsymbol{\rho}_1$, and $\boldsymbol{\rho}_1'$ and $\mathbf{r}_1'$ must be expressed in terms of $\boldsymbol{\rho}_2'$ and $\mathbf{r}_2'$. We are then led to consider the integral

$$\int(d\mathbf{r}_1)(d\boldsymbol{\rho}_1)(d\boldsymbol{\rho}_2')\,|V_2(\mathbf{r}_2)| \times \left|\int(d\mathbf{r}_2')\mathcal{G}_1(E; \boldsymbol{\rho}_1, \mathbf{r}_1; \boldsymbol{\rho}_1', \mathbf{r}_1')\varphi_n(\mathbf{r}_2')\right|^2.$$

Unless φ_n describes a zero-energy bound state of angular momentum one or two, φ_n satisfies (3.5).[22] Hence (4.29) and (4.30) together with the estimates of Appendix C show that the above integrals converge absolutely. Thus each term in (5.5) is in HS. Therefore, so is Ω'_{12}.

The same arguments apply if in Ω'_{12} we replace v_2 by v_3, i.e., to

$$v_3\Gamma'_{12}u_2 = v_3G_1V_1G'_2u_2. \tag{5.7}$$

We conclude that $v_3\Gamma'_{12}u_2$ too is in HS.

6. THE OPERATOR Ω''_{12}

We must now examine the operator Ω''_{12} of (5.6), which is given more explicitly by

$$\begin{aligned}\Omega''_{12} &= v_2G_1(E)V_1\sum_{n=1}^{N}P^{(r)}_{n2}u_2g^{(\rho)}_{02}(E-E_n)\\ &= v_2G_1(E)V_1P_2G_2(E)u_2.\end{aligned} \tag{6.1}$$

This effect of the bound states in the (1, 3) system is not as well behaved as those previously considered. Indeed, it is clear that any operator that contains $g^{(\rho)}_0(E)$, with $E \gtrsim 0$, as a right-hand factor, is unbounded.

We proceed as outlined in Sec. 1, following (1.18), noting that Ω''_{12} can be written as in (1.19), or

$$\Omega''_{12} = \tilde{\Omega}_{12}\tilde{\Omega}_2, \tag{6.2}$$

where

$$\tilde{\Omega}_{12} = v_2G_1V_1P_2S_2, \tag{6.3}$$

$$\tilde{\Omega}_2 = S_2^{-1}P_2G_2u_2. \tag{6.4}$$

The operator S_2 is a multiple of unity on $\mathcal{K}^{(2)}_r$ and multiplicative on $\mathcal{K}^{(2)}_\rho$. It is given by

$$S_2 = (\rho_2 + \rho_0)^{\frac{7}{4}}, \tag{6.5}$$

ρ_0 being an arbitrary positive constant. It must be shown that the operators $\tilde{\Omega}_{12}$, $\tilde{\Omega}_{12}\Omega'_{12}$, and $\tilde{\Omega}_2\tilde{\Omega}_{12}$ are in HS for the lemma of Appendix F to be applicable.

Let us first consider the operator

$$\begin{aligned}C_{12} &\equiv S_2\tilde{\Omega}_2\tilde{\Omega}_{12}S_2^{-1} = P_2G_2V_2G_1V_1P_2\\ &= \sum_n P^{(r)}_{2n}g^{(\rho)}_{02}(E-E_n)V_2G_1(E)V_1P_2\end{aligned} \tag{6.6}$$

and write out its kernel explicitly:

$$\begin{aligned}&C_{12}(\boldsymbol{\rho}_2, \mathbf{r}_2; \boldsymbol{\rho}'_2, \mathbf{r}'_2)\\ &= \sum_{n,m}\varphi_n(\mathbf{r}_2)\varphi^*_m(\mathbf{r}'_2)\int(d\mathbf{r}''_2)(d\mathbf{r}'''_2)(d\boldsymbol{\rho}''_2)\varphi^*_n(\mathbf{r}''_2)\varphi_m(\mathbf{r}'''_2)V_2(\mathbf{r}''_2)\\ &\quad\times g_{02}(E-E_n; \boldsymbol{\rho}_2, \boldsymbol{\rho}''_2)G_1(E; \boldsymbol{\rho}''_1, \mathbf{r}''_1; \boldsymbol{\rho}'''_1, \mathbf{r}'''_1)V_1(\mathbf{r}'''_1),\end{aligned} \tag{6.7}$$

where $\mathbf{r}'''_1$ and $\boldsymbol{\rho}'''_1$ have to be expressed by (2.5) in terms of $\boldsymbol{\rho}'_2$ and $\mathbf{r}'''_2$; and $\boldsymbol{\rho}''_1$ and $\mathbf{r}''_1$ in terms of $\boldsymbol{\rho}''_2$ and $\mathbf{r}''_2$.

Note that the $\mathbf{r}''_2$ and $\mathbf{r}'''_2$ integrals are so strongly damped that they do not require any decrease from g_{02} and G_1. The estimates of Appendix D show that G_1 contributes a decrease at least as $\rho''^{-\frac{17}{8}}$, and g_{02} goes as ρ''^{-1}_2. Thus the $\boldsymbol{\rho}''_2$ integral converges absolutely and is bounded as a function of $\boldsymbol{\rho}_2$. Left multiplication by S_2^{-1} therefore makes it square integrable in $\boldsymbol{\rho}_2$. On the other hand, the factor $V_1(\mathbf{r}'''_1)$ produces sufficient decrease as a function of $\boldsymbol{\rho}'_2$, if (3.5) is satisfied, to make even $C_{12}S_2$ square integrable as a function of $\boldsymbol{\rho}'_2$.[23] As a function of $\mathbf{r}_2$ and $\mathbf{r}'_2$, C_{12} is square integrable by virtue of the outside factors φ_n and φ^*_m. Thus the kernel of $S_2^{-1}C_{12}S_2 = \tilde{\Omega}_2\tilde{\Omega}_{12}$ is in $\mathfrak{L}^2$.

The results of Appendix D show that the operator whose kernel is $f(\boldsymbol{\rho}_1)g(\boldsymbol{\rho}'_1)(G_1v_1)(\boldsymbol{\rho}_1, \mathbf{r}_1; \boldsymbol{\rho}'_1, \mathbf{r}'_1)$ is in $\mathfrak{L}^2$ if $|f|^2$ and $|g|^2$ obey (3.5). The damping role of f and g in (6.3) is played by v_2 and P_2, and the factor S_2, expressed in terms of $\mathbf{r}_1$ and $\boldsymbol{\rho}_1$, is damped out by $u_1(\mathbf{r}_1)$. Thus the operator $\tilde{\Omega}_{12}$ is in $\mathfrak{L}^2$. The same result holds if v_2 in (6.3) is replaced by v_3.

It remains to study the product $\tilde{\Omega}_2\Omega'_{12}$ or, explicitly by (5.5),

$$\begin{aligned}&S_2^{-1}P_2G_2u_2\Omega'_{12}\\ &= S_2^{-1}\sum_n P^{(r)}_{2n}u_2g^{(\rho)}_{02}(E-E_n)\Omega'_{12}\\ &= S_2^{-1}\sum_n P^{(r)}_{2n}V_2g^{(\rho)}_{02}(E-E_n)\mathfrak{G}_1(E)[u_2M'_2(E) - P_2u_2].\end{aligned} \tag{6.8}$$

A look at (4.2) shows that we therefore need the product $g^{(\rho)}_{02}(E')g^{(\rho)}_{01}(E'')$. It is shown in Appendix B that the kernel of this operator product is given by

$$\begin{aligned}&[g^{(\rho)}_{02}(E')g^{(\rho)}_{01}(E'')](\boldsymbol{\rho}_1, \mathbf{r}_1; \boldsymbol{\rho}'_1, \mathbf{r}'_1)\\ &\quad= \kappa_{12}^3g_0[E', \kappa_{12}(\mathbf{r}_1 - \mathbf{r}'_1)]g_0[E'', \kappa_{12}(\mathbf{r}_2 - \mathbf{r}'_2)]\end{aligned} \tag{6.9}$$

with $\kappa_{12} = (\tilde{\mu}_1/\mu_2)^{\frac{1}{2}}$. Thus in the calculation of $g^{(\rho)}_{02}(E-E_n)\mathfrak{G}_1(E)$ we first look at [see (4.4)]

$$\begin{aligned}&(g^{(\rho)}_{02}I_{1+})(\boldsymbol{\rho}_1, \mathbf{r}_1; \boldsymbol{\rho}'_1, \mathbf{r}'_1)\\ &\quad= -\frac{1}{4\pi}\int(d\mathbf{r})\frac{\exp[i\kappa_{12}(E-E_n)^{\frac{1}{2}}|\mathbf{r}-\mathbf{r}_1|]}{|\mathbf{r}-\mathbf{r}_1|}\\ &\qquad\times I'_{1+}(\boldsymbol{\rho}_1, \mathbf{r}; \boldsymbol{\rho}'_1, \mathbf{r}'_1),\end{aligned} \tag{6.10}$$

where I'_{1+} has the same structure as (4.7) except that $\boldsymbol{\rho}$, $\boldsymbol{\rho}'$, and $\mathbf{r}'$ are replaced by $\boldsymbol{\rho}_1$, $\boldsymbol{\rho}'_1$, and $\mathbf{r}'_1$, respectively, and R' now is given by

$$\begin{aligned}R' &= \kappa_{12}|\mathbf{r}_2 - \mathbf{r}'_2|\\ &= |\boldsymbol{\rho}_1 - \boldsymbol{\rho}'_1 + (m_1m_2/Mm_3)^{\frac{1}{2}}(\mathbf{r} - \mathbf{r}'_1)|.\end{aligned}$$

All integrals converge absolutely and uniformly, and the z integral in (4.8) is estimated as in Sec. 6. We arrive at the inequality (4.29), and we must carry out the $\mathbf{r}$ integral in (6.10). We then see that arguments

based on these inequalities fall short by an $r_1'^{-\epsilon}$ to prove the square integrability of $g_{02}^{(\rho)}I_{1+}$ as a function of $\mathbf{r}_1'$. We must therefore make use of the oscillatory nature of the $\mathbf{r}$ integral. This is done in Appendix E, in which it is shown that the $\mathbf{r}_1'$ integral of the square modulus of $g_{02}^{(\rho)}I_{1+}$ exists and is bounded as a function of $\boldsymbol{\rho}_1$, $\boldsymbol{\rho}_1'$, and $\mathbf{r}_1$. The factors $S_2^{-1}P_{2n}^{(r)}V_2$ in (6.8) provide the necessary damping to make the result square integrable in $\mathbf{r}_1$ and $\boldsymbol{\rho}_1$ (or in $\mathbf{r}_2$ and $\boldsymbol{\rho}_2$), and the factors u_2 or P_2u_2 make it square integrable in $\boldsymbol{\rho}_1$. The operator M_2' being bounded, we conclude that the term I_{1+} for $\mathfrak{G}_1$ [see (4.4)] in (6.8) results in an $\mathfrak{L}^2$ kernel. The same holds for I_-. There remains the A term of (4.4′), given by (4.5), inserted in (6.8). The product $g_{02}^{(\rho)}g_{01}^{(\rho)}$ is given in (6.9), and all four variables are strongly damped: $\mathbf{r}_2$ and $\boldsymbol{\rho}_2$ are damped by S_2^{-1} and V_2, and $\mathbf{r}_1'$ and $\boldsymbol{\rho}_1'$ are damped by $P_{1n}^{(r)}$ and u_2 or P_2u_2. Hence the operator product $\tilde{\Omega}_2\Omega_{12}'$ in (6.8) is in HS.

The same argument is applicable if we replace $u_2M_2' - P_2u_2$ in (6.8) by $u_3M_3' - P_3u_3$. Hence $\tilde{\Omega}_2u_2\Gamma_{13}'u_3$ is also in HS.

7. THE OPERATOR Ω_3

We now look at the terms of Ω_3 in (1.22). First we consider Ω_3' of (1.23) and (1.22). The first two terms, Ω_{13}' and Ω_{23}', have already been proved to be in HS.

In the operator $v_3G_2u_2(\mathbb{1} - \Omega_{12})^{-1}v_2\Gamma_{13}'u_3$ we write

$$(\mathbb{1} - \Omega_{12})^{-1} = \mathbb{1} + \Omega_{12}'(\mathbb{1} - \Omega_{12})^{-1} + \tilde{\Omega}_{12}\tilde{\Omega}_2(\mathbb{1} - \Omega_{12})^{-1}, \quad (7.1)$$

so that

$$v_3G_2u_2(\mathbb{1} - \Omega_{12})^{-1}v_2\Gamma_{13}'u_3 = v_3G_2V_2\Gamma_{13}'u_3 + (v_3G_2V_2\Gamma_{12}'u_2)(\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}'u_3) + (v_3\Gamma_{21}V_1P_2S_2)\tilde{\Omega}_2(\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}'u_3). \quad (7.2)$$

It has been shown in Sec. 5 that $v_2\Gamma_{13}'u_3$ is in HS and, in Sec. 6, that $\tilde{\Omega}_2v_2\Gamma_{13}'u_3$ is in HS. Hence by the corollary to the lemma of Appendix F, both $(\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}'u_3)$ and $\tilde{\Omega}_2(\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}'u_3)$ are in HS. The operator $v_3\Gamma_{21}V_1P_2S_2$ is written as

$$v_3\Gamma_{21}V_1P_2S_2 = (v_3\Gamma_{21}'u_1)(v_1P_2S_2) + (v_3G_2V_2P_1S_1)(S_1^{-1}P_1G_1V_1P_2S_2). \quad (7.3)$$

$v_3\Gamma_{21}'u_1$ is in HS, and the operator $v_1P_2S_2$ is not difficult to show to be bounded. Hence the first term in (7.3) is in HS.

The operator $v_3G_2V_2P_1S_1$ was shown in Sec. 6 to be in HS. The operator

$$Q_{12} = S_1^{-1}P_1G_1V_1P_2S_2 \quad (7.4)$$

has the kernel

$$Q_{12}(\boldsymbol{\rho}_1, \mathbf{r}_1; \boldsymbol{\rho}_2', \mathbf{r}_2') = \sum_{n,m}(\rho_1 + \rho_0)^{-\frac{7}{2}}\varphi_n(\mathbf{r}_1) \times \int(d\mathbf{r}_2'')\varphi_n^*(\mathbf{r}_1'')g_{01}(E - E_n; \boldsymbol{\rho}_1 - \boldsymbol{\rho}_1'') \times V_1(\mathbf{r}_1'')\varphi_m(\mathbf{r}_2'')\varphi_m^*(\mathbf{r}_2')(\rho_0 + \rho_2')^{\frac{7}{2}},$$

in which $\boldsymbol{\rho}_1''$ and $\mathbf{r}_1''$ must be expressed in terms of $\boldsymbol{\rho}_2'$ and $\mathbf{r}_2''$. The $\mathbf{r}_2''$ integral converges absolutely and is bounded by $C(\rho_0 + \rho_2')^{-\frac{7}{2}}$. Hence the result is square integrable in the four variables $\boldsymbol{\rho}_1$, $\mathbf{r}_1$, $\boldsymbol{\rho}_2'$, and $\mathbf{r}_2'$. Hence the last term in (7.3) is in HS.

The only terms in (7.2) that remain are

$$v_3G_2V_2\Gamma_{13}'u_3 = v_3\mathfrak{G}_2V_2\mathfrak{G}_1(u_3M_3' - P_3u_3) \quad (7.5)$$

and

$$v_3G_2V_2\Gamma_{12}'u_2 = v_3G_2V_2\mathfrak{G}_1(u_2M_2' - P_2u_2). \quad (7.5')$$

We must examine $v_3G_2V_2\mathfrak{G}_1$.

If we expand $G_2(E)$ as in (4.2), we arrive at the analog of (4.4),

$$G_2(E) = \sum_{n=1}^{N} g_{02}^{(\rho)}(E - E_n)P_{2n}^{(r)} + \frac{1}{2\pi i}\int_0^\infty dz'\,g_{02}^{(\rho)}(E - z') \times [g_2^{(r)-}(z') - g_2^{(r)+}(z')]. \quad (7.6)$$

The first term, from the (1, 3) bound states, leads to the exact analog of (6.8), the only difference being the replacement of S_2^{-1} by v_3. This term, used in $v_3G_2V_2\mathfrak{G}_1$, therefore leads to an HS operator. As for the z' integral in (7.6), we may divide it into two pieces, one for $0 \leq z' \leq Z$, $Z > E$, and the other for $z' > Z$. In the latter part, $g_{02}^{(\rho)}(E - z')$ is the Green's function for negative energy, whose kernel decreases exponentially as a function of ρ. The factor v_3 may then be used to dampen the $\mathbf{r}_2$ dependence of $g_2^{(r)\pm}$, making the result square integrable.

We are then left with the z' integral from 0 to Z, which we may write

$$\hat{G}_2 = \int_0^Z dP_2^{(r)}(z')g_{02}^{(\rho)}(E - z'). \quad (7.7)$$

Here $dP_2^{(r)}(z')$ is the spectral projection for $h_2^{(r)}$, which is such that

$$\int_0^\infty dP_2^{(r)}(z) + P_2 = \mathbb{1}.$$

It follows that $\int_0^\infty dP_2^{(r)}(z)f(z)$ is a bounded operator if $f(z)$ is a bounded function. We now treat

$$X = v_3\int_0^Z dP_2^{(r)}(z')V_2g_{02}^{(\rho)}(E - z')\mathfrak{G}_1u_3$$

and we did (6.8), using (6.10) and the result of Appendix E, according to which the kernel of $g_{02}^{(\rho)}I_{1+}$ is such that the $\mathbf{r}_1'$ integral of its square modulus exists and is bounded as a function of $\boldsymbol{\rho}_1$, $\boldsymbol{\rho}_1'$, and $\mathbf{r}_1$. The factors $v_3\int_0^Z dP_2^{(r)}(z')V_2$ on the left and u_3, P_3u_3, u_2, or P_2u_2 on the right thus make the contribution from I_+ in $\mathfrak{S}_1$ to the kernel of X square integrable. The same holds for the contribution from I_-. The contribution from A of (4.5) is again handled by (6.9) and seen to have the same property as $g_{02}^{(\rho)}I_{1+}$. Thus X is in HS.

As a result the operator product on the left-hand side of (7.2) is in HS, and, of course, so is

$$v_3G_1u_1(\mathbb{1} - \Omega_{21})^{-1}v_1\Gamma_{23}u_3.$$

The next term of (1.22) to be considered is

$$\begin{aligned}(v_3\Gamma_{12}u_2)(\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}'u_3)\\ = (v_3\Gamma_{12}'u_2)(\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}'u_3)\\ + (v_3G_1V_1P_2S_2)\tilde{\Omega}_2(\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}'u_3). \quad (7.8)\end{aligned}$$

The first term on the right is a product of two operators that were shown to be in HS and of a bounded operator. The second term consists of two factors, the first of which, $v_3G_1V_1P_2S_2$, differs from $\tilde{\Omega}_{12}$ only by the substitution of v_3 for v_2. It is shown in Sec. 6 to be in HS. The second, $\tilde{\Omega}_2(\mathbb{1} - \Omega_{12})^{-1}(v_2\Gamma_{13}'u_3)$, has already been shown to be in HS. The same argument, of course, applies to the product

$$v_3\Gamma_{21}u_1(\mathbb{1} - \Omega_{21})^{-1}v_1\Gamma_{23}'u_3.$$

We have therefore shown that Ω_3' of (1.22) and (1.23) is an HS operator. To complete the argument of Sec. 1, we must now demonstrate that $\tilde{\Omega}_3$, $\tilde{\Omega}_3\Omega_3$, and $\tilde{\Omega}_3\tilde{\Omega}_3$ are also in HS.

The operator $\tilde{\Omega}_3$ is given in (1.25). The first two terms are $\tilde{\Omega}_{13}$ and $\tilde{\Omega}_{23}$, and these have already been shown to be in HS. The other two terms differ from the corresponding two terms in Ω_3' only by the substitution of $v_1G_2V_2P_3S_3$ and $v_2G_1V_1P_3S_3$ for $v_1\Gamma_{23}'u_3$ and $v_2\Gamma_{13}'u_3$, respectively. But these terms, in turn, have already been shown to be in HS, and their ranges include the domains of $\tilde{\Omega}_1$ and $\tilde{\Omega}_2$, respectively. Hence the arguments given above, to show that Ω_3' is in HS, carry over to the demonstration that $\tilde{\Omega}_3$ is also in HS.

Next, there is the operator $\tilde{\Omega}_3\Omega_3'$. The first two terms are $\tilde{\Omega}_3\Omega_{13}'$ and $\tilde{\Omega}_3\Omega_{23}'$, and these have already been shown to be in HS. Then there is $\tilde{\Omega}_3$ right-multiplied by the operator of (7.2). The first factor of the last term of (7.2) is analyzed in (7.3) and, when left-multiplied by $\tilde{\Omega}_3$, is seen to be in HS, by previous arguments. The other two terms of (7.2) lead to

$$\tilde{\Omega}_3v_3G_2V_2\Gamma_{13}'u_3 = (S_3^{-1}P_3\Gamma_{32}u_2)(v_2\Gamma_{13}'u_3) \quad (7.9)$$

and

$$\tilde{\Omega}_3v_3G_2V_2\Gamma_{12}'u_2 = (S_3^{-1}P_3\Gamma_{32}u_2)\Omega_{12}'. \quad (7.10)$$

Now the kernel of $S_3^{-1}\Gamma_{32}'u_2$ is in $\mathfrak{L}^2$ just as $v_2\Gamma_{32}'u_2$ is; S_3^{-1} provides the same ρ_3 damping as v_2. The (1, 3) bound-state contributions to Γ_{32} give rise to

$$(S_3^{-1}P_3\Gamma_{32}''u_2) = Q_{32}\tilde{\Omega}_2, \quad (7.11)$$

where Q_{32} is given by the analog of (7.4). It was shown to be in HS, and so was $\tilde{\Omega}_2(v_2\Gamma_{13}'u_3)$. Hence the operator of (7.9) is in HS, and so is the operator of (7.10). Consequently, (7.2), when left-multiplied by $\tilde{\Omega}_3$, is in HS, and, similarly,

$$\tilde{\Omega}_3v_3G_1u_1(\mathbb{1} - \Omega_{21})^{-1}(v_1\Gamma_{23}u_3).$$

The only remaining terms are (7.8) left-multiplied by $\tilde{\Omega}_3$, and the same with 1 and 2 exchanged. In both terms on the right-hand side of (7.8), the left-hand parentheses are operators of the same structure as the left-hand parentheses of (7.3), which have already been argued to be in HS when left-multiplied by $\tilde{\Omega}_3$. The other factors in (7.8) are in HS. Hence the operator of (7.8), left-multiplied by $\tilde{\Omega}_3$, is in HS, and so is, by the same arguments, $\tilde{\Omega}_3v_3\Gamma_{21}u_1(\mathbb{1} - \Omega_{21})^{-1}v_1\Gamma_{23}u_3$. Therefore, $\tilde{\Omega}_3\Omega_3'$ is in HS.

Finally, there is the product $\tilde{\Omega}_3\tilde{\Omega}_3$, with $\tilde{\Omega}_3$ given by (1.25). The first two terms are $\tilde{\Omega}_3\tilde{\Omega}_{13}$ and $\tilde{\Omega}_3\tilde{\Omega}_{23}$ and, hence, in HS. The arguments for the remaining terms are exactly like the corresponding ones for $\tilde{\Omega}_3\Omega_3'$. The only difference is that the right-hand factors $v_1\Gamma_{23}'u_3$ and $v_2\Gamma_{13}'u_3$ are replaced by other terms which have already been shown to be in HS and whose ranges include the domains of $\tilde{\Omega}_1$ and $\tilde{\Omega}_2$, respectively. Hence all the arguments used in the examination of $\tilde{\Omega}_3\Omega_3'$ carry over to $\tilde{\Omega}_3\tilde{\Omega}_3$, and $\tilde{\Omega}_3\tilde{\Omega}_3$ is in HS.

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APPENDIX A

In this appendix we construct the free Green's function on $\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_\rho$, using the same technique as in (4.2)–(4.4):

$$\begin{aligned}G_0(E) &= \frac{1}{2\pi i}\int_C dz\, g_0^{(\rho)}(E - z)g_0^{(r)}(z)\\ &= \frac{1}{2\pi i}\int_0^\infty dz\, g_0^{(\rho)}(E - z)[g_0^{(r)-}(z) - g_0^{(r)+}(z)]\end{aligned}$$

or, explicitly,

$$G_0(E;\boldsymbol{\rho},\mathbf{r};\boldsymbol{\rho}',\mathbf{r}') = -\frac{1}{2(2\pi)^3}\frac{1}{|\mathbf{r}-\mathbf{r}'|\,|\boldsymbol{\rho}-\boldsymbol{\rho}'|}\int_0^\infty dz \times e^{iR'(E-z)^{\frac{1}{2}}}\sin(z^{\frac{1}{2}}R),$$

where R' is given by (4.9) and R is now

$$R = |\mathbf{r}-\mathbf{r}'|.$$

As in (4.8), the integral runs *below* the point $z = E$. It is the same as in (4.19), and its value is given by (4.22):

$$G_0(E;\boldsymbol{\rho},\mathbf{r};\boldsymbol{\rho}',\mathbf{r}') = -(Ei/16\pi^2\bar{R}^2)H_2^{(1)}(E^{\frac{1}{2}}\bar{R}), \quad \text{(A1)}$$

where $\bar{R}^2 = R^2 + R'^2$. Since

$$H_2^{(1)}(z) = O(z^{-2}) \quad \text{as} \quad z \to 0$$
$$= O(z^{-\frac{1}{2}}) \quad \text{as} \quad z \to \infty$$

for real z, there exists a constant C such that

$$|H_2^{(1)}(z)| \leq C(z^{-\frac{1}{2}} + z^{-2}).$$

Consequently,

$$|G_0(E;\boldsymbol{\rho},\mathbf{r};\boldsymbol{\rho}',\mathbf{r}')| \leq C(\bar{R}^{-4} + \bar{R}^{-\frac{5}{2}}E^{\frac{3}{4}}), \quad \text{(A2)}$$

where C is independent of E. As $r \to \infty$, all other variables being fixed, this leads to

$$G_0 = O(r^{-\frac{5}{2}}). \quad \text{(A3)}$$

APPENDIX B

We evaluate here the product of two Green's functions. According to (2.5),

$$\begin{aligned}
&\langle \mathbf{r}_2\boldsymbol{\rho}_2|\, g_{02}^{(\rho)} g_{01}^{(\rho)}\, |\mathbf{r}_1'\boldsymbol{\rho}_1'\rangle \\
&= \int (d\mathbf{r}_1'')(d\mathbf{r}_2'')(d\boldsymbol{\rho}_1'')(d\boldsymbol{\rho}_2'') \\
&\quad \times \langle \mathbf{r}_2\boldsymbol{\rho}_2|\, g_{02}^{(\rho)}\, |\mathbf{r}_2''\boldsymbol{\rho}_2''\rangle\langle \mathbf{r}_2''\boldsymbol{\rho}_2''\,|\,\mathbf{r}_1''\boldsymbol{\rho}_1''\rangle\langle \mathbf{r}_1''\boldsymbol{\rho}_1''|\, g_{01}^{(\rho)}\, |\mathbf{r}_1'\boldsymbol{\rho}_1'\rangle \\
&= \int (d\mathbf{r}_1'')(d\mathbf{r}_2'')(d\boldsymbol{\rho}_1'')(d\boldsymbol{\rho}_2'') \\
&\quad \times g_{02}(\boldsymbol{\rho}_2 - \boldsymbol{\rho}_2'')\delta(\mathbf{r}_2 - \mathbf{r}_2'')g_{01}(\boldsymbol{\rho}_1'' - \boldsymbol{\rho}_1') \\
&\quad \times \delta(\mathbf{r}_1'' - \mathbf{r}_1')\delta(\mathbf{r}_2'' + a\mathbf{r}_1'' + b\boldsymbol{\rho}_1'')\delta(\boldsymbol{\rho}_2'' - c\mathbf{r}_1'' + a\boldsymbol{\rho}_1'') \\
&= \int (d\boldsymbol{\rho}_1'')\delta(\mathbf{r}_2 + a\mathbf{r}_1' + b\boldsymbol{\rho}_1'') \\
&\quad \times g_{02}(\boldsymbol{\rho}_2 - c\mathbf{r}_1' + a\boldsymbol{\rho}_1'')g_{01}(\boldsymbol{\rho}_1'' - \boldsymbol{\rho}_1') \\
&= \kappa_{12}^3 g_{02}[\kappa_{12}(\mathbf{r}_1 - \mathbf{r}_1')]g_{01}[\kappa_{12}(\mathbf{r}_2 - \mathbf{r}_2')], \quad \text{(B1)}
\end{aligned}$$

where $a = (\mu_1\mu_2)^{\frac{1}{2}}/m_3$, $b = (\mu_2/\bar{\mu}_1)^{\frac{1}{2}}$, $c = (\mu_1/\bar{\mu}_2)^{\frac{1}{2}}$, and $\kappa_{12} = (\bar{\mu}_1/\mu_2)^{\frac{1}{2}}$ and where $\mathbf{r}_2'$ and $\mathbf{r}_1$ are to be expressed in terms of $\mathbf{r}_1'$, $\boldsymbol{\rho}_1'$ and $\mathbf{r}_2$, $\boldsymbol{\rho}_2$, respectively, by (2.5).

APPENDIX C

Let us first consider the integral

$$f(\mathbf{r}) = \int \frac{(d\mathbf{r}')(r_0 + r')^{-n}}{|\mathbf{r}' - \mathbf{r}|^\beta}$$

for $0 \leq \beta < 3$ and $n > 3$. We can carry out the angle integration

$$\begin{aligned}
f(\mathbf{r}) &= 2\pi\int_0^\infty dr'r'^2(r_0 + r')^{-n} \\
&\quad \times \int_{-1}^1 du(r^2 + r'^2 - 2rr'u)^{-\frac{1}{2}\beta} \\
&= \frac{2\pi}{2-\beta}\frac{1}{r}\int_0^\infty dr'r'(r_0 + r')^{-n} \\
&\quad \times |(r + r')^{2-\beta} - |r - r'|^{2-\beta}|
\end{aligned}$$

and we have

$$\int_0^a dr'r'(r_0 + r')^{-n}\,|(r + r')^{2-\beta} - |r - r'|^{2-\beta}| \leq Cr^{1-\beta}$$

$$\int_a^\infty dr' \cdots \leq r^{4-\beta-n}\int_{a/r}^\infty dx x^{1-n} \times |(1 + x)^{2-\beta} - |1 - x|^{2-\beta}| \leq Cr^{1-\beta}.$$

Since $f(\mathbf{r})$ is bounded for all finite $\mathbf{r}$, we conclude that

$$\int \frac{(d\mathbf{r}')(r_0 + r')^{-n}}{|\mathbf{r}' - \mathbf{r}|^\beta} \leq C(r_0 + r)^{-\beta}. \quad \text{(C1)}$$

We now study the integral

$$f(\mathbf{r},\mathbf{r}') = \int \frac{(d\mathbf{r}'')(r_0 + r'')^{-n}}{|\mathbf{r}'' - \mathbf{r}|\,|\mathbf{r}'' - \mathbf{r}'|\,(|\mathbf{r}'' - \mathbf{r}| + |\mathbf{r}'' - \mathbf{r}'|)^\alpha} \quad \text{(C2)}$$

for $\alpha = \frac{3}{2}, 2$. Since

$$|\mathbf{r}'' - \mathbf{r}| + |\mathbf{r}'' - \mathbf{r}'| \geq \begin{cases} |\mathbf{r} - \mathbf{r}'| \\ |\mathbf{r}'' - \mathbf{r}|, \\ |\mathbf{r}'' - \mathbf{r}'| \end{cases}$$

we have

$$\begin{aligned}
f(\mathbf{r},\mathbf{r}') &\leq \frac{1}{|\mathbf{r} - \mathbf{r}'|^{\alpha-\frac{3}{4}}}\int \frac{(d\mathbf{r}'')(r_0 + r'')^{-n}}{|\mathbf{r}'' - \mathbf{r}|^{\frac{11}{8}}\,|\mathbf{r}'' - \mathbf{r}'|^{\frac{11}{8}}} \\
&\leq \frac{1}{|\mathbf{r} - \mathbf{r}'|^{\alpha-\frac{3}{4}}}\left(\int \frac{(d\mathbf{r}'')(r_0 + r'')^{-n}}{|\mathbf{r}'' - \mathbf{r}|^{\frac{11}{4}}}\right)^{\frac{1}{2}} \\
&\quad \times \left(\int \frac{(d\mathbf{r}'')(r_0 + r'')^{-n}}{|\mathbf{r}'' - \mathbf{r}'|^{\frac{11}{4}}}\right)^{\frac{1}{2}}
\end{aligned}$$

by Schwarz's inequality. Therefore, by (C1),

$$f(\mathbf{r},\mathbf{r}') \leq C/[|\mathbf{r} - \mathbf{r}'|^{\alpha-\frac{3}{4}}(r_0 + r)^{\frac{11}{8}}(r_0 + r')^{\frac{11}{8}}]. \quad \text{(C3)}$$

The next integral we need is

$$g(\mathbf{r},\mathbf{r}') = \int \frac{(d\mathbf{r}'')(d\mathbf{r}''')(r_0 + r'')^{-n}(r_0 + r''')^{-n}}{|\mathbf{r}'' - \mathbf{r}|\,|\mathbf{r}''' - \mathbf{r}'|\,(|\mathbf{r}'' - \mathbf{r}| + |\mathbf{r}''' - \mathbf{r}'|)^\alpha}, \quad \text{(C4)}$$

in which we use

$$\mathbf{r}'' - \mathbf{r}| + |\mathbf{r}''' - \mathbf{r}'| \geq (|\mathbf{r}'' - \mathbf{r}|\,|\mathbf{r}''' - \mathbf{r}'|)^{\frac{1}{2}}$$

and then use (C1):

$$g(\mathbf{r},\mathbf{r}') \le C\int \frac{(d\mathbf{r}'')(r_0+r'')^{-n}}{|\mathbf{r}''-\mathbf{r}|^{1+\frac{1}{2}\alpha}}\int \frac{(d\mathbf{r}''')(r_0+r''')^{-n}}{|\mathbf{r}'''-\mathbf{r}'|^{1+\frac{1}{2}\alpha}}$$
$$\le C(r_0+r)^{-1-\frac{1}{2}\alpha}(r_0+r')^{-1-\frac{1}{2}\alpha}. \qquad \text{(C5)}$$

Another integral needed is

$$h(\mathbf{r},\mathbf{r}')$$
$$=\int \frac{(d\mathbf{r}'')(d\mathbf{r}''')(r_0+r'')^{-n}(r_0+r''')^{-n}}{|\mathbf{r}''-\mathbf{r}|\,|\mathbf{r}'''-\mathbf{r}'|\,|\mathbf{r}'''-\mathbf{r}''|\,(|\mathbf{r}''-\mathbf{r}|+|\mathbf{r}'''-\mathbf{r}'|)^{\alpha}}$$
$$\le\int \frac{(d\mathbf{r}''')(r_0+r''')^{-n}}{|\mathbf{r}'''-\mathbf{r}'|^{1+\frac{1}{2}\alpha}}\int \frac{(d\mathbf{r}'')(r_0+r'')^{-n}}{|\mathbf{r}''-\mathbf{r}|^{1+\frac{1}{2}\alpha}|\mathbf{r}''-\mathbf{r}'''|}. \qquad \text{(C6)}$$

Doing the $\mathbf{r}''$ integral, we insert

$$1 \le (|\mathbf{r}''-\mathbf{r}|+|\mathbf{r}''-\mathbf{r}'''|)/|\mathbf{r}-\mathbf{r}'''|$$

and then have the two integrals

$$\int \frac{(d\mathbf{r}'')(r_0+r'')^{-n}}{|\mathbf{r}''-\mathbf{r}|^{\frac{1}{2}\alpha}|\mathbf{r}''-\mathbf{r}'''|}+\int \frac{(d\mathbf{r}'')(r_0+r'')^{-n}}{|\mathbf{r}''-\mathbf{r}|^{1+\frac{1}{2}\alpha}}.$$

The first is handled by Schwarz's inequality

$$\left(\int \frac{(d\mathbf{r}'')(r_0+r'')^{-n}}{|\mathbf{r}''-\mathbf{r}|^{\frac{1}{2}\alpha}|\mathbf{r}''-\mathbf{r}'''|}\right)^2$$
$$\le\int \frac{(d\mathbf{r}'')(r_0+r'')^{-n}}{|\mathbf{r}''-\mathbf{r}|^{\alpha}}\int \frac{(d\mathbf{r}'')(r_0+r'')^{-n}}{|\mathbf{r}''-\mathbf{r}'''|^2}$$
$$\le C(r_0+r)^{-\alpha}(r_0+r''')^{-2}$$

by (C1). The second integral is also estimated by (C1), so that

$$\int \frac{(d\mathbf{r})(r_0+r'')^{-n}}{|\mathbf{r}''-\mathbf{r}|^{1+\frac{1}{2}\alpha}|\mathbf{r}''-\mathbf{r}'''|}$$
$$\le \frac{C}{|\mathbf{r}-\mathbf{r}'''|\,(r_0+r)^{\frac{1}{2}\alpha}}\left(\frac{1}{r_0+r}+\frac{1}{r_0+r'''}\right).$$

We then have the $\mathbf{r}'''$ integral

$$\int \frac{(d\mathbf{r}''')(r_0+r''')^{-n}}{|\mathbf{r}'''-\mathbf{r}'|^{1+\frac{1}{2}\alpha}|\mathbf{r}'''-\mathbf{r}|}$$
$$\le \frac{C}{|\mathbf{r}-\mathbf{r}'|\,(r_0+r')^{\frac{1}{2}\alpha}}\left(\frac{1}{r_0+r'}+\frac{1}{r_0+r}\right),$$

and hence

$$h(r,r') \le \frac{C}{|\mathbf{r}-\mathbf{r}'|\,(r_0+r')^{\frac{1}{2}\alpha}(r_0+r)^{\frac{1}{2}\alpha}}$$
$$\times\left(\frac{1}{r_0+r}+\frac{1}{r_0+r'}\right). \qquad \text{(C7)}$$

The next question is whether the functions $f(\mathbf{r},\mathbf{r}')$, $g(\mathbf{r},\mathbf{r}')$, and $h(\mathbf{r},\mathbf{r}')$ are $\mathfrak{L}^2$ in both variables. According to (C3), (C5), and (C7),

$$\|f\|_2^2 \le C\int (d\mathbf{r})(d\mathbf{r}')\,|\mathbf{r}-\mathbf{r}'|^{\frac{3}{2}-2\alpha}$$
$$\times (r_0+r)^{-\frac{11}{4}}(r_0+r')^{-\frac{11}{4}}, \qquad \text{(C8)}$$

$$\|g\|_2^2 \le C\int (d\mathbf{r})(d\mathbf{r}')(r_0+r)^{-2-\alpha}(r_0+r')^{-2-\alpha}, \qquad \text{(C9)}$$

$$\|h\|_2^2 \le C\int (d\mathbf{r})(d\mathbf{r}')\,|\mathbf{r}-\mathbf{r}'|^{-2}\,(r_0+r)^{-1-\alpha}(r_0+r')^{-\alpha}$$
$$\times[(r_0+r)^{-1}+(r_0+r')^{-1}]. \qquad \text{(C10)}$$

The integrals in (C9) obviously converge for $\alpha=\frac{3}{2}$ and $\alpha=2$. In (C8) we do the angle integral

$$A=\int_{-1}^{1} du(r^2+r'^2-2rr'u)^{-\beta}$$
$$=\frac{1}{2(1-\beta)}\frac{1}{rr'}\,|(r+r')^{2-2\beta}-|r-r'|^{2-2\beta}|$$
$$\le Cr^{1-2\beta}r'^{-1}\left|\left(1+\frac{r'}{r}\right)^{2-2\beta}-\left|1-\frac{r'}{r}\right|^{2-2\beta}\right|.$$

For $\alpha=\frac{3}{2}$, we have $\beta=\frac{3}{4}$, and hence

$$A \le C(r+r')^{-\frac{3}{2}} \le Cr^{-\frac{3}{4}}r'^{-\frac{3}{4}}.$$

For $\alpha=2$, $\beta=\frac{5}{4}$, and hence A contains an integrable singularity at $r=r'$. For $r'/r \le a \le 1$, we have $A \le Cr^{-\frac{5}{2}}$ and, for $r'/r \ge b > 1$, $A \le Cr'^{-\frac{5}{2}}$. In both cases (C8) is easily seen to exist.

In (C10) the angle integral is

$$A=\frac{1}{2rr'}\ln[(r+r')/(r-r')]^2$$

so that it too has an integrable singularity, and, for $r'/r \le a < 1$, $A \le Cr^{-2}$ whereas, for $r'/r \ge b > 1$, $A \le Cr'^{-2}$. Hence both for $\alpha=\frac{3}{2}$ and $\alpha=2$, (C10) is seen to exist.

APPENDIX D

We shall here estimate $G(E)u$ in a manner analogous to the estimate of $\mathfrak{G}(E)$ in Sec. 4. The analog of (4.2) now is

$$G(E)u=\frac{1}{2\pi i}\int_C dz g_0^{(\rho)}(E-z)g^{(r)}(z)u, \qquad \text{(D1)}$$

and hence G is split up as $\mathfrak{G}$ in (4.4), where A is the same as in (4.5), and $I_{\pm}$ are given by integrals analogous to (4.7):

$$I_+(\boldsymbol{\rho},\mathbf{r};\boldsymbol{\rho}',\mathbf{r}')$$
$$=\frac{C}{|\boldsymbol{\rho}-\boldsymbol{\rho}'|}\int \frac{(d\mathbf{r}'')u(\mathbf{r}'')}{|\mathbf{r}-\mathbf{r}''|}J(\mathbf{r},\mathbf{r}',\mathbf{r}'',\mathbf{r}';\boldsymbol{\rho},\boldsymbol{\rho}'). \qquad \text{(D2)}$$

J is the same as in (4.8), except with $\mathbf{r}'''=\mathbf{r}'$. We now

insert the inequalities (4.28) in (D2) and obtain

$$|I_+(\rho, \mathbf{r}; \rho', \mathbf{r}')| \leq Cv(\mathbf{r}')(1 + R_0^{\frac{3}{2}}|\rho - \rho'|^{-\frac{3}{2}}) \times \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|^{\frac{5}{2}}} + \int \frac{(d\mathbf{r}'')\,|V(\mathbf{r}'')|}{|\mathbf{r}'' - \mathbf{r}|^{\frac{5}{2}}} + \int \frac{(d\mathbf{r}'')\,|V(\mathbf{r}'')|}{|\mathbf{r}'' - \mathbf{r}|\,|\mathbf{r}'' - \mathbf{r}'|} \frac{1}{(|\mathbf{r}'' - \mathbf{r}'| + |\mathbf{r}'' - \mathbf{r}|)^{\frac{3}{2}}}\right). \tag{D3}$$

These integrals are estimated by (C1) and (C3):

$$|I_+(\rho, \mathbf{r}; \rho', \mathbf{r}')| \leq Cv(\mathbf{r}')(1 + R_0^{\frac{3}{2}}|\rho - \rho'|^{-\frac{3}{2}})[|\mathbf{r} - \mathbf{r}'|^{-\frac{5}{2}} + (r_0 + r)^{-\frac{5}{2}} + |\mathbf{r} - \mathbf{r}'|^{-\frac{3}{4}}(r_0 + r)^{-\frac{11}{8}}(r_0 + r')^{-\frac{11}{8}}]. \tag{D4}$$

The same holds for I_-, and A, by (4.30), is bounded by

$$|A(\rho, \mathbf{r}; \rho', \mathbf{r}')| \leq C(r_0 + r)^{-\frac{7}{4}}(r_0 + r')^{-\frac{7}{4}}/|\rho - \rho'|. \tag{D5}$$

Consequently, $|G(\rho, \mathbf{r}; \rho', \mathbf{r}')u(\mathbf{r}')|$ is bounded by the sum of (D4) and (D5).

APPENDIX E

Let us split the $\mathbf{r}$ integral in (6.10) into two parts,

$$-4\pi g_{02}^{(\rho)} I_{1+} = \int_{r \leq A} (d\mathbf{r}) \cdots + \int_{r > A} (d\mathbf{r}) \cdots, \tag{E1}$$

where $A = A' r_1'^{\gamma}$, $0 < \gamma < 1$, and A' is a constant. Insertion of the inequalities (4.28) shows that the first integral is bounded by $(r_0 + r_1')^{\frac{5}{4}\gamma - \frac{11}{4}}$ and hence it is square integrable in $\mathbf{r}_1'$. In the second integral we insert the asymptotic values (4.25)–(4.27). We then arrive, for large $\mathbf{r}_1'$, at the integral

$$\frac{1}{r_0 + r_1'} \int_{r > A} (d\mathbf{r}) \frac{\exp(ivr + i\hat{\mathbf{n}} \cdot \bar{\mathbf{r}} + iE^{\frac{1}{2}}\bar{R})}{r^2 (r + r_1')^{\frac{3}{2}}} \equiv \frac{r_1'^{-\frac{1}{2}}}{r_0 + r_1'} f(\mathbf{r}_1'), \tag{E2}$$

where $v > 0$ for real E and $\hat{\mathbf{n}} = \mathbf{r}/r$. Changing variables of integration to $\mathbf{x} = \mathbf{r}/r_1'$, we get

$$f(\mathbf{r}_1') = \int d\Omega_x \exp(i\hat{\mathbf{n}} \cdot \bar{\mathbf{r}}) \int_{A/r_1'}^{\infty} dx (x + 1)^{-\frac{3}{2}} \times \exp(ivr_1' x + iE^{\frac{1}{2}}\bar{R}), \tag{E3}$$

$$\bar{R} = \{[\rho_1 - \rho_1' + (m_1 m_2/M m_3)^{\frac{1}{2}} r_1'(\mathbf{x} - \hat{\mathbf{n}}_1')]^2 + r_1'^2 (x + 1)^2\}^{\frac{1}{2}} \simeq r_1'[(x + 1)^2 + (m_1 m_2/M m_3)(\mathbf{x} - \hat{\mathbf{n}}_1')^2]^{\frac{1}{2}} + \frac{(m_1 m_2/M m_3)^{\frac{1}{2}}(\mathbf{x} - \hat{\mathbf{n}}_1') \cdot (\rho_1 - \rho_1')}{[(x + 1)^2 + (m_1 m_2/M m_3)(\mathbf{x} - \hat{\mathbf{n}}_1')^2]^{\frac{1}{2}}} + O(r_1'^{-1}). \tag{E4}$$

Consider the x integral in (E3):

$$\int_{A/r_1'}^{\infty} dx \cdots = \int_0^{\infty} dx (x + 1)^{-\frac{3}{2}} \times \exp[ig(x) + ir_1' h(x)] - \int_0^{A' r_1'^{\gamma - 1}} dx \cdots, \tag{E5}$$

where

$$h(x) = \nu x + [(x + 1)^2 + (m_1 m_2/M m_3)(\mathbf{x} - \hat{\mathbf{n}}_1')^2]^{\frac{1}{2}} E^{\frac{1}{2}}$$

and $g(x)$ is the second term in (E4). The second term in (E5) goes like $r'^{\gamma - 1}$ and hence, with the factor $r_1'^{-\frac{1}{2}}(r_0 + r_1')^{-1}$ in (E2), is square integrable in $\mathbf{r}_1'$. In the first term of (E5) we may use $h(x) = y$ as the new variable of integration. Since $h'(x) \geq \delta \geq 0$ for all x and $(x + 1)^{-\frac{3}{2}}$ is square integrable, the x integral is (one-dimensionally) square integrable as a function of r_1'. The outside factor of $r_1'^{-\frac{1}{2}}(r_0 + r_1')^{-1}$ in (E2), and the fact that since $(x + 1)^{-\frac{3}{2}}$ is integrable, the x integral is bounded for all r_1', makes the result three-dimensionally square integrable as a function of $\mathbf{r}_1'$.

There remains the solid angle integral in (E3). An integral over a finite range, whose integrand is in $\mathfrak{L}^2$ as a function of a parameter, is also in $\mathfrak{L}^2$. This establishes that $g_{02}^{(\rho)} I_{1+}$ is, for each $\mathbf{r}_1$, ρ_1, and ρ_1', square integrable as a function of $\mathbf{r}_1'$. What is more, its $\mathfrak{L}^2$ norm (in $\mathbf{r}_1'$) is bounded as a function of $\mathbf{r}_1$, ρ_1, and ρ_1'.

APPENDIX F

Lemma: Let A and B be Hilbert–Schmidt operators, and let C be such that CA and CB are also in the Hilbert–Schmidt class. Then the operator $D = AC + B$ is such that the Fredholm determinant $\det(\mathbb{1} - \lambda D)$ exists and can be calculated as an absolutely convergent power series in λ for all values of λ by the classical Fredholm theory for $\mathfrak{L}^2$ kernels. The same applies to the calculation of the operator $(\mathbb{1} - \lambda D)^{-1} \det(\mathbb{1} - \lambda D) \equiv \{(\mathbb{1} - \lambda D)^{-1}\}$ which, for every λ, is well defined on the domain of C and a bounded operator on any closed subspace $\mathcal{H}'$ on which C is bounded. Moreover, the range of $\{(\mathbb{1} - \lambda D)^{-1}\}$ (on the domain of C) is included in the domain of C and the operator $C\{(\mathbb{1} - \lambda D)^{-1}\}$ is bounded on $\mathcal{H}'$. ("Fredholm determinant" here means *modified* Fredholm determinant.)

Corollary: If the operator E is in HS such that CE is in HS, then both $\{(\mathbb{1} - \lambda D)^{-1}\}E$ and $C\{(\mathbb{1} - \lambda D)^{-1}\}E$ are in HS for every λ.

Proof: We formally consider[24]

$$f(\lambda,\mu) \equiv \det(\mathbb{1} - \lambda AC - \mu B)$$
$$= \{\det(\mathbb{1} - \lambda AC)[1 - \mu(\mathbb{1} - \lambda AC)^{-1}B]\}$$
$$= g_1(\lambda,\mu)\det(\mathbb{1} - \lambda CA)$$
$$\times \det[\mathbb{1} - \mu B - \mu\lambda A(\mathbb{1} - \lambda CA)^{-1}CB],$$
$$g_1(\lambda,\mu) = \exp\{-\lambda\mu \operatorname{tr}[CBA(\mathbb{1} - \lambda CA)^{-1}]\}$$

in which each determinant is defined by its power series and the indicated inversion of the order of operators is correct term by term. The resulting expression shows $f(\lambda,\mu)$ to be of the form

$$f(\lambda,\mu) = \sum_0^\infty \mu^n f_n(\lambda).$$

Each $f_n(\lambda)$ is an analytic function of λ, regular everywhere except for those values $\lambda = \lambda_i$, $i = 1, 2, \cdots$, for which λCA has the eigenvalue 1, and for each $\lambda \neq \lambda_i$ the power series in μ converges absolutely for all μ. Hence, for each $\lambda \neq \lambda_i$, $f(\lambda,\mu)$ is an entire analytic function of μ.

We may also write

$$f(\lambda,\mu) = \det\{(\mathbb{1} - \mu B)[\mathbb{1} - \lambda AC(\mathbb{1} - \mu B)^{-1}]\}$$
$$= g_2(\lambda,\mu)\det(\mathbb{1} - \mu B)$$
$$\times \det[\mathbb{1} - \lambda CA - \lambda\mu CB(\mathbb{1} - \mu B)^{-1}A],$$
$$g_2(\lambda,\mu) = \exp\{-\lambda\mu \operatorname{tr}[ACB(\mathbb{1} - \mu B)^{-1}]\}$$

thus exhibiting f in the form

$$f(\lambda,\mu) = \sum_0^\infty \lambda^n g_n(\mu).$$

This shows that $f(\lambda,\mu)$ is an entire analytic function of λ for each $\mu \neq \mu_i$, $i = 1, 2, \cdots$, if μ_i^{-1} are the eigenvalues of B.

Thus f is an analytic function of both variables,[25] with singularities possible only at $(\lambda,\mu) = (\lambda_i, \mu_j)$, $i, j = 1, 2, \cdots$. But isolated singularities of an analytic function of two variables are always removable.[26] Hence $f(\lambda,\mu)$ is an entire analytic function of both variables. Therefore, it can be expanded in a power series for $\lambda = \mu$ which converges absolutely for all λ. This is the Fredholm series of $\det(\mathbb{1} - \lambda D)$.

Next we argue similarly for the construction of the resolvents:

$$F(\lambda,\mu) \equiv \{(\mathbb{1} - \lambda AC - \mu B)^{-1}\}$$
$$= \{[\mathbb{1} - \mu B - \mu\lambda A(\mathbb{1} - \lambda CA)^{-1}CB]^{-1}\}$$
$$\times [\mathbb{1}\det(\mathbb{1} - \lambda CA)$$
$$+ \lambda A\{(\mathbb{1} - \lambda CA)^{-1}\}C]g_1(\lambda,\mu)$$
$$= g_2(\lambda,\mu)\{(\mathbb{1} - \mu B)^{-1}\}[\mathbb{1}\det[\mathbb{1} - \lambda CA$$
$$- \lambda\mu CB(\mathbb{1} - \mu B)^{-1}A] + \lambda A\{[\mathbb{1} - \lambda CA$$
$$- \lambda\mu CB(\mathbb{1} - \mu B)^{-1}A]^{-1}\}C(\mathbb{1} - \mu B)^{-1}].$$

On the domain of definition of the operator C, the first equation exhibits the (operator-valued) function $F(\lambda,\mu)$ as an entire function of μ for each $\lambda \neq \lambda_i$, and the second as an entire function of λ for each $\mu \neq \mu_i$. Thus it is an entire analytic function of both λ and μ, and $\{(\mathbb{1} - \lambda D)^{-1}\}\Psi$ exists if $C\Psi$ exists, and it can be expanded in a strongly convergent power series for every λ. Hence the domain of $\{(\mathbb{1} - \lambda D)^{-1}\}$ includes that of C.

Now let $\mathcal{H}'$ be a (closed) subspace on which C is bounded. On it D is completely continuous and hence $(\mathbb{1} - \lambda D)^{-1}$ is a bounded operator on $\mathcal{H}'$ for each λ, except at $\lambda = \lambda_i'$, where $\lambda_i' D$ has the eigenvalue 1. What is more, $(\lambda - \lambda_i')(\mathbb{1} - \lambda D)^{-1}$ is also bounded[27] on $\mathcal{H}'$ at $\lambda = \lambda_i'$, and hence so is $\{(\mathbb{1} - \lambda D)^{-1}\}$ for all λ. Thus,on $\mathcal{H}'$,$\{(\mathbb{1} - \lambda D)^{-1}\}$ is, for every λ, a bounded operator.

Now the same argument may be applied to $CF(\lambda,\mu)$ and it shows that the range of $\{(\mathbb{1} - \lambda D)^{-1}\}$ (on the domain of C) is included in the domain of C. What is more, on $\mathcal{H}'$, $C\{(\mathbb{1} - \lambda D)^{-1}\}$ is bounded.

The corollary follows from the fact that if CE is in HS, then C is bounded on the range of E (which is a closed subspace if E is in HS).

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[1] L. Rosenberg, Phys. Rev. **135**, B715 (1964); R. G. Newton, J. Math. Phys. **8**, 851 (1967).

[2] L. D. Faddeev, *Mathematical Aspects of the Three-Body Problem in Quantum Scattering Theory* (Davey, New York, 1965).

[3] L. D. Faddeev, Zh. Eksp. Teor. Fiz. **39**, 1459 (1960) [Sov. Phys. JETP **12**, 1014 (1961)]; Dokl. Akad. Nauk SSSR **138**, 565 (1961) [Sov. Phys. Doklady **6**, 384 (1961)].

[4] M. Rubin, R. Sugar, and G. Tiktopoulos, Phys. Rev. **159**, 1348 (1967).

[5] Our notation is generally to use small letters for operators on a two-particle Hilbert space [in the center of mass system, so that it is $\mathfrak{L}^2(R^3)$] and capital letters for operators on the three-particle Hilbert space.

[6] K. Meetz, J. Math. Phys. **3**, 690 (1961); J. Schwinger, Proc. Natl. Acad. Sci. (U.S.) **47**, 122 (1961); F. Coester, Phys. Rev. **133**, B1516 (1964); M. Scadron, S. Weinberg, and J. A. Wright, *ibid.* **135**, B202 (1964).

[7] We multiply V_1 by λ_1, V_2 by λ_2, and V_3 by λ_3, and then rule out isolated singularities of the resulting analytic function of three variables.

[8] *Note added in proof:* The author has meanwhile found alternative expressions for the d_{ijk} that do not depend on the factorizations (1.26)–(1.27″). They will be presented in a subsequent publication.

[9] These are the same variables used by C. Lovelace, in *Strong Interactions and High Energy Physics*, edited by R. G. Moorehouse (Oliver and Boyd, London, 1964), p. 437.

[10] See K. Meetz, Ref. 6.

[11] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), p. 281.

[12] C. Zemach and A. Klein, Nuovo Cimento **10**, 1078 (1958).

[13] Ref. 11, p. 284.

[14] An exception to this statement is the case in which $E_n = 0$ and the eigenvector is spherically symmetric. Then there is no bound state even though $k(0)$ has the eigenvalue 1. (Note that this and all our specific statements below concerning the exceptional nature of $E_n = 0$ are based on the assumption that the potentials are spherically symmetric, which otherwise has not been assumed in this paper.)

[15] V. Bargmann, Proc. Natl. Acad. Sci. (U.S.) **38**, 961 (1952).

[16] There are two exceptions to this statement: If there is a "zero-energy resonance," i.e., if the s-wave cross section at zero energy

is infinite; or if there is a zero-energy bound state. In both cases the spectrum of $k(0)$ includes the point 1, but, in the first case, $E = 0$ is not in the point spectrum of h, while in the second case it is. In both cases $m'(0)$ is not a bounded operator and, in fact, it will generally not exist. These two exceptional cases should be kept in mind in all our subsequent results.

[17] If there is a zero-energy resonance or bound state, then $M'(E)$ is a bounded operator only for $E < 0$. The remark of Footnote 16 implies that, for $E \geq 0$, $M'(E)$ is unbounded.

[18] Constants such as C, R_0, r_0, etc., will be used generically, without any implication that they must have the same values when they are used in various contexts.

[19] A. Erdelyi, *Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. I, p. 75.

[20] A. Erdelyi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. II, p. 85.

[21] A. Erdelyi, Ref. 19, Vol. I, p. 16.

[22] If the binding energy is not zero, the bound-state wavefunction is bounded and decreases exponentially; see Ref. 11, pp. 332, 334, and 372–73. If the binding energy is zero (which implies that the angular momentum l is greater than zero) then its decrease is as r^{-l-1}; see Ref. 11, p. 375, Eq. (12.152). Hence, if the potential satisfies (3.5), then so do all the bound-state wavefunctions, except those of P- and D-wave zero-energy bound states. The D-wave case is close enough to (3.5) to make the arguments used here still applicable. Only the P-wave zero-energy bound-state case requires separate consideration. However, these had to be excluded in any case; see Footnote 16.

[23] For this argument to be valid, we must assume that the (1, 3) bound state whose wavefunction is $\varphi_m(\mathbf{r}_3)$ either has nonvanishing binding energy or else, if its binding energy is zero, its angular momentum is at least equal to 2; see Footnote 22. Of course, if V_1 decreases faster than (3.5), then a P-wave zero-energy bound state would be all right.

[24] Note that the determinants are modified Fredholm determinants of $\mathfrak{L}^2$ kernels, so that

$$\det[(\mathbb{1} - A)(\mathbb{1} - B)] = \det(\mathbb{1} - A)\det(\mathbb{1} - B)\exp(-\mathrm{tr}\,AB).$$

[25] See, for example, R. T. Gunning and H. Rossi, *Analytic Functions of Several Complex Variables* (Prentice-Hall, Englewood Cliffs, N.J., 1965), p. 2.

[26] Ref. 25, p. 21.

[27] It is assumed for simplicity that the determinant has a simple zero at $\lambda = \lambda_i'$. If it has a multiple zero, the argument is similar.

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Glauber Amplitudes in Charged Particle Hydrogen Atom Collisions*

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The Glauber scattering amplitudes for the excitation of the ns and np levels of atomic hydrogen by electrons (or protons) incident upon the ground state have been obtained in closed form. In contradistinction to previously quoted results, these new expressions require no numerical integration. For small n, the amplitudes reduce to simple sums of hypergeometric functions. Hence the Glauber amplitudes for these transitions now can be computed with scarcely more difficulty than the Born amplitudes. A selection rule for arbitrary transitions is derived.

I. INTRODUCTION

Recently, the Glauber approximation[1] for scattering amplitudes has been applied, with considerable success, to elastic and inelastic scattering of electrons[2–4] and of protons[5] by atomic hydrogen. In electron–hydrogen collisions especially, the Glauber approximation has been shown to be more useful than the Born approximation for estimating differential and total cross sections. However, the usefulness of the approximation would be appreciably enhanced if these Glauber amplitudes could be expressed in forms more readily computable than those already quoted in the literature.[2,3]

We have, therefore, reconsidered the Glauber scattering amplitudes for the excitation of atomic hydrogen by the impact of arbitrary structureless charged particles. By approaching the amplitude integrals in a slightly novel way, we have been able to obtain closed form expressions for the amplitudes. In contradistinction to the previously quoted results, these new expressions require no numerical integration. Specifically, for the transitions $1s \to ns$, np, the amplitudes reduce to finite sums of hypergeometric functions; when n is small, these sums involve comparatively few terms and are very simple to compute.

The contents of this paper now can be summarized explicitly, as follows. In Sec. II we discuss the reduction of the amplitude integrals corresponding to the two classes of transitions $1s \to ns$ and $1s \to np$, where n is arbitrary; the amplitudes in each class are expressed in terms of a generating function. We conclude Sec. II with several examples from the above classes. In particular we present expressions for the amplitudes $1s \to 1s$, $2s$, $2p$. In Sec. III, a selection rule for arbitrary hydrogenic transitions is derived.

For convenience, certain details of the analysis leading to the aforementioned results are deferred to appendices. In Appendix A we derive a useful and novel (at least to our knowledge) integral representation for the integral

$$\mathfrak{I}_m \equiv \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{im\varphi}(1 + s^2 - 2s\cos\varphi)^{i\eta},$$

is infinite; or if there is a zero-energy bound state. In both cases the spectrum of $k(0)$ includes the point 1, but, in the first case, $E = 0$ is not in the point spectrum of h, while in the second case it is. In both cases $m'(0)$ is not a bounded operator and, in fact, it will generally not exist. These two exceptional cases should be kept in mind in all our subsequent results.

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For convenience, certain details of the analysis leading to the aforementioned results are deferred to appendices. In Appendix A we derive a useful and novel (at least to our knowledge) integral representation for the integral

$$\mathfrak{I}_m \equiv \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{im\varphi}(1 + s^2 - 2s\cos\varphi)^{i\eta},$$

where η is purely real and m is a positive or negative integer. In previous computations[2,3] the integral $\mathfrak{I}_m$ has been expressed as a hypergeometric function, but that simplification did not enable determining a closed form expression for the scattering amplitude, which involves a further integration over the variable s on which $\mathfrak{I}_m$ depends. Use of our new integral representation for $\mathfrak{I}_m$ yields the scattering amplitude in terms of double integrals of the form

$$\mathfrak{K}_{m,r} \equiv \int_0^\infty ds\, s^{1+m}\left(s^2+\frac{q^2}{\lambda^2}\right)^{-2-m-r} \times \int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}\left[J_m(t)J_m(st)\right],$$

where m and r are integers greater than or equal to zero. The reduction of the integrals $\mathfrak{K}_{m,r}$ to closed form hypergeometric functions is given in Appendix B. The results of these two appendices enable us to express the scattering amplitude in closed form as a finite sum of hypergeometric functions. In Appendix C we discuss the behavior of the generating functions, and hence the scattering amplitudes, in the limit of small momentum transfers.

II. THE REDUCTION OF THE GLAUBER AMPLITUDES

In this section we consider the scattering of an arbitrary, structureless, spinless particle of charge Z by ground state atomic hydrogen. Let $\hbar\mathbf{K}_i$, $\hbar\mathbf{K}_f \equiv \mu\mathbf{v}_i$, $\mu\mathbf{v}_f$ define the initial and final momenta of the incident particle in the center of mass system, where μ is the reduced mass of the incident particle–hydrogen atom pair and $\mathbf{v}_i$ and $\mathbf{v}_f$ are respectively the initial and final relative velocities of the colliding particles. If the hydrogen atom is initially at rest, $\mathbf{v}_i$ is just the velocity of the incident particle in the laboratory. Furthermore, define the momentum transfer vector $\mathbf{q}$ by

$$\mathbf{q} \equiv \mathbf{K}_i - \mathbf{K}_f.$$

Then the Glauber approximation to the scattering amplitude $F(i\to f;\mathbf{q})$, in the center of mass system, for collisions in which the atom, initially in some state i, is directly excited to some final state f, is

$$F(i\to f;\mathbf{q}) = \frac{iK_i}{2\pi}\int u_f^*(\mathbf{r})\Gamma(\mathbf{b},\mathbf{r})u_i(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{b}}\,d\mathbf{r}\,d^2b, \quad (1)$$

where u_i and u_f are the initial and final bound state wavefunctions of the atom,

$$\Gamma(\mathbf{b},\mathbf{r}) = 1 - e^{i\chi(\mathbf{b},\mathbf{r})},$$

and the phase shift function χ is defined by

$$\chi(\mathbf{b},\mathbf{r}) = \frac{1}{\hbar v_i}\int_{-\infty}^{\infty} V(\mathbf{b},\mathbf{r};z')\,dz', \quad (2)$$

where $V(\mathbf{b},\mathbf{r};z')$ is the potential seen by the incident particle. In the case of incident electrons, identifying (1) with the scattering amplitude ignores electron exchange (i.e., ignores the effects of particle indistinguishability), as has been discussed previously.[4] In addition, spin-dependent interactions between the incident particle and the hydrogen atom will be ignored, i.e., V is nothing more than the sum of Coulombic interactions between the incident particle and the electron–proton pair.

In Eqs. (1) and (2), $\mathbf{r}'$ and $\mathbf{r}$ denote the coordinates, relative to the atomic nucleus, of the incident particle and the bound electron, respectively, and are expressed as

$$\mathbf{r}' = \mathbf{b} + z'\hat{\boldsymbol{\xi}},$$
$$\mathbf{r} = \mathbf{s} + z\hat{\boldsymbol{\xi}},$$

where $\hat{\boldsymbol{\xi}}$ is the direction in the center of mass system along which the integration in Eq. (2) is performed. To make the five-dimensional integrals of Eq. (1) tractable, we quantize all bound state wavefunctions along the same direction $\hat{\boldsymbol{\xi}}$. Evidently the above relations mean z' and z are the components of $\mathbf{r}'$ and $\mathbf{r}$, respectively, parallel to $\hat{\boldsymbol{\xi}}$, while $\mathbf{b}$ and $\mathbf{s}$ are the projections of $\mathbf{r}'$ and $\mathbf{r}$, respectively, onto the plane perpendicular to $\hat{\boldsymbol{\xi}}$. Furthermore, in Eq. (1) $\mathbf{q}$ is assumed to lie in the plane containing $\mathbf{b}$ and $\mathbf{s}$. For structureless particles of charge Z incident upon atomic hydrogen (with V purely Coulombic, as explained above), it is now readily seen that[2]

$$\chi(\mathbf{b},\mathbf{r}) = 2\eta\ln(|\mathbf{b}-\mathbf{s}|/b),$$

where $\eta = -Ze^2/\hbar v_i$.

A. $1s\to ns$ Amplitudes

The Glauber amplitudes of Eq. (1) for the class of transitions $1s\to ns$ can be considered as a whole; this class includes, of course, elastic scattering from the ground state. The product $u_f^*u_i$ appearing in Eq. (1) then reduces to[6]

$$u_f^*(\mathbf{r})u_i(\mathbf{r}) = -\frac{1}{4\pi}\left(\frac{2}{a_0}\right)^3\frac{1}{2}\left[\frac{(n-1)!}{n^4(n!)^3}\right]^{\frac{1}{2}}e^{-\frac{1}{2}\rho_i}e^{-\frac{1}{2}\rho_f}L_n^1(\rho_f), \quad (3)$$

where $L_n^1(\rho_f)$ is the generalized Laguerre polynomial and

$$\rho_i = \frac{2}{a_0}r, \quad \rho_f = \frac{2}{a_0 n}r, \quad \text{and} \quad r = (s^2+z^2)^{\frac{1}{2}};$$

a_0 is the Bohr radius. The conventional definition of the generalized Laguerre polynomial[6]

$$L_{n+l}^{2l+1}(\rho) = -[(n+l)!]^2 \times \sum_{j=0}^{n-l-1} \frac{(-1)^j \rho^j}{(n-l-1-j)!\,(2l+1+j)!\,j!} \tag{4a}$$

is a bit cumbersome. However, we note that if j has the range of values indicated in Eq. (4a), excluding for the moment $j = 0$, then

$$\begin{aligned}(n-l-1-j)! &= \frac{(n-l-1)!}{(n-l-1)(n-l-2)\cdots(n-l-1-(j-1))} \\ &= \frac{(n-l-1)!}{(-1)^j(-n+l+1)_j},\end{aligned} \tag{4b}$$

where $(a)_j$ is Pochhammer's symbol.[7] Moreover, since $(a)_0 \equiv 1$ for all a, Eq. (4b) is valid for all j in the range of (4a). Inserting (4b) into (4a) and removing a factor $(2l+1)!$ from the denominator of (4a), we obtain a convenient alternative to (4a), namely

$$L_{n+l}^{2l+1}(\rho) = -\frac{[(n+l)!]^2}{(n-l-1)!\,(2l+1)!} \times {}_1F_1(-n+l+1; 2l+2; \rho), \tag{4c}$$

where ${}_1F_1$ is the conventionally defined confluent hypergeometric function.[8] In particular

$$L_n^1(\rho) = -\frac{(n!)^2}{(n-1)!} \sum_{j=0}^{n-1} \frac{(-n+1)_j}{(2)_j j!} \left(\frac{2r}{na_0}\right)^j. \tag{4d}$$

With Eq. (4d), Eq. (3) becomes

$$u_f^* u_i = \frac{1}{4\pi}\left(\frac{2}{a_0}\right)^3 \frac{1}{2}\left(\frac{n!}{n^4(n-1)!}\right)^{\frac{1}{2}} e^{-(1/a_0)(1+1/n)r} \times \sum_{j=0}^{n-1} \frac{(-n+1)_j}{(2)_j j!}\left(\frac{2r}{na_0}\right)^j. \tag{5}$$

By inserting (5) into (1), the amplitude becomes

$$F(1s \to ns; \mathbf{q}) = \frac{iK_i}{(2\pi)^2} A_n \sum_{j=0}^{n-1} \alpha_j(n) \int r^j e^{-(1/a_0)(1+1/n)r} \times \left[1 - \left(\frac{|\mathbf{b}-\mathbf{s}|}{b}\right)^{2i\eta}\right] e^{i\mathbf{q}\cdot\mathbf{b}}\, d\mathbf{r}\, d^2b, \tag{6}$$

where

$$A_n \equiv (2/a_0)^3 \tfrac{1}{4}[n!/n^4(n-1)!]^{\frac{1}{2}} = (2/a_0)^3 \tfrac{1}{4} n^{-\frac{3}{2}}$$

and

$$\alpha_j(n) \equiv [(-n+1)_j/(2)_j j!](2/na_0)^j.$$

Equation (6) can be written in terms of a generating function $I_0(\lambda, q)$ such that

$$F(1s \to ns; \mathbf{q}) = iK_i A_n \left\{\sum_{j=0}^{n-1} \alpha_j(n)(-1)^{j+1} \frac{\partial^{j+1}}{\partial \lambda^{j+1}} I_0(\lambda, q)\right\}\Big|_{\lambda=(1/a_0)[1+(1/n)]},$$

where

$$I_0(\lambda, q) = \frac{1}{(2\pi)^2} \int e^{-\lambda r} \frac{1}{r}\left[1 - \left(\frac{|\mathbf{b}-\mathbf{s}|}{b}\right)^{2i\eta}\right] e^{i\mathbf{q}\cdot\mathbf{b}}\, d\mathbf{r}\, d^2b. \tag{7}$$

Note that the above generating function differs slightly from the generating function $I_0(\lambda, q)$ defined by Eq. (11) of Tai *et al.*[4] The generating function of Eq. (7) contains an extra factor of r^{-1}, which does not affect the convergence properties of the integrals. Now introduce polar coordinates in the plane containing $\mathbf{s}$ and $\mathbf{b}$ such that

$$\mathbf{q}\cdot\mathbf{b} = qb\cos(\varphi_b - \varphi_q)$$

and

$$|\mathbf{b}-\mathbf{s}| = [b^2 + s^2 - 2bs\cos(\varphi_s - \varphi_b)]^{\frac{1}{2}}. \tag{8}$$

Of course, $r = (s^2+z^2)^{\frac{1}{2}}$. Via the periodic properties of the cosine functions, the generating function $I_0(\lambda, q)$ then becomes

$$I_0(\lambda, q) = \frac{1}{(2\pi)^2}\int_0^\infty b\,db \int_0^\infty s\,ds \int_{-\infty}^\infty dz\, \frac{e^{-\lambda(s^2+z^2)^{\frac{1}{2}}}}{(s^2+z^2)^{\frac{1}{2}}} \times \int_0^{2\pi} d\varphi_b e^{iqb\cos\varphi_b} \times \int_0^{2\pi} d\varphi_s \left[1 - \left(\frac{b^2+s^2-2bs\cos\varphi_s}{b^2}\right)^{i\eta}\right] \tag{9}$$

$$= \frac{1}{2\pi}\int_0^\infty b\,db \int_0^\infty s\,ds \int_{-\infty}^\infty dz\, \frac{e^{-\lambda(s^2+z^2)^{\frac{1}{2}}}}{(s^2+z^2)^{\frac{1}{2}}} J_0(qb) \times \int_0^{2\pi} d\varphi_s \left[1 - \left(\frac{b^2+s^2-2bs\cos\varphi_s}{b^2}\right)^{i\eta}\right] \tag{10}$$

$$= \frac{1}{\pi}\int_0^\infty b\,db \int_0^\infty s\,ds K_0(\lambda s) J_0(qb) \times \int_0^{2\pi} d\varphi_s \left[1 - \left(\frac{b^2+s^2-2bs\cos\varphi_s}{b^2}\right)^{i\eta}\right]. \tag{11}$$

The reduction of Eq. (9) to Eq. (11) parallels closely the preliminary reduction of Eq. (11) of Tai *et al.* However, at this point we depart from the analysis of Refs. 2 and 4. In Eq. (11) replace s by bs. The integral over φ_s now is independent of b; moreover, the orders of integration over s and b may be interchanged.

Next, the integral over b may be done by using[9]

$$\int_0^\infty db\, b^3 J_0(qb)K_0(\lambda sb) = \frac{4}{(\lambda s)^4}\, {}_2F_1\left(2, 2; 1; -\frac{q^2}{\lambda^2 s^2}\right).$$

Consequently,

$$I_0(\lambda, q) = 8\int_0^\infty s\, ds(\lambda s)^{-4}\, {}_2F_1\left(2, 2; 1; -\frac{q^2}{\lambda^2 s^2}\right) \times \left(1 - \frac{1}{2\pi}\int_0^{2\pi}(1 + s^2 - 2s\cos\varphi_s)^{i\eta}\, d\varphi_s\right). \tag{12}$$

When q is nonzero, the term in Eq. (12), proportional to the first term in brackets, vanishes. This is seen as follows. Let $z = q^2(\lambda s)^{-2}$ so that $2s^{-3}\, ds = -\lambda^2 q^{-2}\, dz$ and

$$8\int_0^\infty s\, ds(\lambda s)^{-4}\, {}_2F_1\left(2, 2; 1; -\frac{q^2}{\lambda^2 s^2}\right) = \frac{4}{\lambda^2 q^2}\int_0^\infty dz\, {}_2F_1(2, 2; 1; -z). \tag{13a}$$

However,[10]

$$\int_0^\infty {}_2F_1(a, b; c; -z)z^{-s-1}\, dz = \frac{\Gamma(a + s)\Gamma(b + s)\Gamma(c)\Gamma(-s)}{\Gamma(a)\Gamma(b)\Gamma(c + s)}$$

provided $c \neq 0, -1, \cdots$, $\mathrm{Re}\, s < 0$, $\mathrm{Re}\,(a + s)$, $\mathrm{Re}\,(b + s) > 0$. In the right side of (13a), $s = -1$ and the above conditions are satisfied. Moreover, $\Gamma(c + s) = \Gamma(0)$. Hence, for nonzero q

$$8\int_0^\infty s\, ds(\lambda s)^{-4}\, {}_2F_1\left(2, 2; 1; -\frac{q^2}{\lambda^2 s^2}\right) = 0. \tag{13b}$$

One also can verify (13b) directly for nonzero q by explicity expanding the hypergeometric function [see, for example, Eq. (16)] and then integrating over s.

If $q = 0$, the integral over s in the left side of (13a) does not exist; the integral is strongly divergent. Hence, the first term in Eq. (12) diverges at $q = 0$. However, the second term in Eq. (12) diverges absolutely; moreover, the divergence is of the same order as the first term. In fact, the divergence of the integral in (12) at $q = 0$ is of a lower order than either of the first or second terms in (12). Since (13b) is strictly valid for all nonzero q, the only physical way to define $I_0(\lambda, 0)$ is as limit as $q \to 0$ of $I_0(\lambda, q)$, where $I_0(\lambda, q)$ is obtained from Eq. (12) using Eq. (13b). In order to be sure that, in using (13b), we do not neglect a significant contribution to I_0 (and hence the amplitude) at $q = 0$, we have examined the asymptotic behavior of the integrals in Eq. (12) as $q \to 0$. In Appendix C we explicitly show that the asymptotic behavior of Eq. (12) as $q \to 0$ is identical with the asymptotic behavior of our final expression for $I_0(\lambda, q)$ obtained with (13b).

The φ_s integral of Eq. (12) is of the class $\mathfrak{I}_m$ defined in Sec. I and discussed in Appendix A. The case $m = 0$ is of interest in this present subsection. Letting $m = 0$ in Eq. (A6) of Appendix A, we have

$$\frac{1}{2\pi}\int_0^{2\pi}(1 + s^2 - 2s\cos\varphi_s)^{i\eta}\, d\varphi_s = -2^{2i\eta}\frac{\Gamma(1 + i\eta)}{\Gamma(1 - i\eta)}\int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}[J_0(st)J_0(t)]. \tag{14}$$

Integrating by parts does not simplify the right side of (14) [see comments following Eq. (A6)]. With Eqs. (13b) and (14), Eq. (12) becomes

$$I_0(\lambda, q) = 8\int_0^\infty s\, ds(\lambda s)^{-4}\, {}_2F_1\left(2, 2; 1; -\frac{q^2}{\lambda^2 s^2}\right) \times 2^{2i\eta}\frac{\Gamma(1 + i\eta)}{\Gamma(1 - i\eta)}\int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}[J_0(st)J_0(t)]; \tag{15}$$

Eq. (15) can be handled best by expanding the hypergeometric function. Applying the standard analytic continuation formulas[11] for the ${}_2F_1$, we get

$$\begin{aligned} {}_2F_1\left(2, 2; 1; -\frac{q^2}{\lambda^2 s^2}\right) &= \left(1 + \frac{q^2}{\lambda^2 s^2}\right)^{-2}\, {}_2F_1\left(2, -1; 1; \frac{q^2/\lambda^2 s^2}{1 + q^2/\lambda^2 s^2}\right) \\ &= s^4\left(s^2 + \frac{q^2}{\lambda^2}\right)^{-2}\left[1 - \frac{2q^2/\lambda^2}{(s^2 + q^2/\lambda^2)}\right]. \end{aligned} \tag{16}$$

Hence

$$I_0(\lambda, q) = 2^{2i\eta+3}\frac{\Gamma(1 + i\eta)}{\Gamma(1 - i\eta)}\frac{1}{\lambda^4} \times \int_0^\infty s\, ds\left(s^2 + \frac{q^2}{\lambda^2}\right)^{-2}\left[1 - \frac{2q^2/\lambda^2}{s^2 + q^2/\lambda^2}\right] \times \int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}[J_0(st)J_0(t)]. \tag{17}$$

The two terms in (17) are multiple integrals of the class discussed in Appendix B. They are $\mathcal{K}_{0,0}$ and $\mathcal{K}_{0,1}$ as defined by Eq. (B1). Therefore,

$$I_0(\lambda, q) = 2^{2i\eta+3}[\Gamma(1 + i\eta)/\Gamma(1 - i\eta)\lambda^4] \times [\mathcal{K}_{0,0} - 2(q^2/\lambda^2)\mathcal{K}_{0,1}],$$

which reduces, via (B6) or (B7), to

$$I_0(\lambda, q) = -4\lambda^{-2-2i\eta}q^{-2+2i\eta}\Gamma(1 + i\eta)\Gamma(1 - i\eta) \times [{}_2F_1(-i\eta + 1, -i\eta; 1; -\lambda^2/q^2) - (1 - i\eta)\, {}_2F_1(-i\eta + 2, -i\eta; 1; -\lambda^2/q^2)]. \tag{18}$$

The two hypergeometric functions in (18) may be combined via a Gauss recursion relation[12]

$$(\beta - \alpha)\,{}_2F_1(\alpha, \beta; \gamma; z) + \alpha\,{}_2F_1(\alpha + 1, \beta; \gamma; z) - \beta\,{}_2F_1(\alpha, \beta + 1; \gamma; z) = 0.$$

Hence,

$$F(1s \to ns; \mathbf{q}) = iK_i\left(\frac{2}{a_0}\right)^3 \tfrac{1}{4} n^{-\frac{3}{2}} \sum_{j=0}^{n-1} \alpha_j(n)(-1)^{j+1} \times \frac{\partial^{j+1}}{\partial \lambda^{j+1}} I_0(\lambda, q)\Big|_{\lambda=(1/a_0)(1+1/n)}, \quad (19a)$$

where

$$\alpha_j(n) \equiv [(-n+1)_j/(2)_j j!]\left(\frac{2}{na_0}\right)^j, \quad (19b)$$

$$I_0(\lambda, q) = -4i\eta\Gamma(1 + i\eta)\Gamma(1 - i\eta)\lambda^{-2-2i\eta} q^{-2+2i\eta} \times {}_2F_1(-i\eta + 1, -i\eta + 1; 1; -\lambda^2/q^2); \quad (19c)$$

Eq. (19) is the desired closed form expression for $F(1s \to ns; \mathbf{q})$.

B. $1s \to np$ Transitions

The amplitudes for transitions of the class $1s \to np$ can be considered in much the same way as in the previous subsection. Quantizing the atomic wavefunctions along $\hat{\xi}$, we again introduce polar coordinates such that Eqs. (8) are satisfied. Hence the product $u_f^*(\mathbf{r})u_i(\mathbf{r})$ appearing in Eq. (1) becomes

$$u_f^*(\mathbf{r})u_i(\mathbf{r}) = -\frac{1}{4\pi}\left(\frac{3(1-|m|)!}{(1+|m|)!}\right)^{\frac{1}{2}}\left(\frac{2}{a_0}\right)^3 \frac{1}{2}\left(\frac{(n-2)!}{n^4[(n+1)!]^3}\right)^{\frac{1}{2}} \times e^{-\frac{1}{2}(\rho_i+\rho_f)}\rho_f L_{n+1}^3(\rho_f) P_1^{|m|}\left(\frac{\mathbf{r}\cdot\hat{\xi}}{r}\right) e^{-im\varphi_s}, \quad (20)$$

where L_{n+1}^3, ρ_i, and ρ_f are as previously defined and $m = 0, \pm 1$. However, from Eq. (4c),

$$L_{n+1}^3(\rho_f) = -\frac{[(n+1)!]^2}{(n-2)!\,3!}\,{}_1F_1(-n+2; 4; \rho_f), \quad (21a)$$

where $n \geq 2$. Furthermore, we note that

$$\mathbf{r}\cdot\hat{\xi}/r = z/(s^2 + z^2)^{\frac{1}{2}}. \quad (21b)$$

Therefore, using Eqs. (21) in Eq. (20) and expanding the confluent hypergeometric function of (21a), we obtain for the amplitudes of Eq. (1)

$$F(1s \to np_m; \mathbf{q}) = \frac{iK_i}{(2\pi)^2}\frac{\sqrt{3}}{4}\left(\frac{(1-|m|)!}{(1+|m|)!}\right)^{\frac{1}{2}}\left(\frac{2}{a_0}\right)^4 \frac{1}{n}\left[\frac{(n+1)!}{n^4(n-2)!}\right]^{\frac{1}{2}}\frac{1}{3!} \times \sum_{j=0}^{n-2}\beta_j(n)\int_0^\infty b\,db\int_0^{2\pi}d\varphi_b\int_0^{2\pi}d\varphi_s\int_0^\infty s\,ds\int_{-\infty}^\infty dz \times e^{i\mathbf{q}\cdot\mathbf{b}}e^{-(1/a_0)(1+1/n)r_f}r_f^{j+1}\left[P_1^{|m|}\left(\frac{z}{(s^2+z^2)^{\frac{1}{2}}}\right)\right] \times e^{-im\varphi_s}\left[1 - \left(\frac{b^2 + s^2 - 2bs\cos(\varphi_s - \varphi_b)}{b^2}\right)^{i\eta}\right], \quad (22a)$$

where

$$\beta_j(n) = \frac{(-n+2)_j}{j!\,(4)_j}\left(\frac{2}{na_0}\right)^j. \quad (22b)$$

In Eq. (22a), the integral over z is of the form

$$\int_{-\infty}^\infty dz\, f((s^2+z^2)^{\frac{1}{2}})\left[P_1^{|m|}\left(\frac{z}{(s^2+z^2)^{\frac{1}{2}}}\right)\right].$$

However, the parity of the $P_1^{|m|}$ is $(-1)^{1-|m|}$; hence, when $m = 0$,

$$F(1s \to np, m = 0; \mathbf{q}) \equiv 0.$$

Therefore, one only needs to evaluate (22a) for magnetic quantum numbers $m = \pm 1$. As in Subsection A, the amplitude of Eq. (22a) can be expressed in terms of a generating function $I_1(\lambda, q)$. From the periodic properties of the trigonometric functions one can show that

$$F(1s \to np_{\pm 1}; \mathbf{q}) = 2iK_i(\tfrac{3}{2})^{\frac{1}{2}}\frac{1}{4!}\left(\frac{2}{a_0}\right)^4\frac{1}{n^3}\left[\frac{(n+1)!}{(n-2)!}\right]^{\frac{1}{2}} e^{-im\varphi_q} \times \sum_{j=0}^{n-2}\beta_j(n)(-1)^{j+1}\frac{\partial^{j+1}}{\partial\lambda^{j+1}} I_1(\lambda, q)\Big|_{\lambda=(1/a_0)(1+1/n)}, \quad (23a)$$

where

$$I_1(\lambda, q) = \frac{1}{(2\pi)^2}\int_0^\infty b\,db\int_0^\infty s^2\,ds\int_0^\infty dz\,\frac{e^{-\lambda(s^2+z^2)^{\frac{1}{2}}}}{(s^2+z^2)^{\frac{1}{2}}} \times \int_0^{2\pi}d\varphi_b \exp i(qb\cos\varphi_b - m\varphi_b)\int_0^{2\pi}d\varphi_s \times e^{-im\varphi_s}\left[1 - \left(\frac{b^2+s^2-2bs\cos\varphi_s}{b^2}\right)^{i\eta}\right]. \quad (23b)$$

In (23a), φ_q is the polar angle of $\mathbf{q}$ in the plane perpendicular to $\hat{\xi}$. The reduction of Eq. (23b) is similar to

that of Eq. (9). We find, then, that

$$I_1(\lambda, q) = \frac{i}{2\pi}\int_0^\infty b\,db\int_0^\infty s^2\,ds K_0(\lambda s)J_1(qb)\int_0^{2\pi} d\varphi_s \times e^{-im\varphi_s}\left[1-\left(\frac{b^2+s^2-2bs\cos\varphi_s}{b^2}\right)^{i\eta}\right]$$
$$= -\frac{i}{2\pi}\int_0^\infty b^4\,db\int_0^\infty s^2\,ds K_0(\lambda sb)J_1(qb) \times \int_0^{2\pi} d\varphi_s e^{-im\varphi_s}(1+s^2-2s\cos\varphi_s)^{i\eta} \tag{24a}$$

by letting $s \to bs$. The orders of integration over b and s may now be interchanged. Furthermore,[9,11]

$$\int_0^\infty db\, b^4 K_0(\lambda sb)J_1(qb)$$
$$= 2^5(\lambda s)^{-6} q\, {}_2F_1(3,3;2;-q^2/\lambda^2 s^2)$$
$$= 2^5 q(\lambda s)^{-6}\left(1+\frac{q^2}{\lambda^2 s^2}\right)^{-3} {}_2F_1\left(3,-1;2;\frac{q^2/\lambda^2}{s^2+q^2/\lambda^2}\right)$$
$$= 2^5 q\lambda^{-6}\left(s^2+\frac{q^2}{\lambda^2}\right)^{-3}\left(1-\frac{3}{2}\frac{q^2/\lambda^2}{(s^2+q^2/\lambda^2)}\right). \tag{24b}$$

Again the integral over φ_s is of the class $\mathfrak{I}_m$ discussed in Appendix A where $|m| = 1$, so that

$$\frac{1}{2\pi}\int_0^{2\pi} e^{i(\pm 1)\varphi_s}(1+s^2-2s\cos\varphi_s)^{i\eta}\,d\varphi_s = -2^{2i\eta}\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}[J_1(st)J_1(t)].$$

Hence Eq. (24a) becomes

$$I_1(\lambda, q) = i2^{2i\eta+5}\frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}\lambda^{-6}q \times \int_0^\infty s^2\,ds\left(s^2+\frac{q^2}{\lambda^2}\right)^{-3}\left(1-\frac{3}{2}\frac{q^2/\lambda^2}{(s^2+q^2/\lambda^2)}\right) \times \int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}[J_1(st)J_1(t)]$$
$$= i2^{2i\eta+5}[\Gamma(1+i\eta)/\Gamma(1-i\eta)]\lambda^{-6}q \times \{\mathcal{K}_{1,0} - \tfrac{3}{2}(q^2/\lambda^2)\mathcal{K}_{1,1}\}, \tag{25}$$

where $\mathcal{K}_{m,r}$ is defined in Appendix B. Therefore, using Eq. (B7), we have

$$I_1(\lambda, q) = i2^2\Gamma(1+i\eta)\Gamma(-i\eta+2)(i\eta)\lambda^{-2i\eta-2}q^{2i\eta-3} \times \{2\,{}_2F_1(-i\eta+2,-i\eta+1;2;-\lambda^2/q^2) - (-i\eta+2) \times {}_2F_1(-i\eta+3,-i\eta+1;2;-\lambda^2/q^2)\}. \tag{26}$$

The sum of hypergeometric functions in Eq. (26) may be rewritten via the Gauss recursion relations.[12] We, therefore, find that

$$F(1s \to 2p_0; \mathbf{q}) \equiv 0 \tag{27a}$$

and

$$F(1s \to 2p_{\pm 1}; \mathbf{q}) = 2iK_i(\tfrac{3}{2})^{\frac{1}{2}}\frac{1}{4!}\left(\frac{2}{a_0}\right)^4\frac{1}{n^3}\left(\frac{(n+1)!}{(n-2)!}\right)^{\frac{1}{2}}e^{\mp i\varphi_q} \times \sum_{j=0}^{n-2}\beta_j(n)(-1)^{j+1}\frac{\partial^{j+1}}{\partial\lambda^{j+1}}I_1(\lambda, q)\Big|_{\lambda=(1/a_0)(1+1/n)}, \tag{27b}$$

where

$$I_1(\lambda, q) = i4\Gamma(1+i\eta)\Gamma(2-i\eta)(i\eta)\lambda^{-2i\eta-2}q^{2i\eta-3} \times \{-{}_2F_1(-i\eta+2,-i\eta+1;1;-\lambda^2/q^2) + (1+i\eta) \times {}_2F_1(-i\eta+2,-i\eta+1;2;-\lambda^2/q^2)\}, \tag{27c}$$

$$\beta_j(n) = [(-n+2)_j/j!(4)_j](2/na_0)^j. \tag{27d}$$

Equations (27) complete the specification of the general amplitude $F(1s \to np)$.

C. Special Cases

The Glauber amplitudes for the five transitions $1s \to 1s$, $2s$, $2p$, $3s$, $3p$ have been discussed previously in the literature.[2-4] In each case the amplitude has been expressed in the form of a nontrivial integral of a hypergeometric function (or an equivalent double integral) which, heretofore, has been done numerically. Using Eqs. (19) and (27), one can reduce each of these amplitudes to a simple sum of hypergeometric functions which can be readily computed. We evaluate only the first three transition amplitudes as specific examples of the results of Eqs. (19) and (27).

Consider first the s transition amplitudes defined by Eqs. (19). When $n = 1$, Eq. (19a) reduces to

$$F(1s \to 1s; \mathbf{q}) = -iK_i(2/a_0)^3\tfrac{1}{4}\left[\frac{\partial}{\partial\lambda}I_0(\lambda, q)\right]\Big|_{\lambda=2/a_0};$$

I_0 is defined by (19c). The hypergeometric function in I_0 is readily differentiated via[13]

$$\frac{d}{dz}{}_2F_1(\alpha,\beta;\gamma;z) = (\alpha\beta/\gamma)\,{}_2F_1(\alpha+1,\beta+1;\gamma+1;z)$$

so that

$$F(1s \to 1s; \mathbf{q}) = -2iK_i(i\eta)\Gamma(1+i\eta)\Gamma(1-i\eta)(a_0/2)^2(2/a_0q)^{2-2i\eta} \times \{(1+i\eta)\,{}_2F_1(1-i\eta,1-i\eta;1;-4/a_0^2q^2) + (1-i\eta)^2(4/a_0^2q^2) \times {}_2F_1(2-i\eta,2-i\eta;2;-4/a_0^2q^2)\}. \tag{28a}$$

Furthermore, when $n = 2$,

$$F(1s \to 2s; \mathbf{q})$$
$$= -iK_i(2/a_0)^3 \frac{1}{8\sqrt{2}}\left\{\left(1 + \frac{1}{2a_0}\frac{\partial}{\partial\lambda}\right)\frac{\partial}{\partial\lambda} I_0(\lambda, q)\right\}\Big|_{\lambda=3/2a_0}$$
$$= iK_i \frac{4}{\sqrt{2}}(1/a_0)^4\lambda^{-6}(\lambda^2/q^2)^{1-i\eta}\Gamma(1 + i\eta)\Gamma(1 - i\eta)(i\eta)$$
$$\times \{2i\eta(1 + i\eta)\,{}_2F_1(1 - i\eta, 1 - i\eta; 1; -\lambda^2/q^2)$$
$$+ 4i\eta(1 - i\eta)^2(\lambda^2/q^2)$$
$$\times {}_2F_1(2 - i\eta, 2 - i\eta; 2; -\lambda^2/q^2)$$
$$+ (1 - i\eta)^2(2 - i\eta)^2(\lambda^4/q^4)$$
$$\times {}_2F_1(3 - i\eta, 3 - i\eta; 3; -\lambda^2/q^2)\}\big|_{\lambda=3/2a_0}. \quad (28b)$$

The $1s \to 2p$ transition amplitudes are determined by Eqs. (27). Setting $n = 2$, we find, for the nontrivial amplitude $1s \to 2p_{\pm 1}$,

$$F(1s \to 2p_{\pm 1}; \mathbf{q})$$
$$= -iK_i \tfrac{1}{2}(1/a_0)^4 e^{\mp i\varphi_q}\frac{\partial}{\partial\lambda} I_1(\lambda, q)\Big|_{\lambda=3/2a_0}, \quad (29a)$$

so that

$$F(1s \to 2p_{\pm 1}; \mathbf{q})$$
$$= -4K_i(a_0)^{-4}e^{\mp i\varphi_q}\Gamma(1 + i\eta)\Gamma(2 - i\eta)i\eta q^{-3+2i\eta}\lambda^{-2i\eta-3}$$
$$\times \{2(1 + i\eta)\,{}_2F_1(2 - i\eta, 1 - i\eta; 2; -\lambda^2/q^2)$$
$$- (2 - i\eta)(1 + i\eta + 2\lambda^2/q^2)$$
$$\times {}_2F_1(3 - i\eta, 2 - i\eta; 2; -\lambda^2/q^2)\}\big|_{\lambda=3/2a_0}. \quad (29b)$$

Equation (29b) is obtained from (29a) first by performing the indicated differentiation of $I_1(\lambda, q)$ with respect to λ and then by combining the four resulting hypergeometric functions via the Gauss recursion relations.

Our experience, together with the known properties of the Gauss recursion relations,[12] indicates that whenever more than two hypergeometric functions appear in the amplitudes, as determined by Eqs. (19) and (27), the amplitude expressions can be reduced further, via the Gauss relations, to a sum of two hypergeometric functions with coefficients which are rational functions of $i\eta$ and λ^2/q^2. The hypergeometric functions then can be readily computed from their standard expansions when $\lambda^2/q^2 < 1$ and their appropriate analytic continuation when $\lambda^2/q^2 > 1$. It appears, therefore, that these Glauber amplitudes now can be computed with scarcely more difficulty than the Born amplitudes.

III. SELECTION RULE FOR ARBITRARY TRANSITIONS

As one might suspect the results of Sec. II can be generalized to arbitrary excitations in atomic hydrogen. Furthermore, the rudimentary selection rule derived for $1s$, np transitions is fully generalizable. Consider a general transition in which the quantum numbers of the initial and final bound states are respectively nlm and $n'l'm'$. Again quantize the bound state wavefunctions along $\hat{\xi}$; then

$$F(i \to f; \mathbf{q})$$
$$= \frac{iK_i}{2\pi} A(i \to f)\int d^2b\, dr e^{i\mathbf{q}\cdot\mathbf{b}}\Gamma(\mathbf{b}, \mathbf{r})$$
$$\times R_{nl}(r)R_{n'l'}(r)P_l^{|m|}\left(\frac{\mathbf{r}\cdot\hat{\xi}}{r}\right)P_{l'}^{|m'|}\left(\frac{\mathbf{r}\cdot\hat{\xi}}{r}\right)e^{i(m-m')\varphi_s}, \quad (30)$$

where $R_{nl}(r)$ is the usual hydrogenic radial wavefunction and A is a normalization constant. Equations (8) still hold. As in Sec. II, the integrations over φ_s and φ_b may be separated so that

$$F(i \to f; \mathbf{q})$$
$$= \frac{iK_i}{2\pi} Ae^{i(m-m')\varphi_q}\int_0^\infty b\, db\int_0^{2\pi} d\varphi_b$$
$$\times \exp i[qb\cos\varphi_b + (m - m')\varphi_b]$$
$$\times \int_{-\infty}^{\infty} dz\int_0^\infty s\, ds R_{nl}(r)R_{n'l'}(r)P_l^{|m|}\left(\frac{\mathbf{r}\cdot\hat{\xi}}{r}\right)P_{l'}^{|m'|}\left(\frac{\mathbf{r}\cdot\hat{\xi}}{r}\right)$$
$$\times \int_0^{2\pi} d\varphi_s e^{i(m-m')\varphi_s}\left[1 - \left(\frac{b^2 + s^2 - 2bs\cos\varphi_s}{b^2}\right)^{i\eta}\right]. \quad (31)$$

The z integral in (31) immediately yields the Glauber selection rule for induced transitions in atomic hydrogen. Ignoring all other integrations, we have

$$F(i \to f; \mathbf{q}) \propto \int_{-\infty}^{\infty} dz\, f(r)P_l^{|m|}\left(\frac{\mathbf{r}\cdot\hat{\xi}}{r}\right)P_{l'}^{|m'|}\left(\frac{\mathbf{r}\cdot\hat{\xi}}{r}\right), \quad (32)$$

where $f(r)$ is defined by the radial functions and is a purely even function of z since $r = (s^2 + z^2)^{\frac{1}{2}}$. Recall that

$$\frac{\mathbf{r}\cdot\hat{\xi}}{r} = z(s^2 + z^2)^{-\frac{1}{2}}.$$

However, the parity of the associated Legendre polynomial $P_l^{|m|}$ is $l - |m|$; hence Eq. (32) becomes

$$F(i \to f; \mathbf{q})$$
$$\propto \int_0^\infty dz\, f(r)P_l^{|m|}[z(s^2 + z^2)^{-\frac{1}{2}}]P_{l'}^{|m'|}[z(s^2 + z^2)^{-\frac{1}{2}}]$$
$$\times [1 + (-1)^{l+l'-|m|-|m'|}].$$

Therefore, if $l + l' - |m| - |m'|$ is odd, the right side of (32) vanishes.

Hence, when the hydrogen bound state wavefunctions are quantized along $\hat{\xi}$, the Glauber amplitude

$$F(nlm \to n'l'm'; \mathbf{q}) \equiv 0 \tag{33}$$

when $l + l' + |m| + |m'| =$ odd integer. Otherwise, the amplitude is given by Eq. (31).

The techniques of Sec. II can be generalized to perform the reduction of Eq. (31) when $l + l' + |m| + |m'|$ is an arbitrary even integer. In this case, one can reduce (31) to the evaluation of a generating function which is related to the amplitude by an equation similar to, but far more complex than, either Eq. (19a) or Eq. (27b). The general result is given elsewhere.[14]

APPENDIX A: AN EQUIVALENT INTEGRAL FOR $\mathfrak{I}_m$

Whenever the Glauber approximation is applied to charged particle collisions with neutral atoms whose bound state wavefunctions are approximated by-products of hydrogenlike wavefunctions, one encounters integrals of the class

$$\mathfrak{I}_m = \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{im\varphi}(1 + s^2 - 2s\cos\varphi)^{i\eta}, \tag{A1}$$

where m is a positive or negative integer, η is purely real, and $0 \leq s < \infty$. Since $\sin(m\varphi)$ is an odd function, $\mathfrak{I}_m$ can be reduced to

$$\mathfrak{I}_m = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \cos(m\varphi)(1 + s^2 - 2s\cos\varphi)^{i\eta} \tag{A2}$$

and only $m \geq 0$ need be considered. The integral (A2) can be evaluated via[15]

$$\frac{1}{2\pi}\int_0^{2\pi} \frac{\cos(n\varphi)\, d\varphi}{(1 - 2z\cos\varphi + z^2)^{\alpha}} = \frac{\Gamma(\alpha + n)}{\Gamma(\alpha)n!} z^n {}_2F_1(\alpha, \alpha + n; 1 + n; z^2), \tag{A3}$$

provided

$$n = 0, 1, 2, \cdots, \quad \alpha \neq 0, -1, -2, \cdots, \quad |z| < 1.$$

When $s < 1$, (A2) is evaluated by directly applying (A3); when $s > 1$, one first removes a factor of s^2 from the integrand of (A2) and then applies (A3) to the resulting integral. Alternatively, (A2) can be evaluated by expanding $(1 + s^2 - 2s\cos\varphi)^{i\eta}$ in powers of $[2s\cos\varphi/(1 + s^2)]$ and integrating term by term. The hypergeometric function obtained from the latter method can be shown to be equivalent to the results obtained via (A3) by using a standard quadratic transformation.[16] However, the direct integration of (A2) is not particularly useful because it considerably complicates the ensuing integrals over s.

We, therefore, seek an integral representation for $\mathfrak{I}_m$ such that the integral over s is readily doable. This is accomplished as follows. It is known[17] that

$$\int_0^{\infty} t^{\mu-1}J_{\nu}(at)\, dt = 2^{\mu-1}a^{-\mu}\frac{\Gamma(\frac{1}{2}\nu + \frac{1}{2}\mu)}{\Gamma(1 + \frac{1}{2}\nu - \frac{1}{2}\mu)}$$

provided $-\mathrm{Re}\,\nu < \mathrm{Re}\,\mu < \frac{3}{2}$.

If $a \equiv (1 + s^2 - 2s\cos\varphi)^{\frac{1}{2}}$, then

$$a^{2i\eta-1} = 2^{2i\eta}\frac{\Gamma(1 + i\eta)}{\Gamma(1 - i\eta)}\int_0^{\infty} dt\, t^{-2i\eta}J_1(at), \tag{A4}$$

where $\mu = -2i\eta + 1$ and $\nu = 1$, thereby satisfying the above conditions on μ and ν. But

$$J_1(at) = -\frac{1}{a}\frac{d}{dt}J_0(at).$$

Hence

$$\begin{aligned}\mathfrak{I}_m &= \frac{1}{\pi}\int_0^{\pi} d\varphi \cos(m\varphi)(1 + s^2 - 2s\cos\varphi)^{i\eta} \\ &= -2^{2i\eta}\frac{\Gamma(1 + i\eta)}{\Gamma(1 - i\eta)}\frac{1}{\pi}\int_0^{\infty} dt\, t^{-2i\eta}\frac{d}{dt}\int_0^{\pi} d\varphi \cos(m\varphi) \\ &\quad \times J_0([1 + s^2 - 2s\cos\varphi]^{\frac{1}{2}}t).\end{aligned} \tag{A5}$$

To obtain (A5), we have assumed, for the moment, that interchanging the order of integration and differentiation with respect to t with the integration over φ is justified. As we shall ultimately see, this assumption is valid.

Now expand $J_0([1 + s^2 - 2s\cos\varphi]^{\frac{1}{2}}t)$ in the Neumann series[18]

$$J_0(at) = \sum_{n=0}^{\infty}\epsilon_n J_n(st)J_n(t)\cos(n\varphi),$$

where $\epsilon_0 = 1$, $\epsilon_n = 2$ for $n \geq 1$, and perform the integration over φ term by term. One readily finds that $\mathfrak{I}_m$ can be written

$$\begin{aligned}&\frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{im\varphi}(1 + s^2 - 2s\cos\varphi)^{i\eta} \\ &\quad = -2^{2i\eta}\frac{\Gamma(1 + i\eta)}{\Gamma(1 - i\eta)}\int_0^{\infty} dt\, t^{-2i\eta}\frac{d}{dt}[J_{|m|}(st)J_{|m|}(t)]\end{aligned} \tag{A6}$$

for arbitrary (positive or negative) integers m.

Equation (A6) is the desired result. It can be reduced by integrating by parts when $|m| > 0$. When $m = 0$, the first term from such a reduction is proportional to $t^{-2i\eta}J_0(st)J_0(t)$ evaluated at $t = 0$ and $t = \infty$. However, the limit of this term as $t \to 0$ is bounded but not defined. Hence, when $m = 0$, one must perform the indicated differentiation with respect to t in (A6).

Keeping the preceding remarks in mind, one can use the known hypergeometric function results for Weber–Schafheitlin discontinuous integrals[19] to evaluate the right side of (A6). (When $m = 0$, one obtains two hypergeometric functions which can be combined via the Gauss recursion relations.[20]) If these results are compared with those obtained, via (A3), from the left side of (A6), one immediately sees that the integrations on both sides of (A6) yield results identical for all $s \geq 0$. Thus we validate, *a posteriori*, the assumptions which led to equation (A5).

APPENDIX B: THE CLASS OF INTEGRALS $\mathcal{K}_{m,r}$

When the integral representation (A6), derived in Appendix A, is used to evaluate the Glauber amplitudes for arbitrary transitions in atomic hydrogen, one can express the amplitudes as finite sums of integrals $\mathcal{K}_{m,r}$ of the type

$$\mathcal{K}_{m,r} = \int_0^\infty ds\, s^{1+m}\left(s^2 + \frac{q^2}{\lambda^2}\right)^{-2-m-r} \times \int_0^\infty dt\, t^{-2i\eta}\frac{d}{dt}[J_m(t)J_m(st)], \quad \text{(B1)}$$

where m and r are integers greater than or equal to zero. The reduction of (B1) to a form easily computed is accomplished in a relatively straightforward way, provided one keeps in mind the comments following Eq. (A6).

First consider the case $m = 0$. Perform the differentiation as indicated. As long as $q^2/\lambda^2 > 0$, one may interchange the order of integrations so that (B1) becomes

$$\mathcal{K}_{0,r} = -\int_0^\infty dt\, t^{-2i\eta}\left[J_1(t)\int_0^\infty ds\, sJ_0(st)\left(s^2 + \frac{q^2}{\lambda^2}\right)^{-2-r} + J_0(t)\int_0^\infty ds\, s^2 J_1(st)\left(s^2 + \frac{q^2}{\lambda^2}\right)^{-2-r}\right]. \quad \text{(B2)}$$

However,[21]

$$\int_0^\infty dx\, \frac{J_\nu(bx)x^{\nu+1}}{(x^2 + a^2)^{\mu+1}} = \frac{a^{\nu-\mu}b^\mu K_{\nu-\mu}(ab)}{2^\mu\Gamma(\mu+1)}, \quad \text{(B3)}$$

provided $-1 < \operatorname{Re}\nu < \operatorname{Re}(2\mu + \frac{3}{2})$, $a, b > 0$.

Each term in (B2) satisfies the conditions of (B3) for all integers $r \geq 0$. Therefore, since $K_{-n}(z) = K_n(z)$,

$$\mathcal{K}_{0,r} = -\left(\frac{\lambda}{q}\right)^r 2^{-1-r}[\Gamma(2+r)]^{-1} \times \int_0^\infty dt\, t^{-2i\eta+1+r}\left[\frac{\lambda}{q}J_1(t)K_{1+r}\left(\frac{q}{\lambda}t\right) + J_0(t)K_r\left(\frac{q}{\lambda}t\right)\right], \quad \text{(B4)}$$

provided $q^2/\lambda^2 > 0$. Moreover,[9]

$$\int_0^\infty dt\, t^{-\rho}J_\nu(\beta t)K_\mu(\alpha t) = 2^{-1-\rho}\alpha^{\rho-\nu-1}\beta^\nu\Gamma\left(\frac{1+\nu-\rho+\mu}{2}\right)\Gamma\left(\frac{1+\nu-\rho-\mu}{2}\right) \times [\Gamma(1+\nu)]^{-1}\,{}_2F_1\left(\frac{1+\nu-\rho+\mu}{2}, \frac{1+\nu-\rho-\mu}{2}; 1+\nu; -\frac{\beta^2}{\alpha^2}\right)$$

$$\text{provided} \quad \operatorname{Re}(\alpha \pm i\beta) > 0, \quad \operatorname{Re}(\nu - \rho + 1 \pm \mu) > 0. \quad \text{(B5)}$$

Again, the terms in (B4) obey the conditions of (B5) for all $r \geq 0$, so that

$$\mathcal{K}_{0,r} = -2^{-2i\eta-1}(\lambda/q)^{2r+2-2i\eta} \times \Gamma(-i\eta+1+r)\Gamma(-i\eta+1)[\Gamma(2+r)]^{-1} \times \{{}_2F_1(-i\eta+r+1, -i\eta+1; 1; -\lambda^2/q^2) + (\lambda^2/q^2)(-i\eta+r+1) \times {}_2F_1(-i\eta+r+2, -i\eta+1; 2; -\lambda^2/q^2)\}.$$

The hypergeometric functions can be combined via the Gauss recursion relation[20]

$$\gamma\,{}_2F_1(\alpha,\beta;\gamma;z) - \gamma\,{}_2F_1(\alpha,\beta+1;\gamma;z) + \alpha z\,{}_2F_1(\alpha+1,\beta+1;\gamma+1;z) = 0.$$

Therefore, when $m = 0$, the double integral of (B1) reduces to

$$\mathcal{K}_{0,r} = -2^{-2i\eta-1}(\lambda/q)^{2r+2-2i\eta} \times [\Gamma(-i\eta+1+r)\Gamma(-i\eta+1)/\Gamma(2+r)] \times {}_2F_1(-i\eta+r+1, -i\eta; 1; -\lambda^2/q^2). \quad \text{(B6)}$$

When $m > 0$, the reduction of (B1) is simpler. First integrate once by parts with respect to t. Then, after interchanging the orders of integration,

$$\mathcal{K}_{m,r} = (2i\eta)\int_0^\infty dt\, t^{-2i\eta-1}J_m(t) \times \int_0^\infty ds\, s^{1+m}\left(s^2 + \frac{q^2}{\lambda^2}\right)^{-2-m-r}J_m(st).$$

Using (B3), one can perform the integration over s. One finds that

$$\mathcal{K}_{m,r} = 2i\eta\left(\frac{\lambda}{q}\right)^{1+r}\frac{2^{-1-m-r}}{\Gamma(2+m+r)} \times \int_0^\infty dt\, t^{-2i\eta+m+r}J_m(t)K_{1+r}\left(t\frac{q}{\lambda}\right).$$

Since $\operatorname{Re}[1 + 2m - 2i\eta + r \pm (1+r)] \geq 2m > 0$, the final integral over t can be done using (B5).

Therefore,

$$\mathcal{K}_{m,r} = i\eta 2^{-2i\eta-1}(\lambda/q)^{-2i\eta+2m+2r+2}\Gamma(-i\eta+m+r+1) \times \Gamma(-i\eta+m)[\Gamma(1+m)]^{-1}[\Gamma(2+m+r)]^{-1} \times {}_2F_1(-i\eta+m+r+1, -i\eta+m; 1+m; -\lambda^2/q^2) \quad \text{(B7)}$$

when $m > 0$. However, when $m = 0$, (B7) reduces to (B6) since $i\eta\Gamma(-i\eta) = -\Gamma(-i\eta+1)$. Hence (B7) is valid for all integers m and $r \geq 0$.

APPENDIX C: ASYMPTOTIC FORMS OF THE GENERATING FUNCTIONS I_0 AND I_1

In this appendix we discuss the asymptotic behavior of the generating functions $I_0(\lambda, q)$ and $I_1(\lambda, q)$ as $q \to 0$. In particular we examine in detail the asymptotic form of $I_0(\lambda, q)$ as determined by Eq. (12) of Sec. II. We apply Eq. (A3) of Appendix A to evaluate the φ_s integral of Eq. (12); then, via Eq. (16), Eq. (12) becomes

$$I_0(\lambda, q) = 8\lambda^{-4}\Bigg\{\int_0^1 s\,ds\left(s^2+\frac{q^2}{\lambda^2}\right)^{-2} \times \left[1 - 2\frac{q^2}{\lambda^2}\left(s^2+\frac{q^2}{\lambda^2}\right)^{-1}\right] \times [1 - {}_2F_1(-i\eta, -i\eta; 1; s^2)] + \int_1^\infty s\,ds\left(s^2+\frac{q^2}{\lambda^2}\right)^{-2}\left[1 - \frac{2q^2}{\lambda^2}\left(s^2+\frac{q^2}{\lambda^2}\right)^{-1}\right] \times [1 - s^{2i\eta}\,{}_2F_1(-i\eta, -i\eta; 1; s^{-2})]\Bigg\}. \quad \text{(C1)}$$

Since the integral in (C1) over the region $[1, \infty)$ is well behaved as $q \to 0$, the behavior of $I_0(\lambda, q)$ as $q \to 0$ is determined by the integral over the region $[0, 1]$. We expand the hypergeometric function ${}_2F_1(-i\eta, -i\eta; 1; s^2)$ in powers of s^2, retaining only the first few terms, so that

$$[1 - {}_2F_1(-i\eta, -i\eta; 1; s^2)] = -(-i\eta)^2 s^2 \times [1 + \tfrac{1}{4}(1-i\eta)^2 s^2 + \tfrac{1}{36}(1-i\eta)^2(2-i\eta)^2 s^4 + \cdots]$$

and

$$I_0(\lambda, q) \sim -8\lambda^{-4}\int_0^1 s\,ds\left(s^2+\frac{q^2}{\lambda^2}\right)^{-2} \times \left[1 - \frac{2q^2}{\lambda^2}\left(s^2+\frac{q^2}{\lambda^2}\right)^{-1}\right] \times (-i\eta)^2 s^2[1 + \tfrac{1}{4}(1-i\eta)^2 s^2 + \tfrac{1}{36}(1-i\eta)^2(2-i\eta)^2 s^4]. \quad \text{(C2)}$$

Note that, in obtaining Eq. (C2), we already have subtracted off the possible divergence stemming from the first term under the brackets in Eq. (12). Now, let $t = (s^2 + q^2/\lambda^2)$. Then, one can readily show that, as $q \to 0$, the leading term in (C2) is proportional to $\ln(q^2/\lambda^2)$; all other terms are either finite or vanish at $q = 0$. Hence, as $q \to 0$,

$$I_0(\lambda, q) \sim 4\lambda^{-4}(i\eta)^2 \ln(q^2/\lambda^2). \quad \text{(C3)}$$

Equation (C3) is precisely the asymptotic behavior of (19C) obtained by using the standard analytic continuation of the hypergeometric function[22] appearing in (19C) as $q \to 0$. Therefore, Eqs. (19) are valid for all $q \geq 0$.

The logarithmic divergence of $I_0(\lambda, q)$ as $q \to 0$ leads directly to the logarithmic divergence of the elastic scattering amplitude in the forward direction, which has been noted and discussed by Franco.[2] Furthermore, it should be apparent from Eqs. (19) that all amplitudes $F(1s \to ns; \mathbf{q})$ diverge logarithmically as $q \to 0$.

In a fashion similar to that described above, one can obtain from Eqs. (24) the asymptotic behavior of $I_1(\lambda, q)$ as $q \to 0$. However, one now finds that, as $q \to 0$,

$$I_1(\lambda, q) \sim -4\eta\lambda^{-4}q^{-1}. \quad \text{(C4)}$$

As one might suspect, Eq. (C4) agrees with the asymptotic behavior of $I_1(\lambda, q)$ obtained from Eq. (27c). Furthermore (C4) implies that each of the nonzero $1s \to np$ amplitudes of Eq. (27b) diverges as q^{-1} as $q \to 0$.

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On the Two-Dimensional Ising Model with Random Impurities

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The McCoy–Wu treatment of the two-dimensional Ising model with random impurities is generalized to allow both vertical and horizontal interactions to vary randomly from row to row (while still keeping them constant in any row). If the random impurities are narrowly distributed, the order-one term in the specific heat at T_c is infinitely differentiable but nonanalytic.

Recently, McCoy and Wu[1] wrote a series of articles analyzing the Ising model with the horizontal interaction energies fixed and the vertical energies varying randomly from row to row. They found that the specific heat was indefinitely differentiable but nonanalytic at T_c, when the impurities were distributed with a power law distribution function.

Subsequently, McCoy[2] generalized these considerations to any narrow distribution function, and found the same behavior of the specific heat C_M, near T_c.

Does a study of a more general lattice yield similar results? The most obvious way to generalize McCoy–Wu lattice is to allow the horizontal coupling constant to be a random variable keeping each translationably invariant. McCoy[3] has conjectured that the analytic properties of C_M will remain the same. It is the purpose of this article to prove this conjecture by a direct computation.

Consider the Hamiltonian

$$H = -\sum_{n,m=1}^{M} \{E_1(m)\sigma_{m,n}\sigma_{m+1,n} + E_2(m)\sigma_{m,n}\sigma_{m,n+1}\}, \tag{1}$$

where $E_1(m)$ and $E_2(m)$ are random variables distributed symmetrically[4] around a narrow peak, with a distribution function $P(E_1, E_2)$.

Define the new variables

$$z(m) = \coth [2K_2(m)], \quad y(m) = \tanh^2 [K_1(m)] \tag{2}$$

and their distribution function as

$$P(E_1, E_2)\, dE_1\, dE_2 = N^2 D[N(z - z_0), N(y - y_0)]\, dy\, dz, \tag{3}$$

where N is large but finite.

McCoy and Wu[1] located the critical temperature T_c, which is given by

$$0 = \iint dz\, dy\, N^2 D[(N(z - z_0), N(y - y_0)] \times \ln [y(z + 1)(z - 1)^{-1}]. \tag{4}$$

By assuming that $T - T_c = O(N^{-2})$ and expanding (4) in powers of N^{-1}, we obtain

$$y_0(z_0 + 1)(z_0 - 1)^{-1} = 1 + [(1 + \delta)b/2]N^{-2} + o(N^{-2}), \tag{5}$$

where b is given by $b = D_{yy}y_0^{-2} + 4z_0D_{zz}(z_0^2 - 1)^{-2}$, δ is the scaled temperature proportional to $|T - T_c|$, and D_{yz} the second moment of the distribution D with respect to the variables (y, z).

The integral equation[1,2] for the limiting distribution $\nu(x)$ is given by (q is treated as a parameter)

$$\nu(x) = \iiint dz\, dy\, dx' \nu(x') N^2 D[N(z - z_0), N(y - y_0)] \times \delta\left(x - \frac{x'(z - \cos q) + y \sin q}{x' \sin q + y(z + \cos q)}\right). \tag{6}$$

We first carry out the integral over x' to obtain

$$\nu(x) = \iint dy\, dz \left[\nu\left(\frac{y[\sin q - x(z + \cos q)]}{x \sin q - (z - \cos q)}\right) N^2 D[N(z - z_0), N(y - y_0)] \times y\left(\frac{(z + \cos q)[-x \sin q + (z - \cos q)] + \sin q[x(z + \cos q) - \sin q]}{[x \sin q - (z - \cos q)]^2}\right)\right]. \tag{7}$$

Following McCoy,[2] we expand both sides of (7) around the peak of D in powers of N^{-1}, set $\sin q = qN^{-2}$, $\cos q = 1$, and equate orders of N^{-1}. The terms of order one, N^{-1} give identities.

The $O(N^{-2})$ term gives a differential equation for $\tilde{\nu}$ which is our approximation for $\nu(x)$. Explicitly, $\tilde{\nu}$ is given by

$$\tfrac{1}{2}x^2A\frac{d\tilde{\nu}(x)}{dx} + [\tfrac{1}{2}(1 + \delta)bx + 2xB + x^2q(z_0 - 1)^{-1}]\tilde{\nu}(x) = 0, \tag{8}$$

where $A = D_{yy}y_0^{-2} + 4D_{zz}(z_0^2 - 1)^{-2}$ and

$$B = D_{zz}(1 - z_0)(z_0^2 - 1)^{-2} + D_{yz}(z_0 - 1)^{-2}.$$

Let $P = bA^{-1}$; then the solution of (8) is given by

$$\tilde{\nu}(x) = Cx^{-1-\delta P} \exp\{-\tfrac{1}{2}\varphi[y_0^{-\frac{1}{2}}x + y_0^{\frac{1}{2}}x^{-1}]\}, \tag{9}$$

where $\varphi = 4qy_0^{\frac{1}{2}}A^{-1}(z_0 - 1)^{-1}$, the normalization constant C is given by

$$C^{-1} = 2y_0^{-\delta P/2}K_{\delta'}(\varphi) \tag{10}$$

and $K_{\delta'}(\varphi)$ is the Bessel function of the third kind,

and $\delta' = \delta P$. The function $\tilde{v}(x)$ has identical analytical behavior to the case investigated by McCoy.[2] The evaluation of C_M near T_c using our $\tilde{v}(x)$ yield similar results as obtained by McCoy, which we now quote for completeness. The most singular part of C_M is given by

$$C_M \propto \int_0^\infty d\varphi \left\{ \frac{\partial^2}{\partial(\delta')^2} \ln K_{\delta'}(\varphi) - (\varphi + 1)^{-1} \right\} \equiv I(\delta'). \tag{11}$$

$I(\delta')$ does not have a convergent power series for $\delta' \sim 0$ but is infinitely differentiable,[1,2] in agreement with McCoy's conjecture.[3]

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[4] This requirement is made without loss of generality.

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Vector–Scalar Sector Solutions to the Spinor–Spinor Bethe–Salpeter Equation*

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(Received 16 November 1970)

A new method is proposed to discuss the exact $J = 0$ vector–scalar sector solutions to the equal-mass spinor–spinor Bethe–Salpeter equation for the massless-meson exchange ladder model at the vanishing total 4-momentum. Under the assumption that all solutions belonging to a discrete spectrum have a discrete spectral representation in the relative 4-momentum squared, it is proved that no discrete solutions other than the solution (in the vector-coupling case) found by Bastai, Bertocchi, Furlan, and Tonin exist in any case of the scalar, pseudoscalar, and vector couplings. As for the case of the axialvector coupling, it is shown that possible eigenvalues have to belong to one of three exponentially increasing sequences; but the existence of any solution other than Keam's one is quite unlikely. It is mathematically interesting that in the above analysis one encounters some Diophantine equations of the second degree.

1. INTRODUCTION

In spite of its importance, our knowledge on the spinor–spinor Bethe–Salpeter (B–S) equation is yet very little because of its complexity. It is especially difficult to find exact solutions to it even in the ladder model. So far the only manageable case is the case of the vanishing total 4-momentum ($P_\mu = 0$). In this case, the spinor–spinor B–S equation is decomposed into three sectors: pseudoscalar sector, tensor–axialvector sector, and vector–scalar sector, where we assume that both constituent particles have the same mass. If the exchanged mesons are massless, we can find some exact solutions.

In the pseudoscalar sector, which is called the Goldstein equation,[1] we obtain a set of solutions belonging to a continuous spectrum, but there exist no discrete solutions.

In the tensor–axialvector sector, it is remarkable that one of two coupled integral equations becomes trivial in the vector-coupling (V-coupling) case and in the axialvector-coupling (A-coupling) case. In 1964, noting this fact, Kummer[2] found a set of exact solutions belonging to a discrete spectrum in the V-coupling case. Recently, some further analyses of Kummer's solutions have been made on the basis of the $O(4)$ symmetry consideration by Seto[3] and by Ito.[4]

The vector–scalar sector consists of two coupled nontrivial integral equations. Until recently, only one exact solution was known only in the V-coupling case. It was found by Bastai, Bertocchi, Furlan, and Tonin,[5] who employed a technique similar to the proof of the Ward identity. Recently, Keam[6] found a new $J = 0$ solution in the A-coupling case by means of a computer (see Sec. 2 for details).

In the present paper, we make a systematic study of the $J = 0$ vector–scalar sector solutions. Under a reasonable assumption stated in Sec. 3, the problem

and $\delta' = \delta P$. The function $\tilde{v}(x)$ has identical analytical behavior to the case investigated by McCoy.[2] The evaluation of C_M near T_c using our $\tilde{v}(x)$ yield similar results as obtained by McCoy, which we now quote for completeness. The most singular part of C_M is given by

$$C_M \propto \int_0^\infty d\varphi \left\{ \frac{\partial^2}{\partial(\delta')^2} \ln K_{\delta'}(\varphi) - (\varphi + 1)^{-1} \right\} \equiv I(\delta'). \tag{11}$$

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The vector–scalar sector consists of two coupled nontrivial integral equations. Until recently, only one exact solution was known only in the V-coupling case. It was found by Bastai, Bertocchi, Furlan, and Tonin,[5] who employed a technique similar to the proof of the Ward identity. Recently, Keam[6] found a new $J = 0$ solution in the A-coupling case by means of a computer (see Sec. 2 for details).

In the present paper, we make a systematic study of the $J = 0$ vector–scalar sector solutions. Under a reasonable assumption stated in Sec. 3, the problem

of finding the solutions is reduced to a system of recurrence relations for parameters. From it, we encounter some Diophantine equations of the second degree, which are well known in number theory. By investigating them, we prove that no solution exists in the scalar-coupling (S-coupling) case and in the pseudoscalar-coupling (P-coupling) case, that no solution other than that of Bastai *et al.* exists in the V-coupling case, and that possible eigenvalues in the A-coupling case have to belong to one of three exponentially increasing sequences. It is expected that our method is useful also for finding the $J \neq 0$ vector–scalar sector solutions and the tensor–axialvector sector solutions in the S-coupling and P-coupling cases.

2. KNOWN SOLUTIONS

The vector–scalar sector of the equal-mass spinor–spinor B–S equation for the massless-meson-exchange ladder model at $P_\mu = 0$ consists of two coupled integral equations[7]:

$$(1 - p^2)\phi_\mu^{\mathrm{V}}(p) + 2p_\mu p^\nu \phi_\nu^{\mathrm{V}}(p) - 2p_\mu \phi^{\mathrm{S}}(p) = \frac{\lambda^{\mathrm{V}}}{\pi^2 i}\int d^4q \frac{\phi_\mu^{\mathrm{V}}(q)}{-(p-q)^2 - i\epsilon},$$

$$(1 + p^2)\phi^{\mathrm{S}}(p) - 2p^\mu \phi_\mu^{\mathrm{V}}(p) = \frac{\lambda^{\mathrm{S}}}{\pi^2 i}\int d^4q \frac{\phi^{\mathrm{S}}(q)}{-(p-q)^2 - i\epsilon}. \quad (2.1)$$

Here p_μ is the relative 4-momentum of the two constituent particles, whose mass is put equal to unity; $\phi_\mu^{\mathrm{V}}(p)$ and $\phi^{\mathrm{S}}(p)$ denote the vector components and the scalar component of the B–S amplitude, respectively; λ^{V} and λ^{S} are given by Table I, with $\lambda \equiv (g/4\pi)^2$ [$\lambda = -(g/4\pi)^2$ can also occur only in the V-coupling case], g being the coupling constant. Physically, we should have $\lambda > 0$ except for the V-coupling case, but we do not impose this condition because the B–S equation often yields physically unexpected results[7] and because we can construct a model having $\lambda < 0$ by considering nonidentical fermions as constituent particles.

We confine ourselves to the spinless ($J = 0$) case alone, that is, we set

$$\phi_\mu^{\mathrm{V}}(p) = p_\mu V(p^2), \quad \phi^{\mathrm{S}}(p) = S(p^2). \quad (2.2)$$

Then (2.1) reduces to

$$p_\mu[(1 + p^2)V(p^2) - 2S(p^2)] = \frac{\lambda^{\mathrm{V}}}{\pi^2 i}\int d^4q \frac{q_\mu V(q^2)}{-(p-q)^2 - i\epsilon},$$

$$(1 + p^2)S(p^2) - 2p^2 V(p^2) = \frac{\lambda^{\mathrm{S}}}{\pi^2 i}\int d^4q \frac{S(q^2)}{-(p-q)^2 - i\epsilon}. \quad (2.3)$$

TABLE I.

	S-coupling	P-coupling	V-coupling	A-coupling
$\lambda^{\mathrm{V}}/\lambda$	1	1	2	2
$\lambda^{\mathrm{S}}/\lambda$	1	−1	−4	4

Bastai *et al.*[5] found the following solutions to (2.3) in the V-coupling case ($\lambda^{\mathrm{V}} = 2\lambda$ and $\lambda^{\mathrm{S}} = -4\lambda$):

$$\lambda = -\tfrac{1}{2}, \quad V(p^2) = c\frac{3 - p^2}{(1 - p^2 - i\epsilon)^3}, \quad S(p^2) = c\frac{2}{(1 - p^2 - i\epsilon)^3}, \quad (2.4)$$

where c is a constant.

Keam[6] investigated the solutions by analyzing an equivalent fourth-order ordinary differential equation with boundary conditions by means of a computer.[8] His computer test was made for the following ranges: $0 < \lambda \leq 10$ in the S-coupling case, $0 < \lambda < \frac{1}{4}$ in the P-coupling case, $0 < \lambda < \frac{1}{16}$ in the V-coupling case, and $0 < \lambda \leq 50$ in the A-coupling case. (It was argued[9] that no acceptable solutions would exist for $\lambda \geq \frac{1}{4}$ in the P-coupling case and for $\lambda \geq \frac{1}{16}$ in the V-coupling case.) He found only one solution only in the A-coupling case ($\lambda^{\mathrm{V}} = 2\lambda$ and $\lambda^{\mathrm{S}} = 4\lambda$):

$$\lambda = \tfrac{15}{2},$$
$$V(p^2) = c'(-7y^{-8} + 56y^{-9} - 126y^{-10} + 84y^{-11}),$$
$$S(p^2) = c'(2y^{-7} - 28y^{-8} + 112y^{-9} - 168y^{-10} + 84y^{-11}), \quad (2.5)$$

where c' is a constant and

$$y \equiv 1 - p^2 - i\epsilon. \quad (2.6)$$

It is noteworthy that we can rewrite the expressions for $V(p^2)$ and $S(p^2)$ as

$$c'^{-1}V(p^2) = -7y^{-8}F(-3, 8; 3; y^{-1}) = \tfrac{1}{5}y^{-8}C_3^{\frac{5}{2}}(2y^{-1} - 1),$$
$$c'^{-1}S(p^2) = 2y^{-7}F(-4, 7; 2; y^{-1}) = \tfrac{2}{15}y^{-7}C_4^{\frac{3}{2}}(2y^{-1} - 1), \quad (2.7)$$

respectively, where F and C_n^α denote the hypergeometric function and the Gegenbauer polynomial, respectively. It is somewhat remarkable that the above expressions are quite akin to the solutions in the equal-mass Wick–Cutkosky model at $P_\mu = 0$.[7]

3. RECURRENCE FORMULAS

From the known results in the B–S equation,[7] it is natural to conjecture that any solution to the equal-mass B–S equation for the *massless-meson-exchange* ladder model belongs to a discrete spectrum of the eigenvalues if and only if the B–S amplitude has a

discrete spectral representation in p^2. In the present paper, we assume that this conjecture is true. Since each discrete value of the spectral variable in the p^2 spectral representation yields an independent contribution, it is sufficient to consider only the case in which the spectrum consists of only one point α. Since $\alpha \neq 0$ because of the (infrared) convergence condition of the integrals, we can set

$$V(p^2) = \sum_{k=2}^{N} \frac{\alpha^k a_k}{(\alpha - p^2 - i\epsilon)^k},$$
$$S(p^2) = \sum_{k=2}^{N} \frac{\alpha^k b_k}{(\alpha - p^2 - i\epsilon)^k}, \tag{3.1}$$

where a_k and b_k are constants such that

$$|a_N| + |b_N| \neq 0 \tag{3.2}$$

with $N \geq 2$; the term with $k = 1$ has been excluded because of the (ultraviolet) convergence condition of the integrals. Hereafter, we omit $-i\epsilon$ in the denominator for simplicity.

It is straightforward to show that

$$\frac{1}{\pi^2 i}\int \frac{q_\mu d^4q}{[-(p-q)^2](\alpha - q^2)^k} = \frac{p_\mu}{k-1}\int_0^1 \frac{x\,dx}{(\alpha - xp^2)^{k-1}},$$
$$\frac{1}{\pi^2 i}\int \frac{d^4q}{[-(p-q)^2](\alpha - q^2)^k} = \frac{1}{k-1}\int_0^1 \frac{dx}{(\alpha - xp^2)^{k-1}}. \tag{3.3}$$

Therefore, in order that no logarithmic terms appear in the right-hand side of (2.3), it is necessary and sufficient that

$$a_3 = 2a_2, \quad b_2 = 0. \tag{3.4}$$

Indeed,

$$\int_0^1 dx\left(\frac{x}{\alpha - xp^2} + \frac{x\alpha}{(\alpha - xp^2)^2}\right) = \frac{1}{\alpha - p^2},$$
$$\int_0^1 \frac{x\,dx}{(\alpha - xp^2)^{k-1}} = \frac{1}{(k-2)(k-3)}\sum_{j=2}^{k-2}\frac{(j-1)\alpha^{-k+j+1}}{(\alpha - p^2)^j} \quad \text{for } k \geq 4,$$
$$\int_0^1 \frac{dx}{(\alpha - xp^2)^{k-1}} = \frac{1}{k-2}\sum_{j=1}^{k-2}\frac{\alpha^{-k+j+1}}{(\alpha - p^2)^j} \quad \text{for } k \geq 3. \tag{3.5}$$

On substituting (3.1) in (2.3) and using (3.4), (3.3), and (3.5) in the right-hand sides, we obtain

$$(1+\alpha)\sum_{k=2}^{N}\frac{\alpha^k a_k}{(\alpha - p^2)^k} - \sum_{k=1}^{N-1}\frac{\alpha^{k+1}a_{k+1}}{(\alpha - p^2)^k} - 2\sum_{k=2}^{N}\frac{\alpha^k b_k}{(\alpha - p^2)^k}$$
$$= \lambda^{\mathrm{V}}\left(\frac{\alpha^2 a_2}{\alpha - p^2} + \sum_{k=2}^{N-2}\frac{(k-1)\alpha^{k+1}}{(\alpha - p^2)^k} \times \sum_{l=k+2}^{N}\frac{a_l}{(l-1)(l-2)(l-3)}\right), \tag{3.6a}$$

$$(1+\alpha)\sum_{k=2}^{N}\frac{\alpha^k b_k}{(\alpha - p^2)^k} - \sum_{k=1}^{N-1}\frac{\alpha^{k+1}b_{k+1}}{(\alpha - p^2)^k}$$
$$- 2\alpha\sum_{k=2}^{N}\frac{\alpha^k a_k}{(\alpha - p^2)^k} + 2\sum_{k=1}^{N-1}\frac{\alpha^{k+1}a_{k+1}}{(\alpha - p^2)^k}$$
$$= \lambda^{\mathrm{S}}\sum_{k=1}^{N-2}\frac{\alpha^{k+1}}{(\alpha - p^2)^k}\sum_{l=k+2}^{N}\frac{b_l}{(l-1)(l-2)}. \tag{3.6b}$$

Since $N \geq 2$, by comparing the coefficients of $(\alpha - p^2)^{-N}$ in (3.6), we obtain

$$(1+\alpha)a_N - 2b_N = 0, \quad (1+\alpha)b_N - 2\alpha a_N = 0. \tag{3.7}$$

Hence (3.2) implies that

$$\begin{vmatrix} 1+\alpha & -2 \\ -2\alpha & 1+\alpha \end{vmatrix} = (1-\alpha)^2 = 0, \tag{3.8}$$

that is, we have $\alpha = 1$ and therefore, from (3.7) and (3.2),

$$b_N = a_N \equiv a \neq 0. \tag{3.9}$$

Hereafter we set $\alpha = 1$ in (3.6). From (3.4) and (3.9) we see that the only possible solution for $2 \leq N \leq 3$ is (2.4).

For $N \geq 4$, by considering the terms of $(1 - p^2)^{-N+1}$ and $(1 - p^2)^{-N+2}$ in (3.6), we have

$$2a_{N-1} - a_N - 2b_{N-1} = 0,$$
$$2b_{N-1} - b_N - 2a_{N-1} + 2a_N = 0 \tag{3.10}$$

and

$$2a_{N-2} - a_{N-1} - 2b_{N-2} = \frac{\lambda^{\mathrm{V}} a_N}{(N-1)(N-2)},$$
$$2b_{N-2} - b_{N-1} - 2a_{N-2} + 2a_{N-1} = \frac{\lambda^{\mathrm{S}} b_N}{(N-1)(N-2)}, \tag{3.11}$$

respectively. Equations (3.10) are identical because of (3.9), and reduce to

$$a_{N-1} - b_{N-1} = \tfrac{1}{2}a. \tag{3.12}$$

The sum of Eqs. (3.11) reads

$$a_{N-1} - b_{N-1} = (\lambda^{\mathrm{V}} + \lambda^{\mathrm{S}})a/(N-1)(N-2). \tag{3.13}$$

From (3.12) and (3.13), we have

$$\lambda^{\mathrm{V}} + \lambda^{\mathrm{S}} = \tfrac{1}{2}(N-1)(N-2). \tag{3.14}$$

The left-hand side of (3.14) equals 2λ for the S coupling, 0 for the P coupling, -2λ for the V coupling, and 6λ for the A coupling. Therefore, the P-coupling case has no solution.

It is important to note that, in general, a_2 can be nonzero only if $\lambda^{\mathrm{V}} = -1$, as is seen from the coefficients of $(1 - p^2)^{-1}$ in Eq. (3.6a). Because then $\lambda^{\mathrm{V}} + \lambda^{\mathrm{S}} \leq 1$ for any coupling, $N \geq 4$ is incompatible

with $a_2 \neq 0$ as is seen from (3.14). We thus conclude that $a_2 = a_3 = 0$ aside from the solution (2.4) of Bastai *et al.*

The comparison of the coefficients of $(1 - p^2)^{-k}$ in (3.6) yields

$$2(a_k - b_k) - a_{k+1} = \lambda^V(k-1)f_{k+2} \quad \text{for } 2 \leq k \leq N-1, \tag{3.15a}$$

$$-2(a_k - b_k) + 2a_{k+1} - b_{k+1} = \lambda^S g_{k+2} \quad \text{for } 1 \leq k \leq N-1, \tag{3.15b}$$

where $a_1 = b_1 = 0$ and

$$f_m \equiv \sum_{l=m}^{N} \frac{a_l}{(l-1)(l-2)(l-3)}, \quad f_{N+1} \equiv 0,$$

$$g_m \equiv \sum_{l=m}^{N} \frac{b_l}{(l-1)(l-2)}, \quad g_{N+1} \equiv 0. \tag{3.16}$$

The sum of Eqs. (3.15) is

$$a_{k+1} - b_{k+1} = \lambda^V(k-1)f_{k+2} + \lambda^S g_{k+2}. \tag{3.17}$$

By using (3.17) with the replacement of $k+1$ by k, we eliminate $a_k - b_k$ from Eq. (3.15a):

$$(1 - 2\lambda^V/k(k-1))a_{k+1} - [2\lambda^S/k(k-1)]b_{k+1} = \lambda^V(k-3)f_{k+2} + 2\lambda^S g_{k+2}. \tag{3.18}$$

From (3.17) and (3.18), we can uniquely solve a_{k+1} and b_{k+1}, $2 \leq k \leq N-2$, because of (3.14). Thus a_{k+1} and b_{k+1} are expressible in terms of a and λ. The eigenvalue λ is determined by the requirement that two sequences

$$\{a_N, a_{N-1}, \cdots, a_k, \cdots\}$$

and

$$\{b_N, b_{N-1}, \cdots, b_k, \cdots\}$$

have to terminate. This problem is discussed in the next section.

4. DIOPHANTINE EQUATIONS

We rewrite (3.15) by replacing k by $k-1$:

$$2(a_{k-1} - b_{k-1}) - a_k = \lambda^V(k-2)f_{k+2} + \lambda^V a_{k+1}/k(k-1),$$

$$-2(a_{k-1} - b_{k-1}) + 2a_k - b_k = \lambda^S g_{k+2} + \lambda^S b_{k+1}/k(k-1). \tag{4.1}$$

It is straightforward to eliminate f_{k+2} and g_{k+2} from (3.15) and (4.1). We find

$$2(k-1)(a_{k-1} - b_{k-1}) - (3k-5)a_k + 2(k-2)b_k + [(k-2) - \lambda^V/k]a_{k+1} = 0 \quad \text{for } 3 \leq k \leq N-1,$$

$$-2(a_{k-1} - b_{k-1}) + 4a_k - 3b_k - 2a_{k+1} + [1 - \lambda^S/k(k-1)]b_{k+1} = 0 \quad \text{for } 2 \leq k \leq N-1. \tag{4.2}$$

Let n be the greatest integer such that $a_k = b_k = 0$ for all $k \leq n$; of course,

$$2 \leq n \leq N-2. \tag{4.3}$$

Then (4.2) with $k = n$ reads

$$[n(n-2) - \lambda^V]a_{n+1} = 0,$$

$$[n(n-1) - \lambda^S]b_{n+1} = 2n(n-1)a_{n+1}. \tag{4.4}$$

Since $|a_{n+1}| + |b_{n+1}| \neq 0$, we have *either* $a_{n+1} = 0$, $b_{n+1} \neq 0$, and

$$\lambda^S = n(n-1) \tag{4.5}$$

or $a_{n+1} \neq 0$, $b_{n+1} \neq 0$, and

$$\lambda^V = n(n-2). \tag{4.6}$$

If we combine (4.5) and (4.6) with (3.14), we obtain

$$(N-1)(N-2) = \xi n(n-1), \tag{4.7}$$

$$(N-1)(N-2) = \eta n(n-2), \tag{4.8}$$

respectively, where

$$\begin{aligned} &\xi = 4, \quad \eta = 4 \quad \text{for S coupling,} \\ &\xi = 1, \quad \eta = -2 \quad \text{for V coupling,} \\ &\xi = 3, \quad \eta = 6 \quad \text{for A coupling.} \end{aligned} \tag{4.9}$$

Since N and n are unknown integers, (4.7) and (4.8) are nothing but Diophantine equations of the second degree, which are well known in number theory.[10]

It is evident that neither (4.7) nor (4.8) have solutions satisfying (4.3) in the V-coupling case.

Next, we consider the S-coupling case. In (4.7), the discriminant D with respect to n is given by

$$D = N^2 - 3N + 3. \tag{4.10}$$

Since

$$(N-2)^2 < D < (N-1)^2, \tag{4.11}$$

D cannot be a perfect square. Thus (4.7) has no solution in the S-coupling case. In (4.8), the discriminant D with respect to n is given by

$$D = N^2 - 3N + 6. \tag{4.12}$$

Hence (4.11) holds for $N \geq 6$. For $4 \leq N \leq 5$, (4.8) is satisfied by $(N, n) = (5, 3)$. In this case, however, from (4.2) together with (4.4) and (4.6), we have $a_5 = -(\frac{3}{5})b_4$ and $b_5 = -(\frac{3}{15})b_4$ in contradiction with (3.9). Thus there exists no solution to (3.6) in the S-coupling case.

In the A-coupling case, both (4.7) and (4.8) have an infinite number of solutions satisfying (4.3). In order to obtain all solutions, we quote the following results known in the theory of Diophantine equations.[10]

Given a prime p and a positive integer d which is not a perfect square, all solutions (u, v) to the Diophantine equation

$$u^2 - dv^2 = \pm p \tag{4.13}$$

can be written (not uniquely) as

$$u + v\sqrt{d} = \pm(u_0 \pm v_0\sqrt{d})(x \pm y\sqrt{d})^k, \quad k = 0, 1, 2, \cdots, \tag{4.14}$$

with all double signs being independent, where (u_0, v_0) is the smallest positive solution, which always exists, to (4.13) and where (x, y) is the fundamental solution (i.e., the smallest positive solution), which always exists, to an auxiliary Diophantine equation

$$x^2 - dy^2 = 1. \tag{4.15}$$

By setting $N = \frac{1}{2}(u + 3)$ and $n = \frac{1}{2}(v + 1)$, (4.7) with $\xi = 3$ reduces to

$$u^2 - 3v^2 = -2. \tag{4.16}$$

From (4.14), it is easy to see that any *positive* solution to (4.16) is uniquely expressed as

$$u + v\sqrt{3} = (1 + \sqrt{3})(2 + \sqrt{3})^k, \quad k = 0, 1, 2, \cdots. \tag{4.17}$$

In particular, the smallest five solutions are $(N, n) = (2, 1), (4, 2), (11, 6), (37, 21), (134, 77)$, where the first solution is excluded by (4.3).

Next, by setting $N = \frac{1}{2}(u + 3)$ and $n = \frac{1}{2}(v + 2)$, (4.8) with $\eta = 6$ reduces to

$$u^2 - 6v^2 = -23. \tag{4.18}$$

Hence, any positive solution is uniquely expressed as either of

$$\begin{aligned} u + v\sqrt{6} &= (1 + 2\sqrt{6})(5 + 2\sqrt{6})^k, \quad k = 0, 1, 2, \cdots, \\ u + v\sqrt{6} &= (19 + 8\sqrt{6})(5 + 2\sqrt{6})^k, \quad k = 0, 1, 2, \cdots. \end{aligned} \tag{4.19}$$

In particular, the smallest five solutions are $(N, n) = (2, 2), (11, 5), (16, 7), (97, 40), (146, 60)$, where the first solution is excluded by (4.3).

Finally, we discuss whether or not the above solutions to the Diophantine equations lead us to solutions to the original B–S equation. We can uniquely solve (4.2) with respect to a_{k+1} and b_{k+1} for $k > n$ if and only if we do *not* have

$$3k(k - 1) = (N - 1)(N - 2). \tag{4.20}$$

[The exceptional case (4.20) is realized for $k = 6$ in the case $(N, n) = (11, 5)$.] Then all of $a_{n+1}, a_{n+2}, \cdots, a_N$ and $b_{n+1}, b_{n+2}, \cdots, b_N$ are expressible in terms of (and proportional to) $b_{n+1} \neq 0$. Since (3.7) is not included in (3.15), the former implies a relation independent of (4.2). Therefore, we obtain a solution to the original B–S equation if and only if (3.9), namely $a_N = b_N$, is satisfied when a_N and b_N are expressed in terms of b_{n+1}. Since (3.9) is an additional condition, almost all solutions to the Diophantine equations do not lead us to solutions to the original B–S equation. Keam's solution (2.5), which corresponds to $(N, n) = (11, 6)$, is a very fortunate example. It is cumbersome to check (3.9) explicitly for N large, but it is much easier to see whether or not $V(p^2)$ and $S(p^2)$ can be expressed in terms of single hypergeometric functions as in (2.5). It is unlikely that there exists any solution other than Keam's one.[11]

Note added in proof: Keam and his collaborator independently obtained the Diophantine equations by his differential-equation method, and examined the acceptability of two solutions $(N, n) = (37, 21)$ and $(134, 77)$ by a computer (private communication).

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$$b_{n+2}/b_{n+1} = -(n + 1)(5n + 2)/2(n + 2).$$

Except for the first three, the possible values of n already yield complicated fractions. Moreover, if we compute b_{n+3}/b_{n+1}, we find too complicated fractions to believe that they lead us to solutions to the original B–S equation.

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Observables and the Field in Quantum Mechanics

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Corresponding to any irreducible proposition system L in general quantum mechanics there is a division ring D with an anti-automorphism * and a vector space (V, D) over D with a definite sesquilinear form ϕ such that L is isomorphic to the set of ϕ closed subspaces of (V, D). The main task remaining in connecting the general quantum mechanics to the conventional quantum theory in a complex Hilbert space is to give physical arguments which force D to be the complex field. In this paper it is shown that if L admits a certain type of observable (together with other structure which seems to be physically justified), then D contains the real field as a subfield. Steps are then indicated that can be taken to move from the reals to the complexes or quaternions.

1. INTRODUCTION

Using physical arguments, Jauch and Piron[1] have shown that the collection of propositions for a physical system form a complete, atomic, semimodular orthomodular lattice or, as we shall call it, a *propositional system* L. Using standard arguments, one can show that a propositional system can be represented as a direct product of irreducible propositional systems; and Piron[2] has shown that corresponding to any irreducible propositional system L there is a division ring D with an anti-automorphism * and a vector space (V, D) over D with a definite sesquilinear form ϕ such that L is isomorphic to the propositional system $L(V, D)$ of all ϕ closed subspaces of (V, D). As Jauch has said,[3] this forms the bridge which connects the general theory, as an abstract propositional system, with conventional quantum theory in a complex Hilbert space. However, this bridge is not yet complete in the sense that there are no convincing empirical grounds why our Hilbert space should be constructed over the field of complex numbers. In this paper we attempt to close this gap and complete the bridge.

Some progress has been made in determining the division ring D,[4] and work has been done on quantum mechanical theories over real[5] and quaternionic[6] Hilbert spaces and even vector spaces over certain algebras.[7] It seems to us as though the propositional system L alone does not contain enough empirical structure to expose the division ring D. It thus seems likely that more physical data must be included in L to restrict the choice of D. In this paper we show that if L admits a certain type of observable (together with the other structure which seems to be physically justified), then D contains the real field R as a subfield. We then indicate steps that can be taken to move from the reals to the complexes or quaternions.

2. SMOOTH MAXIMAL OBSERVABLES

Recall that a *state*[8] is a map $m: L \to [0, 1] \subset R$ that satisfies: (S1) $m(1) = 1$; (S2) $m(\bigvee a_i) = \Sigma m(a_i)$ if $a_i \perp a_j$, $i \neq j$; (S3) if $m(a) = m(b) = 1$, then $m(a \wedge b) = 1$. We denote the set of all states on L by S. We say that L satisfies the *first Gleason theorem* if a state m is pure if and only if there is an atom $a \in L$ such that $m(a) = 1$. It clearly follows from Gleason's theorem[9] that the lattice of closed subspaces of a separable complex Hilbert space satisfies this condition. In the sequel we shall assume that L satisfies the first Gleason theorem. We shall also assume that S is a *separating* set of states; that is, if $a \neq b$, there is an $m \in S$ such that $m(a) \neq m(b)$.

Let $\mathcal{S}$ be a set and B a Boolean σ-algebra of subsets of $\mathcal{S}$. A map $X: B \to L$ is an *observable on* $(\mathcal{S}, B)$ if (O1) $X(\mathcal{S}) = 1$, (O2) $E, F \in B$ and $E \cap F = \phi$ implies $X(E) \perp X(F)$, (O3) $X(\cup E_i) = \bigvee X(E_i)$ if E_i is a sequence of mutually disjoint sets in B. Now let μ be a measure on B.[10] To eliminate certain pathologies, we shall always assume that there are three mutually disjoints $E_i \in B$ of positive measure such that $X(E_i) \neq 0$, $i = 1, 2, 3$. It seems that this condition only eliminates the case in which there are only two essential points in $\mathcal{S}$, that is, physically those systems in which only a two-valued observable is considered. We say that an observable X on $(\mathcal{S}, B, \mu)$ is *smooth*[11] if $\mu(E) = 0$ whenever $X(E) = 0$. We will show in Theorem 1, Sec. 3, that all reasonable physical systems admit a smooth observable.

All physical systems contain the following mathematical structure. There is a locally compact, second

countable, Hausdorff space $\mathcal{S}$, which we call a *physical space* and a locally compact, second countable Hausdorff group G, which we call a *symmetry group* acting as a continuous, transitive, transformation group[12] on $\mathcal{S}$. Furthermore, there is a representation $g \to W_g$ of G on the group of automorphisms aut (L) of L which is continuous in the sense that $g \to m(W_g a)$ is a continuous function for all $m \in S$, $a \in L$. The Borel σ-algebra of $\mathcal{S}$ being denoted by $B(\mathcal{S})$, all physical systems admit an observable $X: B(\mathcal{S}) \to L$ that satisfies $X(gE) = W_g X(E)$, for all $E \in B(\mathcal{S})$, $g \in G$.[13] We call such observables *covariant*. One example of a covariant observable is the position observable. However, X need not be a position observable in the ordinary sense. $\mathcal{S}$ could be a momentum space, an energy space, a charge space, or a coordinate-spin space for example. A nontrivial σ-finite measure μ on $B(\mathcal{S})$ is *quasi-invariant* if $\mu(E) = 0$ if and only if $\mu(gE) = 0$ for all $E \in B(\mathcal{S})$, $g \in G$. It can be shown that there exist quasi-invariant measures on $B(\mathcal{S})$.[14]

Let X be an observable on any measure space $(\mathcal{S}, B, \mu)$. We now consider a requirement in which X is maximal in a certain sense. Denoting the range of X by $R(X)$, maximality relative to a set of states $M \subseteq S$ means (roughly) that $R(X)$ is so large that states on $R(X)$ can be uniquely extended to states in M, that superpositions of states on $R(X)$ correspond to superpositions in M, and that compatibility of states on $R(X)$ corresponds to compatibility in M. We now make the above vague statements mathematically precise. If m is a state with domain $R(X)$, then clearly m defines a probability measure $E \to m(X(E))$ on B. For this reason we call such states *probability measures* on $R(X)$. We first assume that there is a set of pure states $M \subseteq S$ such that every probability measure ν on $R(X)$ has a unique extension $\tilde{\nu} \in M$. Now for every pure state m there is a *unique* atom $a(m)$ such that $m(a(m)) = 1$ since if $m(a_1) = m(a_2) = 1$ for distinct atoms a_1, a_2, then $m(a_1 \wedge a_2) = 1$ and hence $a_1 \wedge a_2 = a_1$ so that $a_1 \leq a_2$ which implies $a_1 = a_2$, a contradiction. If m_1, m_2 are distinct pure states, we say that a pure state m_3 is a *superposition* of m_1 and m_2 if $a(m_3) < a(m_1) \vee a(m_2)$ ($a < b$ means $a \leq b$ but $a \neq b$). We must now define what is meant by a superposition of probability measures on $R(X)$. Suppose ν_1, ν_2, and ν_3 are distinct probability measures on $R(X)$ that are absolutely continuous relative to μ.[15] If there exist real numbers α, β such that $(d\nu_3/d\mu)^{\frac{1}{2}} = \alpha(d\nu_1/d\mu)^{\frac{1}{2}} + \beta(d\nu_2/d\mu)^{\frac{1}{2}}$, we say that ν_3 is a *superposition* of ν_1 and ν_2. Our next assumption is that if ν_3 is a superposition of ν_1 and ν_2, then $\tilde{\nu}_3$ is a superposition of $\tilde{\nu}_1$ and $\tilde{\nu}_2$. Finally we say that two distinct probability measures ν_1 and ν_2 that are absolutely continuous relative to μ are *compatible* if $[(\frac{1}{2}d\nu_1/d\mu)^{\frac{1}{2}} + (\frac{1}{2}d\nu_2/d\mu)^{\frac{1}{2}}]^2$ is a density function for a probability measure, and we assume that if ν_1 and ν_2 are compatible, then so are $a(\tilde{\nu}_1)$ and $a(\tilde{\nu}_2)$.[16] The motivation for this definition of compatibility stems from the fact that if ν_1 and ν_2 are compatible, then

$$1 = \int [(\tfrac{1}{2}d\nu_1/d\mu)^{\frac{1}{2}} + (\tfrac{1}{2}d\nu_2/d\mu)^{\frac{1}{2}}]\, d\mu$$

$$= 1 + \tfrac{1}{2}\int (d\nu_1/d\mu)^{\frac{1}{2}}(d\nu_2/d\mu)^{\frac{1}{2}}\, d\mu$$

which implies that $(d\nu_1/d\mu)^{\frac{1}{2}}$ and $(d\nu_2/d\mu)^{\frac{1}{2}}$ are orthogonal normalized functions in $L_2(\mathcal{S}, \mu)$. Now unit vectors in $L_2(\mathcal{S}, \mu)$ correspond to atoms and distinct atoms in a proposition system are compatible if and only if they are orthogonal.

It turns out that we need more than the conditions in the previous paragraph. We need these conditions to hold not just for probability measures on $R(X)$ but for signed probability measures on $R(X)$. We say that a signed measure ν on $R(X)$ is a *signed probability measure* if the total variation measure $|\nu|$ is a probability measure on $R(X)$.[17] It follows from the Jordan decomposition theorem[18] that every signed probability measure ν on $R(X)$ that is not a measure has the unique form $\nu = c\nu^+ - (1 - c)\nu^-$, where $0 < c < 1$ and ν^+ and ν^- are mutually singular [i.e., $\nu^+(a) = \nu^-(b) = 1$ for some $a \perp b$] probability measures on $R(X)$. Besides ν^+ and ν^-, a third important probability measure associated with ν is $\nu^* = (1 - c)\nu^+ + c\nu^-$. Now we have seen that if ν is a probability measure on $R(X)$, there is an associated atom $a(\nu) \equiv a(\tilde{\nu}) \in L$. In a similar way, if ν is a signed probability measure on $R(X)$ that is not a measure, we associate with it the atom $a(\nu) = [a(\nu^+) \vee a(\nu^*)] \wedge a(\nu^*)'$.[19] That $a(\nu)$ is an atom is demonstrated in the proof of Theorem 2 in Sec. 4. We now generalize the conditions of the previous paragraph to include signed probability measures. We thus say that an observable X on $(\mathcal{S}, B, \mu)$ is *maximal* relative to a set of pure states $M \subseteq S$ if the following conditions hold:

(1) Every probability measure ν on $R(X)$ has a unique extension $\tilde{\nu} \in M$.

(2) Let ν_1, ν_2, ν_3 be distinct (i.e., $\nu_i \neq \pm\nu_j$, $i \neq j = 1, 2, 3$) signed probability measures on $R(X)$ that are absolutely continuous relative to μ. If $(d\nu_3/d\mu)^{\frac{1}{2}} = \alpha(d\nu_1/d\mu)^{\frac{1}{2}} + \beta(d\nu_2/d\mu)^{\frac{1}{2}}$ for some $\alpha, \beta \in R$, then $a(\nu_3) < a(\nu_1) \vee a(\nu_2)$. If $\alpha = \beta = (2)^{-\frac{1}{2}}$, then $a(\nu_1) \leftrightarrow a(\nu_2)$. (We define $\alpha^{\frac{1}{2}} = \alpha/|\alpha|^{\frac{1}{2}}$ for $0 \neq \alpha \in R$ and $O^{\frac{1}{2}} = 0$.)

We now give an example of a smooth maximal observable. This is the usual formulation of a spinless, nonrelativistic particle moving in one-dimensional

space. The proposition system L is the lattice of closed subspaces (or equivalently, the lattice of orthogonal projectors) of the complex Hilbert space $L_2(R, \mu)$, where μ is Lebesgue measure and the real line R is the physical space. The observable is given by

$$(X(E)f)(\lambda) = \chi_E(\lambda)f(\lambda),$$

where χ_E is the characteristic function of $E \in B(R)$. Clearly X is a smooth observable. Also X is the covariant position observable relative to the representation of R given by $W_\alpha P = U_\alpha P U_\alpha^{-1}$ for all $P \in L$, $\alpha \in R$, where $(U_\alpha f)(\lambda) = f(\lambda - \alpha)$, $f \in L_2(R, \mu)$. Let M be the set of pure states of the form $m_f(P) = \langle f, Pf\rangle$, where $f \in L_2(R, \mu)$, $\|f\| = 1$ and $f \geq 0$. We now show that X is maximal relative to M. We first check condition (1). Let ν be a probability measure on $R(X)$ and define $\nu_0(E) = \nu(X(E))$, $E \in B(R)$. Then ν_0 is a measure on $B(R)$ that is absolutely continuous relative to μ so by the Radon–Nikodym theorem there is a unique $f \in L_1(R, \mu)$, $f \geq 0$ such that $\nu_0(E) = \int_E f\,d\mu$ for all $E \in B(R)$. Let $g = f^{\frac{1}{2}}$ so that $\nu_0(E) = \int_E g^2\,d\mu = \int_R \chi_E g^2\,d\mu = \langle g, X(E)g\rangle$. Therefore, $m_g \in M$ and, since $m_g(X(E)) = \nu(X(E))$, we see that m_g is the unique extension of ν in M. We now verify condition (2). Let ν_1, ν_2, ν_3 be distinct signed probability measures on $R(X)$, or equivalently on $B(R)$, that are absolutely continuous relative to μ, and suppose $(d\nu_3/d\mu)^{\frac{1}{2}} = \alpha(d\nu_1/d\mu)^{\frac{1}{2}} + \beta(d\nu_2/d\mu)^{\frac{1}{2}}$ for some $\alpha, \beta \in R$. Now $(d\nu_i/d\mu)^{\frac{1}{2}} \in L_2(R, \mu)$, $i = 1, 2, 3$, and, if we denote the ray generated by a unit vector f by $[f]$, we obtain

$$[d\nu_3/d\mu)^{\frac{1}{2}}] < [d\nu_1/d\mu)^{\frac{1}{2}}] \vee [(d\nu_2/d\mu)^{\frac{1}{2}}].$$

If ν_1, ν_2, ν_3 are probability measures, we have $a(\nu_3) < a(\nu_1) \vee a(\nu_2)$. Now any real unit vector f admits the unique representation $f = cf^+ - (1 - c)f^-$, where f^+, f^- are nonnegative, orthogonal, unit vectors and $0 < c < 1$. By defining $f^* = (1 - c)f^- + cf^+$, it is clear that if $0 \leq c \leq 1$, then $[f] = ([f^+] \vee [f^*]) \wedge [f^*]'$. Thus, if $d\nu_1/d\mu$, say, is not nonnegative, we have

$$\begin{aligned}
&[(d\nu_1/d\mu)^{\frac{1}{2}}] \\
&\quad = \{[((d\nu_1/d\mu)^+)^{\frac{1}{2}}] \vee [((d\nu_1/d\mu)^*)^{\frac{1}{2}}]\} \wedge [((d\nu_1/d\mu)^*)^{\frac{1}{2}}]' \\
&\quad = \{[(d\nu_1^+/d\mu)^{\frac{1}{2}}] \vee [(d\nu_1^*/d\mu)^{\frac{1}{2}}]\} \wedge [(d\nu_1^*/d\mu)^{\frac{1}{2}}]' \\
&\quad = [a(\nu_1^+) \vee a(\nu_1^*)] \wedge a(\nu_1^*)' = a(\nu_1).
\end{aligned}$$

We then obtain for every case that $a(\nu_3) < a(\nu_1) \vee a(\nu_2)$. Finally, if $\alpha = \beta = (2)^{-\frac{1}{2}}$, then $(d\nu_1/d\mu)^{\frac{1}{2}} \perp (d\nu_2/d\mu)^{\frac{1}{2}}$ so that $a(\nu_1) \perp a(\nu_2)$ and hence $a(\nu_1) \leftrightarrow a(\nu_2)$.

A smooth maximal observable need not have a continuous spectrum as in the previous example; it may have a discrete spectrum consisting of a finite number of points. Let us consider, for example, the three-valued magnetic moment with values $\lambda_1 = -1$, $\lambda_2 = 0$, $\lambda_3 = 1$. The space $S = \{-1, 0, 1\}$ and the measure is given by $\mu(\{-1\}) = \mu(\{0\}) = \mu(\{1\}) = \frac{1}{3}$. The proposition system is the lattice of subspaces (or lattice of projectors) in three-dimensional complex Hilbert space C^3. Let $\phi_1 = (1, 0, 0)$, $\phi_2 = (0, 1, 0)$, $\phi_3 = (0, 0, 1)$ be the usual orthonormal basis. Define the observable X by $X(E) = \bigvee\{\phi_i: \lambda_i \in E\}$, $E \subseteq \{-1, 0, 1\}$. Clearly X is smooth. Let M be the set of pure states of the form $m_\alpha(P) = \langle \alpha, P\alpha\rangle$ where $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in C^3$, $\|\alpha\| = 1$, $a_i \geq 0$, $i = 1, 2, 3$. Any probability measure ν on $R(X)$ is given by three nonnegative numbers α_1, α_2, α_3, where $\nu([\phi_i]) = \alpha_i$ and $\sum_{i=1}^3 \alpha_i = 1$. Letting $\phi_\alpha \in C^3$ be defined by $\phi_\alpha = (\alpha_1^{\frac{1}{2}}, \alpha_2^{\frac{1}{2}}, \alpha_3^{\frac{1}{2}})$, we see that $m_{\phi_\alpha} \in M$ and

$$\begin{aligned}
\nu(X(E)) &= \sum\{\nu([\phi_i]): \lambda_i \in E\} = \sum\{\alpha_i: \phi_i \in E\} \\
&= \langle \phi_\alpha, X(E)\phi_\alpha\rangle = m_{\phi_\alpha}(X(E))
\end{aligned}$$

so that m_{ϕ_α} is the unique extension of ν to M. We thus see that this example is just a special case of the previous one and the demonstration that X is maximal relative to M is similar (and easier) to the previous example. It is also clear that the Hilbert space need not be C^3 but could be some infinite-dimensional Hilbert space.

3. THE FIELD IN QUANTUM MECHANICS

We first show that any reasonable physical system admits a smooth observable.

Theorem 1: Let S be a physical space, G a symmetry group on S, $g \to W_g$ a continuous representation of G on aut (L), and μ a quasi-invariant measure. If $X: B(S) \to L$ is a covariant observable satisfying condition (1), then there is a set $F \in B(S)$ with $\mu(F) \neq 0$ such that $X: B(F) \to L$ is smooth.

We shall give the proof of this theorem in Sec. 4. Note that $F \in B(S)$ in Theorem 1 gives the spectrum of X.

We now state our main result.

Theorem 2: Let L be a proposition system that admits a smooth maximal observable on a measure space (S, B, μ). Then there is a lattice monomorphism[20] from the lattice of finite-dimensional subspaces of the real Hilbert space $L_2(S, \mu)$ to the lattice of finite elements of L that maps atoms to atoms.

The proof of this theorem is given in Sec. 4. Upon examining the proof one can see that the theorem is true under slightly weaker conditions. We can eliminate condition (S3) for states and the requirement that

Gleason's first theorem holds if we impose the condition that for each pure state m [satisfying (S1) and (S2)] there is a unique atom $a(m)$ such that $m(b) = 1$ implies $a(m) \leq b$ and different pure states correspond to different atoms. Besides being useful in determining the field, Theorem 2 has an interest in its own right since it gives a correspondence between certain subspaces of the Hilbert space $L_2(\mathcal{S}, \mu)$ and elements of L.

Let us now suppose that L is irreducible so that it may be represented as the closed subspaces $L(V', D')$ of a vector space (V', D') over a division ring D'. Our next theorem is now applicable.

Theorem 3: Let (V, D) and (V', D') be vector spaces over division rings with $\dim V \geq 3$. Let ξ be a lattice monomorphism from the lattice of finite-dimensional subspaces of (V, D) to the lattice of finite-dimensional subspaces of (V', D') that maps atoms of (V, D) to atoms of (V', D'). Then there is an injection $T: V \to V'$ and a map $\sigma\ (c \to c^\sigma): D \to D'$ such that $T(x_1 + x_2) = Tx_1 + Tx_2$, $T(cx) = c^\sigma Tx$, $\xi(Dx) = D'Tx$.

The proof of this last theorem is very similar to the proof of the stronger result when ξ is an isomorphism given, for example, in Varadarajan.[21] It is easy to show that $\sigma: D \to D'$ is a field monomorphism. Indeed, if $c_1 \neq c_2 \in D$ and $0 \neq x \in V$, then $c_1x \neq c_2x$ so that $c_1^\sigma Tx = T(c_1x) \neq T(c_2x) = c_2^\sigma Tx$ and $c_1^\sigma \neq c_2^\sigma$. If c_1, c_2 are now arbitrary elements of D and $0 \neq x \in V$, then $Tx \neq 0$ and $(c_1 + c_2)^\sigma Tx = T((c_1 + c_2)x) = T(c_1x) + T(c_2x) = (c_1^\sigma + c_2^\sigma)Tx$ so that $(c_1 + c_2)^\sigma = c_1^\sigma + c_2^\sigma$. Similarly

$$(c_1c_2)^\sigma Tx = T((c_1(c_2x)) = c_1^\sigma T(c_2x) = c_1^\sigma c_2^\sigma Tx$$

so that $(c_1c_2)^\sigma = c_1^\sigma c_2^\sigma$.

The next theorem now follows.

Theorem 4: Let $L = L(V, D)$ be an irreducible proposition system that admits a smooth maximal observable. Then D contains the real field R as a subfield.

Strictly speaking, of course, we should say that D contains a subfield that is isomorphic to R.

We thus see that if an irreducible proposition system $L(V, D)$ admits a smooth maximal observable, then D is an extension of R. It seems physically reasonable that D should be a finite extension of R since otherwise elements of D would not be accessible from elements of R using a finite number of steps. We now quote a theorem of Frobenius whose proof, for example, is in Pontryagin.[22]

Theorem 5: If D is a division ring which contains the reals in its center and is a finite extension of the reals (i.e., there are $e_1, \cdots, e_k \in D$ such that every $x \in D$ has a unique representation

$$x = d_0 + d_1e_1 + \cdots + d_ke_k,$$

$d_i \in R$, $i = 1, \cdots, k$), then D is the reals, complexes, or quaternions.

Finally we conclude that under physically reasonable circumstances, if an irreducible proposition system $L(V, D)$ admits a smooth maximal observable, then D is the reals, complexes, or quaternions. Other physical criteria must be used to determine which of these three fields is the correct one.

4. PROOFS OF THEOREMS

Proof of Theorem 1: If $m \in M$ then $E \to m(X(E))$, $E \in B(\mathcal{S})$, is absolutely continuous relative to μ by Lemma II.2 Gudder.[23] By the Radon–Nikodym theorem there exists a unique $f \in L_1(\mathcal{S}, \mu)$, $f \geq 0$, such that $m(X(E)) = \int_E f\, d\mu$ for all $R \in B(\mathcal{S})$. Let $\hat{m} = f^{\frac{1}{2}}$; then $\hat{m} \in L_2(\mathcal{S}, \mu)$, $\|\hat{m}\| = 1$, $\hat{m} \geq 0$. Let $V = \overline{sp}\{\hat{m}: m \in M\}$, the closed span of $\{\hat{m}: m \in M\}$. Let $E_0 \in B(\mathcal{S})$ and $m \in M$. If $m(X(E_0)) = 0$, then $\hat{m} = 0$ a.e. on E_0 so that $\hat{m}\chi_{E_0} = 0 \in V$. If $m(X(E_0)) \neq 0$, define ν on $R(X)$ by $\nu(X(E)) = m(X(E \cap E_0))/m(X(E_0))$. Then ν is a probability measure on $R(X)$. Hence

$$\begin{aligned}\int_E \tilde{\nu}\hat{m}^2\, d\mu &= m(X(E \cap E_0))/m(X(E_0)) \\ &= m(X(E_0))^{-1}\int_{E\cap E_0} \hat{m}^2\, d\mu = \int_E \hat{m}^2\chi_{E_0}/m(X(E_0))\, d\mu\end{aligned}$$

so that $\tilde{\nu}\hat{m} = [m(X(E_0))]^{\frac{1}{2}}\hat{m}\chi_{E_0}$ and again $\hat{m}\chi_{E_0} \in V$. Thus, if $f \in V$, we have $\chi_{E_0}f \in V$. Since multiplication by characteristic functions forms a maximal set of projections, it follows that $V = L_2(F, \mu)$ for some $F \in B(\mathcal{S})$. Now $\mu(F) \neq 0$ since for $m_0 \in M$ we have $1 = m_0(X(\mathcal{S})) = \int_{\mathcal{S}} \hat{m}_0^2\, d\mu = \int_F \hat{m}_0^2\, d\mu$. To show X is smooth, suppose $X(E) = 0$. Then $m(X(E)) = 0$ for all $m \in M$ and hence $\hat{m} = 0$ a.e. on E for all $m \in M$. Hence $g = 0$ a.e. on E for all $g \in V$ which implies $\mu(E) = 0$.

Proof of Theorem 2: Let $[f]$, $f \in L_2(\mathcal{S}, \mu)$, $\|f\| = 1$, $f \geq 0$ be a positive ray. Consider the function $X(E) \to \int_E f^2\, d\mu$, $E \in B$. This is a well-defined function on $R(X)$. Indeed suppose $X(E) = X(F)$, $E, F \in B$. Let $E\Delta F = (E - F) \cup (F - E)$ be the symmetric difference of E and F. Then $X(E\Delta F) = (X(E) - X(F)) \vee (X(F) - X(E)) = 0$ and, since X is smooth, $\mu(E\Delta F) = 0$. It follows that $\int_E f^2\, d\mu = \int_F f^2\, d\mu$. It is now clear that $X(E) \to \int_E f^2\, d\mu$ is a probability measure on $R(X)$. Applying condition (1), we have a unique

$m_f \in M$ such that $m_f(X(E)) = \int_E f^2\,d\mu$ for all $E \in B$. Define $\psi[f] = a(m_f)$. If $[f] \neq [g]$ are positive rays, then $\int_E f^2\,d\mu \neq \int_E g^2\,d\mu$ for some $E \in B$ and hence $m_f \neq m_g$. It follows that $a(m_f) \neq a(m_g)$ since otherwise $(\frac{1}{2}m_f + \frac{1}{2}m_g)(a(m_f)) = 1$, which contradicts Gleason's first theorem. Thus ψ is injective. Now suppose $[f] \perp [g]$ are positive rays and hence $f \perp g$. Then there exist $F_1, F_2 \in B$ such that $F_1 \cap F_2 = \phi$, $F_1 \cup F_2 = S$, $f = 0$ a.e. on F_2 and $g = 0$ a.e. on F_1. Now $X(F_1) \perp X(F_2)$ and $m_f(X(F_1)) = m_g(X(F_2)) = 1$. Since $m_f(a(m_f) \wedge X(F_1)) = 1$, it follows that $a(m_f) \leq X(F_1)$. Similarly $a(m_g) \leq X(F_2)$ and hence $a(m_f) \perp a(m_g)$ or $\psi[f] \perp \psi[g]$. Thus ψ preserves orthogonality. We now extend these results to arbitrary rays. We first prove that if $p \neq q \in L$ are atoms, then $a = (p \vee q) \wedge q'$ is an atom. Indeed $a \vee q = ((p \vee q) \wedge q') \vee q = p \vee q$ by weak modularity. Hence by semimodularity (the covering law) $p \vee q$ covers a. Now $a \neq 0$ since otherwise $p \vee q$ is an atom which would imply $p = p \vee q = q$, a contradiction. Now suppose a is not an atom. Then there exists an atom $r < a$ and $a = r \vee (a \wedge r')$ and so there is an atom $r_1 \perp r$ such that $r \vee r_1 \leq a$. Now $r \vee q$ covers q since $r \perp q$ and $r_1 \vee (r \vee q)$ covers $r \vee q$ since $r_1 \perp r$ and $r_1 \perp q$, which implies $r_1 \perp r \vee q$. We thus have $q < r \vee q < r_1 \vee r \vee q \leq p \vee q$, which contradicts the fact that $p \vee q$ covers q. Thus $(p \wedge q) \wedge q'$ is an atom. Now let $[f]$ be a ray generated by a nonpositive (by this we mean f takes positive *and* negative values on sets of positive measure) unit vector $f \in L_2(S, \mu)$. We can write $f = \alpha f^+ - (1 - \alpha^2)^{\frac{1}{2}} f^-$, where $f^+ = \max(f, 0)/\|\max(f, 0)\|$ and $f^- = \max(-f, 0)/\|\max(-f, 0)\|$, $0 < \alpha < 1$. Thus f^+ and f^- are orthogonal positive unit vectors. If $f^* = (1 - \alpha^2)^{\frac{1}{2}} f^+ + \alpha f^-$, we see that f^* is a positive unit vector orthogonal to f. Define $\psi[f] = (\psi[f^+] \vee \psi[f^*]) \wedge \psi[f^*]'$, which is an atom in L. Now ψ thus extended is defined on all rays of $L_2(S, \mu)$ and has range a subset of the atoms of L. We now show that ψ is injective. If $\psi[f] = \psi[g]$, where f, g are nonpositive unit vectors in $L_2(S, \mu)$, then $(\psi[f^+] \vee \psi[f^*]) \wedge \psi[f^*]' = (\psi[g^+] \vee \psi[g^*]) \wedge \psi[g^*]'$, where $f = \alpha f^+ - (1 - \alpha^2)^{\frac{1}{2}} f^-$ and $g = \beta g^+ - (1 - \beta^2)^{\frac{1}{2}} g^-$. Define $\nu_1^{\pm}(X(E)) = \int_E (f^{\pm})^2\,d\mu$, $\nu_2^{\pm}(X(E)) = \int_E (g^{\pm})^2\,d\mu$ for all $E \in B$ and let $\nu_1 = \alpha^2\nu_1^+ - (1 - \alpha^2)\nu_1^-$ and $\nu_2 = \beta^2\nu_2^+ - (1 - \beta^2)\nu_2^-$. Now since $f^* = (1 - \alpha^2)^{\frac{1}{2}} f^+ + \alpha f^-$, $g^* = (1 - \beta^2)^{\frac{1}{2}} g^+ + \beta g^-$, we have

$$\begin{aligned}\int_E (f^*)^2\,d\mu &= (1 - \alpha^2)\int_E (f^+)^2\,d\mu + \alpha^2\int_E (f^-)^2\,d\mu \\ &= (1 - \alpha^2)\nu_1^+(X(E)) + \alpha^2\nu_1^-(X(E)) = \nu_1^*(X(E))\end{aligned}$$

and hence $\psi[f^*] = a(\nu_1^*)$. Similarly, $\psi[g^*] = a(\nu_2^*)$, $\psi[f^+] = a(\nu_1^+)$, $\psi[g^+] = a(\nu_2^+)$. Thus $a(\nu_1) = a(\nu_2)$. Now there are real numbers α, β such that $\alpha(d\nu_1/d\mu)^{\frac{1}{2}} + \beta(d\nu_2/d\mu)^{\frac{1}{2}} = (d\nu_3/d\mu)^{\frac{1}{2}}$, where ν_3 is some signed probability measure on $R(X)$. Now, if $\nu_1 \neq \pm\nu_2$, applying condition (2), we have $a(\nu_3) < a(\nu_1) \vee a(\nu_2) = a(\nu_1)$, a contradiction. Thus $\nu_1 = \pm\nu_2$. It follows that $\alpha^2(f^+)^2 - (1 - \alpha^2)(f^-)^2 = \pm[\beta^2(g^+)^2 - (1 - \beta^2)(g^-)^2]$ a.e. (μ). Now let $E_1 = \{\omega \in S: f^+(\omega), g^+(\omega) > 0\}$, $E_2 = \{\omega \in S:\ f^-(\omega),\ g^-(\omega) > 0\}$, $E_3 = \{\omega \in S:\ f^+(\omega),\ g^-(\omega) > 0\}$, and $E_4 = \{\omega \in S:\ f^-(\omega),\ g^+(\omega) > 0\}$. Suppose the plus sign holds. Then, on E_1, $\alpha^2(f^+)^2 = \beta^2(g^+)^2$ so that $\alpha f^+ = \beta g^+$ on E_1 and hence $f = \alpha f^+ - (1 - \alpha^2)^{\frac{1}{2}} f^- = \beta g^+ - (1 - \beta^2)^{\frac{1}{2}} g^- = g$ on E_1. In a similar way, $f = g$ on E_2. Now on E_3 we have $\alpha^2(f^+)^2 = -(1 - \beta^2)(g^-)^2$ so that $E_3 = \phi$. Similarly $E_4 = \phi$ so $f = g$ a.e. (μ). If the negative sign holds, we obtain $E_1 = E_2 = \phi$ and $f = -g$ on $E_3 \cup E_4$ so that $f = -g$ a.e. (μ). We finally obtain $[f] = [g]$ and ψ is injective. To show that ψ preserves orthogonality, suppose $f \perp g$. Then $\alpha f^+ - (1 - \alpha^2)^{\frac{1}{2}} f^- \perp \beta g^+ - (1 - \beta^2)^{\frac{1}{2}} g^-$, which implies that $(\frac{1}{2}d\nu_1/d\mu)^{\frac{1}{2}} + (\frac{1}{2}d\nu_2/d\mu)^{\frac{1}{2}}$ is a unit vector. Via condition (2), it follows that $\psi[f] \leftrightarrow \psi[g]$. Now $\psi[f] \neq \psi[g]$ since ψ is injective and the only other way for two atoms to be compatible is that $\psi[f] \perp \psi[g]$. Denote the lattice of finite-dimensional subspaces of $L_2(S, \mu)$ by $PL_2(S, \mu)$. We extend ψ to $PL_2(S, \mu)$ as follows: If $a \in PL_2(S, \mu)$ and $\{e_\alpha\}$ is the set of rays in a, define $\psi(a) = V_\alpha \psi(e_\alpha)$. To show that ψ preserves suprema, let $a, b \in PL_2(S, \mu)$. Then

$$\begin{aligned}\psi(a \vee b) &= V\{\psi(e): e \leq a \vee b, e \text{ an atom}\} \\ &\geq V\{\psi(f): f \leq a, f \text{ an atom}\} \vee V\{\psi(g): \\ &\quad g \leq b, g \text{ an atom}\} \\ &= \psi(a) \vee \psi(b).\end{aligned}$$

Now suppose e is an atom and $e \leq a \vee b$. Then there are atoms f, g such that $f \leq a$, $g \leq b$ and $e \leq f \vee g$. By applying condition (2) as above it follows that $\psi(e) \leq \psi(f) \vee \psi(g) \leq \psi(a) \vee \psi(b)$ and hence $\psi(a \vee b) = \psi(a) \vee \psi(b)$. Now it is clear that ψ preserves orthogonality on $PL_2(S, \mu)$ and, if $a \leq b \in PL_2(S, \mu)$, then $a \perp (b - a)$ so that $\psi(a) \perp \psi(b - a)$ and $\psi(b - a) \leq \psi(a)'$. Hence $\psi(b) \wedge \psi(a)' = [\psi(a) \vee \psi(b - a)] \wedge \psi(a)' = \psi(b - a) \wedge \psi(a)' = \psi(b - a)$. To show ψ preserves infima, let $a, b \in PL_2(S, \mu)$ and define $c^\circ = a \vee b - c$ for any $c \in [0, a \vee b]$. Since $'$ is an orthocomplementation on the orthomodular lattice of closed subspaces of $L_2(S, \mu)$, it follows that $\circ$ is an orthocomplementation which makes $[0, a \vee b]$ into an orthomodular lattice. Hence

$$\begin{aligned}\psi(a \wedge b) &= \psi((a^\circ \vee b^\circ)^\circ) = \psi(a \vee b) \wedge \psi(a^\circ \vee b^\circ)' \\ &= \psi(a \vee b) \wedge [\psi(a^\circ) \vee \psi(b^\circ)]' \\ &= \psi(a \vee b) \wedge \psi(a^\circ)' \wedge \psi(b^\circ)' \\ &= [\psi(a \vee b) \wedge \psi(a^\circ)'] \wedge [\psi(a \vee b) \wedge \psi(b^\circ)'] \\ &= \psi(a^{\circ\circ}) \wedge \psi(b^{\circ\circ}) = \psi(a) \wedge \psi(b).\end{aligned}$$

We finally show that this extended ψ is injective. First, if $\psi(a) = 0$, it is clear that $a = 0$. If $\psi(a) = \psi(b)$, $a, b \in PL_2(8, \mu)$, then

$$\begin{aligned}\psi(a - a \wedge b) &= \psi(a) \wedge (\psi(a \wedge b))' \\ &= \psi(a) \wedge (\psi(a)' \vee \psi(b)') \\ &= \psi(a) \wedge \psi(a)' = 0.\end{aligned}$$

By orthomodularity $a = (a \wedge b) \vee (a - a \wedge b) = a \wedge b$ so $a \leq b$. Similarly $b \leq a$ so $a = b$.

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[10] When an observable is defined on a measure space, we always assume that sets which are equal almost everywhere are identified. This amounts to taking the σ-algebra to be B modulo sets of measure zero.
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[12] V. Varadarajan, *Geometry of Quantum Theory* (Van Nostrand, Princeton, N.J., 1970), Vol. II; see also Ref. 11.
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[15] A. Friedman, *Foundations of Modern Analysis* (Holt, Rinehart and Winston, New York, 1970).
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[19] One motivation for this definition is seen in the example of the next paragraph.
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Modification Rules and Products of Irreducible Representations of the Unitary, Orthogonal, and Symplectic Groups

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Modification rules, expressible in terms of the removal of continuous boundary hooks, are derived which relate nonstandard irreducible representations (IR's) of the unitary, orthogonal, and symplectic groups in n dimensions to standard IR's. Tensorial methods are used to derive procedures for reducing the outer products of IR's of $U(n)$, $O(n)$, and $Sp(n)$, and for reducing general IR's of $U(n)$ specified by composite Young tableaux with respect to the subgroups $O(n)$ and $Sp(n)$. In these derivations the conjugacy relationship between the orthogonal and the symplectic groups is fully exploited. The results taken in conjunction with the modification rules are valid for all n.

1. INTRODUCTION

The inequivalent, standard, irreducible representations, IR's, of the unitary group in n dimensions, $U(n)$, may be denoted by $\{\nu; \mu\}_a^b$. They are specified by means of the composite Young tableaux[1] associated with the partitions $(\mu)_a = (\mu_1, \mu_2, \cdots, \mu_p)$ and $(\nu)_b = (\nu_1, \nu_2, \cdots, \nu_r)$, with $\mu_1 + \mu_2 + \cdots + \mu_p = a$ and $\nu_1 + \nu_2 + \cdots + \nu_r = b$, subject to the condition $p + r \leq n$. However, if this condition is violated, the composite tableau is said to be inadmissible and to define a nonstandard IR of $U(n)$. It has been pointed out[2] that there exist equivalence relations between inadmissible and admissible tableaux. These relations enable nonstandard IR's to be defined in terms of standard IR's. In Sec. 2 of this paper the modification rules which lead to these equivalence relations are derived. They are stated in a manner which involves only the removal of continuous boundary hooks from the appropriate composite tableau.

Similarly the inequivalent, standard IR's of the orthogonal and symplectic groups in n dimensions, $O(n)$ and $Sp(n)$, may be denoted by $[\mu]_a$ and $\langle\mu\rangle_a$ respectively. They are both specified by the Young tableau[3-5] associated with the partition $(\mu)_a = (\mu_1, \mu_2, \cdots, \mu_p)$, with $\mu_1 + \mu_2 + \cdots + \mu_p = a$, subject to the condition $p \leq k$ for the groups $O(2k)$, $O(2k + 1)$, and $Sp(2k)$. If this condition is violated, the tableau specifies a nonstandard IR which is defined in terms of a standard IR by means of an equivalence relation.[4,6] These equivalence relations

We finally show that this extended ψ is injective. First, if $\psi(a) = 0$, it is clear that $a = 0$. If $\psi(a) = \psi(b)$, $a, b \in PL_2(8, \mu)$, then

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By orthomodularity $a = (a \wedge b) \vee (a - a \wedge b) = a \wedge b$ so $a \leq b$. Similarly $b \leq a$ so $a = b$.

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1. INTRODUCTION

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Similarly the inequivalent, standard IR's of the orthogonal and symplectic groups in n dimensions, $O(n)$ and $Sp(n)$, may be denoted by $[\mu]_a$ and $\langle\mu\rangle_a$ respectively. They are both specified by the Young tableau[3-5] associated with the partition $(\mu)_a = (\mu_1, \mu_2, \cdots, \mu_p)$, with $\mu_1 + \mu_2 + \cdots + \mu_p = a$, subject to the condition $p \leq k$ for the groups $O(2k)$, $O(2k + 1)$, and $Sp(2k)$. If this condition is violated, the tableau specifies a nonstandard IR which is defined in terms of a standard IR by means of an equivalence relation.[4,6] These equivalence relations

are themselves defined by three modification rules[6] appropriate to $O(2k)$, $O(2k+1)$, and $Sp(2k)$, which are very easy to use if the portion of the tableau below the kth row contains more columns than rows. In other cases they have to be used with care.[7] In Sec. 3 of this paper the same equivalence relations are defined by means of just two modification rules appropriate to $O(n)$ and $Sp(n)$. These rules are analogous to those appropriate to $U(n)$, and involve only the removal of continuous boundary hooks from the appropriate Young tableau.

The introduction of composite tableaux to specify IR's of $U(n)$ was motivated in the first instance by the desire to mirror the quark–antiquark structure of elementary particles in the theory of the representations of the approximate symmetry group of the interactions of these particles. The associated problem of decomposing the outer product of two standard IRs of $U(n)$ specified by composite tableaux was solved in terms of a five stage procedure.[1] However, a greatly simplified procedure for carrying out such decompositions was conjectured by Abramsky.[8] In Sec. 4 of this paper this conjecture is proved to be valid when taken in conjunction with the modification rules of Sec. 2. The tensorial methods used in this derivation are then applied to the problem of decomposing the outer products of IR's of $O(n)$ and $Sp(n)$. The resulting procedural rules associated with these decompositions correspond to those derived by Newell[6] and Littlewood,[9] but are slightly simpler to use.

Finally, in Sec. 5, procedures are given for decomposing an IR of $U(n)$ specified by a composite tableau into IR's of $O(n)$ and $Sp(n)$. In the derivation of these procedural rules, use is made of the conjugacy[10,11] of $O(n)$ and $Sp(n)$.

2. MODIFICATION RULES FOR $U(n)$

A finite-dimensional regular IR of $U(n)$ may be denoted by[1]

$$\begin{aligned}\{\nu,\mu\}_a^b &= \{\nu_1,\nu_2,\cdots,\nu_r;\mu_1,\mu_2,\cdots,\mu_p\}\\ &= \{\nu_s',\cdots,\nu_2',\nu_1';\mu_1',\mu_2',\cdots,\mu_q'\}',\end{aligned}\quad(2.1)$$

where

$$\sum_{i=1}^{p}\mu_i=\sum_{j=1}^{q}\mu_j'=a,$$

$$\sum_{k=1}^{r}\nu_k=\sum_{l=1}^{s}\nu_l'=b,$$

and

$$\mu_1\geq\mu_2\geq\cdots\geq\mu_p>0,\quad \mu_1'\geq\mu_2'\geq\cdots\geq\mu_q'>0.$$
$$\nu_1\geq\nu_2\geq\cdots\geq\nu_r>0,\quad \nu_1'\geq\nu_2'\geq\cdots\geq\nu_s'>0,$$

with $p=\mu_1'$, $q=\mu_1$, $r=\nu_1'$, and $s=\nu_1$. This IR is defined to be standard if

$$p+r\leq n.\quad(2.2)$$

The basis of such an IR is a set of traceless mixed tensors whose index symmetry is specified by the IR's of the symmetric group associated with the partitions $(\mu)_a$ and $(\nu)_b$. Diagrammatically (2.1) is defined by a composite tableau formed by joining back-to-back an undotted and a dotted Young tableau, the row lengths of these tableaux are determined by the partitions $(\mu)_a$ and $(\nu)_b$, and the column lengths by the conjugate partions $(\mu')_a$ and $(\nu')_b$, respectively. The corresponding tensors take the form

$$T^{(\beta)_b}_{(\alpha)_a}=T^{(\beta_1\beta_2\cdots\beta_{\nu_1'})(\beta_{\nu_1'+1}\cdots\beta_{\nu_1'+\nu_2'})\cdots(\cdots\beta_b)}_{(\alpha_1\alpha_2\cdots\alpha_{\mu_1'})(\alpha_{\mu_1'+1}\cdots\alpha_{\mu_1'+\mu_2'})\cdots(\cdots\alpha_a)},\quad(2.3)$$

where each of the indices α_i and β_j may take on the values $1,2,\cdots,n$ and the brackets $(\cdots)$ indicate antisymmetrization.

Contraction with the fundamental totally antisymmetric pseudotensor $\epsilon_{\gamma_1\gamma_2\cdots\gamma_n}$ then gives rise to the tensors

$$S^{(\beta)_{b-r}}_{(\alpha)_{a+n-r}}=\epsilon_{\beta_1\beta_2\cdots\beta_r\alpha_{a+1}\alpha_{a+2}\cdots\alpha_{a+n-r}}T^{(\beta)_b}_{(\alpha)_a},\quad(2.4)$$

with $r=\nu_1'$. Just as the tensors (2.3) form the basis of the IR (2.1), so the tensors (2.4) form the basis of the IR

$$\begin{aligned}\{\rho;\lambda\}_c^d &= \{\rho_1,\rho_2,\cdots;\lambda_1,\lambda_2,\cdots\}\\ &= \{\nu_s',\cdots,\nu_2';n-\nu_1',\mu_1',\mu_2',\cdots,\mu_q'\}',\end{aligned}\quad(2.5)$$

with $c=a+n-r$ and $d=b-r$. For the group $SU(n)$, the IR's (2.1) and (2.5) are equivalent, whereas, for $U(n)$, the properties of the pseudotensor $\epsilon_{\gamma_1\gamma_2\cdots\gamma_n}$ are such that they are inequivalent but related by the equivalence formula

$$\{\nu;\mu\}_a^b=\epsilon\{\rho;\lambda\}_c^d,$$

where ϵ is the determinant of the matrix in this IR of the particular group element being considered.

Repeated application of this technique of lowering indices, and the exactly analogous technique of raising indices, then leads to the set of equivalence relations

$$\begin{aligned}\{\nu;\mu\}_a^b &= \{\nu_s',\cdots,\nu_2',\nu_1';\mu_1',\mu_2',\cdots,\mu_q'\}'\\ &= \epsilon^{l}\{\nu_s',\cdots,\nu_{l+1}';n-\nu_l',\cdots,n-\nu_2',\\ &\quad n-\nu_1',\mu_1',\mu_2',\cdots,\mu_q'\}'\\ &= \epsilon^{-j}\{\nu_s',\cdots,\nu_2',\nu_1',n-\mu_1',\\ &\quad n-\mu_2',\cdots,n-\mu_j';\mu_{j+1}',\cdots,\mu_q'\}',\end{aligned}\quad(2.6)$$

with $l=1,2,\cdots,s$ and $j=1,2,\cdots,q$.

For the group $SU(n)$, $\epsilon=1$, so that the complete set of inequivalent standard regular IR's of $SU(n)$ may be specified by conventional regular Young tableaux

associated with covariant tensors. These are obtained from (2.6) by taking the special case $l = s$. More generally, for IR's of $U(n)$,

$$\{\nu;\mu\}_a^b = \epsilon^s\{\lambda\}_c, \tag{2.7}$$

where

$$\{\lambda\}_c = \{\lambda_1, \lambda_2, \cdots, \lambda_{n-\nu_s'}\} = \{\lambda_1', \lambda_2', \cdots, \lambda_{s+q}'\}', \tag{2.8}$$

with $c = ns - b + a$,

$$\begin{aligned}\lambda_g &= s + \mu_g, && \text{if } g = 1, 2, \cdots, p,\\ &= s, && \text{if } g = p+1, p+2, \cdots, n-r,\\ &= s - \nu_{n-g+1}, && \text{if } g = n-r+1, n-r+2, \cdots, n-\nu_s',\end{aligned}$$

and

$$\begin{aligned}\lambda_h' &= n - \nu_{s-h+1}', && \text{if } h = 1, 2, \cdots, s,\\ &= \mu_{h-s}', && \text{if } h = s+1, s+2, \cdots, s+q.\end{aligned}$$

It may be seen from (2.1), (2.7), and (2.8) that if the constraint (2.2) is relaxed so that $p + r > n$, the IR $\{\nu;\mu\}_a^b$ is equivalent to an IR $\{\lambda\}_c$ that is specified by a Young tableau which is irregular in the sense that $\lambda_{s+1}' > \lambda_s'$. For such values of n, the composite tableau corresponding to $\{\nu;\mu\}_a^b$ is said to be inadmissible, and it does not specify a standard IR either of $U(n)$ or of $SU(n)$. This is essentially because the tracelessness condition for the indices of the mixed tensors (2.2) is such that these tensors vanish identically.

However, if an inadmissible tableau occurs, for example, in the reduction of the outer product of standard IR's of $U(n)$, then it is not sufficient that such a tableau be ignored and the corresponding IR deleted from the reduction. The procedural rules given for analysing outer products makes this clear.[1] Unfortunately, the problem of admissibility made it necessary to associate subscripts with the multiplicities of composite tableau in such reductions. These subscripts carried information regarding restrictions for particular values of n. It has been pointed out[2] that the necessity of introducing such subscripts is obviated if use is made of equivalence relations between IR's of $U(n)$.

It is well known[12,13] that if $\{\lambda\}_c = \{\lambda_1, \lambda_2, \cdots\} = \{\lambda_1', \lambda_2', \cdots\}'$, then

$$\{\lambda\}_c = |\{\lambda_i - i + j\}| \tag{2.9}$$

and

$$\{\lambda\}_c = |\{1^{\lambda_j'+i-j}\}|. \tag{2.10}$$

These identities, (2.9) and (2.10), express IR's of $U(n)$ in terms of products of IR's of $U(n)$ whose bases are totally symmetric and totally antisymmetric tensors respectively. The identity (2.9) has been used[14] to attach a meaning to IR's of $U(n)$ defined by irregular Young tableaux for which the rule $\lambda_i \geq \lambda_{i+1}$ is violated for some value of i. In the same way (2.10) serves to give meaning to those IR's of $U(n)$ defined by irregular Young tableaux for which the rule $\lambda_j' \geq \lambda_{j+1}'$ is violated for some value of j. Simple rearrangements of the rows and columns of the determinantal expressions (2.9) and (2.10) lead directly to equivalence relations between IR's of $U(n)$ defined by irregular and regular Young tableaux.

Via (2.10), the fundamental identity is given by

$$\{\lambda_1', \lambda_2, \cdots, \lambda_j', \lambda_{j+1}', \cdots\}' = -\{\lambda_1', \lambda_2', \cdots, \lambda_{j+1}' - 1, \lambda_j' + 1, \cdots\}'. \tag{2.11}$$

From this result it follows immediately that if j takes on the largest value for which $\lambda_j' < \lambda_{j+1}'$, then

$$\{\lambda\}_c = (-1)^x\{\sigma\}_c, \tag{2.12}$$

where the tableaux corresponding to the IR's $\{\lambda\}_c$ and $\{\sigma\}_c$ are both obtained from one and the same augmented tableau corresponding to $\{\mu\}_{c+h}$ by removing, for $\{\lambda\}_c$, a set of h boxes from the jth column and by removing, for $\{\sigma\}_c$, a continuous boundary hook containing h boxes. The hook starts from the jth column and ends in the $(j+x)$th column. The augmented tableau is defined so that $\{\mu\}_{c+h} = \{\mu_1'\mu_2', \cdots, \mu_k', \cdots\}'$ with

$$\begin{aligned}\mu_k' &= \lambda_k', && \text{if } k \neq j,\\ &= \lambda_j' + h, && \text{if } k = j,\end{aligned} \tag{2.13}$$

where h is any integer such that $\lambda_j' + h \geq \lambda_{j+1}'$. The numbers h and x are called the length and depth, respectively, of the hook. If it is not possible to remove a hook of the required length in such a way that the portion of the tableau corresponding to $\{\sigma\}_c$ to the right of the jth column is regular, then $\{\lambda\}_c$ is identically zero. The removal of hooks should be continued until either a regular tableau or zero results. This technique is illustrated in the examples of Fig. 1 which correspond to the equivalences

$$\{7, 1, 5, 4\}' = \{7, 4, 3^2\}' = \{4^3, 2, 1^3\},$$
$$\{7, 1, 5, 3\}' = 0,$$
$$\{2, 1, 5, 4\}' = \{2, 4, 3^2\}' = -\{3^4\}' = -\{4^3\}.$$

Via (2.6), (2.11), and (2.12), it is easy to determine the equivalence relations associated with inadmissible composite tableaux. For IR's of $U(n)$ it follows from (2.6) that

$$\{\nu;\mu\}_a^b = (\nu_s', \cdots, \nu_2', r; p, \mu_2', \cdots, \mu_q')' = \epsilon\{\nu_s', \cdots, \nu_2'; n-r, p, \mu_2', \cdots, \mu_q'\}'. \tag{2.14}$$

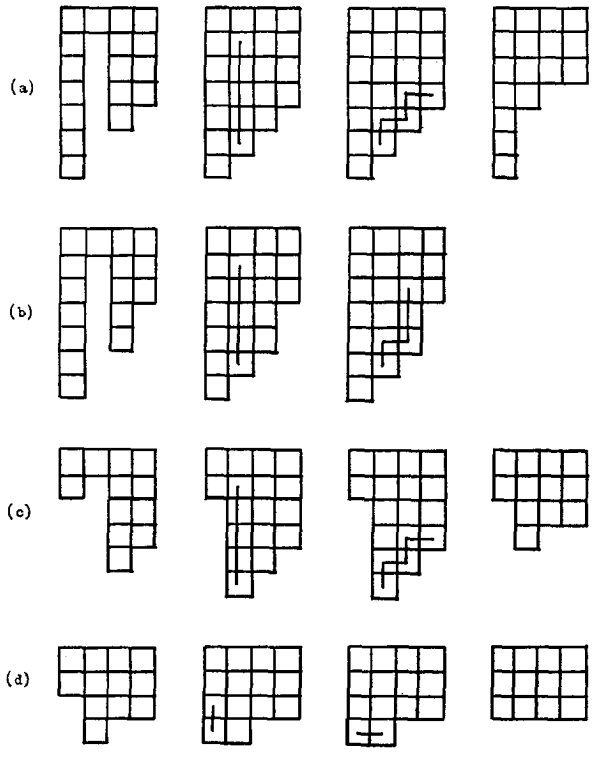

FIG. 1. Regularization of Young tableaux (see Table I).

TABLE I. Regularization of tableaux in accordance with the formula $\{\lambda\}_c = (-1)^x\{\sigma\}_c$. Continuous boundary hooks of length h and depth x are removed from the augmented tableaux denoted by $\{\mu\}_{c+h}$.

	$\{\lambda\}_c$	$\{\mu\}_{c+h}$	h	$\{\sigma\}_c$	x
(a)	$\{7,1,5,4\}'$	$\{7,6,5,4\}'$	5	$\{7,4,3^2\}'$	2
(b)	$\{7,1,5,3\}'$	$\{7,6,5,3\}'$	5	$\{7,4,2,3\}' = 0$	1
(c)	$\{2,1,5,4\}'$	$\{2,6,5,4\}'$	5	$\{2,4,3^2\}'$	2
(d)	$\{2,4,3^2\}'$	$\{4^2,3^2\}'$	2	$\{3^4\}'$	1

Therefore form (2.11)

$$\{\nu;\mu\}_a^b = -\epsilon\{\nu_s', \cdots, \nu_2'; p-1, n-r+1, \mu_2', \cdots, \mu_q'\}', \quad (2.15)$$

so that (2.6) yields the result published earlier[2]:

$$\{\nu;\mu\}_a^b = -\{\nu_s', \cdots, \nu_2', n-p+1; n-r+1, \mu_2', \cdots, \mu_q'\}'. \quad (2.16)$$

Clearly, if $p + r = n + 1$, this identity (2.16) indicates that $\{\nu;\mu\}_a^b = 0$. On the other hand, if $p + r > n + 1$, it follows that

$$\{\nu;\mu\}_a^b = -\{\rho;\lambda\}_c^d, \quad (2.17)$$

with $c = a - p - r + n + 1$, $d = b - p - r + n + 1$, $\rho_1' = n - r + 1$, and $\lambda_1' = n - p + 1$. Thus, if $\{\nu;\mu\}_a^b$ corresponds to an inadmissible composite tableau for which $\nu_1' + \mu_1' = p + r > n + 1$, then $\{\rho;\lambda\}_c^d$ corresponds to an admissible composite tableau since $\rho_1' + \lambda_1' = 2n - p - r + 2 \leq n$. This tableau may however be irregular and need further modification. In fact, the tableaux defined by $\{\lambda\}_c$ and $\{\rho\}_d$ are obtained from what might be called the augmented tableaux defined by $\{\mu\}_a$ and $\{\nu\}_b$ by the removal of $(p + r - n - 1)$ boxes from the first columns of these tableaux. Finally (2.12) leads to the modification rule

$$\{\nu;\mu\}_a^b = (-1)^{x+y+1}\{\tau;\sigma\}_c^d, \quad (2.18)$$

where the tableaux defined by $\{\sigma\}_c$ and $\{\tau\}_d$ are obtained from those defined by $\{\mu\}_a$ and $\{\nu\}_b$, respectively, by the removal of continuous boundary hooks of length $(p + r - n - 1)$ and depths x and y, starting in the first columns of the dotted and undotted portions of the inadmissible composite tableau. If the resulting tableau is irregular, the corresponding IR vanishes identically. Even if this tableau is regular, it may still, of course, be inadmissible. In this case the hook removal process may be repeated, more than once if necessary, until either an admissible composite tableau or an irregular composite tableau results. At each stage the length of the pair of hooks to be removed is determined by n and the lengths of the first columns of the dotted and undotted portions of the inadmissible composite tableau.

Illustrative examples are given in Fig. 2 corresponding to the equivalences

$$\begin{aligned}\{3^2 21; 2^2 1^4\} &= -\{3^2 2; 2^2 1^3\}, \text{ for } U(8),\\ &= +\{3^2; 2^2 1\}, \text{ for } U(6),\\ &= +\{21; 2\}, \text{ for } U(3),\\ &= 0, \text{ for } U(9), U(7), U(5), U(4), U(2), \text{ and } U(1).\end{aligned} \quad (2.19)$$

These results may be checked by making use of the dimensionality formula[15,16] appropriate to IR's of $U(n)$ specified by composite tableaux. This formula is valid both for admissible and inadmissible tableaux, and gives

$$\begin{aligned}D_n\{3^2 21; 2^2 1^4\} = {} & (n+4)(n+3)^2(n+2)(n+1)^2(n)^3\\ & \times (n-1)^2(n-2)^2(n-4)(n-5)\\ & \times (n-7)(n-9)/7^2 5^4 2^3 3^2 2^3,\end{aligned} \quad (2.20)$$

which is useful for checking (2.19).

It is worth noting that (2.15) includes the well-known result $\{0;\mu\}_a^0 = \{\mu\}_a = 0$, if $p > n$.

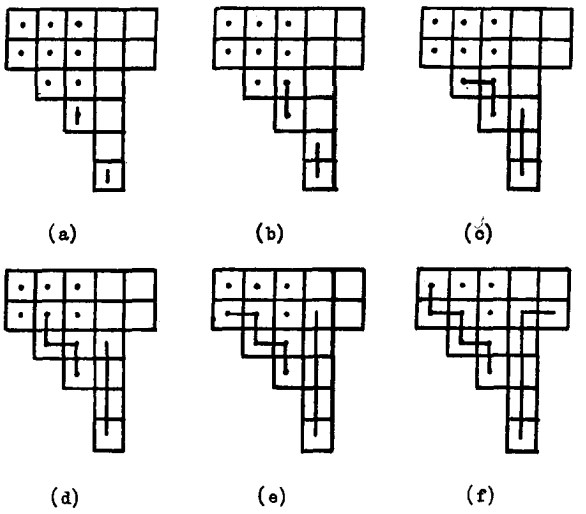

FIG. 2. Standardization of composite tableaux (see Table II).

TABLE II. Standardization of composite tableaux in accordance with the formula $\{\nu;\mu\}_{\cdot} = (-1)^{x+y+1}\{\tau,\sigma\}_c^d$. Continuous boundary hooks of length h and depths x and y are removed from the dotted and undotted parts of the tableau corresponding to the IR of $U(n)$:

$$\{\nu;\mu\}_a^b = \{3^2,2,1;2^2,1^4\} = \{2,3,4;6,2\}'.$$

	n	h	$\{\tau,\sigma\}_c^d$	x	y
(a)	8	1	$\{2,3^2;5,2\}'$	0	0
(b)	7	2	$\{2,3,2;5,2\}' = 0$	0	0
(c)	6	3	$\{2^3;3,2\}'$	1	0
(d)	5	4	$\{2,1,2;2^2\}' = 0$	1	0
(e)	4	5	$\{1^2,2;1,2\}' = 0$	2	0
(f)	3	6	$\{1,2;1^2\}'$	2	1

3. MODIFICATION RULES FOR $O(n)$ AND $Sp(n)$

For the groups $O(n)$ and $Sp(n)$, the group elements are restricted in such a way that there exist invariant metric tensors $g_{\lambda_1\lambda_2}$ and $h_{\lambda_1\lambda_2}$ which are symmetric and antisymmetric, respectively. These metric tensors may be used both to reduce IR's of $U(n)$ with respect to $O(n)$ and $Sp(n)$ and to raise and lower tensor indices.

The IR's of $O(n)$ and $Sp(n)$ associated with the partition $(\lambda)_c = (\lambda_1, \lambda_2, \cdots, \lambda_t)$ are specified by the symbols $[\lambda]_c$ and $\langle\lambda\rangle_c$, respectively. For the groups $O(2k)$, $O(2k+1)$, and $Sp(2k)$, such IR's are said to be standard if $t \leq k$. Newell[6] by generalizing a method due to Murnaghan,[4] has determined three modification rules appropriate to these groups whereby nonstandard IR's, with $t > k$, are defined in terms of standard IR's. However, it is possible to derive two modification rules for $O(n)$ and $Sp(n)$ which are analogous to the rule (2.18) which is appropriate to $U(n)$. To do this, it is first necessary to generalize the identities[17]

$$[\lambda] = |[\lambda_i - i + j] + [\lambda_i - i - j + 2] - \delta_{1j}[\lambda_i - i + 1]|, \quad (3.1)$$

and[18]

$$\langle\lambda\rangle = |\langle\lambda_i - i + j\rangle + \langle\lambda_i - i - j + 2\rangle - \delta_{1j}\langle\lambda_i - i + 1\rangle|. \quad (3.2)$$

The required expressions are

$$[\lambda] = |[1^{\lambda_j'+i-j}] + [1^{\lambda_j'-i-j+2}] - \delta_{i1}[1^{\lambda_j'-i+1}]| \quad (3.3)$$

and

$$\langle\lambda\rangle = |\langle 1^{\lambda_j'+i-j}\rangle + \langle 1^{\lambda_j'-i-j+2}\rangle - \delta_{i1}\langle 1^{\lambda_j'-j+1}\rangle|. \quad (3.4)$$

The identities (3.1) and (3.2) may be used to define IR's of $O(n)$ and $Sp(n)$ specified by irregular Young tableaux for which the rule $\lambda_i \geq \lambda_{i+1}$ is violated, while (3.3) and (3.4) may be used in the cases for which the rule $\lambda_j' \geq \lambda_{j+1}'$ is violated. The fundamental identities which follow from (3.1) and (3.2) are

$$[\lambda_1', \lambda_2', \cdots, \lambda_j', \lambda_{j+1}', \cdots]' = -[\lambda_1', \lambda_2', \cdots, \lambda_{j+1}' - 1, \lambda_j' + 1, \cdots]', \quad (3.5)$$

and

$$\langle\lambda_1', \lambda_2', \cdots, \lambda_j', \lambda_{j+1}', \cdots\rangle' = -\langle\lambda_1', \lambda_2', \cdots, \lambda_{j+1}' - 1, \lambda_j' + 1, \cdots\rangle'. \quad (3.6)$$

These identities, (3.5) and (3.6), are exactly analogous to (2.11), and lead in the notation of (2.12) to the results

$$[\lambda]_c = (-1)^x[\sigma]_c \quad (3.7)$$

and

$$\langle\lambda\rangle_c = (-1)^x\langle\sigma\rangle_c. \quad (3.8)$$

For the groups $O(2k)$ and $O(2k+1)$ the IR $[\mu]_a = [p, \mu_2', \cdots, \mu_q']'$ is nonstandard if $p > k$, and the corresponding tableau is inadmissible. However, it is possible to contract the p antisymmetrised indices associated with the first column of this inadmissible tableau with the pseudotensor $\epsilon^{\gamma_1\gamma_2\cdots\gamma_n}$ and to lower the resulting upper indices by contractions with the metric tensor $g_{\gamma\delta}$. It then follows that

$$[\mu]_a = \epsilon[\lambda]_c, \quad (3.9)$$

where

$$[\lambda]_c = [n - p, \mu_2', \cdots, \mu_q']', \quad (3.10)$$

with $c = a + n - 2p$. The resulting tableau corresponding to $[\lambda]_c$ is then admissible, but it may not be regular. However, the use of (3.7) yields the modification rule

$$[\mu]_a = (-1)^x\epsilon[\sigma]_c, \quad (3.11)$$

where the tableau corresponding to $[\sigma]_c$ is obtained

from the inadmissible tableau corresponding to $[\mu]_a$ by the removal of a continuous boundary hook of length $2p - n$ and the depth x, starting in the first column of the inadmissible tableau.

Repeated application of (3.11) leads either to an admissible tableau or to zero if, at any stage, the removal of the required hook leaves an irregular tableau. Illustrative examples are given in Fig. 3 corresponding to the equivalences

$$\begin{aligned}[3^3, 1] &= \epsilon[3^3], \quad \text{for } O(7),\\ &= \epsilon[3^2], \quad \text{for } O(4),\\ &= -[2], \quad \text{for } O(2),\\ &= 0, \quad \text{for } O(6), O(5), \text{ and } O(3). \end{aligned} \tag{3.12}$$

These results may be checked by making use of the dimensionality formula[11] appropriate to IR's of $O(n)$. This formula is valid both for admissible and inadmissible tableaux, and gives

$$\begin{aligned}D_n[3^3, 1] = (n+4)(n+3)(n+2)^2(n+1)(n)\\ \times (n-1)(n-3)(n-5)(n-6)/\\ 6\cdot 5\cdot 4^2\cdot 3^2\cdot 2, \end{aligned} \tag{3.13}$$

which is useful for checking (3.12).

It should be noted that, for the orthogonal group, $\epsilon = \pm 1$, so that $\epsilon^2 = 1$. Use has been made of this in deriving (3.12).

An interesting special case of (3.9) arises when $n = 2k$ and $p = k$. In this case

$$[\mu_1, \mu_2, \cdots, \mu_k] = \epsilon[\mu_1, \mu_2, \cdots, \mu_k], \tag{3.14}$$

which implies that, for those group elements for which $\epsilon = -1$, the particular characters of $O(2k)$ defined by (3.14) vanish.

For the rotation subgroup $SO(n)$ of $O(n)$, the group elements are restricted by the condition $\epsilon = 1$. Under this restriction the IR's of $O(n)$ remain irreducible except for $n = 2k$, in which case the IR's of $O(n)$ of the form (3.14), with $\mu_k > 0$, reduce into two IR's of $SO(n)$ which are usually denoted[19] by $[\mu_1, \mu_2, \cdots, \mu_{k-1}, \mu_k]$ and $[\mu_1, \mu_2, \cdots, \mu_{k-1}, -\mu_k]$. These IR's of $SO(n)$ have the same dimensions.

The use of $\epsilon_{\gamma_1\gamma_2\cdots,\gamma_n}$ to raise and lower indices of the tensors which form the basis of an IR of $O(n)$ is confined to a single operation, as in (3.9), in contrast to (2.6) which applies to IR's of $U(n)$. This limitation arises as the result of the well-known identity

$$\epsilon_{\alpha_1\alpha_2\cdots\alpha_n}\epsilon_{\beta_1\beta_2\cdots\beta_n} = |g_{\alpha_i\beta_j}|. \tag{3.15}$$

For the group $Sp(n)$, the pseudotensor $\epsilon_{\gamma_1\gamma_2\cdots\gamma_a}$ may itself be written[20] in terms of products of the metric tensor $h_{\alpha\beta}$ so that it is not clear that the fundamental pseudotensor may be used to raise and lower indices. However, the results of Newell[6] for $Sp(n)$ may be obtained by the use of the modification rule

$$\langle\mu\rangle_a = (-1)^{x+1}\langle\sigma\rangle_c, \tag{3.16}$$

where the tableau corresponding to $\langle\sigma\rangle_c$ is obtained from the inadmissible tableau corresponding to $\langle\mu\rangle_a$ by the removal of a continuous boundary hook of length $2p - n - 2$ and depth x, starting in the first column of the inadmissible tableau. Clearly $c = a + n + 2 - 2p$, and use has been made of the fact that for the symplectic group $\epsilon = 1$. Repeated application of (3.16) leads either to an admissible tableau or to zero in the usual way.

Illustrative examples are given in Fig. 4 corresponding to the equivalences

$$\begin{aligned}\langle 4^2, 3, 2, 1^2\rangle &= -\langle 4^2, 3, 2\rangle, \quad \text{for } Sp(8),\\ &= +\langle 4^2, 3\rangle, \quad \text{for } Sp(6),\\ &= 0, \quad \text{for } Sp(10), Sp(4), \text{ and } Sp(2). \end{aligned} \tag{3.17}$$

Use of the dimensionality formula[11] appropriate to IR's of $Sp(n)$ which is valid for both admissible and

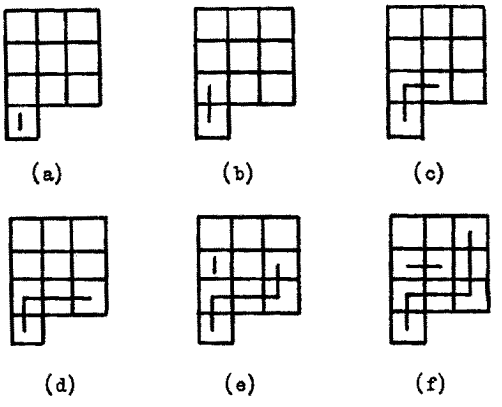

FIG. 3. Standardization of IR's of $O(n)$ (see Table III).

TABLE III. Standardization of IR's of $O(n)$ in accordance with the formula

$$[\mu]_a = (-1)^x\epsilon[\sigma]_c = (-1)^{x+y}[\tau]_d.$$

Continuous boundary hooks of lengths h and l and depths x and y are successively removed from the tableaux corresponding to $[\mu]_a$ and $[\sigma]_c$, with $[\mu]_a = [3^3, 1] = [4, 3^2]'$.

	n	h	$[\sigma]_c$	x	l	$[\tau]_d$	y
(a)	7	1	$[3^3]'$	0			
(b)	6	2	$[2, 3^2]' = 0$	0			
(c)	5	3	$[2^2, 3]' = 0$	1			
(d)	4	4	$[2^3]'$	2			
(e)	3	5	$[2^2, 1]'$	2	1	$[1, 2, 1]'$	0
(f)	2	6	$[2^2]'$	2	2	$[1^2]'$	1

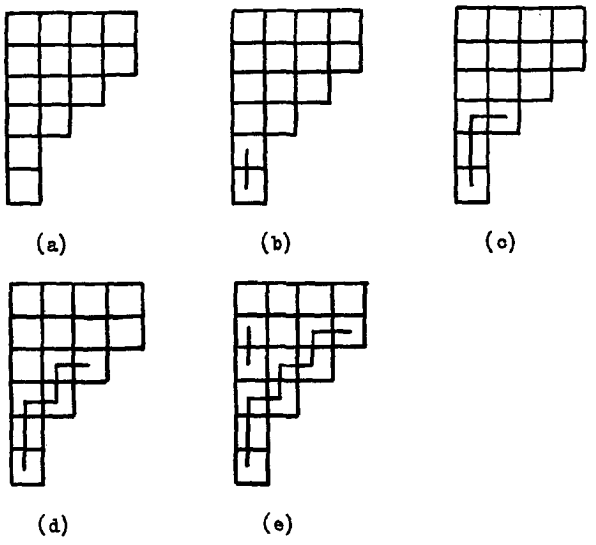

FIG. 4. Standardization of IR's of $Sp(n)$ (see Table IV).

TABLE IV. Standardization of IR's of $Sp(n)$ in accordance with the formula

$$\langle\mu\rangle_a = (-1)^{x+1}\langle\sigma\rangle_c = (-1)^{x+y}\langle\tau\rangle_d.$$

Continuous boundary hooks of lengths h and l and depths x and y are successively removed from the tableaux corresponding to $\langle\mu\rangle_a$ and $\langle\sigma\rangle_c$, with $\langle\mu\rangle_a = \langle 4^2, 3, 2, 1^2\rangle = \langle 6, 4, 3, 2\rangle'$.

	n	h	$\langle\sigma\rangle_c$	x	l	$\langle\tau\rangle_d$	y
(a)	10	0	$\langle 6,4\ 3,2\rangle' = 0$	0			
(b)	8	2	$\langle 4^2, 3, 2\rangle'$	0			
(c)	6	4	$\langle 3^2, 2\rangle'$	1			
(d)	4	6	$\langle 3, 2^2\rangle'$	2	0	$\langle 3, 2^2\rangle' = 0$	0
(e)	2	8	$\langle 3, 2, 1^2\rangle'$	3	2	$\langle 1, 2, 1^2\rangle' = 0$	0

inadmissible tableaux gives

$$D_n\langle 4^2, 3, 2, 1^2\rangle = (n+7)(n+5)(n+4)(n+3) \times (n+2)(n+1)(n)^3(n-2)(n-3)(n-4)(n-5) \times (n-7)(n-10)/9 \cdot 8 \cdot 6^2 \cdot 5 \cdot 4^2 \cdot 3^2 \cdot 2^2. \quad (3.18)$$

This may be used for checking the relations (3.17).

The IR's of $Sp(2k)$ of the form

$$\langle\mu\rangle_a = \langle\mu_1, \mu_2, \cdots, \mu_k, \mu_{k+1}\rangle \quad (3.19)$$

with $\mu_{k+1} > 0$, are such that (3.16) implies

$$\langle\mu\rangle_a = -\langle\mu\rangle_a \quad (3.20)$$

since the appropriate hook length and depth are both zero. Thus the IR's (3.19) vanish identically.

Clearly the fact that the hook length associated with the modification rule (3.16) is $(2p - n - 2)$, rather than $(2p - n)$, requires further study. No explanation in terms of operations on tensor indices is currently available.

4. OUTER PRODUCTS OF IRREDUCIBLE REPRESENTATIONS

The chief motivation for deriving the equivalence relations of Sec. 2 was provided by the desire to simplify the procedure[1] for calculating the multiplicities $m_{\mu\lambda,\sigma}^{\nu\rho,\tau}$ associated with the decomposition of the product of two IR's of $U(n)$ given by

$$\{\nu;\mu\}_a^b \cdot \{\rho;\lambda\}_c^d = \sum_{\sigma,\tau} m_{\mu\lambda,\sigma}^{\nu\rho,\tau}\{\tau;\sigma\}_e^f. \quad (4.1)$$

Abramsky[8] pointed out that if all traces exist, a simplified procedure may be used involving contractions and symmetrizations of the indices of the mixed tensors forming the bases of the IR's. Following the work of Abramsky, to derive the appropriate formula for the multiplicities, it is necessary first to determine the IR's $\{\beta;\alpha\}_{a-t}^{d-t}$ and $\{\delta;\gamma\}_{c-s}^{b-s}$ whose bases are traceless tensors contained in the products[1]

$$\{\mu\}_a \cdot \{\rho\}^d = \sum_{\alpha,\beta} m_{\mu,\alpha}^{\rho,\beta}\{\beta;\alpha\}_{a-t}^{d-t} \quad (4.2)$$

and

$$\{\nu\}^b \cdot \{\lambda\}_c = \sum_{\gamma\delta} m_{\lambda,\gamma}^{\nu,\delta}\{\delta;\gamma\}_{c-s}^{b-s}. \quad (4.3)$$

Then it merely remains to symmetrize uncontracted covariant and contravariant indices separately in accordance with the rules

$$\{\alpha\}_{a-t} \cdot \{\gamma\}_{c-s} = \sum_{\sigma} m_{\alpha\gamma,\sigma}\{\sigma\}_e \quad (4.4)$$

and

$$\{\beta\}^{d-t} \cdot \{\delta\}^{b-s} = \sum_{\tau} m_{\beta\delta,\tau}\{\tau\}^f, \quad (4.5)$$

with $e = a + c - s - t$ and $f = b + d - s - t$. The resulting tensors associated with $\{\tau;\sigma\}_e^f$ are then completely traceless and symmetrized. Thus in (4.1) Abramsky's procedure yields[2,8]

$$m_{\mu\lambda,\sigma}^{\nu\rho,\tau} = \sum_{\substack{\alpha\beta \\ \gamma\delta}} m_{\mu,\alpha}^{\rho,\beta} m_{\lambda,\gamma}^{\nu,\delta} m_{\alpha\gamma,\sigma} m_{\beta\delta,\tau}. \quad (4.6)$$

If n is sufficiently large, it is certainly true that all the relevant traces of sets of s and t indices indicated in (4.2) and (4.3) may be extracted, and all the tableaux defined by the IR's of (4.1)–(4.5) are admissible. It then follows that (4.6) is valid for such values of n and remains valid for all n provided that the modification rules of Sec. 2 are used to express all nonstandard IR's in terms of standard IR's associated with admissible tableaux.

For example, (4.6) leads to the result

$$\{1;1\} \cdot \{1;3,1\} = \{2;4,1\} + \{2;3,2\} + \{2;3,1^2\} + \{1^2;4,1\} + \{1^2;3,2\} + \{1^2;3,1^2\} + \{1;4\} + 3\{1;3,1\} + \{1;2^2\} + \{1;21^2\} + \{0;3\} + \{0;21\}, \quad (4.7)$$

which is appropriate to IR's of $U(n)$ with $n \geq 5$.

However, in the case $n = 3$, (2.18) leads to the equivalence relations

$$\{2; 3, 1^2\} = \{1^2; 4, 1\} = \{1^2; 3, 2\} = \{1; 21^2\} = 0$$

and

$$\{1^2; 3, 1^2\} = -\{1; 3, 1\},$$

so that for IR's of $U(3)$

$$\{1; 1\} \cdot \{1; 31\} = \{2; 4, 1\} + \{2; 3, 2\} + \{1; 4\} + 2\{1; 3, 1\} + \{1; 2^2\} + \{0; 3\} + \{0; 21\}. \quad (4.8)$$

Similarly the modification rules of Sec. 3 are of great use in analyzing the decompositions of the products of IR's of $O(n)$ and of IR's of $Sp(n)$, given by

$$[\mu]_a \cdot [\nu]_b = \sum_\lambda r_{\mu\nu,\lambda}[\lambda]_c \quad (4.9)$$

and

$$\langle\mu\rangle_a \cdot \langle\nu\rangle_b = \sum_\lambda s_{\mu\nu,\lambda}\langle\lambda\rangle_c. \quad (4.10)$$

To determine the multiplicities $r_{\mu\nu,\lambda}$, it is first convenient to use the metric tensor $g^{\gamma_1\gamma_2}$ to raise all the indices of the tensors associated with the IR $[\nu]_b$ and then to define the corresponding IR by $[\nu]^b$. With this notation,

$$[\mu]_a \cdot [\nu]_b = [\mu]_a \cdot [\nu]^b. \quad (4.11)$$

The covariant and contravariant indices of the tensors associated with $[\mu]_a$ and $[\nu]^b$ are, of course, separately traceless. The first step in the reduction of the product (4.11) then corresponds to the removal of traces defined by contractions between the covariant and contravariant indices in accordance with the formula

$$\{\mu\}_a \cdot \{\nu\}^b = \sum_{\sigma,\tau} m^{\nu,\tau}_{\mu,\sigma}\{\tau; \sigma\}^{b-t}_{a-t}. \quad (4.12)$$

It is then possible to write

$$[\mu]_a \cdot [\nu]^b = \sum_{\sigma,\tau} m^{\nu,\tau}_{\mu,\sigma}[\tau; \sigma]^{b-t}_{a-t},$$

where $[\tau; \sigma]^{b-t}_{a-t}$ denotes a representation of $O(n)$ which is in general reducible, but for which the corresponding tensor basis is completely traceless. The contravariant indices may then be lowered by using the metric tensor $g_{\gamma_1\gamma_2}$, and the resulting representation decomposed into IR's of $O(n)$ by carrying out the necessary symmetrizations of indices in accordance with the relation

$$\{\tau\}_{b-t} \cdot \{\sigma\}_{a-t} = \sum_\lambda m_{\tau\sigma,\lambda}\{\lambda\}_c, \quad (4.13)$$

with $c = a + b - 2t$. Thus in (4.9)

$$r_{\mu\nu,\lambda} = \sum_{\sigma,\tau} m^{\nu,\tau}_{\mu,\sigma} m_{\tau\sigma,\lambda}. \quad (4.14)$$

The identity[1]

$$m^{\nu,\tau}_{\mu,\sigma} = \sum_\rho m_{\rho\sigma,\mu} m_{\rho\tau,\nu} \quad (4.15)$$

may be used to show that (4.14) agrees precisely with the formulas derived by Newell[6] and Littlewood.[9]

The following example illustrates the two steps of the procedure based on (4.14) to derive decompositions of the form (4.9). The first step gives for the product $[3, 1] \cdot [2, 1]$ the terms

$$\begin{array}{l} \ldots a\,a + \ldots a\,a + b\,.\,a\,a \\ \quad .\,b \qquad b\not{b} \qquad .\not{b} \\ \quad + \ldots a\not{a} + a\,.\,a\not{a} + b\,.\,a\not{a} + a\,.\,a\not{a} \\ \qquad a\,b \qquad .\,b \qquad a\not{b} \qquad b\not{b} \\ \quad + a\,b\,.\,a\not{a} + a\,b\,.\not{a}\not{a}. \\ \qquad .\not{b} \qquad a\not{b} \end{array} \quad (4.16)$$

The second step gives, for example, from the third term in this expression, the IR's

$$\begin{array}{l} .\,.\,a\,a + .\,.\,a + .\,.\,a + .\,. \quad . \\ \quad . \qquad .\,a \qquad . \qquad .\,a \\ \qquad\qquad\qquad a \qquad a \end{array}$$

The final result is then seen to be

$$[3, 1] \cdot [2, 1] = [5, 2] + [5, 1^2] + [4, 3] + 2[4, 2, 1] + [4, 1^3] + [3^2, 1] + [3, 2^2] + [3, 2, 1^2] + [5] + 3[4, 1] + 3[3, 2] + 3[3, 1^2] + 2[2^2, 1] + [2, 1^3] + 2[3] + 3[2, 1] + [1^3] + [1]. \quad (4.17)$$

This result is valid for $n \geq 8$. For the particular case $n = 4$ it is necessary to apply the modification rule (3.11). This leads to the equivalence relations

$$[5, 1^2] = \epsilon[5], \quad [3, 2^2] = -\epsilon[3, 2],$$
$$[3, 2, 1^2] = -\epsilon[3], \quad [3, 1^2] = \epsilon[3], \quad [1^3] = \epsilon[1],$$

and

$$[4, 2, 1] = [4, 1^3] = [3^2, 1] = [2^2, 1] = [2, 1^3] = 0.$$

Therefore, for $O(4)$,

$$[3, 1] \cdot [2, 1] = [5, 2] + \epsilon[5] + [4, 3] + [5] + 3[4, 1] + 2[3, 2] + 2(1 + \epsilon)[3] + (1 + \epsilon)[1], \quad (4.18)$$

where use has been made of (3.14) to derive the identity

$$(3 - \epsilon)[3, 2] = 2[3, 2].$$

An alternative procedure for deriving an expression for the multiplicities $r_{\mu\nu,\lambda}$ defined by (4.9) involves the identities[21]

$$\{\rho\}_d = \sum_\lambda d_{\rho\lambda}[\lambda]_c = \sum_{\delta\lambda} m_{\delta\lambda,\rho}[\lambda]_c, \quad (4.19)$$

and

$$[\mu]_a = \sum_\sigma c_{\mu\sigma}\{\sigma\}_a = \sum_{\gamma\sigma} (-1)^{e/2} m_{\gamma\sigma,\mu}\{\sigma\}_e, \quad (4.20)$$

where $(\delta)_a$ is a partition into even parts only, and, in Frobenius notation, $(\gamma)_c$ takes the form

$$(\gamma)_c = \begin{bmatrix} c_1 + 1 & c_2 + 1 & \cdots \\ c_1 & c_2 & \cdots \end{bmatrix}. \tag{4.21}$$

The application of (4.20) to (4.9), followed by the use of (4.13) and finally (4.19), yields the result

$$r_{\mu\nu,\lambda} = \sum_{\sigma\tau\rho} c_{\mu\sigma} c_{\nu\tau} m_{\sigma\tau,\rho} d_{\rho\lambda}. \tag{4.22}$$

In order to derive a result analogous to (4.22) for the multiplicities $s_{\mu\nu,\lambda}$ defined by (4.10), it is necessary to use the identities[22]

$$\{\rho\}_d = \sum_{\lambda} b_{\rho\lambda} \langle\lambda\rangle_c = \sum_{\beta\lambda} m_{\beta\lambda,\rho} \langle\lambda\rangle_c, \tag{4.23}$$

and

$$\langle\mu\rangle_a = \sum_{\sigma} a_{\mu\sigma} \{\sigma\}_e = \sum_{\alpha\sigma} (-1)^{a/2} m_{\alpha\sigma,\mu} \{\sigma\}_e, \tag{4.24}$$

where $(\beta)_b$ is the conjugate of a partition into even parts only and $(\alpha)_a$ is the conjugate of a partition of the form (4.21). With this notation

$$s_{\mu\nu,\lambda} = \sum_{\sigma\tau\rho} a_{\mu\sigma} a_{\nu\tau} m_{\sigma\tau,\rho} b_{\rho\lambda}. \tag{4.25}$$

The well-known identity

$$m_{\sigma\tau,\rho} = m_{\sigma'\tau',\rho'} \tag{4.26}$$

leads to the conjugacy relations[11]

$$b_{\rho\lambda} = d_{\rho'\lambda'} \quad \text{and} \quad a_{\mu\sigma} = c_{\mu'\sigma'} \tag{4.27}$$

and, from (4.15), to the identity

$$m^{\nu',\tau'}_{\mu',\sigma'} = m^{\nu,\tau}_{\mu,\sigma}. \tag{4.28}$$

The comparison of (4.22) and (4.25) then yields, using (4.27),

$$s_{\mu\nu,\lambda} = r_{\mu'\nu',\lambda'}, \tag{4.29}$$

while (4.26) and (4.28), when applied to (4.14), give

$$r_{\mu'\nu',\lambda'} = r_{\mu\nu,\lambda}. \tag{4.30}$$

Hence

$$s_{\mu\nu,\lambda} = r_{\mu\nu,\lambda} \tag{4.31}$$

so that, in terms of tableaux, the reduction into IR's of the outer products of IR's of $O(n)$ and of $Sp(n)$ are identical.

It then follows directly, for example, from (4.17) that for IR's of $Sp(n)$

$$\begin{aligned}\langle 3,1\rangle \cdot \langle 2,1\rangle &= \langle 5,2\rangle + \langle 5,1^2\rangle + \langle 4,3\rangle + 2\langle 4,2,1\rangle \\ &+ \langle 4,1^2\rangle + \langle 3^2,1\rangle + \langle 3,2^2\rangle + \langle 3,2,1^2\rangle + \langle 5\rangle \\ &+ 3\langle 4,1\rangle + 3\langle 3,2\rangle + 2\langle 3,1^2\rangle + 2\langle 2^2,1\rangle + \langle 2,1^3\rangle \\ &+ 2\langle 3\rangle + 3\langle 2,1\rangle + \langle 1^3\rangle + \langle 1\rangle. \end{aligned} \tag{4.32}$$

This result is valid for $n \geq 8$. For the particular case $n = 4$ it is necessary to apply the modification rule (3.16); this leads to the equivalence relations

$$\langle 4,1^2\rangle = -\langle 4,1\rangle, \quad \langle 3,2,1^2\rangle = -\langle 3,2\rangle,$$
$$\langle 2,1^3\rangle = -\langle 2,1\rangle,$$

while (3.19) and (3.20) imply that all IR's of $Sp(4)$ specified by tableaux with three rows vanish identically. Therefore, for $Sp(4)$

$$\begin{aligned}\langle 3,1\rangle \cdot \langle 2,1\rangle &= \langle 5,2\rangle + \langle 4,3\rangle + \langle 5\rangle + 2\langle 4,1\rangle \\ &+ 2\langle 3,2\rangle + 2\langle 3\rangle + 2\langle 2,1\rangle + \langle 1\rangle. \end{aligned} \tag{4.33}$$

It should be noted that, by virtue of (4.30) and the analogous result,

$$s_{\mu'\nu',\lambda'} = s_{\mu\nu\lambda}. \tag{4.34}$$

It follows that the products $[2,1^2] \cdot [2,1]$ and $\langle 2,1^2\rangle \cdot \langle 2,1\rangle$ may be written down immediately by taking the conjugate of the terms in (4.17) and (4.32), respectively. These results are valid for $O(n)$ and $Sp(n)$ with $n \geq 5$. The modification rules (3.11) and (3.16) may then be used to derive results appropriate to $n < 5$. It is not valid for $n = 4$ to take, for example, the conjugate of the terms in (4.18) and (4.23). The correct results are

$$\begin{aligned}[2,1^2] \cdot [2,1] &= [4,1] + [3,2] + (1+\epsilon)[3] + [2,1] \\ &+ (1+\epsilon)[1] \end{aligned}$$

and

$$\langle 2,1^2\rangle \cdot \langle 2,1\rangle = 0.$$

They may be derived most conveniently by noting that for $O(4)$ $[2,1^2] = \epsilon[2]$, while, for $Sp(4)$, $\langle 2,1^2\rangle = 0$.

5. THE REDUCTION $U(n) \downarrow O(n)$ AND $U(n) \downarrow Sp(n)$

The decomposition formulas (4.19) and (4.23) may be derived most directly by noting that the covariant tensor basis of an IR of $U(n)$ forms a basis of a reducible representation of $O(n)$ and a basis of a reducible representation of $Sp(n)$. The reduction processes corresponding to $U(n) \downarrow O(n)$ and $U(n) \downarrow Sp(n)$ are carried out by systematically removing trace terms arising out of contractions with the metric tensors $g^{\alpha\beta}$ and $h^{\alpha\beta}$, respectively. Clearly m successive identical contractions with these metric tensors are associated with the symmetric products of m IR's $\{2\}$ and $\{1^2\}$. Such symmetric products are examples of plethysms[23] and are denoted by $\{2\} \otimes \{m\}$ and $\{1^2\} \otimes \{m\}$, respectively. It has been shown that,[24] in the notation of Sec. 4,

$$\{2\} \otimes \{m\} = \sum_{\delta} \{\delta\}_d, \tag{5.1}$$

and

$$\{1^2\} \otimes \{m\} = \sum_{\beta} \{\beta\}_b, \tag{5.2}$$

with $d = b = 2m$. The reduction formulas (4.19) and (4.25) then follow immediately.

This interpretation of the reduction $U(n) \downarrow O(n)$ and $U(n) \downarrow Sp(n)$ in terms of contractions with the appropriate metric tensor leads directly to the following rules, D and B, for evaluating the coefficients $d_{\rho\lambda}$ and $b_{\rho\lambda}$ contained in (4.19) and (4.23).

D: Write down the tableau corresponding to $\{\rho\}_d$ with the d boxes replaced by dots. Superpose $2m_1$ letters a, $2m_2$ letters b, $2m_3$ letters c, $\cdots$, one by one, alphabetically, on the dots of the figure in all possible ways such that at each stage in this procedure: D(i) the resulting figure corresponds to a regular tableau if each dot not superposed by a letter is interpreted as a box, D(ii) the resulting figure contains no two identical letters in the same column, D(iii) the series of letters obtained from the resulting figure by reading the superposed letters from left to right along each row taken in turn from bottom to top is a lattice permutation of those letters.

The coefficient $d_{\rho\lambda}$ is just the number of distinctly labeled figures corresponding to $\{\lambda\}_c$ obtained by means of this procedure, where $c = d - 2m$ and $m = (m_1 + m_2 + m_3 + \cdots)$.

B: Similarly the simplest way of defining the procedure B is to state that B is identical with D except that the rules D(ii) and D(iii) are replaced by: B(ii) the resulting figure contains no two identical letters in the same row, B(iii) the series of letters obtained from the resulting figure by reading the superposed letters from top to bottom along each column taken in turn from right to left is a lattice permutation of those letters.

The coefficient $b_{\rho\lambda}$ is just the number of distinctly labeled figures corresponding to $\{\lambda\}_c$ obtained by means of this procedure.

For example application of the procedures D and B to the tableau corresponding to {4, 2, 1} give rise to the figures

```
.... .... ...a ...a ..aa
..   .a   ..   .a   ..
.    a    a    .    .
..aa ...b ..bb .baa
.a   ba   .a   ba
a    a    a    a
```

and

```
.... .... ...a ...a ..ba ...a
..   .a   ..   .a   .a   ba
.    a    a    .    b    b.
```

Hence, for $U(n) \downarrow O(n)$

$$\{4, 2, 1\} = [4, 2, 1] + [4, 1] + [3, 2] + [3, 1^2] + [2^2, 1] + [3] + 2[2, 1] + [1], \quad (5.3)$$

and for $U(n) \downarrow Sp(n)$

$$\{4, 2, 1\} = \langle 4, 2, 1\rangle + \langle 4, 1\rangle + \langle 3, 2\rangle + \langle 3, 1^2\rangle + \langle 3\rangle + \langle 2, 1\rangle. \quad (5.4)$$

Application of (4.27) then indicates that

$$\{3, 2, 1^2\} = [3, 2, 1^2] + [3, 1^2] + [2^2, 1] + [2, 1^3] + [2, 1] + [1^3] \quad (5.5)$$

and

$$\{3, 2, 1^2\} = \langle 3, 2, 1^2\rangle + \langle 3, 2\rangle + \langle 3, 1^2\rangle + \langle 2^2, 1\rangle + \langle 2, 1^3\rangle + 2\langle 2, 1\rangle + \langle 1^3\rangle + \langle 1\rangle. \quad (5.6)$$

The decomposition formulas (4.19) and (4.23) are, of course, well known; however, the procedures D and B for carrying out these decompositions are new. Their particular merit lies in the fact that they fully exploit both the step-by-step nature of the trace removal process and the conjugacy of IR's of $O(n)$ and $Sp(n)$.

To solve completely the reduction problem, it is necessary to consider the IR of $U(n)$ denoted by $\{\nu; \mu\}_a^b$ and specified by a regular composite tableau. Since the tensors (2.3) forming the basis of such an IR of $U(n)$ are traceless, it is merely necessary to remove trace terms arising out of contractions of the metric tensors either with covariant indices or with contravariant indices. This step is followed by the lowering of the uncontracted contravariant indices using the metric tensor, and the subsequent symmetrization of these lowered indices with the uncontracted covariant indices. It follows that for the reduction $U(n) \downarrow O(n)$

$$\{\nu; \mu\}_a^b = \sum_{\sigma\tau\rho} d_{\nu\sigma} d_{\mu\tau} m_{\sigma\tau,\rho} [\rho]_e, \quad (5.7)$$

while for the reduction $U(n) \downarrow Sp(n)$

$$\{\nu; \mu\}_a^b = \sum_{\sigma\tau\rho} b_{\nu\sigma} b_{\mu\tau} m_{\sigma\tau,\rho} \langle\rho\rangle_e. \quad (5.8)$$

In practice it is often more convenient to use (5.7) and (5.8), which are valid for all n, when taken in conjunction with the modification rules of Sec. 3, rather than to use (2.7) for a particular value of n followed by either (4.19) or (4.23). This latter method would lead to the results

$$\{\nu; \mu\}_a^b = \sum_{\rho} \epsilon^s d_{\lambda\rho} [\rho]_e, \quad (5.9)$$

and

$$\{\nu; \mu\}_a^b = \sum_{\rho} b_{\lambda\rho} \langle\rho\rangle_e, \quad (5.10)$$

where, of course, for the particular value of n under consideration, the modification rules of Sec. 3 must be used.

An alternative procedure for deriving expressions equivalent to (5.7) and (5.8) which are valid for all n involves using the identity[1]

$$\{\nu;\mu\}_a^b = \sum (-1)^t m_{\mu,\sigma}^{\nu',\tau'} \{\sigma\}_{a-t} \cdot \{\tau\}^{b-t}, \quad (5.11)$$

followed by (4.19) or (4.23) and then (4.9) or (4.10). This method is very tedious in general but, by virtue of the conjugacy relations (4.26) and (4.27), provides a method of deriving (5.8) from (5.7).

For the IR $\{3,1;2,1\}$ of $U(n)$, the first steps appropriate to (5.7) and (5.8) give rise, using the procedures D and B, to the figures

$$\begin{array}{llll} \ldots & \ldots a & .a\,a, & \ldots .a \\ . & a & . & . \quad a \end{array}$$

and

$$\begin{array}{llll} \ldots & \ldots a, & & \ldots .a, \\ . & a & & . \quad a \end{array}$$

respectively. Taking the products of the appropriate terms in accordance with (4.4) then gives

$$\begin{aligned} \{3,1;21\} = {} & [5,2] + [5,1^2] + [4,3] + 2[4,2,1] \\ & + [4,1^3] + [3^2,1] + [3,2^2] + [3,2,1^2] \\ & + 2[4,1] + 3[3,2] + 3[3,1^2] + 2[2^2,1] \\ & + [2,1^4] + [3] + 2[2,1] + [1^3] \end{aligned}$$

and

$$\begin{aligned} \{3,1;2,1\} = {} & \langle 5,2\rangle + \langle 5,1^2\rangle + \langle 4,3\rangle + 2\langle 4,2,1\rangle \\ & + \langle 4,1^3\rangle + \langle 3^2,1\rangle + \langle 3,2^2\rangle + \langle 3,2,1^2\rangle \\ & + 2\langle 4,1\rangle + 2\langle 3,2\rangle + 2\langle 3,1^2\rangle \\ & + \langle 2^2,1\rangle + \langle 3\rangle + \langle 2,1\rangle. \end{aligned}$$

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[13] The notation used here is closest to that of Robinson, Ref. 12, p. 43. In the notation of Weyl, Ref. 3, p. 203, the IR $\{\lambda\}$ of $U(n)$ has character $\chi(\lambda_1,\lambda_2,\cdots) = |p_{l-n+2}\cdots, p_l|$, where l, in the ith row of the determinant, is given by $l_i = \lambda_i + n - i$, and p_m is the character of the IR $\{m\}$. Murnaghan, Ref. 4, p. 121, uses a similar notation whereby the character of the IR's $\{m\}$ and $\{1^m\}$ are denoted by p_m and σ_m, respectively, so that

$$\{\lambda\} = |p_{\lambda_i - i + j}| = |\sigma_{\lambda_j + i - j'}|.$$

Littlewood, Ref. 5, p. 88, adopts a notation in which these characters or S functions are given by $\{m\} = h_m$ and $\{1^m\} = a_m$, so that

$$\{\lambda\} = |h_{\lambda_i - i + j}| = |a_{\lambda_j + i - j'}|.$$

[14] See Ref. 3, p. 214, and Ref. 5, p. 98.
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$$\chi^{(\lambda)} = |q_{\lambda_i - i + 1}, q_{\lambda_i - i} + q_{\lambda_i - i + 2}, \cdots, q_{\lambda_i - i - k + 2} + q_{\lambda_i - i + k}|.$$

The third term in the element of the determinant specified in (3.1) is inserted to cancel out the second term of the elements if and only if it lies in the first column.
[18] In the notation of Weyl, Ref. 3, p. 219, the IR $\langle\lambda\rangle$ of $Sp(2k)$ has character

$$\chi(\lambda_1,\lambda_2,\cdots) = |p_{l-k+1}, p_{l-k+2} + p_{l-k}, \cdots, p_l + p_{l-2k+2}|,$$

where l, in the ith row of this determinant is given by $l_i = \lambda_i + k - i$, and p_m is the character of the IR $\langle m\rangle$. The third term in the element of the determinant specified in (3.2) is inserted to cancel out the second term of the element if and only if it lies in the first column.
[19] See Ref. 15, p. 262, in which Boerner labels IR's of $SO(n)$ by means of their highest weights, so that the IR $[\mu]$ of $SO(n)$ is denoted by ${}^nD_{\mu_1\mu_2}\ldots$.
[20] See Ref. 16, p. 406.
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Matrix Elements for the Most Degenerate Continuous Principal Series of Representations of $SO(p, 1)$

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The matrix elements for finite group transformations of the most degenerate continuous principal series of unitary irreducible representations of $SO(p, 1)$ are calculated. They are shown to agree with special cases already known.

INTRODUCTION

Representation theory for the noncompact rotation groups $SO(p, 1)$ has been described at length in the literature. For the special cases $p = 2, 3$, there is the now famous work of Bargmann,[1] Gel'fand, Minlos, Shapiro,[2] and Naimark.[3] For the case $p = 4$, the de Sitter group $SO(4, 1)$, there is most notably the work of Thomas, Newton, and Dixmier.[4] More generally, representations of $SO(p, 1)$ of the most degenerate type have been discussed by Vilenkin,[5] Bander and Itzykson,[6] and for $SO(p, q)$ by Raczka, Limic, and Niederle.[7]

In the present work, we give an expression for the matrix elements of finite group transformations for the most degenerate representations of the continuous principal series of the group[8] $SO(p, 1)$. The method used is the integral method used by Ström[9] for the case of $SO(3, 1)$. For certain special cases, we show that our expression reduces to those already known.

1. REVIEW OF REPRESENTATION THEORY

The Lie algebra of the groups $SO(p, 1)$ falls into the Cartan classification $B_{\frac{1}{2}p}$ if p is even and $D_{\frac{1}{2}(p+1)}$ if p is odd; hence, for p even (odd), the number of Casimir invariants [= rank of Lie algebra] is $\frac{1}{2}p[\frac{1}{2}(p+1)]$, respectively. However, if one represents a group G on a Hilbert space of functions whose domain is a homogeneous space S of rank 1, all the Casimir operators except one must vanish.[10] The nonvanishing Casimir operator is just the Laplace–Beltrami operator on S. Such representations are called most degenerate.

If we let $G = SO(p)$ and take the homogeneous space S to be the $(p-1)$-dimensional sphere, $S = S^{(p-1)}$ isomorphic to the coset space $SO(p)/SO(p-1)$, we can construct the so-called quasiregular representation of $SO(p)$. This is a most degenerate representation since $S^{(p-1)}$ is a symmetric space of rank 1. We construct the representation as follows: Let $\mathfrak{L}^2(S^{(p-1)})$ denote the Hilbert space of square-integrable functions over $S^{(p-1)}$, i.e.,

$$\|f\| = \int_{S^{(p-1)}} |f(\Omega_p)|^2 \, d\Omega_p < \infty \qquad (1.1)$$

with the inner product

$$(f_1, f_2) \equiv \int_{S^{(p-1)}} d\Omega_p \bar{f}_1(\Omega_p) f_2(\Omega_p),$$

where $d\Omega_p$ is the invariant measure on $S^{(p-1)}$; and let $L(g)$ be an operator on the space $\mathfrak{L}^2(S^{(p-1)})$ such that for each $g \in SO(p)$ and every $f \in \mathfrak{L}^2(S^{(p-1)})$ we have

$$L(g) f(\Omega) = f(g^{-1}\Omega). \qquad (1.2)$$

It is easily verified that $L(g)$ is a representation of $SO(p)$, and it follows from the invariance of the measure under $SO(p)$ rotations that $L(g)$ is unitary.

However, we can go further if we introduce multiplier or projective representations; we can construct representations of $SO(p, 1)$ on $S^{(p-1)}$. The Cartesian coordinates of $S^{(p-1)}$ are denoted by z^α, where $\alpha = 1, \cdots, p$. The representations of $SO(p, 1)$ are given by

$$T^{\sigma\rho}(g) f(z^\alpha) = [(g^{-1})^0_\beta z^\beta + (g^{-1})^0_0]^\sigma f\left(\frac{(g^{-1})^\alpha_\beta z^\beta + (g^{-1})^\alpha_0}{(g^{-1})^0_\beta z^\beta + (g^{-1})^0_0}\right), \qquad (1.3)$$

where $g \in SO(p, 1)$ and $f \in \mathfrak{L}^2(S^{(p-1)})$. The representation (1.3) can be arrived at formally[11] by constructing a quasiregular representation on the upper sheet of the p-dimensional cone $\xi_0^2 - \xi_1^2 - \cdots \xi_p^2 = 0$, with homogeneous functions of degree σ, the coordinates z^α being the homogeneous coordinates ξ^α/ξ^0. In fact, what this procedure does is just pick out the irreducible subspaces, i.e., $T^{\sigma\rho}(g)$ is an irreducible representation of $SO(p, 1)$. These representations are unitary in $\mathfrak{L}^2(S^{(p-1)})$ if and only if

$$\sigma = -\tfrac{1}{2}(p-1) + i\rho, \quad \rho \text{ real}. \qquad (1.4)$$

We can, however, restrict ρ to be nonnegative since $T^{-\rho}$ and T^ρ are unitarily equivalent. If g is a member of the compact subgroup $SO(p)$, the representation (1.3) reduces to (1.2) as it should.

The canonical basis for $SO(p, 1)$ is given by the decomposition according to maximal compact subgroups,

$$SO(p, 1) \supset SO(p) \supset SO(p-1) \supset \cdots \supset SO(2).$$

As a prelude to this decomposition, one introduces coordinates in which the Laplace–Beltrami operators of the compact subgroups separate. Such coordinates are the spherical coordinates

$$\begin{aligned} z^1 &= \sin\theta_{p-1}\cdots\sin\theta_1,\\ z^2 &= \sin\theta_{p-1}\cdots\sin\theta_2\cos\theta_1,\\ &\cdot\\ &\cdot\\ &\cdot\\ z^{p-1} &= \sin\theta_{p-1}\cos\theta_{p-2},\\ z^p &= \cos\theta_{p-1}, \end{aligned} \tag{1.5}$$

with $0 \leq \theta_1 < 2\pi$ and $0 \leq \theta_i \leq \pi, i = 2, \cdots, p-1$. In this coordinate system, the Laplace–Beltrami operator is

$$\Delta(S^{(p-1)}) = \frac{1}{\sin^{p-2}\theta_{p-1}}\frac{\partial}{\partial\theta_{p-1}}\sin^{p-2}\theta_{p-1}\frac{\partial}{\partial\theta_{p-1}} + \cdots + \frac{1}{\sin^2\theta_{p-1}\cdots\sin^2\theta_2}\frac{\partial^2}{\partial\theta_1^2} \tag{1.6}$$

or perhaps in the more convenient form

$$\Delta(S^{(p-1)}) = \frac{\partial^2}{\partial\theta_{p-1}^2} + (p-2)\cot\theta_{p-1}\frac{\partial}{\partial\theta_{p-1}} + \frac{1}{\sin^2\theta_{p-1}}\Delta(S^{p-2}). \tag{1.7}$$

The polynomial solutions of the eigenvalue equation of (1.6) are given by the generalized spherical harmonics[12]

$$Y_N(\theta_{p-1}\cdots\theta_1) = N_p\prod_{j=1}^{p-2} C_{n_{j+1}-n_j}^{n_j+\frac{1}{2}j}(\cos\theta_{j+1})\sin^{n_j}\theta_{j+1}e^{-in_1\theta_1}, \tag{1.8}$$

where the subscript N denotes $(n_{p-1}, \cdots, n_1)$ and the normalization N_p is given by

$$N_p = \frac{1}{(\sqrt{2\pi})}\prod_{j=1}^{p-2}\Gamma(n_j+\tfrac{1}{2}j)2^{n_j+\frac{1}{2}(j-1)} \times\left(\frac{(n_{j+1}+\frac{1}{2}j)\Gamma(n_{j+1}-n_j+1)}{\pi\Gamma(n_{j+1}+n_j+j)}\right)^{\frac{1}{2}}. \tag{1.9}$$

The orthonormality and completeness properties being well known,[6] we now have a discrete basis in which we can calculate matrix elements of $SO(p, 1)$ group transformations by the inner product $(Y_{N'}, T^{\sigma p}(g)Y_N)$.

2. CALCULATION OF THE MATRIX ELEMENTS

We begin with the parametrization of an arbitrary $SO(p, 1)$ group element

$$g = hg_{0p}h', \tag{2.1}$$

where $h, h' \in SO(p)$ and g_{0p} is a "boost" in the pth direction. Typically, g_{0p} is given by

$$g_{0p} = \begin{pmatrix} \cosh\alpha & 0 & \cdots & 0 & \sinh\alpha\\ 0 & 1 & & & 0\\ \cdot & & \cdot & & \cdot\\ \cdot & & & \cdot & \cdot\\ \cdot & & & & \cdot\\ 0 & & & 1 & 0\\ \sinh\alpha & 0 & \cdots & 0 & \cosh\alpha \end{pmatrix}. \tag{2.2}$$

The decomposition (2.1) gives for the operators in the representation space

$$T^{\sigma p}(g) = L^p(h)T^{\sigma p}(g_{0p})L^p(h'). \tag{2.3}$$

Now the operators $L^p(h)$ are not irreducible in $SO(p)$, but their decomposition into irreducible parts is well known.[5] The matrix elements for an irreducible representation of $SO(p)$ have been given[2,13] for $p \leq 5$. It is interesting to note that due to the representation (1.3) the matrix elements for an $SO(p, 1)$ "boost" in the pth direction are much easier to calculate than the corresponding rotation for $SO(p+1)$.

The calculation of the matrix elements for a boost in the pth direction follows Ström's[9] work closely. Using Eqs. (1.3), (1.5), and (2.2), we find

$$T^{\sigma p}(\alpha)Y_N(\theta_{p-1}, \cdots, \theta_1) = (\cosh\alpha - \sinh\alpha\cos\theta_{p-1})^\sigma Y_N(\theta'_{p-1}, \theta_{p-2}, \cdots, \theta_1), \tag{2.4}$$

where

$$\cos\theta'_{p-1} = \frac{\cosh\alpha\cos\theta_{p-1} - \sinh\alpha}{\cosh\alpha - \sinh\alpha\cos\theta_{p-1}}.$$

The relevant matrix elements are given by the inner product

$$(Y_N(\theta_{p-1}, \cdots, \theta_1), T^{\sigma p}(\alpha)Y_{N'}(\theta_{p-1}, \cdots, \theta_1)) \equiv T^{\sigma p}_{NN'}(\alpha). \tag{2.5}$$

The integrations over $\theta_1, \cdots, \theta_{p-2}$ are trivial, yielding

$$T^{\sigma p}_{NN'} \propto \delta_{n'_1,n_1}\cdots\delta_{n'_{p-2},n_{p-2}}. \tag{2.6}$$

The remaining integral is

$$\begin{aligned} T^{\sigma p}_{NN'}(\alpha) = {} & \delta_{n'_1,n}\cdots\delta_{n'_{p-2},n_{p-2}}2^{2n_{p-2}+p-3}[\Gamma(n_{p-2}+\tfrac{1}{2}(p-2))]^2\{[n_{p-1}+\tfrac{1}{2}(p-2)][n'_{p-1}+\tfrac{1}{2}(p-2)]\}^{\frac{1}{2}}\\ & \times\frac{1}{\pi}\left(\frac{(n_{p-1}-n_{p-2})!\,(n'_{p-1}-n_{p-2})!}{(n_{p-1}+n_{p-2}+p-3)!\,(n'_{p-1}+n_{p-2}+p-3)!}\right)^{\frac{1}{2}}\int_0^\pi\sin^{p-2}\theta_{p-1}\,d\theta_{p-1}\\ & \times(\sin\theta_{p-1})^{n_{p-2}}C^{n_{p-2}+\frac{1}{2}(p-2)}_{n_{p-1}-n_{p-2}}(\cos\theta_{p-1})(\sin\theta'_{p-1})^{n_{p-2}}\\ & \times C^{n_{p-2}+\frac{1}{2}(p-2)}_{n'_{p-1}-n_{p-2}}(\cos\theta'_{p-1})(\cosh\alpha - \cos\theta_{p-1}\sinh\alpha)^\sigma. \end{aligned} \tag{2.7}$$

By letting $x = \cos\theta_{p-1}$ and $x' = \cos\theta'_{p-1}$ and noting that

$$\sin\theta'_{p-1} = \sin\theta_{p-1}/(\cosh\alpha - \sinh\alpha\cos\theta_{p-1}),$$

the above integral becomes

$$\int_{-1}^{1} dx(1-x^2)^{n_{p-2}+\frac{1}{2}(p-3)} C^{n_{p-2}+\frac{1}{2}(p-2)}_{n_{p-1}-n_{p-2}}(x) C^{n_{p-2}+\frac{1}{2}(p-2)}_{n'_{p-1}-n_{p-2}}(x')\,(\cosh\alpha - x\sinh\alpha)^{\sigma}. \tag{2.8}$$

To perform this integral, we write the Gegenbauer polynomials as Jacobi polynomials[14]

$$C_n^{(\alpha)}(x) = \frac{\Gamma(\alpha+\frac{1}{2})\Gamma(2\alpha+n)}{\Gamma(2\alpha)\Gamma(\alpha+n+\frac{1}{2})} P_n^{(\alpha-\frac{1}{2},\alpha-\frac{1}{2})}(x),$$

and, using the expansion for Jacobi polynomials[12]

$$P_n^{(\alpha,\beta)}(x) = 2^{-n}\sum_{m=0}^{n}\binom{n+\alpha}{m}\binom{n+\beta}{n-m}(x-1)^{n-m}(x+1)^m,$$

we find

$$C^{n_{p-2}+\frac{1}{2}(p-2)}_{n_{p-1}-n_{p-2}}(x) = \frac{\Gamma(n_{p-1}+n_{p-2}+p-2)\Gamma(n_{p-2}+\frac{1}{2}(p-1))\Gamma(n_{p-1}+\frac{1}{2}(p-1))}{\Gamma(2n_{p-2}+p-2)2^{n_{p-1}-n_{p-2}}}$$
$$\times \sum_{k=0}^{n_{p-1}-n_{p-2}} \frac{(-1)^{n_{p-1}-n_{p-2}-k}(1+x)^k(1-x)^{n_{p-1}-n_{p-2}-k}}{k!\,\Gamma(n_{p-1}+\frac{1}{2}(p-1)-k)\Gamma(n_{p-2}+\frac{1}{2}(p-1)+k)\Gamma(n_{p-1}-n_{p-2}+1-k)}. \tag{2.9}$$

Using

$$1-x' = \frac{e^{\alpha}(1-x)}{\cosh\alpha - x\sinh\alpha}, \quad 1+x' = \frac{e^{-\alpha}(1+x)}{\cosh\alpha - x\sinh\alpha} \tag{2.10}$$

and putting Eq. (2.9) into Eq. (2.8), we obtain

$$\frac{\Gamma(n_{p-1}+n_{p-2}+p-2)[\Gamma(n_{p-1}+\frac{1}{2}(p-1))]^2\Gamma(n'_{p-1}+n_{p-2}+p-2)[\Gamma(n'_{p-1}+\frac{1}{2}(p-1))]^2}{2^{n_{p-1}+n'_{p-1}-2n_{p-2}}[\Gamma(2n_{p-2}+p-2)]^2}$$
$$\times \sum_{k=0}^{n_{p-1}-n_{p-1}} \sum_{k'=0}^{n'_{p-1}-n_{p-2}} \frac{(-1)^{n'_{p-1}+n_{p-1}-2n_{p-2}-k-k'} e^{\alpha(n'_{p-1}-n_{p-2}-2k')}}{k'!\,k!\,\Gamma(n_{p-1}+\frac{1}{2}(p-1)-k)\Gamma(n'_{p-1}+\frac{1}{2}(p-1)-k')}$$
$$\times \frac{1}{\Gamma(n_{p-2}+\frac{1}{2}(p-1)+k)\Gamma(n_{p-2}+\frac{1}{2}(p-1)+k')\Gamma(n_{p-1}-n_{p-2}+1-k)\Gamma(n'_{p-1}-n_{p-2}+1-k')}$$
$$\times \int_{-1}^{1} dx(1-x)^{n'_{p-1}+n_{p-1}-n_{p-2}+\frac{1}{2}(p-3)-k-k'}(1+x)^{n_{p-2}+\frac{1}{2}(p-3)+k+k'}(\cosh\alpha - x\sinh\alpha)^{\sigma-n'_{p-1}}. \tag{2.11}$$

By changing variables from x to $t = \frac{1}{2}(1+x)$, the above integral becomes

$$2^{n'_{p-1}+n_{p-1}+p-3} e^{\alpha(\sigma-n'_{p-1})} \int_0^1 dt\, t^{n_{p-2}+\frac{1}{2}(p-3)+k+k'}(1-t)^{n'_{p-1}+n_{p-1}-n_{p-2}+\frac{1}{2}(p-3)-k-k'}(1-(1-e^{-2\alpha})t)^{\sigma-n'_{p-1}}.$$

Using Euler's integral representation of the hypergeometric function[15]

$${}_2F_1(a,b;c;z) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}\,dt, \tag{2.12}$$

we finally arrive at

$$T^{\sigma p}_{NN'}(\alpha) = N_1 \sum_{k=0}^{n_{p-1}-n_{p-2}} \sum_{k'=0}^{n'_{p-1}-n_{p-2}} \frac{(-1)^{k+k'} e^{\alpha(\sigma-n_{p-2}-2k')}}{k'!\,k!\,\Gamma(n_{p-1}+\frac{1}{2}(p-1)-k)}$$
$$\times \frac{\Gamma(n_{p-2}+\frac{1}{2}(p-1)+k+k')\Gamma(n'_{p-1}+n_{p-1}-n_{p-2}+\frac{1}{2}(p-1)-k-k')}{\Gamma(n'_{p-1}+\frac{1}{2}(p-1)-k')\Gamma(n_{p-2}+\frac{1}{2}(p-1)+k)}$$
$$\times \frac{{}_2F_1(n'_{p-1}-\sigma, n_{p-2}+\frac{1}{2}(p-1)+k+k'; n'_{p-1}+n_{p-1}+p-1; 1-e^{-2\alpha})}{\Gamma(n_{p-2}+\frac{1}{2}(p-1)+k')\Gamma(n_{p-1}-n_{p-2}+1-k)\Gamma(n'_{p-1}-n_{p-2}+1-k')}, \tag{2.13}$$

where

$$N_1 = \delta_{n_1,n_1'}\cdots\delta_{n_{p-2},n'_{p-2}}[(n_{p-1}-n_{p-2})!\,(n'_{p-1}-n_{p-2})!\,(n_{p-1}+n_{p-2}+p-3)!\,(n'_{p-1}+n_{p-2}+p-3)!]^{\frac{1}{2}} \times (-1)^{n'_{p-1}+n_{p-1}} \times \frac{[\Gamma(n_{p-1}+\frac{1}{2}(p-1))\Gamma(n'_{p-1}+\frac{1}{2}(p-1))]\{[n_{p-1}+\frac{1}{2}(p-2)][n'_{p-1}+\frac{1}{2}(p-2)]\}^{\frac{1}{2}}}{(n_{p-1}+n'_{p-1}+p-2)!}.$$

As in Ref. 9, one of the sums in Eq. (2.13) can be eliminated by changing the sums over k and k' to sums over k' and $j = k + k'$ and summing over k', yielding

$$T^{\sigma p}_{NN'}(\alpha) = N_2 e^{-\alpha(n_{p-1}-\sigma)} \sum_j \frac{(-1)^j\Gamma(n'_{p-1}+n_{p-1}-n_{p-2}+\frac{1}{2}(p-1)-j)}{j!\,(n_{p-1}-n_{p-2}-j)!} \times \frac{{}_2F_1(n'_{p-1}-\sigma, n_{p-2}+\frac{1}{2}(p-1)+j; n'_{p-1}+n_{p-1}+p-1; 1-e^{-2\alpha})}{\Gamma(n_{p-1}+\frac{1}{2}(p-1)-j)} \times {}_4F_3\left[\begin{matrix}-j, -n'_{p-1}-\frac{1}{2}(p-3), -n_{p-2}-\frac{1}{2}(p-3)-j, -n'_{p-1}+n_{p-2} \\ n_{p-1}+\frac{1}{2}(p-1)-j, n_{p-2}+\frac{1}{2}(p-1), n_{p-1}-n_{p-2}+1-j\end{matrix}; \; e^{-2\alpha}\right], \quad (2.14)$$

where

$$N_2 = N_1[\Gamma(n'_{p-1}+\tfrac{1}{2}(p-1))\Gamma(n_{p-2}+\tfrac{1}{2}(p-1))\Gamma(n'_{p-1}-n_{p-2}+1)]^{-1}$$

and ${}_pF_q$ is the generalized hypergeometric function defined in Ref. 15.

It is easily seen that $T^{\sigma p}_{NN'}(\alpha)$ agrees for $p = 3$ with the expression given in Ref. 9. Moreover, for the special case $N = (0, 0, \cdots, 0)$ and $N' = (n'_{p-1}, 0, \cdots, 0)$ Vilenkin[5] has expressed $T^{\sigma p}_{ON'}(\alpha)$ in terms of Legendre functions. By using the expression derived in the Appendix

$$e^{\sigma\alpha}\sum_{k=0}^{n}\frac{(-1)^k e^{-2\alpha k}F(n-\sigma, \frac{1}{2}(p-1)+k; n+p-1; 1-e^{-2\alpha})}{k!\,(n-k)!} = \frac{(-1)^{n_2}{}^{2n+\frac{1}{2}(p-2)}(p-1+\sigma)_n\Gamma(n+\frac{1}{2}p)}{n!\,(n+p-1)_n(\sinh\alpha)^{\frac{1}{2}(p-2)}}P^{\frac{1}{2}(2-p)-n}_{\alpha+\frac{1}{2}(p-2)}(\cosh\alpha), \quad (2.15)$$

where $(a)_n = \Gamma(a+n)/\Gamma(a)$ is Pockhammer's symbol, it is seen that Eq. (2.13) reduces to Vilenkin's result,

$$T^{\sigma p}_{ON}(\alpha) = 2^{\frac{1}{2}(p-4)}\frac{\Gamma(\frac{1}{2}(p-2))}{\Gamma(p-2)}(p-1+\sigma)_n\left(\frac{(2n+p-2)\Gamma(n+p-2)\Gamma(p-1)}{n!}\right)^{\frac{1}{2}}\frac{P^{\frac{1}{2}(2-p)-n}_{\sigma+\frac{1}{2}(p-2)}(\cosh\alpha)}{(\sinh\alpha)^{\frac{1}{2}(p-2)}}. \quad (2.16)$$

APPENDIX

We derive the expression (2.15). By expanding the hypergeometric function in (2.15) in a power series and making use of

$$(\tfrac{1}{2}(p-1)+k)_i = (\tfrac{1}{2}(p-1))_i\frac{(\frac{1}{2}(p-1)+i)_k}{(\frac{1}{2}(p-1))_k},$$

the equation becomes

$$(z^{-\sigma})^{\frac{1}{2}}\sum_{k=0}^{n}\frac{(-1)^k}{k!\,(n-k)!} \times z^k F(n-\sigma, \tfrac{1}{2}(p-1)+k; n+p-1; 1-z) = \sum_{i=0}^{\infty}\frac{(n-\sigma)_i(\frac{1}{2}(p-1))_i(1-z)^i}{i!\,(n-p-1)_i} \times F(-n, \tfrac{1}{2}(p-1)+i; \tfrac{1}{2}(p-1); z), \quad (A1)$$

but $F(-n, \frac{1}{2}(p-1)+i; \frac{1}{2}(p-1); z)$ is a polynomial in z of degree n given by[15]

$$F(-n, \tfrac{1}{2}(n-1)+i; \tfrac{1}{2}(p-1); z) = \frac{-(1-z)^{n-i}z^{-\frac{1}{2}(p-3)}}{(\frac{1}{2}(p-1))_n}\frac{d^n}{dz^n}[z^{n+\frac{1}{2}(p-3)}(1-z)^i]; \quad (A2)$$

thus the right-hand side of (A1) becomes

$$\frac{z^{-\frac{1}{2}(p-3)}}{(\frac{1}{2}(p-1))_n}(1-z)^n\frac{d^n}{dz^n} \times [z^{n+\frac{1}{2}(p-3)}F(n-\sigma, \tfrac{1}{2}(p-1); n+p-1; 1-z)]. \quad (A3)$$

Via the differentiation formula[15] for hypergeometric functions,

$$\frac{d^n}{dz^n}[(1-z)^{a+n-1}F(a, b; c; z)] = \frac{(-1)^n(a)_n(c-b)_n(1-z)^{a-1}}{(c)_n} \times F(a+n, b; c+n; z), \quad (A4)$$

Eq. (A1) becomes

$$e^{\alpha\sigma}\sum_{k=0}^{n}\frac{(-1)^k e^{-2\alpha k}}{k!\,(n-k)!}\times F(n-\sigma,\tfrac{1}{2}(p-1)+k;n+p-1;1-e^{-2\alpha})$$
$$=\frac{(-1)^n(p-1+\sigma)_n}{n!\,(n+p-1)_n}e^{\sigma\alpha}(1-e^{-2\alpha})^n\times F(n-\sigma,n+\tfrac{1}{2}(p-1);2n+p-1;1-e^{-2\alpha}). \quad \text{(A5)}$$

It is now a simple task to arrive at Eq. (2.15), by noticing that the hypergeometric function in (A5) is expressible in terms of Legendre functions.

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Thermodynamical Theory of Directed Curves*

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A nonlinear thermodynamical theory of directed curves is obtained by postulating an energy balance, an entropy production inequality, and invariance requirements under superposed rigid body motions. Constitutive equations for a class of simple materials without memory are presented.

1. INTRODUCTION

A directed curve is defined as a curve at each point of which is associated a triad of deformable vectors, called directors. The application of this one-dimensional continuum to rod theory was first investigated by E. and F. Cosserat[1] and later by Ericksen and Truesdell,[2] who developed nonlinear theories of strain for both rods and shells. The latter work is incomplete in the sense that constitutive equations were not considered.

Several investigations into complete theories of directed curves have recently been made. Based on principles of virtual work and material frame indifference, Cohen[3] developed a statical nonlinear theory of elastic directed curves. A dynamical theory of elastic directed curves was obtained by Whitman and DeSilva[4] from a Hamilton's principle and invariance of the action density function under rigid body variations. An explicit form of the director inertia terms was determined by making a constitutive postulate on the form of the action density function. In addition, the general nonlinear theory was reduced for the case of a Cosserat curve, i.e., a directed curve whose directors are constrained to be a rigid triad (but with three rotational degrees of freedom). Further results were obtained by Whitman and DeSilva,[5] who considered plane motions and dynamical stability of elastic Cosserat curves. In particular, it was shown that the nonlinear theory yields a generalization of the classical elastica theory while the linear theory generalizes Timoshenko beam theory.

A thermodynamical theory of rods was obtained by Green and Laws,[6] who defined a rod to be a curve with two, rather than three, directors defined at each point. These authors postulated an entropy production inequality and an energy balance and employed the methods of Green and Rivlin[7,8] to obtain the governing equations. Working from the theory of Ref. 6, Green, Laws, and Naghdi[9] presented a linear theory of straight elastic rods, and Green, Knops, and Laws[10] considered small deformations superposed on finite deformations and stability of elastic rods.

Eq. (A1) becomes

$$e^{\alpha\sigma}\sum_{k=0}^{n}\frac{(-1)^k e^{-2\alpha k}}{k!\,(n-k)!}\times F(n-\sigma,\tfrac{1}{2}(p-1)+k;n+p-1;1-e^{-2\alpha})$$
$$=\frac{(-1)^n(p-1+\sigma)_n}{n!\,(n+p-1)_n}e^{\sigma\alpha}(1-e^{-2\alpha})^n\times F(n-\sigma,n+\tfrac{1}{2}(p-1);2n+p-1;1-e^{-2\alpha}). \quad \text{(A5)}$$

It is now a simple task to arrive at Eq. (2.15), by noticing that the hypergeometric function in (A5) is expressible in terms of Legendre functions.

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Thermodynamical Theory of Directed Curves*

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A nonlinear thermodynamical theory of directed curves is obtained by postulating an energy balance, an entropy production inequality, and invariance requirements under superposed rigid body motions. Constitutive equations for a class of simple materials without memory are presented.

1. INTRODUCTION

A directed curve is defined as a curve at each point of which is associated a triad of deformable vectors, called directors. The application of this one-dimensional continuum to rod theory was first investigated by E. and F. Cosserat[1] and later by Ericksen and Truesdell,[2] who developed nonlinear theories of strain for both rods and shells. The latter work is incomplete in the sense that constitutive equations were not considered.

Several investigations into complete theories of directed curves have recently been made. Based on principles of virtual work and material frame indifference, Cohen[3] developed a statical nonlinear theory of elastic directed curves. A dynamical theory of elastic directed curves was obtained by Whitman and DeSilva[4] from a Hamilton's principle and invariance of the action density function under rigid body variations. An explicit form of the director inertia terms was determined by making a constitutive postulate on the form of the action density function. In addition, the general nonlinear theory was reduced for the case of a Cosserat curve, i.e., a directed curve whose directors are constrained to be a rigid triad (but with three rotational degrees of freedom). Further results were obtained by Whitman and DeSilva,[5] who considered plane motions and dynamical stability of elastic Cosserat curves. In particular, it was shown that the nonlinear theory yields a generalization of the classical elastica theory while the linear theory generalizes Timoshenko beam theory.

A thermodynamical theory of rods was obtained by Green and Laws,[6] who defined a rod to be a curve with two, rather than three, directors defined at each point. These authors postulated an entropy production inequality and an energy balance and employed the methods of Green and Rivlin[7,8] to obtain the governing equations. Working from the theory of Ref. 6, Green, Laws, and Naghdi[9] presented a linear theory of straight elastic rods, and Green, Knops, and Laws[10] considered small deformations superposed on finite deformations and stability of elastic rods.

In the present paper, the authors develop a nonlinear thermodynamical theory of directed curves which generalizes the theory of Ref. 4. The kinematics of directed curves are briefly reviewed in Sec. 2. We obtain the governing equations in Sec. 3 by postulating an energy balance, an entropy production inequality, and invariance requirements under superimposed rigid body motions, but with a definition for director momentum density different than that adopted in Ref. 6. In Sec. 4 we develop constitutive equations for a class of simple materials without memory. Finally, in Sec. 5 we discuss a separate but equivalent set of balance postulates and the relationship of the assumed form of the director momentum density to that employed in Ref. 6.

2. KINEMATICS

In this section we summarize the essential kinematics of a directed curve. A deformed configuration of the directed curve at time t is defined by the functions

$$\mathbf{r} = \mathbf{r}(s, t), \quad \mathbf{d}_\alpha = \mathbf{d}_\alpha(s, t), \quad \alpha = 1, 2, 3, \quad (2.1)$$

where $\mathbf{r}$ is the position vector of points on the curve c, $\mathbf{d}_\alpha$ are the deformed directors (assumed noncoplanar), and s is the arc length along the curve. We define a fixed reference configuration at $t = 0$ such that

$$\mathbf{R}(S) = \mathbf{r}|_{t=0}, \quad \mathbf{D}_\alpha(S) = \mathbf{d}_\alpha|_{t=0}, \quad (2.2)$$

where $\mathbf{R}$, $\mathbf{D}_\alpha$, and S denote respectively the position vector, directors, and arc length in the reference configuration. A family of deformations is then defined by a smooth function

$$s = s(S, t). \quad (2.3)$$

The stretch $\lambda = \partial s/\partial S$ is assumed to be bounded and positive, implying that (2.3) can be inverted to yield $S = S(s, t)$.

Introducing a single fixed curvilinear coordinate system x^i with metric $\mathbf{g}$, we define a set of reciprocal directors $\mathbf{d}^\alpha$ such that

$$d_\alpha^i d_i^\beta = \delta_\alpha^\beta, \quad d_\alpha^i d_j^\alpha = \delta_j^i, \quad (2.4)$$

where $\boldsymbol{\delta}$ is the Kronecker delta and diagonally repeated indices are summed over the range 1, 2, 3. With the definitions (2.4), it is possible to define components of tensors with respect to either the base vectors $\mathbf{g}_i$ or the directors $\mathbf{d}_\alpha$. For a second-order tensor $\mathbf{U}$, the tensor components U_{ij}, U^{ij} (with respect to $\mathbf{g}_i$) are related to the anholonomic components $U_{\alpha\beta}$, $U^{\alpha\beta}$ (with respect to $\mathbf{d}_\alpha$) by identities of the form

$$U_{ij} = U^{\alpha\beta} d_{\alpha i} d_{\beta j} = U_{\alpha\beta} d_i^\alpha d_j^\beta,$$
$$U^{\alpha\beta} = U^{ij} d_i^\alpha d_j^\beta = U_{ij} d^{\alpha i} d^{\beta j}.$$

Differentiation with respect to arc lengths s and S will be denoted by

$$(\check{}) = \frac{\partial(\ )}{\partial s}, \quad (\hat{}) = \frac{\partial(\ )}{\partial S}.$$

For a vector $\mathbf{u}$ with tensor components $u^i = \mathbf{u} \cdot \mathbf{g}^i$, the component form of the arc derivative $\check{\mathbf{u}}$ is defined by

$$\check{u}^i = \frac{\partial u^i}{\partial s} + u^m \Gamma^i_{mn} \frac{\partial x^n}{\partial s},$$

where the Christoffel symbol Γ^i_{mn} is evaluated along the curve. Consistent with this notation we define

$$\check{u}^\alpha = \frac{\partial u^\alpha}{\partial s}, \quad \hat{u}^\alpha = \frac{\partial u^\alpha}{\partial S}.$$

We define the Ericksen–Truesdell deformation measures for a directed curve in the form:

$$y_\alpha = \mathbf{d}_\alpha \cdot \check{\mathbf{r}}, \quad C_{\alpha\beta} = \mathbf{d}_\alpha \cdot \mathbf{d}_\beta, \quad F_{\alpha\beta} = \mathbf{d}_\alpha \cdot \hat{\mathbf{d}}_\beta. \quad (2.5)$$

These quantities completely describe the strain of a directed curve, as shown in Ref. 2. From the above definitions, it is easy to show that

$$\hat{C}_{\alpha\beta} = F_{(\alpha\beta)}, \quad (2.6)$$

where $F_{(\alpha\beta)} = \frac{1}{2}(F_{\alpha\beta} + F_{\beta\alpha})$ is the symmetric part of $F_{\alpha\beta}$. We note that y_α, $C_{\alpha\beta}$, $F_{\alpha\beta}$ are simply anholonomic components of the vectors $\check{\mathbf{r}}$, $\mathbf{d}_\beta$, $\hat{\mathbf{d}}_\beta$.

The velocity vector $\mathbf{v}$ of a point on c and the director velocities $\mathbf{w}_\alpha$ are defined by

$$\mathbf{v} = \dot{\mathbf{r}}, \quad \mathbf{w}_\alpha = \dot{\mathbf{d}}_\alpha, \quad (2.7)$$

where $\dot{(\ )} = \partial(\ )/\partial t|_S$ is the usual material derivative. As kinematical measures of the director motions, we introduce the anholonomic components of the director velocities $\mathbf{w}_\alpha$ such that

$$W_{\alpha\beta} = \mathbf{w}_\alpha \cdot \mathbf{d}_\beta, \quad \mathbf{w}_\alpha = W_{\alpha\beta}\mathbf{d}^\beta. \quad (2.8)$$

The tensor components associated with $W_{\alpha\beta}$ are defined by

$$W_{mn} = W_{\alpha\beta} d_m^\alpha d_n^\beta = d_m^\alpha w_{\alpha n}. \quad (2.9)$$

By the definitions of $C_{\alpha\beta}$ and $W_{\alpha\beta}$ it follows that

$$\dot{C}_{\alpha\beta} = 2W_{(\alpha\beta)}. \quad (2.10)$$

Since the quantities $C_{\alpha\beta}$ are instantaneous measures of the lengths of the directors and the angles between them, (2.10) implies that $W_{(\alpha\beta)}$ is a measure of the deformation rates of the directors. In particular, $W_{(\alpha\beta)} = 0$ when the directors form a rigid triad. Defining a rotational velocity $\boldsymbol{\Omega}$ of the director triad

$$2\boldsymbol{\Omega} = \mathbf{d}^\alpha \times \mathbf{w}_\alpha,$$

then we can show that

$$W_{[\alpha\beta]} = \epsilon_{\alpha\beta\delta}\Omega^\delta, \quad (2.11)$$

where $W_{[\alpha\beta]} = \frac{1}{2}(W_{\alpha\beta} - W_{\beta\alpha})$ is the skew-symmetric part of $W_{\alpha\beta}$, and the anholonomic components of the alternating tensor $\boldsymbol{\epsilon}$ are given by

$$\epsilon_{\alpha\beta\delta} = \epsilon_{ijk} d^i_\alpha d^j_\beta d^k_\delta = \mathbf{d}_\alpha \cdot \mathbf{d}_\beta \times \mathbf{d}_\delta .$$

From (2.11) we see that $W_{[\alpha\beta]}$ is a measure of the rate of rotation of the director triad. The above interpretations were given in terms of the tensor components W_{mn} by Allen and DeSilva.[11] Finally, from (2.5) and (2.8) $F_{(\alpha\beta)}$ and $W_{(\alpha\beta)}$ are related by the equation

$$\dot{F}_{(\alpha\beta)} = \hat{W}_{(\alpha\beta)} . \tag{2.12}$$

3. GENERAL THEORY OF A DIRECTED CURVE

In this section we develop the field equations governing a thermodynamical motion of a directed curve by generalizing the energy balance obtained by Whitman and DeSilva[4] for the isothermal theory and by postulating invariance requirements on certain kinematic and thermodynamic quantities under superimposed rigid body motions.

Let an arbitrary deforming segment of the directed curve be defined by the interval $s_1 \leq s \leq s_2$. At each point of this interval we define a body force vector $\mathbf{f}$ and a body force $\mathbf{h}^\alpha$ associated with each director $\mathbf{d}_\alpha$. At the ends of the curve segment we define a stress vector $\boldsymbol{\tau}$ and a set of director stress vectors $\boldsymbol{\mu}^\alpha$. We now postulate that the energy balance for the curve segment is given by

$$\frac{d}{dt}\int_{s_1}^{s_2} \rho E \, ds = \int_{s_1}^{s_2} \rho(Q + f^i v_i + h^{\alpha i} w_{\alpha i}) \, ds + [\tau^i v_i + \mu^{\alpha i} w_{\alpha i} - q]_{s_1}^{s_2}, \tag{3.1}$$

where the energy density E is defined as

$$E = e + \tfrac{1}{2} v^i v_i + \tfrac{1}{2} A^{\alpha\beta} w_{\alpha i} w^i_\beta . \tag{3.2}$$

In the above equations ρ is the mass density, e is the internal energy density, Q is the heat supply density per unit time, and q is the heat flux per unit time from the curve segment to the surroundings. The quantity $A^{\alpha\beta}$ in (3.2) expresses the kinetic energy associated with the directors in a general form and can be taken as symmetric without loss of generality. We assume that $A^{\alpha\beta}$ is a positive-definite matrix, which implies that an arbitrary director motion gives rise to a positive contribution to the total kinetic energy. Finally, we allow $A^{\alpha\beta}$ to be time dependent.

Using (3.2), we can write (3.1) in the form

$$\int_{s_1}^{s_2} \rho[\dot{e} - Q - (f^i - \dot{v}^i)v_i - (h^{\alpha i} - \omega^{\alpha i})w_{\alpha i} - \tfrac{1}{2}\dot{A}^{\alpha\beta} w_{\alpha i} w^i_\beta] \, ds + \int_{s_1}^{s_2} E\rho \, \overset{\cdot}{\overline{ds}} = [\tau^i v_i + \mu^{\alpha i} w_{\alpha i} - q]_{s_1}^{s_2}, \tag{3.3}$$

where the director momentum density $\boldsymbol{\omega}^\alpha$ is defined as

$$\boldsymbol{\omega}^\alpha = A^{\alpha\beta} \mathbf{w}_\beta . \tag{3.4}$$

This definition is consistent with that adopted in Ref. 4.

We now superimpose an arbitrary translational velocity $\mathbf{a}(t)$ upon the motion of the curve at time $t^* = t + b$ such that

$$\mathbf{v}^* = \mathbf{v} + \mathbf{a}, \quad \mathbf{w}^*_\alpha = \mathbf{w}_\alpha .$$

Under this combined motion we require ρ, e, Q, q, $\boldsymbol{\tau}$, $\boldsymbol{\mu}^\alpha$, $A^{\alpha\beta}$, $(\mathbf{f} - \dot{\mathbf{v}})$, and $(\mathbf{h}^\alpha - \dot{\boldsymbol{\omega}}^\alpha)$ to be invariant, i.e., $\rho^* = \rho$, etc. The energy balance (3.3) is now applied to the combined motion. Then, by the usual arguments, we can show that

$$\dot{\rho} + \rho \check{v}^i \check{x}_i = 0, \tag{3.5}$$

$$\tau^i + \rho f^i = \rho \dot{v}^i . \tag{3.6}$$

Equations (3.5) and (3.6) express the local conservation of mass and the local balance of linear momentum, respectively.

We now superimpose an arbitrary rigid body rotation $\Omega_{ij}(t)$ at time $t^* = t + b$ such that

$$v^*_i = v_i + \Omega_{ij} x^j, \quad w^*_{\alpha i} = w_{\alpha i} + \Omega_{ij} d^j_\alpha, \quad \Omega_{ij} = -\Omega_{ji} .$$

By requiring the invariance of the quantities given previously under the above superimposed motion, we obtain from (3.3) [as modified by (3.5) and (3.6)]

$$-\Omega_{ij}\left(\int_{s_1}^{s_2} [\tau^i \check{x}^j + \rho(h^{\alpha i} - \dot{\omega}^{\alpha i}) d^j_\alpha + \rho A^{\alpha\beta} w^i_\alpha d^j_\beta] \, ds + [\mu^{\alpha i} d^j_\alpha]_{s_1}^{s_2}\right) - \tfrac{1}{2}\Omega^m{}_i \Omega_{mj} \int_{s_1}^{s_2} \rho \psi^{ij} \, ds = 0, \tag{3.7}$$

where ψ^{ij} are the tensor components of $\dot{A}^{\alpha\beta}$:

$$\psi^{ij} = \dot{A}^{\alpha\beta} d^i_\alpha d^j_\beta = \psi^{ji} . \tag{3.8}$$

Since $\boldsymbol{\Omega}$ is an arbitrary skew-symmetric tensor and noting that $\Omega^m{}_i \Omega_{mn}$ is symmetric, Eq. (3.7) is satisfied if and only if

$$\psi^{(ij)} = 0, \tag{3.9}$$

$$\overset{\vee}{\overline{(d^{[i}_\alpha \mu^{\alpha j]})}} - \tau^{[i} \check{x}^{j]} + \rho d^{[i}_\alpha h^{\alpha j]} = \rho d^{[i}_\alpha \dot{\omega}^{\alpha j]} . \tag{3.10}$$

Equation (3.9) implies ψ^{ij} must vanish, since by definition (3.8) $\psi^{[ij]}$ vanishes identically. But ψ^{ij} vanishes if and only if

$$\dot{A}^{\alpha\beta} = 0. \tag{3.11}$$

If one interprets the directed curve as representing a one-dimensional continuum with substructure, then

(3.11) implies a balance law for substructure mass distribution. Indeed, one could make the separate postulate

$$\frac{d}{dt}\int_{s_1}^{s_2}\rho A^{\alpha\beta}\,ds = 0, \tag{3.12}$$

which is obviously equivalent to (3.11) provided $\overset{\cdot}{\rho\,ds} = 0$. In terms of the tensor components of $A^{\alpha\beta}$, i.e.,

$$A^{ij} = A^{\alpha\beta}d^i_\alpha d^j_\beta = A^{ji},$$

it can be shown that $\psi^{ij} = 0$ implies the following set of differential equations for A^{ij}:

$$\dot{A}^{ij} = 2A^{(im}W_m{}^{j)}. \tag{3.13}$$

If we define the components of a double force tensor $\mathbf{m}$ such that

$$m^{ij} = \overset{\vee}{(d^i_\alpha\mu^{\alpha j})} - \tau^i\check{x}^j + \rho d^i_\alpha h^{\alpha j} - \rho d^i_\alpha\dot{\omega}^{\alpha j}, \tag{3.14}$$

then, by (3.10), m^{ij} is symmetric and an alternate form of (3.10) is

$$m^{[ij]} = 0. \tag{3.15}$$

In order to recover the form of the director momentum balance as recorded in Ref. 4, we define a tensor $\boldsymbol{\varphi}$ such that

$$\varphi^{ij} = m^{ij} - \check{d}^i_\alpha\mu^{\alpha j} + \tau^i\check{x}^j. \tag{3.16}$$

Applying (3.14) to (3.16), we obtain

$$\varphi^{ij} = d^i_\alpha(\check{\mu}^{\alpha j} + \rho h^{\alpha j} - \rho\dot{\omega}^{\alpha j}). \tag{3.17}$$

Defining a set of vectors $\boldsymbol{\varphi}^\alpha$ such that $\varphi^{ij} = d^i_\alpha\varphi^\alpha_j$, we can write (3.17) in the form

$$\check{\boldsymbol{\mu}}^\alpha - \boldsymbol{\varphi}^\alpha + \rho\mathbf{h}^\alpha = \rho\dot{\boldsymbol{\omega}}^\alpha, \tag{3.18}$$

which is the director momentum equation as given by Whitman and DeSilva.[4] If we apply the condition (3.15) to (3.16), we obtain

$$\varphi^{[ij]} + \check{d}^{[i}_\alpha\mu^{\alpha j]} - \tau^{[i}\check{x}^{j]} = 0. \tag{3.19}$$

This equation can be interpreted as the local balance of moment of momentum and arose in Ref. 4 by requiring the action density function to be invariant under rigid body rotations.

It can now be shown that by making suitable definitions of tensor and anholonomic components, all the forms of the field equations presented in Ref. 4 can be obtained. For example, if we set

$$\mu^{ij} = d^i_\alpha\mu^{\alpha j}, \quad h^{ij} = d^i_\alpha h^{\alpha j}, \quad \omega^{ij} = d^i_\alpha\omega^{\alpha j},$$

then (3.10) yields the couple stress equation of motion [see (4.7) in Ref. 4]:

$$\check{\mu}^{[ij]} - \tau^{[i}\check{x}^{j]} + \rho h^{[ij]} = \rho\dot{\omega}^{[ij]}. \tag{3.20}$$

Alternatively, if we define $\mathbf{m}$, $\mathbf{l}$, $\boldsymbol{\alpha}$ to be the axial vectors

$$m_i = \epsilon_{imn}\mu^{mn}, \quad l_i = \epsilon_{imn}h^{mn}, \quad \alpha_i = \epsilon_{imn}\omega^{mn},$$

then (3.20) becomes

$$\check{m}_i - \epsilon_{imn}\tau^m\check{x}^n + \rho l_i = \rho\dot{\alpha}_i. \tag{3.21}$$

The double stress equation of motion follows directly from (3.18):

$$\check{\mu}^{(ij)} - \check{d}^{(i}_\alpha\mu^{\alpha j)} - \varphi^{(ij)} + \rho h^{(ij)} = \rho\dot{\omega}^{(ij)} - A^{mn}W_m{}^iW_n{}^j. \tag{3.22}$$

Hence, the field equations consist of (3.7), (3.8), (3.20) or (3.21) and (3.22).

The anholonomic forms of the equations of motion follow by defining anholonomic components $\tau_\alpha = \mathbf{d}_\alpha\cdot\boldsymbol{\tau}$, $\mu^{\alpha\beta} = \boldsymbol{\mu}^\alpha\cdot\mathbf{d}^\beta$, etc. Then equations (3.6), (3.21), and (3.22) can be put into the forms

$$\begin{aligned}
&\check{\tau}_\alpha - w^\beta{}_\alpha\tau_\beta + \rho f_\alpha = \rho\dot{v}_\alpha - \rho W_\alpha{}^\beta v_\beta,\\
&\check{m}^\alpha + w^\alpha{}_\beta m^\beta - \epsilon^{\alpha\beta\delta}\tau_\beta t_\delta + \rho l^\alpha = \rho\dot{\alpha}^\alpha + \rho W_\beta{}^\alpha\alpha^\beta,\\
&\check{\mu}^{(\alpha\beta)} + \mu^{(\alpha\delta}w^{\beta)}{}_\delta - \varphi^{(\alpha\beta)} + \rho h^{(\alpha\beta)} = \rho\dot{\omega}^{(\alpha\beta)} + \rho\omega^{(\alpha\delta}W_\delta{}^{\beta)},
\end{aligned} \tag{3.23}$$

where

$$w^\alpha{}_\beta = (1/\lambda)F^\alpha{}_\beta \quad\text{and}\quad t_\alpha = (1/\lambda)y_\alpha.$$

Finally, by using (3.11) and (3.18) in (3.3) as modified previously, we can show that the local balance of energy reduces to the form

$$\rho\dot{e} - (\rho Q - \check{q}) = \tau^i\check{v}_i + \varphi^{\alpha i}w_{\alpha i} + \mu^{\alpha i}\check{w}_{\alpha i}. \tag{3.24}$$

When $Q = \check{q} = 0$ and e is identified with the strain energy function ϵ, then (3.24) reduces to the form obtained in Ref. 4. An alternate form of (3.24) can be obtained by applying (3.16) and the inverse to (2.9), i.e., $w_{\alpha n} = d^m_\alpha W_{mn}$. Hence,

$$\begin{aligned}
&\rho\dot{e} - (\rho Q - \check{q})\\
&\quad = \tau^i(\check{v}_i + \check{x}^jW_{ij}) + m^{ij}W_{(ij)} + \mu^{ij}\check{W}_{ij}.
\end{aligned} \tag{3.25}$$

To complete the general theory, we postulate the Clausius–Duhem inequality in the form

$$\frac{d}{dt}\int_{s_1}^{s_2}\rho\eta\,ds - \int_{s_1}^{s_2}\frac{\rho Q}{\vartheta}\,ds + \left[\frac{q}{\vartheta}\right]_{s_1}^{s_2} \geq 0, \tag{3.26}$$

where η is the entropy density and $\vartheta > 0$ is the temperature. Making the usual smoothness assumptions and applying the conservation of mass (3.5), we obtain from (3.26)

$$\rho\vartheta\dot{\eta} - \rho Q + \check{q} - q\check{\vartheta}/\vartheta \geq 0. \tag{3.27}$$

If we define the Helmholtz free energy function $\psi = e - \vartheta\eta$, then the energy equation (3.24) becomes

$$\rho\vartheta\dot{\eta} - \rho Q + \check{q} = \tau^i\check{v}_i + \varphi^{\alpha i}w_{\alpha i} + \mu^{\alpha i}\check{w}_{\alpha i} - \rho(\dot{\psi} + \dot{\vartheta}\eta). \quad (3.28)$$

Using this equation in (3.27), we obtain an alternate form of the entropy production inequality

$$\tau^i\check{v}_i + \varphi^{\alpha i}w_{\alpha i} + \mu^{\alpha i}\check{w}_{\alpha i} - \rho(\dot{\psi} + \dot{\vartheta}\eta) - (q\check{\vartheta}/\vartheta) \geq 0. \quad (3.29)$$

4. CONSTITUTIVE EQUATIONS

We consider here constitutive equations, appropriate for directed curves, for a class of simple materials without memory. By applying the arguments of Coleman and Mizel,[12] as adapted to simple directed media by Kline,[13] we obtain restrictions on the constitutive equations imposed by the Clasius–Duhem inequality. Further restrictions are then obtained by applying the principle of material frame indifference. This principle, also called the principle of objectivity, is discussed in the treatise by Truesdell and Noll.[14]

For a directed curve we define a simple material without memory as one for which ψ, η, q, $\boldsymbol{\tau}$, $\boldsymbol{\varphi}^\alpha$, and $\boldsymbol{\mu}^\alpha$ are sufficiently smooth functions of the following set of kinematical and thermodynamical measures:

$$\mathcal{S} = \{\hat{x}^i, d^i_\alpha, \hat{d}^i_\alpha, \vartheta, \hat{v}^i, w^i_\alpha, \hat{w}^i_\alpha, \hat{\vartheta}\}. \quad (4.1)$$

That is, we postulate a complete set of constitutive equations in the form

$$\psi = \psi(\mathcal{S}), \quad \eta = \eta(\mathcal{S}), \quad q = q(\mathcal{S}),$$
$$\boldsymbol{\tau} = \boldsymbol{\tau}(\mathcal{S}), \quad \boldsymbol{\varphi}^\alpha = \boldsymbol{\varphi}^\alpha(\mathcal{S}), \quad \boldsymbol{\mu}^\alpha = \boldsymbol{\mu}^\alpha(\mathcal{S}). \quad (4.2)$$

Guided by the arguments in Refs. 12 and 13, we can show that, under the assumptions (4.2), the entropy production inequality (3.29) is satisfied for arbitrary thermodynamical processes[15] if and only if

$$\frac{\partial\psi}{\partial\hat{v}^i} = \frac{\partial\psi}{\partial w^i_\alpha} = \frac{\partial\psi}{\partial\hat{w}^i_\alpha} = \frac{\partial\psi}{\partial\hat{\vartheta}} = 0, \quad (4.3)$$

$$\eta = -\frac{\partial\psi}{\partial\vartheta}, \quad (4.4)$$

$$\left(\frac{1}{\lambda}\tau_i - \rho\frac{\partial\psi}{\partial\hat{x}^i}\right)\hat{v}^i + \left(\varphi^\alpha_i - \rho\frac{\partial\psi}{\partial d^i_\alpha}\right)w^i_\alpha + \left(\frac{1}{\lambda}\mu^\alpha_i - \rho\frac{\partial\psi}{\partial\hat{d}^i_\alpha}\right)w^i_\alpha - \frac{q\hat{\vartheta}}{\lambda\vartheta} \geq 0. \quad (4.5)$$

From (4.3) we see that

$$\psi = \psi(\mathcal{S}_0), \quad (4.6)$$

where $\mathcal{S}_0$ is the subset of $\mathcal{S}$ defined by

$$\mathcal{S}_0 = \{\hat{x}^i, d^i_\alpha, \hat{d}^i_\alpha, \vartheta\}. \quad (4.7)$$

Equations (4.6), (4.4), and (4.5) are respectively the caloric equation of state, the entropy–temperature relation, and the reduced form of the entropy–production inequality.

Following Ref. 12, we assume that the stresses[16] $\boldsymbol{\tau}$, $\boldsymbol{\varphi}^\alpha$, $\boldsymbol{\mu}^\alpha$ can be written in the form

$$\begin{aligned}\boldsymbol{\tau}(\mathcal{S}) &= \boldsymbol{\tau}_{(0)}(\mathcal{S}_0) + \boldsymbol{\tau}_{(D)}(\mathcal{S}),\\ \boldsymbol{\varphi}^\alpha(\mathcal{S}) &= \boldsymbol{\varphi}^\alpha_{(0)}(\mathcal{S}_0) + \boldsymbol{\varphi}^\alpha_{(D)}(\mathcal{S}),\\ \boldsymbol{\mu}^\alpha(\mathcal{S}) &= \boldsymbol{\mu}^\alpha_{(0)}(\mathcal{S}_0) + \boldsymbol{\mu}^\alpha_{(D)}(\mathcal{S}),\end{aligned} \quad (4.8)$$

where $\boldsymbol{\tau}_{(0)}$, $\boldsymbol{\mu}^\alpha_{(0)}$, $\boldsymbol{\mu}^\alpha_{(0)}$ denote the stresses in thermal and mechanical equilibrium, i.e., that state defined by the vanishing of $\hat{\mathbf{v}}$, $\mathbf{w}_\alpha$, $\hat{\mathbf{w}}_\alpha$, and $\hat{\vartheta}$. Thus,

$$\boldsymbol{\tau}_{(0)} = \boldsymbol{\tau}(\hat{x}^i, d^i_\alpha, \hat{d}^i_\alpha, \vartheta, 0, 0, 0, 0) = \boldsymbol{\tau}_{(0)}(\mathcal{S}_0).$$

The functions $\boldsymbol{\tau}_{(D)}$, $\boldsymbol{\varphi}^\alpha_{(D)}$, $\boldsymbol{\mu}^\alpha_{(D)}$ are extra or dissipative stresses which vanish in the equilibrium state. Then from (4.5) and (4.8) we obtain the following results:

$$\tau_{(0)i} = \rho\lambda\frac{\partial\psi}{\partial\hat{x}^i}, \quad \varphi^\alpha_{(0)i} = \rho\frac{\partial\psi}{\partial d^i_\alpha}, \quad \mu^\alpha_{(0)i} = \rho\lambda\frac{\partial\psi}{\partial\hat{d}^i_\alpha}, \quad (4.9)$$

$$\boldsymbol{\tau}_{(D)}\cdot\hat{\mathbf{v}} + \lambda\boldsymbol{\varphi}^\alpha_{(D)}\cdot\mathbf{w}_\alpha + \boldsymbol{\mu}^\alpha_{(D)}\cdot\hat{\mathbf{w}}_\alpha - q\hat{\vartheta}/\vartheta \geq 0. \quad (4.10)$$

Thus the equilibrium stresses are specified when the equation of state (4.6) is known. We call (4.10) the general dissipation inequality. The constitutive equations (4.2) now take the form

$$\begin{aligned}&\psi = \psi(\mathcal{S}_0), \quad \eta = \eta(\mathcal{S}_0), \quad q = q(\mathcal{S}),\\ &\boldsymbol{\tau} = \boldsymbol{\tau}_{(0)}(\mathcal{S}_0) + \boldsymbol{\tau}_{(D)}(\mathcal{S}), \quad \boldsymbol{\varphi}^\alpha = \boldsymbol{\varphi}^\alpha_{(0)}(\mathcal{S}_0) + \boldsymbol{\varphi}^\alpha_{(D)}(\mathcal{S}),\\ &\boldsymbol{\mu}^\alpha = \boldsymbol{\mu}^\alpha_{(0)}(\mathcal{S}_0) + \boldsymbol{\mu}^\alpha_{(D)}(\mathcal{S}).\end{aligned} \quad (4.11)$$

Using (4.4), (4.6), (4.8), and (4.9) in the energy equation (3.28), we obtain

$$\rho\vartheta\dot{\eta} - \rho Q + \check{q} = \boldsymbol{\tau}_{(D)}\cdot\check{\mathbf{v}} + \boldsymbol{\varphi}^\alpha_{(D)}\cdot\mathbf{w}_\alpha + \boldsymbol{\mu}^\alpha_{(D)}\cdot\check{\mathbf{w}}_\alpha. \quad (4.12)$$

For the special case when the dissipative stresses and heat flux are independent of $\check{\mathbf{v}}$, $\mathbf{w}_\alpha$, $\check{\mathbf{w}}_\alpha$, (4.10) implies

$$\tau^\alpha_{(D)}(\mathcal{S}_0, \vartheta) = \boldsymbol{\varphi}^\alpha_{(D)}(\mathcal{S}_0, \vartheta) = \boldsymbol{\mu}^\alpha_{(D)}(\mathcal{S}_0, \vartheta) = 0, \quad (4.13)$$

$$\hat{\vartheta}q(\mathcal{S}_0, \hat{\vartheta}) \leq 0. \quad (4.14)$$

Then, from (4.8), (4.9), and (4.13), the stresses depend only on the equation of state (4.6) and are given by

$$\tau_i = \rho\lambda\frac{\partial\psi}{\partial\hat{x}^i}, \quad \psi^\alpha_i = \rho\frac{\partial\psi}{\partial d^i_\alpha}, \quad \mu^\alpha_i = \rho\lambda\frac{\partial\psi}{\partial\hat{d}^i_\alpha}, \quad (4.15)$$

where $\psi = \psi(\mathcal{S}_0)$. These constitutive equations (4.15) can be regarded as defining the thermoelastic response of a directed curve and generalize those given by Whitman and DeSilva[4] for the isothermal theory. In addition to (4.15), a constitutive equation for the heat flux must be specified such that (4.14) is satisfied.

In addition to the entropy production inequality, we postulate that the constitutive equations (4.11) must satisfy the principle of material frame indifference. For convenience we shall employ Cartesian tensor notation. Then a change in frame is defined by the equations

$$x_i^* = Q_{ij}(t)x_j + c_i(t), \quad d_{\alpha i}^* = Q_{ij}(t)d_{\alpha j}, \tag{4.16}$$

where $\mathbf{c}(t)$ is an arbitrary vector, and $\mathbf{Q}(t)$ is an arbitrary orthogonal tensor:

$$Q_{im}Q_{jm} = Q_{mi}Q_{mj} = \delta_{ij}. \tag{4.17}$$

Under the change in frame (4.16), the quantities ψ, $\eta, q, \boldsymbol{\tau}, \boldsymbol{\varphi}^\alpha, \boldsymbol{\mu}^\alpha$ are required to be frame indifferent, i.e.,

$$\begin{aligned} &\psi^* = \psi, \quad \eta^* = \eta, \quad q^* = q, \\ &\tau_i^* = Q_{ij}\tau_j, \quad \varphi_i^{\alpha *} = Q_{ij}\varphi_j^\alpha, \quad \mu_i^{\alpha *} = Q_{ij}\mu_j^\alpha. \end{aligned} \tag{4.18}$$

Applying the change in frame (4.16) to the quantities in $\mathcal{S}$, we find that $\hat{x}_i$, $d_{\alpha i}$, $\hat{d}_{\alpha i}$, ϑ, $\hat{\vartheta}$ are all frame indifferent, whereas $\hat{v}_i$, $w_{\alpha i}$, $\hat{w}_{\alpha i}$ are not. Guided by the local energy balance in the mixed component form (3.24) and the tensor form (3.25), we define the argument set $\bar{\mathcal{S}}$ such that

$$\bar{\mathcal{S}} = \{\mathcal{S}_0, V_i, W_{(ij)}, \hat{W}_{ij}, \hat{\vartheta}\}, \tag{4.19}$$

where the vector $\mathbf{V}$ is defined as

$$V_i = \hat{v}_i + \hat{x}_j W_{ij}. \tag{4.20}$$

It can easily be seen that all the arguments of the set $\bar{\mathcal{S}}$ are frame indifferent. Hence, if $\boldsymbol{\tau}, \boldsymbol{\varphi}^\alpha, \boldsymbol{\mu}^\alpha, q$ are taken as functions of $\bar{\mathcal{S}}$ with ψ, η functions of $\mathcal{S}_0$, then Eqs. (4.18) imply that these quantities are isotropic tensor functions of their arguments.[14]

We now seek forms of the constitutive equations which are sufficient to satisfy (4.18). To this end we define the argument sets $\tilde{\mathcal{S}}_0$ and $\tilde{\mathcal{S}}$ such that

$$\tilde{\mathcal{S}}_0 = \{y_\alpha, C_{\alpha\beta}, F_{\alpha\beta}, \vartheta\}, \tag{4.21}$$

$$\tilde{\mathcal{S}} = \{\tilde{\mathcal{S}}_0, \dot{y}_\alpha, \dot{C}_{\alpha\beta}, \dot{F}_{\alpha\beta}, \hat{\vartheta}\}, \tag{4.22}$$

where $y_\alpha, C_{\alpha\beta}, F_{\alpha\beta}$ are defined by (2.5). It can be shown that under a change of frame all the arguments of the sets $\tilde{\mathcal{S}}_0$ and $\tilde{\mathcal{S}}$ transform as scalars, i.e., $\tilde{\mathcal{S}}_0^* = \tilde{\mathcal{S}}_0$, $\tilde{\mathcal{S}}^* = \tilde{\mathcal{S}}$. Hence, to satisfy (4.18) we rewrite (4.11) in the form

$$\begin{aligned} &\psi = \psi(\tilde{\mathcal{S}}_0), \quad \eta = \eta(\tilde{\mathcal{S}}_0), \quad q = q(\tilde{\mathcal{S}}), \\ &\boldsymbol{\tau} = \mathbf{d}_\alpha[\tau_{(0)}^\alpha(\tilde{\mathcal{S}}_0) + \tau_{(D)}^\alpha(\tilde{\mathcal{S}})], \\ &\boldsymbol{\varphi}^\alpha = \mathbf{d}_\beta[\varphi_{(0)}^{\alpha\beta}(\tilde{\mathcal{S}}_0) + \varphi_{(D)}^{\alpha\beta}(\tilde{\mathcal{S}})], \\ &\boldsymbol{\mu}^\alpha = \mathbf{d}_\beta[\mu_{(0)}^{\alpha\beta}(\tilde{\mathcal{S}}_0) + \mu_{(D)}^{\alpha\beta}(\tilde{\mathcal{S}})]. \end{aligned} \tag{4.23}$$

These forms of the constitutive equations imply that conditions (4.18) are identically satisified. We remark that the argument set $\tilde{\mathcal{S}}$ in (4.23) can be replaced by the set

$$\{\mathcal{S}_0, V_\alpha, W_{(\alpha\beta)}, \hat{W}_{\alpha\beta}, \hat{\vartheta}\}, \tag{4.24}$$

where $V_\alpha = \mathbf{d}_\alpha \cdot \mathbf{V}$. This set of arguments also transforms as scalars under change of frame, and hence (4.23) with $\tilde{\mathcal{S}}$ replaced by (4.24) will satisfy (4.18).

The equilibrium stresses (4.9) take an alternate form in terms of the set $\tilde{\mathcal{S}}_0$. Using (2.5), (4.9) and $(4.23)_1$, we obtain

$$\begin{aligned} &\boldsymbol{\tau}_{(0)} = \rho\lambda\frac{\partial\psi}{\partial y_\alpha}\mathbf{d}_\alpha, \quad \boldsymbol{\mu}_{(0)}^\alpha = \rho\lambda\frac{\partial\psi}{\partial F_{\beta\alpha}}\mathbf{d}_\beta, \\ &\boldsymbol{\varphi}_{(0)}^\alpha = \rho\left(\frac{\partial\psi}{\partial y_\alpha}\hat{\mathbf{r}} + 2\frac{\partial\psi}{\partial C_{\alpha\beta}}\mathbf{d}_\beta + \frac{\partial\psi}{\partial F_{\alpha\beta}}\hat{\mathbf{d}}_\beta\right), \end{aligned} \tag{4.25}$$

where $\psi = \psi(y_\alpha, C_{\alpha\beta}, F_{\alpha\beta}, \vartheta)$. Recalling that equations (4.9) and (4.15) are identical in form, it is clear that (4.25) also apply to the case of thermoelasticity.

In summary, the constitutive equations for a simple directed curve without memory are given by (4.23), where the dissipative stresses must satisfy the general dissipation inequality (4.10) and the equilibrium stresses are given by (4.25).

5. DISCUSSION

By the use of the energy balance equation, invariance under a rigid body translation yields (i) the mass balance equation for a material point $\mathbf{r}$ and (ii) the linear momentum balance equation for a material point $\mathbf{r}$. Invariance under a rigid body rotation yields (i) a mass balance equation for the directors $\mathbf{d}_\alpha$ at $\mathbf{r}$ and (ii) an angular momentum balance equation. The director mass balance or continuity equation is $\psi^{ij} = \dot{A}^{\alpha\beta} = 0$. It is interesting to note that the complete set of field equations as given in Sec. 3 are obtainable from the separate postulates:

(i) mass balance:

$$\frac{d}{dt}\int_{s_1}^{s_2}\rho\, ds = 0; \tag{5.1}$$

(ii) director mass balance:

$$\frac{d}{dt}\int_{s_1}^{s_2}\rho A^{\alpha\beta}\, ds = 0; \tag{5.2}$$

(iii) linear momentum balance:

$$\frac{d}{dt}\int_{s_1}^{s_2}\rho\mathbf{v}\,ds=\int_{s_1}^{s_2}\rho\mathbf{f}\,ds+[\boldsymbol{\tau}]_{s_1}^{s_2};\tag{5.3}$$

(iv) linear director momentum balance:

$$\frac{d}{dt}\int_{s_1}^{s_2}\rho\boldsymbol{\omega}^{\alpha}\,ds=\int_{s_1}^{s_2}(\rho\mathbf{h}^{\alpha}-\boldsymbol{\varphi}^{\alpha})\,ds+[\boldsymbol{\mu}^{\alpha}]_{s_1}^{s_2};\tag{5.4}$$

(v) momentum of momentum balance:

$$\frac{d}{dt}\int_{s_1}^{s_2}\rho(\mathbf{r}\times\mathbf{v}+\mathbf{d}_{\alpha}\times\boldsymbol{\omega}^{\alpha})\,ds=\int_{s_1}^{s_2}\rho(\mathbf{r}\times\mathbf{f}+\mathbf{d}_{\alpha}\times\mathbf{h}^{\alpha})\,ds+[\mathbf{r}\times\boldsymbol{\tau}+\mathbf{d}_{\alpha}\times\boldsymbol{\mu}^{\alpha}]_{s_1}^{s_2}.\tag{5.5}$$

It is of interest to point out that Green and Laws[6] developed a theory for rods, using a one-dimensional continuum with two directors, in which they had $\dot{A}^{\alpha\beta}\neq 0$. In their notation, $y^{\alpha\beta}$ is equivalent to our $A^{\alpha\beta}$. When these authors treated invariance under a rigid body rotation, they were able to obtain only the angular momentum equation. We can recover the result of Green and Laws if we modify our Eq. (3.4) to read

$$\boldsymbol{\omega}^{\alpha}=A^{\alpha\beta}\mathbf{w}_{\beta}-\tfrac{1}{2}\int\dot{A}^{\alpha\beta}\mathbf{w}_{\beta}\,dt.\tag{5.6}$$

We emphasize that (3.4) is a more natural form than the above; moreover, as derived in Ref. 4, there is no restriction placed on $A^{\alpha\beta}$, i.e., $\dot{A}^{\alpha\beta}\neq 0$ in (3.4).

In a subsequent paper, Green, Laws, and Naghdi[17] developed theories of rods and shells using the three-dimensional theory of classical continuum mechanics as a starting point. The (three-dimensional) energy equation is reduced to a one-dimensional form which is a generalization of that postulated by Green and Laws. In this one-dimensional energy equation they derive coefficients $k^{\alpha_1\cdots\alpha_n;\,\beta_1\cdots\beta_m}$ which generalize the $y^{\alpha\beta}$ (our $A^{\alpha\beta}$) of the earlier work of Green and Laws. These coefficients $\mathbf{k}$ are all independent of time: See Eq. (6.14), p. 907, of Ref. 17.

This result bears out our conclusion that $\dot{y}^{\alpha\beta}=0$ is a result which can be proved. Green and Laws very naturally defined in their Eqs. (3.12), p. 149,

$$\mathbf{q}^{\alpha}=\mathbf{l}^{\alpha}-\tfrac{1}{2}\dot{y}^{\alpha\beta}\mathbf{w}_{\beta}-y^{\alpha\beta}\dot{\mathbf{w}}_{\beta}.$$

If they had defined instead $\mathbf{q}^{\alpha}=\mathbf{l}^{\alpha}-y^{\alpha\beta}\dot{\mathbf{w}}_{\beta}$ and modified the integrand on the right side of their Eq. (3.11) to read

$$\int_{\vartheta_1}^{\vartheta_2}\rho(r+\mathbf{f}\cdot\mathbf{v}+\mathbf{q}^{\alpha}\cdot\mathbf{w}_{\alpha}-\tfrac{1}{2}\dot{y}^{\alpha\beta}\mathbf{w}_{\alpha}\cdot\mathbf{w}_{\beta})(a_{33})^{\frac{1}{2}}\,d\vartheta,$$

then, using the argument of invariance under a superposed rigid body rotation, they would have obtained, in addition to their Eq. (3.14), p. 149, the result $\dot{y}^{\alpha\beta}=0$. Hence, they would have anticipated the result on the coefficients $\mathbf{k}$ of Green, Laws, and Naghdi, obtained by expanding the displacement in an infinite series about a curve c.

In the energy approach, the question of the uniqueness of the expression for $\mathbf{q}^{\alpha}$ arises naturally: Why our suggested form given above and not that of Green and Laws? We can answer only by repeating that (3.4) seems more reasonable than (5.6) for the director momentum density; moreover, in Ref. 4, (3.4) followed from a derived constitutive equation.

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Regge Trajectories at High Energies for a Class of Analytic Potentials

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We consider scattering by nonsingular, energy-independent, central potentials $V(r)$ which are analytic in r in a sector of half-angle θ about the real positive axis. Simple considerations show that at high energies all Regge trajectories leave the sector of the angular momentum plane given by $|\arg l| \leq \theta$. One finds in general, however, that Regge trajectories remain in the right half l plane at sufficiently high energies for potentials of the above type. The Wood–Saxon potential is analyzed numerically. It is found that Regge trajectories which represent bound states remain in the right half l plane at high energies.

1. INTRODUCTION

It is well understood that in scattering from central potentials $V(r)$ of Yukawa type (i.e., analytic in the right half r plane) the corresponding Regge trajectories $l(k)$ at high energies either (1) approach $l = -n$, where n is a positive integer, or (2) approach the point at infinity along such a path that $\mathrm{Re}\, l \to -\infty$. The fact that Regge trajectories all leave the right half l plane is intimately connected with the fact that the scattering amplitude here satisfies the Mandelstam representation with a finite number of subtractions in momentum transfer.

Here we will consider scattering from central potentials $V(r)$ which, while not of Yakawa type in general, are analytic in r (and vanish at infinity) in some sector of the real r axis of half angle θ. A simple example is the Gaussian potential

$$V(r) = g \exp(-r^2),$$

which is analytic and asymptotically decreasing in a sector of half-angle $\pi/4 - \epsilon$. We are interested in the behavior of the Regge trajectories at large energies for this type of potential. The Mandelstam representation is not expected to hold for this class of potentials because of singularities at complex momentum transfer or at infinity. The scattering amplitude will, however, be analytic in the "large Lehmann ellipse" if the potential is of finite range.

It is straightforward to show directly from the Schrödinger equation that, for potentials analytic and asymptotically decreasing in a sector of half-angle θ, there can be no Regge trajectories at sufficiently high energies in the complex l plane in a sector of half-angle θ about the real l axis.[1] In addition, Barut and Dilley have used Langer's theory of asymptotic behavior of differential equations to obtain the following asymptotic form of the scattering amplitude valid in the limit $|\lambda| \to \infty$ away from the negative real axis for fixed[2] k:

$$f_\lambda(k) \sim i \frac{\lambda^{\frac{1}{2}}}{\sqrt{2}\, k^2} V\left(\frac{\lambda}{k}\right), \quad \lambda = l + \tfrac{1}{2}. \tag{1.1}$$

It is not clear from the context to what extent this result is asymptotically correct in the limit as $|\lambda| \to \infty$ and $k \to \infty$, although simple examples suggest that it may well be valid there. (In particular, see Sec. 4 here.) Indeed, the asymptotic result (1.1) applied to a sector-analytic potential is certainly consistent with the above-mentioned fact that all Regge trajectories leave the region $|\arg l| \leq \theta$ at high energies.

Our approach is to examine the Fredholm determinant $\Delta(\lambda, k)$ of the Lippman–Schwinger equation,[3] the Jost function. From the asymptotic form of Δ at large energies we will calculate the asymptotic position of its zeros in a representative case. In this way we locate the Regge trajectories asymptotically; we find that in general they remain in the right half l plane.

In addition, we have written a search program to determine the location of Regge trajectories by numerical integration of the Schrödinger equation. The program was used for the Wood–Saxon potential familiar in nuclear physics.[4] The results are in general agreement with Eq. (1.1) above.

2. FORMALISM; THE CLASS OF POTENTIALS

We consider scattering by energy independent central potentials for which $\int_0^\infty dr\, r\, |V(r)|$ is a convergent integral. Froissart[5] has shown that for such potentials the scattering amplitude $f(\lambda, k)$, considered for complex angular momentum λ and positive real momentum k, is meromorphic in λ at finite λ except possibly at the points

$$\lambda = -n + (m/2)(s - 2);$$

m and n are positive integers and s is an element of the set of singularities of the integral[6]

$$u(\sigma) = \int_0^1 dr V(r) r^{\sigma - 1}.$$

We restrict considerations to the class of potentials for which $\mu(\sigma)$ is analytic in σ for $\operatorname{Re}\sigma \geq 2$. This condition is not very stringent—it can easily be insured by reasonable assumptions about $V(r)$ for real r. For this class of potentials the scattering amplitude will consequently be meromorphic for finite λ in the right half λ plane.[7]

Under the above conditions we can represent $rV(r)$ for real positive r by the Fourier integral

$$\begin{aligned} rV(r) &= V_+(r) + V_-(r) \\ &= \int_0^\infty ds[f(s)e^{-isr} + f^*(s)e^{isr}]. \end{aligned} \tag{2.1}$$

We impose analyticity upon V by requiring that $f(s)$ be analytic in the wedge-shaped region $\operatorname{Re} s > 0$, $|\arg s| < \theta$, $0 < \theta \leq \pi/2$. Let us also require that $sf(s) \to 0$ as $s \to \infty$ within this region. Then we can distort the contours of integration to write

$$V_+(r) = \int_0^\infty dp g_+(p) \exp\left[-pre^{i(\pi/2-\theta)}\right], \tag{2.2a}$$

$$V_-(r) = \int_0^\infty dp g_-(p) \exp\left[-pre^{-i(\pi/2-\theta)}\right], \tag{2.2b}$$

where $g_+(p) = e^{-i\theta}f(pe^{-i\theta})$ and $g_-(p) = [g_+(p)]^*$. We will place some constraints on the moments of $g_\pm(p)$ in this work. These constraints will be sufficient to guarantee that $V(r)$ is analytic and asymptotically decreasing in a wedge of half-angle θ.

Let us give an example of a potential which is of the above type but which is not analytic and asymptotically decreasing in the entire right half r plane:

$$V(r) = \mu/(r^4 + b^4), \tag{2.3}$$

for which

$$f(s) = (\mu/4b^2)\{e^{-bs\sqrt{-i}} - e^{-bs\sqrt{i}}\}, \tag{2.4}$$

where we make the convention $\sqrt{\pm i} = e^{\pm i\pi/4}$. In this case $f(s)$ is suitably analytic and decreasing in s in a sector of half angle $\theta < \pi/4$ about the real s axis.

We now review construction of the Fredholm determinant and the scattering amplitude at real energies and complex angular momentum. The Froissart–Gribov analytic continuation of the Fredholm determinant $\Delta_\lambda(k)$ is given by

$$\Delta_\lambda(k) = 1 + \sum_{N=1}^{\infty} \Delta_N(\lambda, k), \tag{2.5}$$

where

$$\Delta_N(\lambda, k) = \int_0^\infty \prod_{i=1}^{N} dr_i r_i V(r_i) \cdot \det_N \begin{Bmatrix} K_\lambda(r_j, r_k) \\ j = 1 \cdots N \\ k = 1 \cdots N \end{Bmatrix}, \tag{2.6}$$

with the kernel K_λ expressed through the integral representation[8]

$$K_\lambda(r, r') = \int_0^\infty \frac{k'\,dk'}{k'^2 - k^2 - i\epsilon} J_\lambda(k'r)J_\lambda(k'r'). \tag{2.7}$$

In this context the partial wave S matrix is given by

$$S_\lambda(k) = [\Delta_{\lambda^*}(k)]^*/\Delta_\lambda(k) \tag{2.8}$$

and the scattering amplitude is defined by

$$f_\lambda(k) = [S_\lambda(k) - 1]/2ik. \tag{2.9}$$

We now discuss the location of Regge trajectories at asymptotic energies for potentials of the above type.

3. ASYMPTOTIC TRAJECTORIES

We wish to study the asymptotic behavior of Regge trajectories corresponding to potentials which are analytic in a sector about the real r axis. We can locate Regge trajectories by finding the curve $\lambda(k)$ along which $\Delta_\lambda(k) = 0$, where $\Delta_\lambda(k)$ is defined in (2.5).

In Appendix A we will use the representation (2.2) to obtain a useful representation of Δ_1, the contribution to the Fredholm determinant which is first order in potential strength. This first-order contribution separates naturally into two types of terms. One type of term is expressed as an integral over p of $g_\pm(p)$ multiplied by a Legendre function Q_l of complex order and argument. The second type of term, while not evaluated explicitly, is shown for reasonable weight functions $g_\pm(p)$ to be small in the limit as the momentum k approaches infinity through real values *uniformly* in any region of angular momentum λ, not including the integers. As a result one obtains the asymptotic limit[9]

$$\begin{aligned} &1 + \Delta_1(\lambda, k) \\ &\simeq 1 - \frac{e^{-i\pi\lambda}}{2k \sin \pi\lambda} \int_0^\infty dp \left[g_+(p)Q_l\left(1 + \frac{p^2}{2k^2} e^{2i\theta}\right) \right. \\ &\qquad \left. + g_-(p)Q_l\left(1 + \frac{p^2}{2k^2} e^{-2i\theta}\right)\right]. \end{aligned} \tag{3.1}$$

In general the detailed behavior of Δ_1 depends upon the specific weight functions $g_\pm$. However, one certainly cannot conclude from the asymptotic properties of Q_l *alone* that, for example, Δ_1 becomes small as $k \to \infty$ for $\operatorname{Re}\lambda > 0$, $\operatorname{Im}\lambda > 0$.

Let us consider the behavior of the first-order expression for the Fredholm determinant for the special case of the potential

$$V(r) = \frac{g}{r}(e^{-\mu re^{i\theta}} + e^{-\mu re^{-i\theta}}). \tag{3.2}$$

For this potential the weight functions g_+ and g_- are delta functions. In Appendix B we will obtain the asymptotic location of the solutions of the equation

$$1 + \Delta_1(\lambda, k) = 0 \tag{3.3}$$

in the limit of large real momentum k.

One finds an infinite number of solutions in this limit which lie at $|\lambda|$ large. These trajectories all individually approach the line $\arg \lambda = \pi - \theta$. However, at any finite, though large, momentum k an infinite number of these trajectories lie asymptotically close to the line $\arg \lambda = \pi/2 - \theta$.

The solutions of (3.3) would be the asymptotic locations of Regge trajectories if the terms in the Fredholm determinant which are of higher order in the potential strength are in some sense negligible. It is shown in Appendix C that the contribution to the Fredholm determinant of second order in potential strength may be neglected in determining the asymptotic zeros of the Fredholm determinant. Reasons are also given there for neglecting all the terms Δ_n for $n > 2$

Consequently we have shown that if one has a potential $V(r)$ which is analytic and asymptotically decreasing only in a wedge-shaped region of half-angle $\theta < \pi/2$, one in general cannot expect that all Regge trajectories leave the right half λ plane at some large, though finite, energy. This conclusion is, of course, consistent with the analysis of Barut and Dilley.[2]

4. THE SEARCH PROGRAM

We will now describe a search program for finding Regge trajectories corresponding to any central potential $V(r)$.[10] The corresponding radial Schrödinger equation is

$$-\frac{\partial^2\psi}{\partial r^2} + \frac{\lambda^2 - \frac{1}{4}}{r^2}\psi + V\psi = k^2\psi. \tag{4.1}$$

First we pick a trail value of complex angular momentum λ as an estimate of the location of a Regge pole at a given momentum k. We integrate the Schrödinger equation numerically from $r = 0$, generating a function $\psi_{\text{out}}(r)$ such that

$$\psi_{\text{out}}(r) \sim r^{\lambda+\frac{1}{2}} \tag{4.2}$$

for small r.[11] Next we integrate the equation inward from large r to generate $\psi_{\text{in}}(r)$, which at large r has the form[12]

$$\psi_{\text{in}}(r) \sim \left(\frac{\pi k r}{2}\right)^{\frac{1}{2}} e^{i\pi(\lambda+\frac{1}{2})} H_\lambda^{(1)}(kr). \tag{4.3}$$

The next step is to compute the logarithmic derivatives of a_{in} and a_{out} at an intermediate point r_0:

$$a_{\substack{\text{in}\\\text{out}}}(r_0) = \frac{\partial}{\partial r} \log \psi_{\substack{\text{in}\\\text{out}}}(r_0)\Big|_{r=r_0}. \tag{4.4}$$

We then calculate the quantity

$$P(\lambda, k) = \left|\frac{a_{\text{in}} - a_{\text{out}}}{a_{\text{in}} + a_{\text{out}}}\right|^2. \tag{4.5}$$

One then searches for the value of λ for which the corresponding function P is equal to zero. This value of λ gives the location of a Regge pole at momentum k. One can trace out Regge trajectories by increasing k somewhat and finding the location of the corresponding Regge pole.

This search program was applied to the Wood–Saxon potential

$$V(r) = \frac{U}{1 + e^{(r-r_0)/a}}. \tag{4.6}$$

We used the parameters

$$U = -2.40, \quad a = 0.58, \quad r = 3.30.$$

The locations of the leading and second Regge trajectory are listed in Table I. Note that each trajectory does rise roughly linearly in momentum k; both the real and imaginary parts of angular momentum have this property. The leading trajectory at larger values of k makes an angle of 24° with the real λ axis when the trajectory is plotted in the λ plane parametrically in k. The corresponding angle for the second trajectory is 43°.

Let us compare the above results of numerical calculations at intermediate energies with the predictions obtained by application of expression (1.1) to the Wood–Saxon potential. The Wood–Saxon potential has poles at the following complex values of r:

$$r(n) = r_0 + i(2n + 1)\pi a,$$

where n is any integer. One is thus led by (1.1) to

TABLE I

Leading Trajectory			Second Trajectory		
k	Re	Im	k	Re	Im
0.3	2.98	0.01	0.3	1.24	0.25
0.6	3.44	0.13	0.6	1.50	0.66
0.9	4.08	0.40	0.9	1.84	1.10
1.2	4.80	0.78	1.2	2.26	1.55
1.5	5.57	1.22	1.5	2.76	2.00
1.8	6.38	1.71	1.8	3.30	2.50
2.1	7.21	2.23	2.1	3.99	3.06
2.4	8.07	2.75			
2.7	8.89	3.33			
3.0	9.85	3.76			

predict that Regge trajectories should asymptotically obey the relation

$$\lambda(n) = kr_0 + i(2n + 1)ka\pi. \tag{4.7}$$

Expression (4.7), by way of comparison, predicts that the leading ($n = 0$) trajectory should approach the asymptotic line $\arg \lambda = 29°$, whereas the second trajectory should approach $\arg \lambda = 59°$. One can see that (4.7) is in rough qualitative agreement with the results of the numerical calculation of Regge trajectories.

Finally we note that numerical calculations indicate that these infinitely rising trajectories for the Wood–Saxon potential also contain bound state poles at positive integer angular momenta when analytically continued to negative energies.

The leading trajectory corresponds to $l = 0$, 1, and 2 bound states; the second trajectory has only an $l = 0$ bound state. We know of no explanation as to why the bound state trajectories happen to be infinitely rising here. In the case of the pure Yukawa potential it is found in numerical calculations that the bound state trajectories approach negative integer angular momenta at high energies.[13]

ACKNOWLEDGMENTS

I would like to thank Professor L. S. Kisslinger of Carnegie–Mellon University for helpful suggestions and interest in this work. The questions considered here arose in discussions with Professor Kisslinger. I would like to thank Mrs. M. Ratner for assistance in the search program.

APPENDIX A

Here we will calculate the high energy limit of the function $\Delta_1(\lambda, k)$:

$$\Delta_1(\lambda, k) = \int_0^\infty drrV(r)K_\lambda(r, r). \tag{A1}$$

We are interested in this function for the class of potentials $V(r)$ which are analytic in a sector of half-angle θ about the real r axis, and which can be represented in this sector by the following absolutely convergent integral representation:

$$rV(r) = \int_0^\infty dp[g_+(p)e^{-pre^{i\theta}} + g_-(p)e^{-pre^{-i\theta}}]. \tag{A2}$$

The function Δ may be expressed as the sum of Δ_+ and Δ_-,

$$\Delta_\pm = \int_0^\infty dpg_\pm(p)\int_0^\infty dre^{-pre^{\pm i\theta}}K_\lambda(r, r). \tag{A3}$$

One can write the kernel K_λ explicitly in terms of Bessel functions:

$$K_\lambda(r, r) = \frac{\pi}{2 \sin \pi\lambda}[J_\lambda(kr)J_{-\lambda}(kr) - e^{-i\pi\lambda}J_\lambda(kr)J_\lambda(kr)],$$

as a result one obtains for Δ_ϵ ($\epsilon = \pm 1$) the expression

$$\Delta_\epsilon = \int_0^\infty dpg_\epsilon(p)[I_1(\epsilon, p, k, \lambda) + I_2(\epsilon, p, k, \lambda)] = \Delta_{\epsilon 1} + \Delta_{\epsilon 2}, \tag{A4}$$

where[14]

$$I_1 = -\frac{e^{-i\pi\lambda}}{2k \sin \pi\lambda} Q_l\left(1 + \frac{p^2}{2k^2} e^{2i\epsilon\theta}\right) \tag{A5}$$

and

$$I_2 = \frac{\pi}{2 \sin \pi\lambda}\int_0^\infty drJ_\lambda(kr)J_{-\lambda}(kr)e^{-pre^{i\epsilon\theta}}. \tag{A6}$$

We are interested in the limit of $\Delta_\pm$ for large, real momenta k, where λ is bounded away from the real axis but not necessarily finite. We will show that in this limit I_2 is uniformly small compared to unity. In fact, I_2 may be transformed into the form[14]

$$I_2 = \frac{1}{2 \sin \pi\lambda}\int_0^{\pi/2} \frac{d\omega \cos 2\lambda\omega}{[k^2 \cos^2 \omega + (p^2/4)e^{2i\epsilon\theta}]^{\frac{1}{2}}}. \tag{A7}$$

Integration by parts yields

$$I_2 = \frac{\cos \pi\lambda}{2 \sin \pi\lambda}\int_0^{\pi/2} \frac{d\omega}{[k^2 \cos^2 \omega + (p^2/4)e^{2i\epsilon\theta}]^{\frac{1}{2}}} - \int_0^{\pi/2} \frac{d\omega}{[k^2 \cos^2 \omega + (p^2/4)e^{2i\epsilon\theta}]^{\frac{1}{2}}} \times \left[\frac{\cos \pi\lambda - \cos 2\lambda\omega}{2 \sin \pi\lambda}\right]. \tag{A8}$$

One can easily see that both terms in (A8) are uniformly small for $p > 0$, so that simple restrictions upon $g_\epsilon(p)$ will guarantee that the term $\Delta_{\epsilon 2}$ will make a negligible contribution to (A4) in the above large k limit.

The quantities $\Delta_{\epsilon 1}$, being the contribution to (A4) by integration over the term containing I_1, are, of course, not negligible in general for $\mathrm{Re}\ \lambda > 0$ because the Legendre function $Q_l(z)$ has highly nonuniform dependence upon its arguments as $l \to \infty$ and $z \to 1$.

APPENDIX B

Here we will calculate the "weak coupling" limit of the Fredholm determinant for the potential given in Eq. (3.2). Substitution of this form into the high

energy limiting form Eq. (3.1) yields the equation

$$1 + \Delta_l(\lambda_l k) = 1 + \frac{ig}{k}\left(\frac{-e^{-i\pi\lambda}}{2i \sin \pi\lambda}\right)\left\{Q_l\left(1 + \frac{\mu^2}{2k^2} e^{2i\theta}\right) + Q_l\left(1 + \frac{\mu^2}{2k^2} e^{-2i\theta}\right)\right\}. \quad \text{(B1)}$$

One can easily show that in scattering from nonsingular, energy-independent potentials, Regge trajectories either leave the right half λ plane at high energies or go to infinity there in such a way that $\text{Im}\,\lambda \to +\infty$. We are interested in the latter case, in which the factor $-e^{-i\pi\lambda}/2i \sin \pi\lambda$ approaches unity. In order to find the zeros of the expression (B1), we need some knowledge of the behavior of the Legendre function $Q_l(z)$ in the limit $l \to \infty$ and $z \to 1$. The Legendre function is in fact nonuniform in this limit, so that one must treat the limiting process carefully in searching for the zeros of (B1).

Let us represent the Legendre function by a standard expression:

$$Q_l(z) = \tfrac{1}{2}\int_{-\infty}^{\infty} d\varphi/[z + (z^2 - 1)^{\frac{1}{2}} \cosh \varphi]^{l+1}. \quad \text{(B2)}$$

One can carry out a stationary phase approximation to obtain an asymptotic limit valid for complex l and z. If one imposes the constraint z finite, $|l \cdot (z - 1)| \ll 1$, one obtains the asymptotic result

$$Q_l(z) \sim (\pi/2l)^{\frac{1}{2}}(z^2 - 1)^{-\frac{1}{4}}[z + (z^2 - 1)^{-\frac{1}{2}}]^{l+\frac{1}{2}}. \quad \text{(B3)}$$

Let us use (B3) to determine the asymptotic location of the zeros of (B1). It is convenient to express the angular momentum through its magnitude and phase:

$$l = l_0 e^{i\varphi}.$$

The Legendre functions in braces in (B1) may be replaced by their asymptotic forms, which, as $k \to \infty$, are

$$Q_l(1 + (\mu^2/2k^2)e^{\pm 2i\theta}) = (\pi k/2\mu l_0)^{\frac{1}{2}} e^{-i(\varphi \pm \theta/2)} \times e^{-(\mu l_0/k)[\cos(\theta \pm \varphi) + i \sin(\theta \pm \varphi)]}. \quad \text{(B4)}$$

We are interested in the regime of parameters $0 < \theta < \pi/2$ and $0 < \varphi < \pi$—the upper half l plane. In this regime it is clear that the factor $-\cos(\theta + \varphi)$ is larger than $-\cos(\theta - \varphi)$, so that the second Legendre function in (B1) may be dropped.

It is straightforward to insert (B3) in (B1) and determine the asymptotic zeros of (B1). One obtains the result that at large k the zeros of (B1) are expressed by the equations

$$l_0 = (-1/\cos(\theta + \varphi))(k \ln k/\mu)[1 + o(1)], \quad \text{(B5a)}$$

$$2\pi n = -\pi/2 - (\theta + \varphi)/2 - (\mu l_0/k) \sin(\theta + \varphi), \quad \text{(B5b)}$$

where n is an integer. Note that the factor $\cos(\theta + \varphi)$ must be negative, so that $\pi/2 - \theta < \varphi < 3\pi/2 - \theta$. One can also conclude from (B5) that the ratio l_0/k becomes infinite at large k.

One can parametrize each trajectory by the integer n. If one fixes attention upon a particular trajectory and considers the limit $k \to \infty$, one obtains its asymptote[15]

$$l \sim (k/\mu)e^{i(\pi-\theta)}[\ln k + \tfrac{1}{2} \ln \ln k + 2\pi i n + \ln(2/\pi)^{\frac{1}{2}}(1/g)]. \quad \text{(B6)}$$

On the other hand, if one fixes k at a large value and allows the trajectory number n to approach infinity, one obtains

$$l \sim (2\pi nk/\mu)e^{i(\pi/2-\theta)} - (k/2\mu)e^{-i\theta} \ln n. \quad \text{(B7)}$$

In summary, one can say that for $0 < \theta < \pi/2$ the solutions of (B1) asymptotically approach the line $\arg l = \pi - \theta$ in the second quadrant of the l plane, but that at any finite energy an infinite number of them lie near an angle $\arg l = \pi/2 - \theta$ in the first quadrant.

The special limiting case of the potential (3.2) for $V(r)$ is the simple Yukawa potential. It is informative to carry through the determination of the asymptotic zeros of (3.3) for this special case. One obtains an analogous result: There are an infinite number of trajectories which approach infinity at asymptotic energies. These trajectories individually approach the asymptotic curve

$$\begin{aligned} \text{Re}\, l &\simeq -k \ln k/\mu, \\ \text{Im}\, l &\simeq C(n)k, \end{aligned} \quad \text{(B8)}$$

where $C(n)$ is a constant depending upon the trajectory number but not on k. On the other hand, if one remains at large, fixed k and allows the trajectory number n to approach infinity, one obtains the asymptotic trajectory

$$\begin{aligned} \text{Re}\, l &\simeq -(k/2\mu) \ln n, \\ \text{Im}\, l &\simeq (2\pi/\mu)nk. \end{aligned} \quad \text{(B9)}$$

One can see therefore that at any large, though finite, energy there are an infinite number of Regge trajectories which lie asymptotically near an angle $\arg l = \pi/2$. It is a well known result in scattering from Yukawa potentials at sufficiently high energies that the scattering amplitude $S(\lambda, k)$ is analytic in λ and asymptotically equal to unity in the region of the complex angular momentum plane given by $\text{Re}\,\lambda > -n$, provided that one excludes a small sector about the negative real λ axis.[16] It has, however, *never* been shown that the scattering amplitude at high energies is analytic in the sector of the angular momentum plane

given by $|\arg \lambda| \leq \pi/2 + \epsilon$ for *any* number $\epsilon > 0$. The above "first-order" calculation with a simple Yukawa potential is in accord with the former result, and at the same time it implies that one cannot enlarge the sector of analyticity in the above way.

One can view the generalization (3.2) of the Yukawa potential as an analytic continuation such that the range of the potential becomes complex, while the potential itself remains a real analytic function of r. In this analytic continuation to $\theta \neq 0$ *some* zeros of the Jost function, which at $\theta = 0$ lie asymptotically near the line $\arg \lambda = \pi/2$ at high energies, move into the first quadrant of the λ plane to lie near the line $\arg \lambda = \pi/2 - \theta$ at large, though finite, energies. This "weak coupling" result is in qualitative agreement with the asymptotic form (1.1) obtained by Barut and Dilley.

APPENDIX C

Here we will study the second-order Fredholm term in the limit $k \to \infty$ while $\operatorname{Im} \lambda > 0$. One can explicitly calculate the kernel K_λ given by (2.7) to obtain

$$K_\lambda(r, r') = K_1 + K_2$$
$$= (\pi/2 \sin \pi\lambda)[J_\lambda(kr_<)J_{-\lambda}(kr_>) - e^{-i\pi\lambda}J_\lambda(kr)J_\lambda(kr')], \tag{C1}$$

where $r_<$ is the smaller of r and r' and $r_>$ is the larger. In this case one can write Δ_2 as follows:

$$\Delta_2 = \tfrac{1}{2}\int_0^\infty drrV(r)\int_0^\infty dr'r' \times V(r')[K_\lambda(r, r)K_\lambda(r', r') - K_\lambda(r, r')K_\lambda(r, r')]. \tag{C2}$$

The term Δ_2 may thus be expressed through (2.6) as the sum

$$\Delta_2 = A_+ + A_-,$$

where

$$A_\pm(\lambda, k) = (\pi^2/8 \sin^2 \pi\lambda)\int_0^\infty drrV(r) \times \int_0^\infty dr'r'V(r')H_\pm(r, r'), \tag{C3}$$

with

$$H_+(r, r') = J_\lambda(kr)J_{-\lambda}(kr)J_\lambda(kr')J_{-\lambda}(kr') - 2e^{-i\pi\lambda}J_\lambda^2(kr)J_\lambda(kr')J_{-\lambda}(kr') \tag{C4}$$

and

$$H_-(r, r') = [J_\lambda(kr_<)J_{-\lambda}(kr_>)]^2 - 2e^{-i\pi\lambda}J_\lambda(kr)J_\lambda(kr')[J_\lambda(kr_<)J_{-\lambda}(kr_>)]. \tag{C5}$$

It is crucial to note that the contributions to Δ_2 in (C2) involving four Bessel functions each of order λ identically vanish.

Notice also that one can calculate $A_+(\lambda, k)$ explicitly because the kernel H_+ is relatively simple. One can express the answer in terms of $\Delta_{\epsilon 1}$ and $\Delta_{\epsilon 2}$, which are defined in Eq. (A4). The result is

$$A_+(\lambda, k) = (\Delta_{+2} + \Delta_{-2})[(\Delta_{+1} + \Delta_{-1}) + \tfrac{1}{2}(\Delta_{+2} + \Delta_{-2})]. \tag{C6}$$

We have seen in Appendix A that Δ_{+2} and Δ_{-2} are asymptotically small at large k. The Regge poles obtained by solving Eq. (3.3) occur in a region in which $\Delta_{+1} + \Delta_{-1}$ is of order unity; therefore, in the vicinity of these poles the second-order term $A_+(\lambda, k)$ is small compared with unity.

The term $A_-(\lambda, k)$ is more difficult to handle than $A_+(\lambda, k)$ because the kernel H_- is more complicated than H_+. We have analyzed A_- for the case of the "generalized Yukawa potential" given in (3.2). In that case we have been able to show that $A_-(\lambda, k)$ is negligible in comparison to unity when $\Delta_{+1} + \Delta_{-1}$ is comparable to unity. The procedure for showing this involves a stationary phase integration of (C3). The dominant contribution comes from $r \sim r'$. The result follows from the fact that[17] $J_\lambda(x)J_{-\lambda}(x)/\sin \pi\lambda$, when analytically continued to λ away from the real axis with $|\lambda| \sim |x|$ large, is small in comparison with $J_\lambda(x) \cdot J_\lambda(x)$.

We have written the kernel K_λ in (C1) as the sum of K_1 and K_2, where K_2 is separable. Because of the separability of K_2, the contribution to Δ_2 of second order in K_2 vanishes identically.

In Eq. (2.6) we write $\Delta_n(\lambda, k)$, the contribution to the Fredholm determinant of nth order in the potential, as the integral over an nth-order determinant involving the K_λ. Since K_2 is a separable kernel, the contributions to Δ_n of second or higher order in K_2 vanish identically. Thus one can represent Δ_n by expressions which are generalizations of (C3). One expects in analogy to the above that it should be straightforward to show that $\sum_{n=3}^\infty \Delta_n(\lambda, k)$ is negligible for calculating the asymptotic Regge trajectories for the cases considered here.

[1] R. G. Newton, *The Complex J Plane* (Benjamin, New York, 1964), pp. 53ff. Actually, no trajectories can be in the fourth quadrant of the l plane for positive energy.

[2] A. O, Barut and J. Dilley, J. Math. Phys. **4**, 1401 (1963). See also J. Math. Phys. **7**, 64 (1966).

[3] For reference see R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), pp. 346ff.

[4] R. Santa and C. S. Shastry [Phys. Rev. **176**, 1254 (1968)] have interpolated Regge trajectories between compound nuclear resonances and compared the resultant cross sections with experiment in α nucleon scattering. Their Regge trajectories also rise.

[5] M. Froissart, J. Math. Phys. **3**, 922 (1962). Froissart obtains a domain of meromorphy in k under the restriction that $V(r)$ decreases

at least exponentially in r for r real, positive, and large. Since we are restricted to real k, it is not necessary for us to impose this large r behavior upon V.

[6] The upper limit of the integral may be replaced by any positive number.

[7] For example, if $V(r)$ is analytic in the domain $|r| < 1$, $u(\sigma)$ is analytic for finite σ except perhaps for simple poles at negative integers.

[8] $J_\lambda(x)$ is the Bessel function of real argument x and complex order λ. Our convention for this and other special functions is the same as that of the *Higher Transcendental Functions*, edited by A. Erdélyi *et al.* (McGraw-Hill, New York, 1953).

[9] Q_l is the Legendre function of the second kind.

[10] A program to calculate Regge trajectories has previously been constructed by Lovelace and Masson [Nuovo Cimento **26**, 472 (1962)]. This program requires less computation than ours. However, their method is applicable only if $rV(r)$ is an entire function of r. We have checked our numbers against theirs for a simple Yukawa potential.

[11] Since for complex λ the factor $r^{\lambda+\frac{1}{2}}$ has a rapidly changing phase at small r, it is desirable to factor out this phase in numerical integration of (4.1).

[12] This procedure is subject to numerical instabilities unless the potential $V(r)$ is of finite range. $H_\lambda^{(1)}$ is a Hankel function.

[13] The Wood–Saxon potential has trajectories which approach every negative integer except $l = -1$. See Bethe and Kinoshita, Phys. Rev. **128**, 1418 (1962).

[14] G. N. Watson, *Theory of Bessel Functions* (Cambridge U.P., Cambridge, 1966), p. 390.

[15] Note that (B3) is a valid asymptotic expression for $Q_l(z)$ in this domain.

[16] S. Mandelstam, Ann. Phys. **19**, 254 (1962).

[17] Another manifestation of this relation between $J_\lambda(x)$ and $J_{-\lambda}(x)$ is the fact that their Wronksian is $\sin \pi\lambda$ for all complex λ.

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Complex 2-Form Representation of the Einstein Equations: The Petrov Type III Solutions

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The geometric structure equations of a manifold satisfying the vacuum Einstein equations are expressed in terms of a complexification of the space of 2-forms adapted to the Petrov classification. The Petrov type III problem is invariantly reduced to the solution of one partial differential equation. Examples of solutions containing one arbitrary function are given, corresponding to spaces with groups of motions of dimensions 0, 1, and 2.

INTRODUCTION

This paper makes use of the techniques of a complex 2-form representation of the geometry of a Lorentz manifold, providing a natural formalism in which to analyze the Einstein equations.[1–3] An extensive introduction and survey of this approach may be found in a paper by Israel.[4] Here this formalism is used to obtain the complete reduction of the Petrov type III problem to the solution of one equation in one real function of three real independent variables, $r(x, y, u)$,

$$\nabla^2(e^{-r}\nabla^2 r) = 0, \tag{1}$$

where $\nabla^2 \equiv \partial^2/\partial x^2 + \partial^2/\partial y^2$. Given the most general solution to (1), the most general type III metric may be computed by algebraic quadratures. Further, different solutions for r that are not related to each other by a certain equivalence relationship (46) produce essentially different metrics, i.e., metrics that are not coordinate transforms of each other. The most general solution to (1) has not been explicitly obtained, but a class of solutions depending on one arbitrary function is stated, Eq. (48). Finally, the criterion for the metric to possess a symmetry group is given and particular solutions for r are stated corresponding to symmetry groups of dimensions 0, 1, 2, respectively. When applied to algebraically special metrics, as in this paper, this formalism is, of course, related to widely used techniques which express the metric in terms of the principal null directions.[5]

FORMALISM

The formalism involves the expression of the metric in terms of a Lorentz-orthonormal frame of 1-forms ω^a,

$$ds^2 = \eta_{ab}\omega^a\omega^b, \quad a, b = 0, \cdots, 3, \tag{2}$$

where $\eta_{ab} = \text{diag}\,(-1, +1, +1, +1)$. The geometric content of this metric is then expressed in the structure equations

$$d\omega^a = \omega^b \wedge \omega_b^a, \quad \omega_{ab} + \omega_{ba} = 0,$$
$$d\omega_b^a + \omega_c^a \wedge \omega_b^c = \tfrac{1}{2}R_{bcd}^a\omega^c \wedge \omega^d. \tag{3}$$

The first of these defines the connection forms ω_b^a, and the second gives the components of the Riemann

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$$d\omega_b^a + \omega_c^a \wedge \omega_b^c = \tfrac{1}{2}R_{bcd}^a\omega^c \wedge \omega^d. \tag{3}$$

The first of these defines the connection forms ω_b^a, and the second gives the components of the Riemann

curvature tensor. The expression of the metric (2) determines the frame ω^a only up to homogeneous Lorentz transformations; so in order to get a one-to-one correspondence between a geometry and the frame ω^a, it is necessary to find out just how strongly the geometry can be made to determine the ω^a. This is, of course, just the problem of determining the invariants of the geometry and can be shown to reduce to the problem of finding the algebraic invariants of the components of the curvature tensor and its covariant derivatives. Petrov solved this problem for the Riemann tensor itself for those geometries satisfying the Einstein empty space equations.[6,7]

In attacking this algebraic problem it soon becomes apparent that the most natural formalism to use is one involving a complexification of the space of 2-forms (antisymmetric tensors of rank two). It is apparent, then, that it might be helpful to express the entire structure equations in terms of these 2-forms. Thus, define the three complex forms e^i, $i = 1, 2, 3$, by

$$e^i = I\omega^0 \wedge \omega^i + \omega^j \wedge \omega^k, \quad i,j,k = \text{cyclic}, \qquad I^2 \equiv -1, \quad (4)$$

and their complex conjugates $\bar{e}^i$, noting that the ω^a are real. Lorentz transformations of the ω^a result in complex orthogonal transformations of the e^i, so that the e^i may be modified by such transformations without changing the metric (2). The connection forms may be translated in similar manner:

$$\Gamma^i_j = I\omega^k_0 + \omega^i_j. \quad (5)$$

The structure equations then become

$$de^i = -\Gamma^i_m \wedge e^m, \quad \Gamma^i_j + \Gamma^j_i = 0, \quad (6)$$

$$d\Gamma^i_j + \Gamma^i_m \wedge \Gamma^m_j = Q_{km}e^m + E_{km}\bar{e}^m. \quad (7)$$

Here Q_{km} and E_{km} are complex 3×3 matrices, with Q_{km} being linear combinations of the components of the Weyl tensor and the curvature scalar, and E_{km} of the Einstein tensor $R_{ab} - (\frac{1}{4})\eta_{ab}R$. Thus the Einstein equations $R_{ab} = 0$ become

$$E_{ij} = 0, \quad Q_{ii} = 0. \quad (8)$$

The Petrov problem is that of establishing a canonical form for Q_{ij} by means of complex-orthogonal transformations on the e^i. As is well known, there results a division into three discrete types. This paper will deal only with type III, which in this notation means

$$Q_{12} = Q_{21} = 1, \quad Q_{23} = Q_{32} = I, \qquad \text{other } Q_{ij} = 0, \quad E_{ij} = 0. \quad (9)$$

In this case there is no degeneracy so that the e^i are uniquely determined by the condition (9).

Thus we have the result that a metric described by the ω^a as in (2) and satisfying the Einstein equations for Petrov type III produces a complex basis e^i, which satisfy (6), (7), and (9). The converse question is now important since we wish to concentrate on solving these differential equations and then reconstruct the metric from the ω^a gotten from the inverse to (4). Clearly, if (4) is satisfied, then

$$e^i \wedge e^j = I\delta^{ij}\Omega, \quad e^i \wedge \bar{e}^j = 0, \quad (10)$$

where Ω is a nonzero real 4-form (volume element). On the other hand, it can be shown that if (10) is satisfied, then either e^i or Ie^i can be written in the form (4) with the ω^a real and independent 1-forms. Further, these are then determined up to the inversion, $\omega^a \to -\omega^a$. Thus, a set of complex 2-forms satisfying (6), (7), (9), and (10) is equivalent (up to the inversion) to the family of Petrov type III metrics. The fact that it may be necessary to replace e^i by Ie^i in determining the ω^a from e^i corresponds to the fact that the structure equations are invariant under $e^i \to Ce^i$, $Q_{ij} \to Q_{ij}/C$, where C is an arbitrary nonzero complex constant. The corresponding change in Q_{ij} is from a matrix of a given Petrov type to another of the same type but with relabeled symbols, and is thus of no significance. An equivalent statement is that the ω^a may be obtained from the e^i either from (4) or (11):

$$e^i = -\omega^0 \wedge \omega^i + I\omega^j \wedge \omega^k. \quad (11)$$

ANALYSIS OF TYPE III

Now we will use this formalism to analyze the type III problem. For convenience, define

$$X = \Gamma^2_3 + I\Gamma^1_2, \quad Y = (\Gamma^2_3 - I\Gamma^1_2)/2, \quad Z = I\Gamma^3_1,$$
$$f^1 = -e^3 + Ie^1, \quad f^3 = e^3 + Ie^1, \quad f^2 = e^2. \quad (12)$$

Equations (6), (7), and (9) become

$$dX + Z \wedge X = 0, \quad (13)$$

$$dY - Z \wedge Y = f^2, \quad (14)$$

$$dZ - X \wedge Y = f^1, \quad (15)$$

$$df^1 = -Z \wedge f^1 - X \wedge f^2, \quad (16)$$

$$df^2 = -(\tfrac{1}{2})X \wedge f^3 + Y \wedge f^1, \quad (17)$$

$$df^3 = Z \wedge f^3 + 2Y \wedge f^2. \quad (18)$$

The algebraic conditions (10) become

$$f^1 \wedge f^3 = -2f^2 \wedge f^2 = -2I\Omega, \quad \text{other zero}. \quad (19)$$

To these we add their integrability conditions

$$X \wedge f^1 = 0, \tag{20}$$

$$4Y \wedge f^1 - X \wedge f^3 - 2Z \wedge f^2 = 0, \tag{21}$$

$$Z \wedge f^1 + 2X \wedge f^2 = 0. \tag{22}$$

The relative simplicity of these equations indicates the usefulness of the approach, and similar equations may be obtained for the other Petrov types. The procedure for solving these equations is outlined in the Appendix. The result is that coordinates, $(z, \bar{z}, u, v)$, z complex and u, v, real, may be defined so that

$$f^1 = (e^k/v)\, dz \wedge du, \tag{23}$$

$$f^2 = (v^2 e^{-k}/2)\, dz \wedge dF + v(e^g - \dot{k})\, dz \wedge du + dv \wedge du, \tag{24}$$

$$\begin{aligned} f^3 = {} & 4v^3 e^{g-k}\, dg \wedge du - v^4 e^{-2k}\, dk \wedge dF \\ & + 2v^3 e^{-2k}\, dv \wedge dF + 2v^2 e^{g-k}\, dv \wedge du \\ & - 2\dot{k} v^2 e^{-k}\, dv \wedge du + v^2 e^{-k}\, dh \wedge dz \\ & - v^4 e^{g-2k}\, dz \wedge dF + v^3 e^{-k}(2\dot{k} e^g - 2\ddot{k} + F \\ & - 3e^{2g})\, dz \wedge du. \end{aligned} \tag{25}$$

Here k is a complex function of z and u, with $\dot{k} \equiv \partial k/\partial z$, and F and h are arbitrary complex functions. Finally, the imposition of the purely algebraic conditions of (19) results in the following equations, which, considering the apparent complexity of f^3 are surprisingly simple:

$$\frac{\partial F}{\partial v} = 0, \tag{26}$$

$$e^{-k}\frac{\partial F}{\partial \bar{z}} = \pm e^s, \quad r = \text{real}, \tag{27}$$

$$h = -v^2 e^{-k}\frac{\partial F}{\partial z}, \tag{28}$$

$$e^g = -\frac{v}{4}e^{-k}\frac{\partial F}{\partial u} + G, \tag{29}$$

$$G = \left(\frac{\partial^2 F}{\partial \bar{z}\partial z}\right) \Big/ 2\left(\frac{\partial F}{\partial \bar{z}}\right), \tag{30}$$

$$F + \frac{4\partial G}{\partial z} - 4G^2 + 4G\dot{k} - \dot{k}^2 - 2\ddot{k} = 0. \tag{31}$$

Finally, decomposing the complex coordinate z into the real x and y, $z = x + Iy$, and noting that

$$\frac{4\partial^2}{\partial \bar{z}\partial z} = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2},$$

we can see that Eqs. (26)–(31) are equivalent to the condition that r be a real function of x, y, u, which solves (1), and that F is related to it by

$$F = \left(\frac{\partial r}{\partial z}\right)^2 - 2\frac{\partial^2 r}{\partial z^2}. \tag{32}$$

Finally, in order to reconstruct the metric, it is necessary to decompose the complex 2-forms into the real 1-forms. In this case, (11) and (12) can be translated into more convenient form

$$\begin{aligned} & f^1 = \sigma^1 \wedge \sigma^3, \quad f^3 = \sigma^2 \wedge \bar{\sigma}^3, \\ & f^2 = \tfrac{1}{2}(\sigma^2 \wedge \sigma^1 + \bar{\sigma}^3 \wedge \sigma^3), \end{aligned} \tag{33}$$

where σ^1 and σ^2 are real null 1-forms and σ^3 is complex isotropic. Thus,

$$ds^2 = \sigma^1\sigma^2 + \sigma^3\bar{\sigma}^3. \tag{34}$$

For f^i as given in (23)–(32), the σ's must be of the form

$$\sigma^1 = b\, du, \quad b = \text{real}, \tag{35}$$

$$\sigma^2 = \alpha\, dz + \beta\, du + \gamma\, d\bar{z} + \delta\, dv, \tag{36}$$

$$\sigma^3 = A\, dz + B\, du, \tag{37}$$

where the coefficients are determined from the components of f^i by

$$A\bar{A} = 2f^2_{\bar{z}z}, \tag{38}$$

$$b = -f^1_{zu}/A = \bar{b}, \tag{39}$$

$$\delta = 2/b, \tag{40}$$

$$\alpha = f^3_{z\bar{z}}/\bar{A}, \tag{41}$$

$$B = \bar{f}^3_{\bar{z}u}/\bar{\alpha} \tag{42}$$

$$\gamma = -\bar{A}B/b, \tag{43}$$

$$\beta = f^3_{u\bar{z}}/A + \gamma\bar{B}. \tag{44}$$

The coordinates $(z, \bar{z}, u, v)$, used in the expression for the f^i, and thus the metric, are not unique but subject to the following transformations, leaving the form of the f^i invariant:

$$z \to \varphi(z), \quad u \to \psi(u) \tag{45}$$

$$r \to r(\varphi(z), \overline{\varphi(z)}, \psi(u))\dot{\psi}^2/\dot{\varphi}\bar{\dot{\varphi}}. \tag{46}$$

It is easy to check that (1) is invariant under this transformation. *Thus all Petrov type III metrics may be obtained by algebraic quadratures described in* (23)–(44) *from r's solving* (1). *Different r's not related by a transformation as in* (46) *then result in truly distinct metrics.*

Via the complex notation, it is easy to show that (1) is equivalent to

$$\frac{e^{-r}\partial^2 r}{\partial z \partial \bar{z}} = E(z, u) + \overline{E(z, u)}, \tag{47}$$

where $E(z, u)$ is an arbitrary (differentiable) complex function of z and u. The most general solution to (47) has not yet been explicitly obtained, but a particular solution may be written in terms of this arbitrary E as

$$r = -3 \ln (E + \bar{E}) + \ln \dot{E} + \ln \dot{\bar{E}} + \ln 3. \tag{48}$$

Thus (48) gives a class of solutions to (1) depending on one arbitrary function E.

MOTIONS: EXAMPLES OF SOLUTIONS

Since the type III curvature tensor is nondegenerate and uniquely determines the f^i, the only possible motions are essentially translations. If the Killing vector for a motion has components M^α, then the invariance of f^i under the group implies the vanishing of the Lie derivatives of these forms:

$$f^i_{\alpha\beta,\mu} M^\mu + f^i_{\mu\beta} M^\mu{}_{,\alpha} + f^i_{\alpha\mu} M^\mu{}_{,\beta} = 0. \tag{49}$$

These equations can then be shown to imply that the motion in this case must essentially be a translation:

$$\begin{aligned} &M^z = M^z(z), \quad M^{\bar{z}} = M^{\bar{z}}(\bar{z}), \\ &M^u = M^u(u), \quad M^v = vM^u{}_{,u}. \end{aligned} \tag{50}$$

Since the metric is fully determined by r and its derivatives, it can be shown that the remaining condition is the invariance of r (r is not a scalar) which becomes

$$r_{,z} M^z + r_{,\bar{z}} M^{\bar{z}} + r_{,u} M^u + \dot{M}^z + \dot{M}^{\bar{z}} - 2\dot{M}^u = 0. \tag{51}$$

Thus, as is known, the group must have dimension 0, 1, or 2.

In order to produce solutions with motions, use may be made of the coordinate freedom in z and u to require that the components M^α be constants, and (51) becomes

$$r_{,z} a + r_{,\bar{z}} \bar{a} + r_{,u} b = 0, \quad a, b = \text{const}, \quad b = \text{real}. \tag{52}$$

For example, if E which gives r from (48) is chosen to be ze^{cu}, with $c = \text{const} \neq 0$, then the only Killing vectors will be of the form

$$M^\alpha = (I, -I, 0, 0). \tag{53}$$

However, if $c = 0$, the group is two dimensional, generated by

$$M^\alpha = (I, -I, 0, 0) \quad \text{and} \quad M^\alpha = (0, 0, 1, 0). \tag{54}$$

On the other hand, in order to produce solutions having no motions, it is sufficient to choose E so that it is *not* of the form

$$E = E(\varphi(x) + \psi(u))\dot{\psi}^2 \dot{\varphi}, \tag{55}$$

for some complex function φ and real ψ. As an example, if

$$E = e^{zu}, \tag{56}$$

so that (55) is not satisfied and

$$r = -3 \ln (e^{zu} + e^{\bar{z}u}) + zu + \bar{z}u + 2 \ln u + \ln 3, \tag{57}$$

then the corresponding metric will permit no motions and will have no symmetry group.

APPENDIX

From (13) and (20), it is clear that

$$X = e^\alpha \, dz, \tag{A1}$$

$$Z = -d\alpha + e^g \, dz, \tag{A2}$$

$$f^1 = dz \wedge \omega, \tag{A3}$$

where z, α, and g are complex functions, ω is a 1-form not containing dz and z, $\bar{z}$ may be chosen as complex coordinates. Next, (15) gives

$$Y = -e^{g-\alpha} \, dg - e^{-\alpha}\omega + e^\mu \, dz, \tag{A4}$$

where μ is arbitrary. From the exterior derivative of (15), it follows that

$$dz \wedge (d\omega - (\tfrac{1}{2}) \, d\alpha \wedge \omega) = 0, \tag{A5}$$

from which it may be shown that the real coordinates u, v may be chosen so that

$$\omega = (e^k/v) \, du, \quad e^\alpha = e^k/v^2, \quad k = k(z, u). \tag{A6}$$

Next, (14) determines f^2:

$$f^2 = (\tfrac{1}{2})v^2 e^{-k} \, dz \wedge dF + ve^g \, dz \wedge du - v \, dk \wedge du + dv \wedge du, \tag{A7}$$

where

$$F \equiv e^{2g} - 2e^{\mu+\alpha}. \tag{A8}$$

Finally, Eqs. (17), (18), and (21) give f^3, as described in (25), with the introduction of the new function h.

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Relativistic Wave Equations: Proper Lorentz Invariance and Invariance under Discrete Transformations

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Considering the standard form $i\partial\psi/\partial t = H\psi$ [with ψ transforming according to $D(0, s) \oplus D(s, 0)$] of wave equations for free particles of arbitrary spin, we determined in a recent paper the admissible forms of H consistent with invariance of the equation under the Poincaré group and under T, C, and P. Here we show that even if T and C invariance is not imposed, the admissible Hamiltonians are the same (apart from one extra possibility $H = E$). Expressed differently, except for the trivial case $H = E$, invariance of free-particle equations under the connected Poincaré group and P implies T and C also.

1. INTRODUCTION

In a recent paper[1] we observed that the Schrödinger form

$$i\frac{\partial\psi}{\partial t} = H\psi \tag{1}$$

of the equation of motion for free relativistic particles of any given spin s and nonzero mass m is a standard form to which the familiar manifestly covariant equations[2] can be reduced, though (1) is not *manifestly* covariant. We emphasized that this reduced form is most convenient for analyzing the restrictions on the equation of motion imposed by the various invariance conditions, and then proceeded to determine the most general forms of H consistent with invariance of (1) under the connected Poincaré group and under T, C, and P. Here we show that only these same Hamiltonians are admissible (apart from the trivial one $H = E$) even if we drop the requirement of T and C invariance. The proof is on the same lines as in Ref. 1, though the starting point, the most general form of H permitted by translational, rotational and space-inversion invariance,[3] is more complicated than before:

$$H = \sum_\nu b_\nu B_\nu + \sum_\nu c_\nu C_\nu + \rho_1 \sum_\nu b'_\nu B_\nu + \rho_1 \sum_\nu c'_\nu C_\nu. \tag{2}$$

Here $B_\nu = \Lambda_\nu + \Lambda_{-\nu}$ and $C_\nu = \Lambda_\nu - \Lambda_{-\nu}$, where Λ_ν is the projection operator to the eigenvalue ν, $\nu = s, s-1, \cdots, -s$, of

$$\lambda_p \equiv \boldsymbol{\lambda}\cdot\mathbf{p}/p \equiv \rho_3\mathbf{S}\cdot\mathbf{p}/p,$$

$\mathbf{S}$ being the spin matrix. The summation in (2) is over nonnegative values of ν. Further, ρ_i, $i = 1, 2, 3$, are the Pauli matrices, and θ is defined by $\sinh\theta = p/m$ and $\cosh\theta = E/m$. (For further details of notation, Ref. 1 or Ref. 3 may be consulted.) It is known that if C and T invariance is required, then the coefficients b_ν and *either* the b'_ν *or* the c'_ν in (2) must vanish.[3] What we now show is that even without imposing such invariance, the same result follows from the requirement of boost invariance on (1), namely

$$[H, \mathbf{K}] = i\mathbf{P}, \tag{3}$$

where $\mathbf{K}$ and $\mathbf{P}$ are the boost and translation generators. The nonvanishing coefficients in (2) must then necessarily have the same values as determined in Ref. 1. In other words, Poincaré and P invariance implies also T and C invariance.[4]

2. DETERMINATION OF THE HAMILTONIAN

Since the approach to be employed closely follows that of Ref. 1, we shall not present any calculational details here. We shall merely quote the basic results we need, and outline the salient points of the proof.

The requirements which remain to be satisfied by the Hamiltonian (2) are the mass condition

$$H^2 = E^2 \equiv \mathbf{p}^2 + m^2, \tag{4}$$

and the boost-invariance condition (3). Equation (4) demands that either

$$b_\nu = 0, \quad c_\nu^2 + b_\nu'^2 - c_\nu'^2 = E^2 \quad \text{for all } \nu \tag{5}$$

or

$$b_\nu = E, \quad c_\nu = b'_\nu = c'_\nu = 0 \quad \text{for all } \nu. \tag{6}$$

The latter leads to the trivial Hamiltonian $H = E$, which will not be considered further. To determine the c_ν, b'_ν, c'_ν in the former case, Eq. (5), we employ the boost invariance condition (3), re-expressed in the form[1]

$$H\nabla_p H = [H, \boldsymbol{\lambda}] + \mathbf{p}. \tag{7}$$

To solve this equation following the procedure of Ref. 1, both sides of (7) are reduced to linear combinations of the linearly independent[6] quantities $C_\nu\boldsymbol{\lambda}$, $\rho_3 B_\nu(\boldsymbol{\lambda}\times\mathbf{p})$, $B_\nu\mathbf{p}$, $\rho_1 B_\nu\boldsymbol{\lambda}$, $\rho_2 C_\nu(\boldsymbol{\lambda}\times\mathbf{p})$, and $\rho_1 C_\nu\mathbf{p}$, whose coefficients on the two sides are then equated.

In the present case the resulting equations are

$$E^2 - c_\nu c_{\nu-1} - b'_\nu b'_{\nu-1} + c'_\nu c'_{\nu-1} = p(c_\nu - c_{\nu-1}), \quad (8a)$$

$$c_\nu b'_{\nu-1} - b'_\nu c_{\nu-1} = p(b'_\nu + b'_{\nu-1}), \quad (8b)$$

$$c_\nu c'_{\nu-1} - c'_\nu c_{\nu-1} = p(c'_\nu + c'_{\nu-1}), \quad (8c)$$

$$c'_\nu b'_{\nu-1} - b'_\nu c'_{\nu-1} = 0, \quad (8d)$$

$$b'_\nu \frac{dc_\nu}{dp} - c_\nu \frac{db'_\nu}{dp} = 2\nu b'_\nu, \quad (8e)$$

$$c'_\nu \frac{dc_\nu}{dp} - c_\nu \frac{dc'_\nu}{dp} = 2\nu c'_\nu, \quad (8f)$$

for all $\nu > \nu_0$, where $\nu_0 = \frac{1}{2}$ or 0 according as the spin is half-integral or integral. The solution of these coupled equations is fairly straightforward. Multiplying (8b) by $(c_\nu - p)$ and (8c) by c'_ν and subtracting, we get

$$(c_\nu - p)(b'_\nu b'_{\nu-1} - c'_\nu c'_{\nu-1}) = (c_{\nu-1} + p)(E^2 - c_\nu^2), \quad (9)$$

where Eqs. (8b) and (5) have been used to simplify the right-hand side. Next, multiplying (8a) by $(c_\nu - p)$ and then introducing (9), we find after some algebra that

$$\frac{c_\nu}{E} = \frac{(c_{\nu-1}/E) + \tanh 2\theta}{1 + (c_{\nu-1}/E)\tanh 2\theta}, \quad (10)$$

with θ as defined below Eq. (2). From (10) it follows that either

$$c_\nu = E \tanh 2\nu\theta \quad (11a)$$

or

$$c_\nu = E \coth 2\nu\theta, \quad \nu = s, s-1, \cdots, \nu_0. \quad (11b)$$

At this point we have to consider the equations for $\nu = \nu_0$. Taking for instance the half-integral spin case ($\nu_0 = \frac{1}{2}$), we observe that the relevant equations are obtained from Eqs. (8) by merely interpreting the symbols $c_{-\frac{1}{2}}$, $c'_{-\frac{1}{2}}$, and $b'_{-\frac{1}{2}}$ as $-c_{\frac{1}{2}}$, $-c'_{\frac{1}{2}}$, and $b'_{\frac{1}{2}}$, respectively, as explained in Ref. 1. Equation (8a) then becomes

$$(c_{\frac{1}{2}})^2 - (b'_{\frac{1}{2}})^2 - (c'_{\frac{1}{2}})^2 = 2pc_{\frac{1}{2}} - E^2, \quad (12)$$

which, together with (5), shows that

$$b'_{\frac{1}{2}} = E \operatorname{sech} \theta \quad \text{and} \quad c'_{\frac{1}{2}} = 0, \quad (13a)$$

if (11a) is adopted for c_ν, and

$$b'_{\frac{1}{2}} = 0 \quad \text{and} \quad c'_{\frac{1}{2}} = E \operatorname{csch} \theta, \quad (13b)$$

if the alternative possibility (11b) is taken for c_ν. It is easily seen from Eqs. (8) that if a b' (or c') is zero for one value of ν, then all the b' (or all the c') are zero. Thus we find that there are only two possible solutions, leading to the alternative expressions

$$H = E \sum_\nu \tanh 2\nu\theta C_\nu + E\rho_1 \sum_\nu \operatorname{sech} 2\nu\theta B_\nu \quad (14a)$$

or

$$H = E \sum_\nu \coth 2\nu\theta C_\nu + E\rho_1 \sum_\nu \operatorname{csch} 2\nu\theta C_\nu \quad (14b)$$

for the Hamiltonian. A similar calculation for the integer spin case shows that again there are only two solutions for H and they are identical with (14).

3. DISCUSSION

A word of explanation may be in order as to why P invariance was imposed rather than T or C. The reason is simply that the form (2) of the Hamiltonian to which the consideration of Ref. 1 could be directly applied would not be the most general one if P were violated.

As already noted, the solutions (14) coincide with those obtained in Ref. 1, where the *additional* condition of T and C invariance was invoked. This provides a demonstration of the power of the boost invariance requirement which extends so far as to imply even some invariance properties under discrete transformations. No explicit and general demonstration of this kind seems to have been given before, though one would perhaps suspect some such thing from the well-known particular cases like the Dirac equation where T, C, and P invariance holds without being demanded in the first place. On the other hand, it may well be that in such examples this property is a consequence not so much of Lorentz invariance *per se* but rather of the extra constraints on the form of the equation, especially that of *manifest* covariance. In fact, it is known that such constraints (which may be desirable but not essential) on the *form* of the wave equation can bring in invariance properties which were not explicitly demanded. A discussion of this point may be found in a recent paper by one of us.[5] By not demanding manifest covariance, locality, etc., in our work we have tried to minimize such unintended side effects. Incidentally, it appears from further investigations by two of us (P. M. M. and M. S.) that invariance under the Poincaré group and the combined operation TCP quite generally implies separate T, C, P invariance in the case of free field equations. Though the treatment is similar in spirit to the present one, differences in the general form of the Hamiltonian, referred to earlier in this section, make the details quite different, and the work will therefore be reported separately.

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[4] The one exception to this statement, as already indicated, is $H = E$ which violates C but not T invariance (and hence violates TCP). It may be noted, incidentially, that since the wavefunctions that we use transform according to the (reducible) self-conjugate representation $D(0, s) \oplus D(s, 0)$ of the homogeneous Lorentz group, the operations C, T, P can all be defined on them, though the wave *equation* may not be invariant. Certain aspects of the invariance of linear wave equations under discrete transformations are discussed in Ref. 5.
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Lattice Green's Functions for the Rectangular and the Square Lattices at Arbitrary Points

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The lattice Green's functions of the rectangular and the square lattices

$$I_{\rm rect}(a; m, n; \alpha, \beta) \equiv \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos mx \cos ny\, dx\, dy}{a - i\epsilon - \alpha\cos x - \beta\cos y},$$

$$I_{\rm sq}(a; m, n) \equiv I_{\rm rect}(a; m, n; 1, 1)$$

are considered. The integral $I_{\rm rect}(a, m, n; \alpha, \beta)$ for $a > \alpha + \beta$ is evaluated and expressed in terms of the generalized hypergeometric function F_4. Expressions of $I_{\rm sq}(a; m, n)$ for $a > 2$, $a < 2$, and $a \sim 2$, and $I_{\rm rect}(a; m, m; \alpha, \beta)$ in terms of ${}_pF_{p-1}$ are presented by the method of the analytic continuation using the Mellin–Barnes type integral. They are useful for the understanding of the nature of the singularity and for numerical calculation. The behaviors of $I_{\rm sq}(a; m, n)$ are shown in figures.

1. INTRODUCTION

We consider the lattice Green's functions for the rectangular lattice

$$I_{\rm rect}(a; m, n; \alpha, \beta) = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos mx \cos ny\, dx\, dy}{a - i\epsilon - \alpha\cos x - \beta\cos y} \quad (1.1)$$

and for the square lattice

$$I_{\rm sq}(a; m, n) \equiv I_{\rm rect}(a; m, n; 1, 1) \quad (1.2)$$

at an arbitrary lattice point (m, n). In the function (1.1) α and β are force constants in the x and y directions in the rectangular lattice. The real part of $I_{\rm rect}(a; m, n; \alpha, \beta)$ is an odd or even function of a and the imaginary part is an even or odd function of a, according as $m + n$ is even or odd. We assume $0 \le \beta \le \alpha$ and $0 \le a$ without loss of generality. Though $\mathrm{Im}\, I_{\rm rect}(a < \alpha + \beta; 0, 0; \alpha, \beta)$ have been obtained by Montroll,[1] general calculations for an arbitrary m, n, α, and β are not found.[2] In this paper $I_{\rm rect}(a; m, n; \alpha, \beta)$ is calculated in terms of F_4, and $I_{\rm sq}(a; m, n)$ for $a > 2$, $a < 2$, and $a \sim 2$ is studied by the method of the analytic continuation[3,4] using the Mellin–Barnes type integral.

It is to be noted that Eq. (1.1) can be regarded as a two-body lattice Green's function[5] for the isotropic square lattice, where $\alpha = \cos K_x/2$, $\beta = \cos K_y/2$ (K_x and K_y are the x and y components of the total momentum of the two-body system).

2. $I_{\rm rect}(a; m, n; \alpha, \beta)$

Equation (1.1) is transformed into

$$I_{\rm rect}(a > \alpha + \beta; m, n; \alpha, \beta) = i^{m+n+1}\int_0^\infty e^{-i(a - i\epsilon)t} J_m(\alpha t) J_n(\beta t)\, dt \quad (2.1)$$

$$= i^{m+n+1}(\tfrac{1}{2}\pi a)^{\frac{1}{2}}\int_0^\infty t^{\frac{1}{2}} J_m(\alpha t) J_n(\beta t) \times [J_{-\frac{1}{2}}(at) - iJ_{\frac{1}{2}}(at)]\, dt. \quad (2.2)$$

They can be expressed in terms of Appell's double

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[1] M. Seetharaman, J. Jayaraman, and P. M. Mathews, J. Math. Phys. **12**, 835 (1971).
[2] The Dirac, Fierz–Pauli, Rarita–Schwinger, Bargman–Wigner, and other forms discussed, for example, in E. M. Corson, *Introduction to Tensors, Spinors and Relativistic Wave Equations* (Hafner, New York, 1953).
[3] P. M. Mathews, Phys. Rev. **143**, 978 (1966).
[4] The one exception to this statement, as already indicated, is $H = E$ which violates C but not T invariance (and hence violates TCP). It may be noted, incidentially, that since the wavefunctions that we use transform according to the (reducible) self-conjugate representation $D(0, s) \oplus D(s, 0)$ of the homogeneous Lorentz group, the operations C, T, P can all be defined on them, though the wave *equation* may not be invariant. Certain aspects of the invariance of linear wave equations under discrete transformations are discussed in Ref. 5.
[5] P. M. Mathews, J. Math. Phys. **11**, 1360 (1970).
[6] See Ref. 1, Appendix B.

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Lattice Green's Functions for the Rectangular and the Square Lattices at Arbitrary Points

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The lattice Green's functions of the rectangular and the square lattices

$$I_{\rm rect}(a; m, n; \alpha, \beta) \equiv \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos mx \cos ny\, dx\, dy}{a - i\epsilon - \alpha\cos x - \beta\cos y},$$

$$I_{\rm sq}(a; m, n) \equiv I_{\rm rect}(a; m, n; 1, 1)$$

are considered. The integral $I_{\rm rect}(a, m, n; \alpha, \beta)$ for $a > \alpha + \beta$ is evaluated and expressed in terms of the generalized hypergeometric function F_4. Expressions of $I_{\rm sq}(a; m, n)$ for $a > 2$, $a < 2$, and $a \sim 2$, and $I_{\rm rect}(a; m, m; \alpha, \beta)$ in terms of ${}_pF_{p-1}$ are presented by the method of the analytic continuation using the Mellin–Barnes type integral. They are useful for the understanding of the nature of the singularity and for numerical calculation. The behaviors of $I_{\rm sq}(a; m, n)$ are shown in figures.

1. INTRODUCTION

We consider the lattice Green's functions for the rectangular lattice

$$I_{\rm rect}(a; m, n; \alpha, \beta) = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \frac{\cos mx \cos ny\, dx\, dy}{a - i\epsilon - \alpha\cos x - \beta\cos y} \quad (1.1)$$

and for the square lattice

$$I_{\rm sq}(a; m, n) \equiv I_{\rm rect}(a; m, n; 1, 1) \quad (1.2)$$

at an arbitrary lattice point (m, n). In the function (1.1) α and β are force constants in the x and y directions in the rectangular lattice. The real part of $I_{\rm rect}(a; m, n; \alpha, \beta)$ is an odd or even function of a and the imaginary part is an even or odd function of a, according as $m + n$ is even or odd. We assume $0 \le \beta \le \alpha$ and $0 \le a$ without loss of generality. Though $\mathrm{Im}\, I_{\rm rect}(a < \alpha + \beta; 0, 0; \alpha, \beta)$ have been obtained by Montroll,[1] general calculations for an arbitrary m, n, α, and β are not found.[2] In this paper $I_{\rm rect}(a; m, n; \alpha, \beta)$ is calculated in terms of F_4, and $I_{\rm sq}(a; m, n)$ for $a > 2$, $a < 2$, and $a \sim 2$ is studied by the method of the analytic continuation[3,4] using the Mellin–Barnes type integral.

It is to be noted that Eq. (1.1) can be regarded as a two-body lattice Green's function[5] for the isotropic square lattice, where $\alpha = \cos K_x/2$, $\beta = \cos K_y/2$ (K_x and K_y are the x and y components of the total momentum of the two-body system).

2. $I_{\rm rect}(a; m, n; \alpha, \beta)$

Equation (1.1) is transformed into

$$I_{\rm rect}(a > \alpha + \beta; m, n; \alpha, \beta) = i^{m+n+1}\int_0^\infty e^{-i(a - i\epsilon)t} J_m(\alpha t) J_n(\beta t)\, dt \quad (2.1)$$

$$= i^{m+n+1}(\tfrac{1}{2}\pi a)^{\frac{1}{2}}\int_0^\infty t^{\frac{1}{2}} J_m(\alpha t) J_n(\beta t) \times [J_{-\frac{1}{2}}(at) - iJ_{\frac{1}{2}}(at)]\, dt. \quad (2.2)$$

They can be expressed in terms of Appell's double

hypergeometric function F_4:

$$(2.2) = \frac{1}{2^{m+n}} \frac{(m+n)!}{m!\,n!} \frac{1}{a}\left(\frac{\alpha}{a}\right)^m \left(\frac{\beta}{a}\right)^n F_4\left[\tfrac{1}{2}(m+n+1),\ \tfrac{1}{2}(m+n)+1; m+1; n+1; \left(\frac{\alpha}{a}\right)^2, \left(\frac{\beta}{a}\right)^2\right]. \quad (2.3)$$

Equation (2.3) is convergent for $a > \alpha + \beta$. Here we used the formula[6]

$$\int_0^\infty t^{\lambda-1} J_\mu(at) J_\nu(bt) J_\rho(ct)\, dt = \frac{2^{\lambda-1} a^\mu b^\nu}{c^{\lambda+\mu+\nu}} \times \frac{\Gamma[\frac{1}{2}(\lambda+\mu+\nu+\rho)]}{\Gamma(\mu+1)\Gamma(\nu+1)\Gamma[1-\frac{1}{2}(\lambda+\mu+\nu-\rho)]} \times F_4\left(\tfrac{1}{2}(\lambda+\mu+\nu-\rho), \tfrac{1}{2}(\lambda+\mu+\nu+\rho); \mu+1, \nu+1; \frac{a^2}{c^2}, \frac{b^2}{c^2}\right), \quad (2.4)$$

where

$$\mathrm{Re}\,(\lambda+\mu+\nu+\rho) > 0, \quad \mathrm{Re}\,(\lambda) < \tfrac{5}{2}, \quad c > a+b, \quad a, b, c > 0.$$

3. $I_{sq}(a > 2; m, n)$

In the case of equal arguments the function F_4 is reduced to ${}_4F_3$:

$$F_4(\alpha, \beta; \gamma, \gamma'; z, z) = {}_4F_3\left[\begin{matrix}\alpha, \beta, \frac{1}{2}(\gamma+\gamma')-\frac{1}{2}, \frac{1}{2}(\gamma+\gamma'); \\ \gamma, \gamma', \gamma+\gamma'-1\end{matrix} 4z\right]. \quad (3.1)$$

Though the formula is not found in the literature, we omit the proof which can be given straightforwardly. Hence $I_{sq}(a > 2; m, n)$ can be expressed in terms of ${}_4F_3$:

$$I_{sq}(a > 2; m, n) = \frac{1}{2^{m+n}} \frac{1}{a^{m+n+1}} \frac{(m+n)!}{m!\,n!} {}_4F_3\left[\begin{matrix}\frac{1}{2}(m+n+1), \frac{1}{2}(m+n+1), \frac{1}{2}(m+n)+1, \frac{1}{2}(m+n)+1; \\ m+1, n+1, m+n+1\end{matrix} (2/a)^2\right]. \quad (3.2)$$

Equation (3.2) is simplified in the following cases:

$$I_{sq}(a > 2; m, m) = \frac{(2m)!}{2^{2m} a^{2m+1} (m!)^2} \times {}_2F_1\left(m+\tfrac{1}{2}, m+\tfrac{1}{2}; 2m+1; \left(\frac{2}{a}\right)^2\right), \quad (3.3)$$

$$I_{sq}(a > 2; m, m-1) = \frac{(2m-1)!}{2^{2m-1} a^{2m} m!\,(m-1)!} \times {}_3F_2\left[\begin{matrix}m, m+\frac{1}{2}, m+\frac{1}{2}; \\ m+1, 2m\end{matrix} (2/a)^2\right]. \quad (3.4)$$

For $a > 2$, Eqs. (3.2)–(3.4) can be used directly for the numerical calculation. The analytic continuation to the regions $a \sim 0$ and $a \sim 2$ will be given in next sections.

When we use the functional relation[7,2]

$$\alpha I_{rect}(a; m+1, n; \alpha, \beta) + \alpha I_{rect}(a; m-1, n; \alpha, \beta) + \beta I_{rect}(a; m, n+1; \alpha, \beta) + \beta I_{rect}(a; m, n-1; \alpha, \beta) - 2a I_{rect}(a; m, n; \alpha, \beta) = -2\delta_{m0}\delta_{n0} \quad (3.5)$$

and

$$I_{sq}(a; m, n) = I_{sq}(a; n, m), \quad (3.6)$$

$$I_{rect}(a; m, n; \alpha, \beta) = I_{rect}(a; m, -n; \alpha, \beta), \quad I_{rect}(a; m, n; \alpha, \beta) = I_{rect}(a; -m, n; \alpha, \beta), \quad (3.7)$$

all $I_{sq}(a; m, n)$ can be obtained from $I_{sq}(a; m, m)$ successively. That is,

$$I_{10} = \frac{a}{2} I_{00} - \tfrac{1}{2}, \quad (3.8a)$$

$$I_{n+1,n} = a I_{nn} - I_{n,n-1}, \quad n = 1, 2, \cdots, \quad (3.8b)$$

$$I_{p0} = 2a I_{p-1,0} - I_{p-2,0} - 2I_{p-1,1}, \quad p = 2, 3, \cdots, \quad (3.8c)$$

$$I_{n+p,n} = 2a I_{n+p-1,n} - I_{n+p-2,n} - I_{n+p-1,n+1} - I_{n+p-1,n-1}, \quad n = 1, 2, \cdots. \quad (3.8d)$$

Since Eq. (3.6) does not hold for the rectangular lattice, all $I_{rect}(a; m, n; \alpha, \beta)$ cannot be obtained only from the diagonal element $I_{rect}(a; m, m; \alpha, \beta)$. Morita[8] pointed out that all $I_{rect}(a; m, n; \alpha, \beta)$ can be obtained from the element on the axis $I_{rect}(a; m, 0; \alpha, \beta)$ and the relations (3.5) and (3.6) and that $I_{rect}(a; m, 0; \alpha, \beta)$ can, in principle, be expressed as a linear combination of elliptic integrals.

4. $I_{sq}(a < 2; m, n)$

For $0 < a < 2$, the analytic continuation of ${}_4F_3$ gives the useful expansion. Transforming the generalized hypergeometric function in Eq. (3.2) into a Mellin–Barnes integral,[9] we have

$$I_{sq}(a; m, n) = \frac{1}{2\pi}\left(\frac{2}{a}\right)^{m+n+1} \frac{1}{2\pi i} \int_{-\epsilon-i\infty}^{-\epsilon+i\infty} ds \frac{\Gamma(-s)\{\Gamma[\frac{1}{2}(m+n+1)+s]\}^2 \{\Gamma[\frac{1}{2}(m+n)+1+s]\}^2 (-4/a^2)^s}{\Gamma(m+n+1+s)\Gamma(m+1+s)\Gamma(n+1+s)}, \quad (4.1)$$

where ϵ is a small positive number. Now the integration is carried out by collecting the contribution from the poles in the left half s plane. We assume $m \geq n$ without loss of generality.

When $m + n$ is even, double poles appear at an infinite number of negative half-odd-integer sites,

$$s = -\tfrac{1}{2}(m + n + 1) - p, \quad p = 0, 1, 2, \cdots,$$

and simple poles appear at finite number of integer sites

$$s = -\tfrac{1}{2}(m + n) - 1 - p,$$
$$p = 0, 1, 2, \cdots, \tfrac{1}{2}(m - n) - 1.$$

Then the sum of these residues leads to

$$\begin{aligned} &I_{sq}(a < 2; m, n) \\ &= \frac{i}{2\pi^2} \sum_{p=0}^{\infty} \frac{\Gamma[\frac{1}{2} + p + \frac{1}{2}(m+n)]\Gamma[\frac{1}{2} + p - \frac{1}{2}(m+n)]\Gamma[\frac{1}{2} + p + \frac{1}{2}(m-n)]\Gamma[\frac{1}{2} - p + \frac{1}{2}(m-n)]}{(p!)^2[\Gamma(\frac{1}{2} + p)]^2} \left(\frac{a}{2}\right)^{2p} \\ &\quad \times \{2\psi(1+p) + 2\psi(\tfrac{1}{2} + p) - \psi[\tfrac{1}{2} + p + \tfrac{1}{2}(m+n)] - \psi[\tfrac{1}{2} + p - \tfrac{1}{2}(m+n)] \\ &\quad - \psi[\tfrac{1}{2} + p + \tfrac{1}{2}(m-n)] - \psi[\tfrac{1}{2} + p - \tfrac{1}{2}(m-n)] - i\pi - 2\log \tfrac{1}{2}a\} \\ &\quad + (-1)^{m+1}\tfrac{1}{2}\pi \sum_{p=0}^{\frac{1}{2}(m-n)-1} \frac{\Gamma[\frac{1}{2}(m+n) + 1 + p]\Gamma(\frac{1}{2}(m-n) + 1 + p)(\frac{1}{2}a)^{2p+1}}{(p!)^2[\Gamma(\frac{3}{2} + p)]^2\Gamma[\frac{1}{2}(m+n) - p]\Gamma[\frac{1}{2}(m-n) - p]} \end{aligned} \tag{4.2}$$

for $m + n$ even.

When $m + n$ is odd, double poles appear at an infinite number of negative half-odd integer sites,

$$s = -\tfrac{1}{2}(m + n) - 1 - p, \quad p = 0, 1, 2, \cdots,$$

and simple poles appear at finite number of negative integer sites,

$$s = -\tfrac{1}{2}(m + n + 1) - p, \qquad p = 0, 1, 2, \cdots, \tfrac{1}{2}(m - n - 1).$$

Collecting the contribution from these poles, we obtain

$$\begin{aligned} &I_{sq}(a < 2; m, n) \\ &= \frac{i}{2\pi^2} \sum_{p=0}^{\infty} \frac{\Gamma[p + 1 + \frac{1}{2}(m+n)]\Gamma[p + 1 - \frac{1}{2}(m+n)]\Gamma[p + 1 + \frac{1}{2}(m-n)]\Gamma[p + 1 - \frac{1}{2}(m-n)]}{(p!)^2[\Gamma(\frac{3}{2} + p)]^2} (\tfrac{1}{2}a)^{2p+1} \\ &\quad \times \{2\psi(p+1) + 2\psi(\tfrac{3}{2} + p) - \psi[p + 1 + \tfrac{1}{2}(m+n)] - \psi[p + 1 - \tfrac{1}{2}(m+n)] \\ &\quad - \psi[p + 1 + \tfrac{1}{2}(m-n)] - \psi[p + 1 - \tfrac{1}{2}(m-n)] - i\pi - 2\log \tfrac{1}{2}a\} \\ &\quad + (-)^m \tfrac{1}{2}\pi \sum_{p=0}^{\frac{1}{2}(m-n-1)} \frac{\Gamma[\frac{1}{2}(m+n+1) + p]\Gamma[\frac{1}{2}(m-n+1) + p]}{(p!)^2[\Gamma(\frac{1}{2} + p)]^2\Gamma[\frac{1}{2}(m+n+1) - p]\Gamma[\frac{1}{2}(m-n+1) - p]} (\tfrac{1}{2}a)^{2p} \end{aligned} \tag{4.3}$$

for $m + n$ odd.

In treating the case $-2 < a < 2$, the expression $-i\pi - 2\log \frac{1}{2}a$ in Eqs. (4.2) and (4.3) is replaced by $-i\pi \operatorname{sgn}(a) - 2\log|\frac{1}{2}a|$.

Now we define the function ${}_p\tilde{F}_{p-1}(a_1, a_2, \cdots, a_p; b_1, b_2, \cdots, b_{p-1}; z)$ for nonintegral values of a_i and b_i and real value of z:

$$\begin{aligned} {}_p\tilde{F}_{p-1}\left[\begin{matrix} a_1, a_2, \cdots, a_p; \\ b_1, b_2, \cdots, b_{p-1} \end{matrix} z\right] &= \frac{1}{\pi} \sum_{r=}^{\infty} \frac{(a_1)_r(a_2)_r \cdots (a_p)_r}{r!\,(b_1)_r(b_2)_r \cdots (b_{p-1})_r} z^r \\ &\quad \times [\psi(1+r) + \psi(b_1 + r) + \cdots + \psi(b_{p-1} + r) - \psi(a_1 + r) - \psi(a_2 + r) - \cdots - \psi(a_p + r) - \log|z|]. \end{aligned} \tag{4.4}$$

One of the useful formulas in terms of ${}_p\tilde{F}_{p-1}$ is

$${}_2F_1(a, b; a + b; z) = [\pi\Gamma(a + b)/\Gamma(a)\Gamma(b)]\, {}_2\tilde{F}_1(a, b; 1; 1 - z) \tag{4.5}$$

for half-integral values of a_i and b_i, and for real positive value of z such that $0 \leq z \leq 1$.

The real part and the imaginary part of $I_{sq}(a; m, n)$ are expressed in terms of ${}_4F_3$ and ${}_4\tilde{F}_3$ functions:

$$\begin{aligned}\operatorname{Re} I_{sq}(a; m,n) &= \frac{(-)^m}{2}\,{}_4F_3\left[\begin{matrix}\frac{1}{2}+\frac{1}{2}(m+n), \frac{1}{2}+\frac{1}{2}(m+n), \frac{1}{2}+\frac{1}{2}(m-n), \frac{1}{2}-\frac{1}{2}(m-n); (\frac{1}{2}a)^2 \\ 1, \frac{1}{2}, \frac{1}{2}\end{matrix}\right] + \tfrac{1}{2}[(-)^{m+1}(m^2-n^2)]\tfrac{1}{2}a \\ &\quad \times {}_4F_3\left[\begin{matrix}1+\frac{1}{2}(m+n), 1-\frac{1}{2}(m-n), 1-\frac{1}{2}(m+n), 1-\frac{1}{2}(m-n); (\frac{1}{2}a)^2 \\ 1, \frac{3}{2}, \frac{3}{2}\end{matrix}\right], \qquad (4.6a)\end{aligned}$$

$$\operatorname{Im} I_{sq}(a; m, n) = \tfrac{1}{2}(-)^m\,{}_4\tilde{F}_3\left[\begin{matrix}\frac{1}{2}+\frac{1}{2}(m+n), \frac{1}{2}-\frac{1}{2}(m+n), \frac{1}{2}+\frac{1}{2}(m-n), \frac{1}{2}-\frac{1}{2}(m-n); (\frac{1}{2}a)^2 \\ 1, \frac{1}{2}, \frac{1}{2}\end{matrix}\right] \qquad (4.6b)$$

for even $m + n$, and

$$\begin{aligned}\operatorname{Re} I_{sp}(a; m, n) &= \tfrac{1}{2}[(-)^{m+1}(m^2-n^2)]\tfrac{1}{2}a\,{}_4F_3\left[\begin{matrix}1+\frac{1}{2}(m+n), 1-\frac{1}{2}(m+n), 1+\frac{1}{2}(m-n), 1-\frac{1}{2}(m-n); (\frac{1}{2}a)^2 \\ 1, \frac{3}{2}, \frac{3}{2}\end{matrix}\right] \\ &\quad + \tfrac{1}{2}(-)^m\,{}_4F_3\left[\begin{matrix}\frac{1}{2}(m+n+1), \frac{1}{2}(m-n+1), \frac{1}{2}(1-m-n), \frac{1}{2}(1-m+n); (\frac{1}{2}a)^2 \\ 1, \frac{1}{2}, \frac{1}{2}\end{matrix}\right], \qquad (4.7a)\end{aligned}$$

$$\operatorname{Im} I_{sq}(a; m, n) = \tfrac{1}{2}[(-)^{m+1}(m^2-n^2)]\tfrac{1}{2}a\,{}_4\tilde{F}_3\left[\begin{matrix}1+\frac{1}{2}(m+n), 1-\frac{1}{2}(m+n), 1+\frac{1}{2}(m+n), 1-\frac{1}{2}(m-n); (\frac{1}{2}a)^2 \\ 1, \frac{3}{2}, \frac{3}{2}\end{matrix}\right]$$

for odd $m + n$. (4.7b)

For $n = m - 1$ and $n = m$, ${}_4F_3$, and ${}_4\tilde{F}_3$ are reduced to ${}_3F_2$ and ${}_2F_1$, respectively. In particular

$$\operatorname{Re} I_{sq}(a; m, m) = \tfrac{1}{2}(-)^m\,{}_2F_1(\tfrac{1}{2}+m, \tfrac{1}{2}-m; 1; (\tfrac{1}{2}a)^2), \qquad (4.8a)$$

$$\operatorname{Im} I_{sq}(a; m, m) = \tfrac{1}{2}(-)^m\,{}_2\tilde{F}_1(\tfrac{1}{2}+m, \tfrac{1}{2}-m; 1; (\tfrac{1}{2}a)^2). \qquad (4.8b)$$

Equation (4.8) can also be obtained directly from Eq. (3.3).

We can obtain the expression of $I_{rect}(a < |\alpha - \beta|; m, n; \alpha, \beta)$ in terms of F_4 from Eq. (2.3). The real part of $I_{rect}(a < |\alpha - \beta|; m, n; \alpha, \beta)$ is proved to vanish irrespective of the parity of $m + n$.

5. $I_{sq}(a \sim 2; m, n)$

Now a generalized hypergeometric function ${}_nF_{n-1}$ is expanded in terms of a hypergeometric function of a lower order[10] ${}_{n-1}F_{n-2}$:

$$\begin{aligned}{}_nF_{n-1}\left[\begin{matrix}a_1, a_2, \cdots, a_n \\ b_1, b_2, \cdots, b_{n-1}\end{matrix}\; z\right] &= \frac{\Gamma(b_{n-1})\Gamma(b_{n-2})}{\Gamma(a_n)\Gamma(b_{n-1}+b_{n-2}-a_n)} \\ &\quad \times \sum_{p=0}^{\infty} \frac{(b_{n-1}-a_n)_p (b_{n-2}-a_n)_p}{p!\,(b_{n-1}+b_{n-2}-a_n)_p}\,{}_{n-1}F_{n-2}\left[\begin{matrix}a_1, a_2, \cdots, a_{n-1}; z \\ b_1, b_2, \cdots, b_{n-3}, b_{n-1}+b_{n-2}-a_n+p\end{matrix}\right], \quad \operatorname{Re} a_n > 0, \qquad (5.1)\end{aligned}$$

Applying the formula repeatedly, we expand the hypergeometric function ${}_4F_3$ in Eq. (3.2) in terms of ${}_2F_1$:

$$\begin{aligned}&{}_4F_3\left[\begin{matrix}\frac{1}{2}(m+n+1), \frac{1}{2}(m+n+1), \frac{1}{2}(m+n)+1, \frac{1}{2}(m+n)+1 \\ m+n+1, m+1, n+1\end{matrix}\; 4/a^2\right] \\ &\quad = \frac{m!\,n!\,(m+n)!}{\{\Gamma[\frac{1}{2}(m+n)+1]\}^2} \sum_{p=0}^{\frac{1}{2}(m-n)} \sum_{q=0}^{\infty} \frac{[\frac{1}{2}(m-n)]_p [-\frac{1}{2}(m-n)]_p [\frac{1}{2}(m+n)]_q (p)_q}{p!\,q!\,\Gamma(m+n+1+p+q)} \\ &\qquad \times {}_2F_1\left(\tfrac{1}{2}(m+n+1), \tfrac{1}{2}(m+n+1); m+n+1+p+q; \frac{4}{a^2}\right), \quad m+n \text{ even}, \qquad (5.2a) \\ &\quad = \frac{m!\,n!\,(m+n)!}{\{\Gamma[\frac{1}{2}(m+n+1)]\}^2} \sum_{p=0}^{\frac{1}{2}(m-n-1)} \sum_{q=0}^{\infty} \frac{[\frac{1}{2}(m-n+1)]_p [-\frac{1}{2}(m+n+1)]_p [\frac{1}{2}(m+n+1)]_q (1+p)_q}{p!\,q!\,\Gamma(m+n+2+p+q)} \\ &\qquad \times {}_2F_1\left(\tfrac{1}{2}(m+n)+1, \tfrac{1}{2}(m+n)+1; m+n+2+p+q; \frac{4}{a^2}\right), \quad m+n \text{ odd}. \qquad (5.2b)\end{aligned}$$

These expansion formulas are valid for large values of a, i.e., for $|a^2| > 4$. The hypergeometric function ${}_2F_1$ is analytically continued according to the formula

$$\frac{1}{\Gamma(a+b+l)}\,{}_2F_1(a,b;a+b+l;z)$$
$$=\frac{\Gamma(l)}{\Gamma(a+l)\Gamma(b+l)}\sum_{r=0}^{l-1}\frac{(a)_r(b)_r}{(1-l)_r\,r!}(1-z)^r+\frac{(-1)^l\Gamma(a+b+l)}{\Gamma(a)\Gamma(b)}(1-z)^l\sum_{r=0}^{\infty}\frac{(a+l)_r(b+l)_r}{r!\,(r+l)!}(1-z)^r$$
$$\times[\psi(r+1)+\psi(r+l+1)-\psi(a+l+r)-\psi(b+l+r)-\log(1-z)], \quad (5.3)$$

where l is a positive integer or zero. (When l is zero, the first term in the right-hand side is omitted.)

Equation (5.3) is a useful formula to continue the value from $z\sim 0$ to $z \lesssim 1$. Another formula which is useful to continue from $z\sim 0$ to $z \gtrsim 1$ is

$$\begin{aligned}{}_2F_1(a,b;a+b+l;z)=&\frac{\Gamma(a+b+l)\Gamma(l)}{\Gamma(a+l)\Gamma(b+l)}z^{-a}\sum_{r=0}^{l-1}\frac{(a)_r(1-l-b)_r}{r!\,(1-l)_r}\left(1-\frac{1}{z}\right)^r\\&+\frac{\Gamma(a+b+l)}{\Gamma(a)\Gamma(b)}z^{-a}\left(1-\frac{1}{z}\right)^l\sum_{r=0}^{\infty}\frac{(a+l)_r(1-b)_r}{r!\,(r+l)!}\left(1-\frac{1}{z}\right)^r\\&\times[\psi(1+r)+\psi(1+r+l)-\psi(1-b+r)-\psi(a+l+r)\\&+\pi\operatorname{ctn}\pi b-\log(z^{-1}-1)],\quad -\pi<\arg z<\pi. \end{aligned}\quad (5.4)$$

Equation (5.4), which is not found in the literature, can be proved by taking the limit to the corresponding formula for nonlogarithmic case.

Substitution of Eq. (5.4) into Eq. (5.2) leads to a type of expansion of I_{sq} around $a = 2$. When $m + n$ is even,

$$I_{sq}(a;m,n)=\frac{1}{2\pi}\sum_{p=0}^{\frac{1}{2}(m-n)}\sum_{q=0}^{\infty}\frac{[\frac{1}{2}(m-n)]_p[-\frac{1}{2}(m-n)]_p[\frac{1}{2}(m+n)]_q(p)_q}{p!\,q!}H^e(m,n;p+q;\tfrac{1}{4}a^2-1), \quad (5.5a)$$

where

$$\begin{aligned}&H^e(m,n;p+q;z)\\&=\frac{\Gamma(p+q)}{\{[\frac{1}{2}(m+n+1)]_{p+q}\}^2}\sum_{r=0}^{p+q-1}\frac{[\frac{1}{2}(m+n+1)]_r[\frac{1}{2}(1-m-n)-p-q]_r}{r!\,(1-p-q)_r}(-z)^r\\&+\sum_{r=0}^{\infty}\frac{[\frac{1}{2}(m+n+1)+p+q]_r[-\frac{1}{2}(m+n-1)]_r}{r!\,(p+q+r)!}(-z)^{p+q+r}\\&\times\{\psi(1+r)+\psi(1+p+q+r)-\psi[\tfrac{1}{2}(m+n+1)+p+q+r]-\psi[\tfrac{1}{2}(1-m-n)+r]-\log z\},\end{aligned}\quad (5.6a)$$

and, when $m + n$ is odd,

$$I_{sq}(a;m,n)=\frac{a}{4\pi}\sum_{p=0}^{\frac{1}{2}(m-n-1)}\sum_{q=0}^{\infty}\frac{[\frac{1}{2}(m-n+1)]_p[\frac{1}{2}(1-m+n)]_p[\frac{1}{2}(m+n+1)]_q(1+p)_q}{p!\,q!}H^o(m,n,p+q;\tfrac{1}{4}a^2-1), \quad (5.5b)$$

where

$$\begin{aligned}&H^o(m,n;p+q;z)\\&=\frac{\Gamma(p+q)}{\{[\frac{1}{2}(m+n)+1]_{p+q}\}^2}\sum_{r=0}^{p+q-1}\frac{[\frac{1}{2}(m+n)+1]_r[-\frac{1}{2}(m+n)-p-q]_r}{r!\,(1-p-q)_r}(-z)^r\\&+\sum_{r=0}^{\infty}\frac{[-\frac{1}{2}(m+n)]_r[\frac{1}{2}(m+n)+p+q+1]_r}{r!\,(p+q+r)!}(-z)^{p+q+r}\\&\times\{\psi(1+r)+\psi(1+p+q+r)-\psi[\tfrac{1}{2}(m+n)+1+p+q+r]-\psi[-\tfrac{1}{2}(m+n)+r]-\log z\}.\end{aligned}\quad (5.6b)$$

Equations (5.5a) and (5.5b) are transformed into

$$
\begin{aligned}
&I_{\mathrm{sq}}(a;m,n)\\
&=\frac{1}{2\pi}\sum_{r=0}^{\infty}\frac{[\tfrac{1}{2}(m+n+1)]_r}{r!}(1-\tfrac{1}{4}a^2)^r\\
&\quad\times\Bigg(\sum_{p=0}^{r}\sum_{q=0}^{r-p}\frac{[\tfrac{1}{2}(m-n)]_p[-\tfrac{1}{2}(m-n)]_p[\tfrac{1}{2}(m+n)]_q(p)_q[-\tfrac{1}{2}(m+n-1)]_{r-p-q}}{p!\,[\tfrac{1}{2}(m+n+1)]_p q!\,[\tfrac{1}{2}(m+n+1)+p]_q(r-p-q)!}\\
&\quad\times\{-\log(\tfrac{1}{4}a^2-1)-\psi[\tfrac{1}{2}(m+n+1)+r]-\psi[\tfrac{1}{2}(1-m-n)+r-p-q]+\psi(1+r)+\psi(1+r-p-q)\}\\
&\quad+\sum_{p=1}^{\frac{1}{2}(m-n)\geq 1}\sum_{\substack{q\geq 0\\ q\geq r+1-p}}^{\infty}\frac{[\tfrac{1}{2}(m-n)]_p[-\tfrac{1}{2}(m-n)]_p[\tfrac{1}{2}(m+n)]_q(p)_q\Gamma(p+q-r)}{p!\,[\tfrac{1}{2}(m+n+1)]_p q!\,[\tfrac{1}{2}(m+n+1)+p]_q[\tfrac{1}{2}(m+n+1)]_{p+q-r}}\Bigg)
\end{aligned}
\tag{5.7a}
$$

for $m+n$ even, and

$$
\begin{aligned}
&I_{\mathrm{sq}}(a;m,n)\\
&=\frac{a}{4\pi}\sum_{r=0}^{\infty}\frac{[\tfrac{1}{2}(m+n)+1]_r}{r!}(1-\tfrac{1}{4}a^2)^r\\
&\quad\times\Bigg(\sum_{p=0}^{r}\sum_{q=0}^{r-p}\frac{[\tfrac{1}{2}(m-n+1)]_p[\tfrac{1}{2}(1-m+n)]_p(1+p)_q[\tfrac{1}{2}(m+n+1)]_q[-\tfrac{1}{2}(m+n)]_{r-p-q}}{p!\,[\tfrac{1}{2}(m+n)+1]_p q!\,[\tfrac{1}{2}(m+n)+1+p]_q(r-p-q)!}\\
&\quad\times\{-\log(\tfrac{1}{4}a^2-1)-\psi[\tfrac{1}{2}(m+n)+1+r]-\psi[-\tfrac{1}{2}(m+n)+r-p-q]+\psi(1+r)+\psi(1+r-p-q)\}\\
&\quad+\sum_{p=0}^{\frac{1}{2}(m-n-1)}\sum_{\substack{q\geq 0\\ q\geq r+1-p}}^{\infty}\frac{[\tfrac{1}{2}(m-n+1)]_p[\tfrac{1}{2}(1-m+n)]_p(1+p)_q[\tfrac{1}{2}(m+n+1)]_q\Gamma(p+q-r)}{p!\,[\tfrac{1}{2}(m+n)+1]_p q!\,[\tfrac{1}{2}(m+n)+1+p]_q[\tfrac{1}{2}(m+n)+1]_{p+q-r}}\Bigg)
\end{aligned}
\tag{5.7b}
$$

for $m+n$ odd. Equation (5.7) converges for $0<a<2\sqrt{2}$. It is real for $2<a<2\sqrt{2}$ and complex for $0<a<2$, since $-\log(\frac{1}{4}a^2-1)=i\pi-\log(1-\frac{1}{4}a^2)$ for that region.

The lowest- and the second lowest-order terms are given by

$$
\begin{aligned}
I_{\mathrm{sq}}(a;m,n)\sim&\frac{1}{2\pi}\{-\log(\tfrac{1}{4}a^2-1)+2\psi(1)-2\psi[\tfrac{1}{2}(m+n+1)]\}\\
&+\frac{1}{2\pi}\sum_{p=1}^{\frac{1}{2}(m-n)\geq 1}\frac{[\tfrac{1}{2}(m-n)]_p[-\tfrac{1}{2}(m-n)]_p}{p\{[\tfrac{1}{2}(m+n+1)]_p\}^2}\,{}_3F_2\left[\begin{matrix}\tfrac{1}{2}(m+n),\,p,\,p;\,1\\ \tfrac{1}{2}(m+n+1)+p,\,\tfrac{1}{2}(m+n+1)+p\end{matrix}\right],
\end{aligned}
\tag{5.8a}
$$

for $m+n$ even, and

$$
\begin{aligned}
I_{\mathrm{sq}}(a;m,n)\sim&\frac{1}{2\pi}\{-\log(\tfrac{1}{4}a^2-1)+2\psi(1)-2\psi[\tfrac{1}{2}(m+n)+1]\}\\
&+\frac{1}{2\pi}\frac{2(m+n+1)}{(m+n+2)^2}\,{}_3F_2\left[\begin{matrix}\tfrac{1}{2}(m+n+1)+1,\,1,\,1;\,1\\ \tfrac{1}{2}(m+n)+2,\,\tfrac{1}{2}(m+n)+2\end{matrix}\right]\\
&+\frac{1}{2\pi}\sum_{p=1}^{\frac{1}{2}(m-n-1)\geq 1}\frac{[\tfrac{1}{2}(m-n+1)]_p[\tfrac{1}{2}(1-m+n)]_p}{p\{[\tfrac{1}{2}(m+n)+1]_p\}^2}\,{}_3F_2\left[\begin{matrix}\tfrac{1}{2}(m+n+1),\,p+1,\,p;\,1\\ \tfrac{1}{2}(m+n)+1+p,\,\tfrac{1}{2}(m+n)+1+p\end{matrix}\right],
\end{aligned}
\tag{5.8b}
$$

for $m+n$ odd.

For $m=n$, only terms of $p=q=0$ in Eq. (5.7a) remain, and we have

$$
\mathrm{Re}\,I_{\mathrm{sq}}(a;m,m)=\tfrac{1}{2}\,{}_2\tilde{F}_1(\tfrac{1}{2}+m,\tfrac{1}{2}-m;1;1-\tfrac{1}{4}a^2),\qquad 0<a<2\sqrt{2},\tag{5.9a}
$$

$$
\mathrm{Im}\,I_{\mathrm{sq}}(a;m,m)=\tfrac{1}{2}\,{}_2F_1(\tfrac{1}{2}+m,\tfrac{1}{2}-m;1;1-\tfrac{1}{4}a^2),\qquad 0<a<2.\tag{5.9b}
$$

Equation (5.9) can also be obtained from Eq. (3.3).

When we start from Eq. (5.3), similar expansions to Eqs. (5.7) and (5.8) with independent variable $1-4/a^2$ are obtained, and the leading terms of the expansion are shown to be in agreement with Eqs. (5.8a) and (5.8b) after replacing $\log(1-4/a^2)$ by $\log(\frac{1}{4}a^2-1)$.

The expansion for arbitrary m and n are omitted here and only the case $m=n$ where the expansion

takes a closed form is shown in the following:

$$\mathrm{Re}\, I_{\mathrm{sq}}(a; m, m) = \frac{1}{2}\left(\frac{2}{a}\right)^{2m+1} {}_2\tilde{F}_1\left(\tfrac{1}{2}+m, \tfrac{1}{2}+m; 1; 1-\frac{4}{a^2}\right), \quad \sqrt{2} < a < \infty, \tag{5.10a}$$

$$\mathrm{Im}\, I_{\mathrm{sq}}(a; m, m) = \frac{1}{2}\left(\frac{2}{a}\right)^{2m+1} {}_2F_1\left(\tfrac{1}{2}+m, \tfrac{1}{2}+m; 1; 1-\frac{4}{a^2}\right), \quad \sqrt{2} < a < 2. \tag{5.10b}$$

6. $I_{\mathrm{rect}}(a; m, m; \alpha, \beta)$

In the case $m = n$, I_{rect} can be expressed in terms of the hypergeometric function ${}_2F_1$. From Eq. (2.3),

$$I_{\mathrm{rect}}(a; m, m; \alpha, \beta) = \frac{(2m)!}{2^{2m}a^{2m+1}(m!)^2} \times F_4\left(m+\tfrac{1}{2}, m+1; m+1, m+1; \left(\frac{\alpha}{a}\right)^2, \left(\frac{\beta}{a}\right)^2\right). \tag{6.1}$$

Since[9]

$$F_4\left(a, b; b, b; -\frac{x}{(1-x)(1-y)}, -\frac{y}{(1-x)(1-y)}\right) = (1-x)^a(1-y)^a {}_2F_1(a, 1+a-b; b; xy), \tag{6.2}$$

we put

$$(\alpha/a)^2 = -x/(1-x)(1-y), \tag{6.3}$$

$$(\beta/a)^2 = -y/(1-x)(1-y). \tag{6.4}$$

Then we have

$$x = \alpha^2 C, \quad y = \beta^2 C,$$

$$C = \frac{\alpha^2+\beta^2-a^2 \pm [(\alpha^2+\beta^2-a^2)^2 - 4\alpha^2\beta^2]^{\frac{1}{2}}}{2\alpha^2\beta^2},$$

$$xy = \left(\frac{\alpha^2+\beta^2-a^2 \pm [(\alpha^2+\beta^2-a^2)^2 - 4\alpha^2\beta^2]^{\frac{1}{2}}}{2\alpha\beta}\right)^2. \tag{6.5}$$

Further we use[11]

$${}_2F_1(a, b; a-b+1; z) = (1-\sqrt{z})^{-2a} \times {}_2F_1\left(a, a-b+\tfrac{1}{2}; 2a-2b+1; -\frac{4\sqrt{z}}{(1-\sqrt{z})^2}\right). \tag{6.6}$$

Then we obtain

$$I_{\mathrm{rect}}(a; m, m; \alpha, \beta) = [(2m)!/2^{2m}(m!)^2][a^2-(\alpha-\beta)^2]^{-(m+\frac{1}{2})} \times {}_2F_1(m+\tfrac{1}{2}, m+\tfrac{1}{2}; 2m+1; k_1^2), \tag{6.7}$$

where

$$k_1^2 = 4\alpha\beta/[a^2-(\alpha-\beta)^2]. \tag{6.7'}$$

Equation (6.7) is valid for arbitrary a by considering the analytic continuation of ${}_2F_1$. The expressions of the real arguments such that $0 \le z \le 1$, however, are more convenient. By the transformations of the hypergeometric functions, we have

$$I_{\mathrm{rect}}(a; m, m; \alpha, \beta) = [(-)^m/2(\alpha\beta)^{m+\frac{1}{2}}] \times [{}_2F_1(\tfrac{1}{2}+m, \tfrac{1}{2}-m; 1; k_2^2) + i\, {}_2\tilde{F}_1(\tfrac{1}{2}+m, \tfrac{1}{2}-m; 1; k_2^2)], \tag{6.8a}$$

$$= [2(\alpha\beta)^{m+\frac{1}{2}}]^{-1} \times [{}_2\tilde{F}_1(\tfrac{1}{2}+m, \tfrac{1}{2}-m; 1; k_3^2) + i\, {}_2F_1(\tfrac{1}{2}+m, \tfrac{1}{2}-m; 1; k_3^2)], \tag{6.8b}$$

for $\alpha - \beta < a < \alpha + \beta$, where

$$k_2^2 = [a^2-(\alpha-\beta)^2]/4\alpha\beta, \quad k_3^2 = [(\alpha+\beta)^2-a^2]/4\alpha\beta,$$

and

$$I_{\mathrm{rect}}(a; m, m; \alpha, \beta) = i(-)^m 2^m \left(\frac{1}{(\alpha+\beta)^2-a^2}\right)^{m+\frac{1}{2}} \times {}_2\tilde{F}_1(m+\tfrac{1}{2}, m+\tfrac{1}{2}; 1; k_4^2) \tag{6.9a}$$

$$= i(-)^m \frac{(2m)!}{2^{2m}(m!)^2}\left(\frac{1}{(\alpha+\beta)^2-a^2}\right)^{m+\frac{1}{2}} \times {}_2F_1(m+\tfrac{1}{2}, m+\tfrac{1}{2}; 2m+1; k_5^2) \tag{6.9b}$$

for $0 < a < \alpha - \beta$, where

$$k_4^2 = [(\alpha-\beta)^2-a^2]/[(\alpha+\beta)^2-a^2],$$
$$k_5^2 = 4\alpha\beta/[(\alpha+\beta)^2-a^2].$$

In the case $m = n = 0$, ${}_2F_1$ and ${}_2\tilde{F}_1$ in Eqs. (6.7)–(6.9) reduce to $K(k)$ and $K'(k)$, respectively. In deriving Eq. (6.9) we used

$$\begin{aligned} {}_2F_1(a, a+l; c; z) &= \frac{\Gamma(c)}{\Gamma(a+l)\Gamma(c-a)}\left(\frac{1}{1-z}\right)^a \times \sum_{r=0}^{l-1}\frac{(a)_r(c-a-l)_r\Gamma(l-r)}{r!}\left(\frac{1}{z-1}\right)^r \\ &+ (-)^l\frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a-l)}\left(\frac{1}{1-z}\right)^{a+l} \times \sum_{r=0}^{\infty}\frac{(a+l)_r(c-a)_r}{r!\,(l+r)!}\left(\frac{1}{1-z}\right)^r \\ &\times \left(\psi(1+r)+\psi(1+l+r)-\psi(c-a+r)-\psi(a+l+r)-\log\frac{1}{1-z}\right), \end{aligned} \quad -\pi < \arg(1-z) < \pi, \tag{6.10}$$

which can be proved by taking the limit in the corresponding formula in the nonlogarithmic case.

The imaginary parts of Eqs. (6.8) and (6.9) for the case of $m = 0$ reproduce the result by Montroll.[1] Equation (6.7) for the cases $m = 0$ and $m = 1$ reduce to the result by Wortis.[12] Equations (6.7)–(6.9) for the case $m = 0$ are given by Morita and Horiguchi.[13] Morita[8] pointed out that $I_{\text{rect}}(a; m, m; \alpha, \beta)$ can be expressed in terms of elliptic integrals $\mathbf{K}(k)$ and $\mathbf{E}(k)$ using Eq. (6.7) and the contiguous relation of the hypergeometric function. Wortis' result include

$$I_{\text{rect}}(a; 1, 1; \alpha, \beta) = \frac{1}{k_1 \pi \sqrt{(\alpha\beta)}} [(2 - k_1^2)\mathbf{K}(k_1) - 2\mathbf{E}(k_1)], \quad (6.11)$$

$$I_{\text{rect}}(a; 1, 0; \alpha, \beta) = \frac{1}{\alpha\pi\sqrt{(\alpha\beta)}} [(\alpha + \beta)\mathbf{K}(k_1) - (a + \alpha + \beta)\mathbf{\Pi}(-2\alpha/[a^2 - (\alpha - \beta)^2], k_1)], \quad (6.12)$$

where $\mathbf{\Pi}(\nu, k)$ is the complete elliptic integral of the third kind and k_1 is given by Eq. (6.7′).

7. CONCLUSION

The integral of the lattice Green's function of the rectangular lattice $I_{\text{rect}}(a; m, n; \alpha, \beta)$ for $a > \alpha + \beta$ is evaluated and is given by Eq. (2.3). For $\alpha = \beta$, it reduces to that of the square lattice $I_{\text{sq}}(a, m, n)$ given

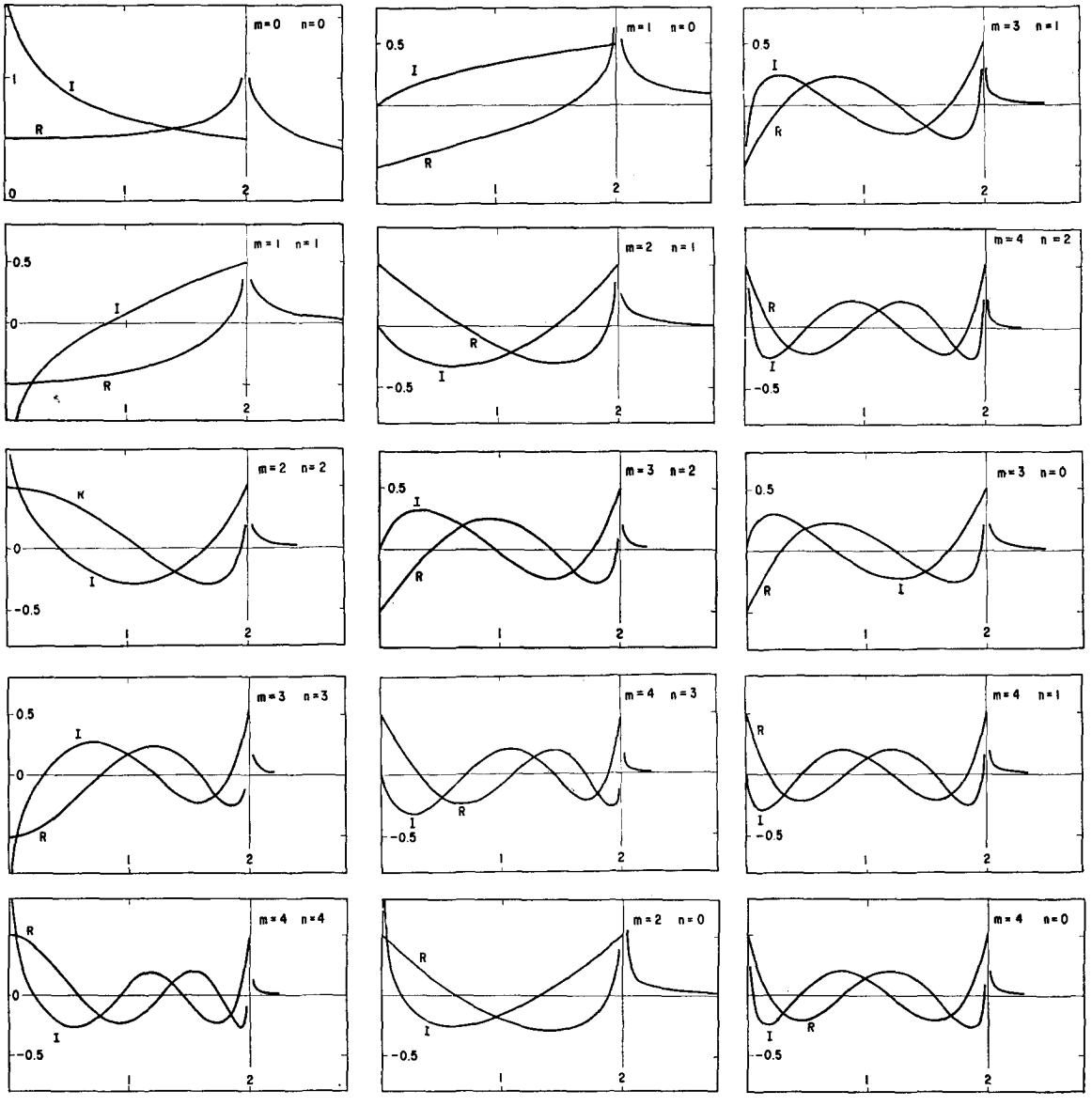

FIG. 1. $I_{\text{sq}}(a; m, n)$. R: Real part, I: Imaginary part. The curve for $a > 2$ is a real part.

by Eq. (3.2) for $a > 2$. By the method of the analytical continuation Eqs. (4.6) and (4.7) for $0 < a < 2$, Eq. (5.7) for $a \sim 2$, are derived. $I_{\text{rect}}(a; m, m; \alpha, \beta)$ is given by Eq. (6.7). These equations are useful to analyze the nature of the singularities and to calculate numerical values.

The singularities of the Green's function of the square lattice arise from two critical points $x = 0$, $y = \pi$ and $x = \pi$, $y = 0$ for $a = 0$ and from a critical point $x = 0$, $y = 0$ for $a = 2$ in the integrand of Eq. (1.1), respectively. When $m = n = 0$, the imaginary part which is proportional to the state density has a logarithmic divergence at $a = 0$ and a discontinuity at $a = 2$, as discussed by van Hove.[14] For the Green's function with arbitrary indices m and n, singular behaviors analogous to the case $m = n = 0$ are generally expected. It is, however, to be noted that when $m + n$ is odd, the contributions from $x = 0$, $y = \pi$ and $x = \pi$, $y = 0$ cancel with each other because of the sign of the numerator and the leading term of the imaginary part is $a \log a$ with no infinities at $a = 0$.

As a result, we obtained $\operatorname{Im} I_{\text{sq}}(a; m, n) \sim \log a$ ($m + n$ even) and $\sim a \log a$ ($m + n$ odd) at $a \sim 0$, and $\operatorname{Re} I_{\text{sq}}(a; m, n) \sim \log |a - 2|$ ($m + n$ even and odd) at $a \sim 2$ and $\operatorname{Im} I_{\text{sq}}(a; m, n) \sim \frac{1}{2} + (zm^2 + 2n^2 - 1)(a - 2)/8$ at $a \sim 2$.

Numerical calculations were carried out using Eqs. (3.3), (4.8), (5.9), and (5.10) for $m = n$ and Eqs. (3.2), (4.6), and (4.7) for $m \neq n$. Values of $\operatorname{Re} I_{\text{sq}}(a; m, n)$ and $\operatorname{Im} I_{\text{sq}}(a; m, n)$ are shown in Fig. 1.

The method in the present paper can be applied to the lattice Green's function for the body-centered cubic lattice at an arbitrary point $I_{\text{bcc}}(a; 1, m, n)$.

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APPENDIX: LATTICE GREEN'S FUNCTION FOR THE LINEAR LATTICE

The real and the imaginary parts of the lattice Green's function of the linear lattice can be obtained by the method of the analytic continuation. It is known that

$$I_{\text{linear}}(a; m) \equiv \frac{1}{\pi} \int_0^{\pi} \frac{\cos mx}{a - \cos x} dx = (a^2 - 1)^{-\frac{1}{2}} [a - (a^2 - 1)^{\frac{1}{2}}]^m, \quad a > 1. \tag{A1}$$

Then

$$I_{\text{linear}}(a - i\epsilon; m) = i(1 - a^2)^{-\frac{1}{2}} [a + i(1 - a^2)^{\frac{1}{2}}]^m, \quad 0 < a < 1. \tag{A2}$$

Hence

$$\operatorname{Im} I_{\text{linear}}(a - i\epsilon; m) = (1 - a^2)^{-\frac{1}{2}} T_m(a) = (1 - a^2)^{-\frac{1}{2}} {}_2F_1(-m, m; \tfrac{1}{2}; \tfrac{1}{2}(1 - a)), \tag{A3}$$

$$\operatorname{Re} I_{\text{linear}}(a - i\epsilon; m) = (1 - a^2)^{-\frac{1}{2}} U_m(a) = m\, {}_2F_1(-m + 1, m + 1; \tfrac{3}{2}; \tfrac{1}{2}(1 - a)), \quad 0 < a < 1, \tag{A4}$$

where $T_m(a)$ and $U_m(a)$ are the Tschebyscheff polynomial of the first and the second order. The results (A3) and (A4) can be obtained as a special case of Eq. (2.3) ($n = 0$, $\alpha = 1$, $\beta = 0$).

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Perturbation Theory of a Nonideal Bose Gas. I*†

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With the pair Hamiltonian model as the starting point, perturbation theory calculations are performed for the average energy and the momentum distribution through second order in the two-body interaction potential. A phenomenological theory of helium II is proposed. The chief underlying feature of this phenomenological theory, which is shown to have a firm basis in the microscopic theory, is the presence of a double quasiparticle spectrum. Phenomenological expressions for the average energy and other quantities of interest are also proposed. Simple prescriptions are obtained for calculating the quasiparticle energies and the chemical potential from the average energy. Via these prescriptions, the quasiparticle energies and the chemical potential are calculated through second order in the interaction potential at $T \neq 0$ °K, and the results are compared with earlier work in the literature.

1. INTRODUCTION

This work concerns itself with the perturbation theoretical studies of a weakly interacting many-boson system at temperatures below the Bose–Einstein transition temperature. The properties of such a system have been investigated extensively in the literature. Our aim in the present study is threefold: (i) to obtain explicit expressions at $T \neq 0$ °K for the average energy and other quantities of interest through second order in the two-body interaction potential V; these results may then constitute a useful check on any detailed realistic microscopic calculations of the equilibrium properties of He II; (ii) to motivate a phenomenological theory of He II; (iii) to supplement the understanding given by the earlier studies. Thus for a dilute hard sphere Bose gas we extend and generalize the $T = 0$ °K results of Wu[1] to $T \neq 0$ °K.

We use the pair Hamiltonian model[2] as the starting point in our calculations. We, therefore, briefly review this model in Sec. 2 in order to establish a double-quasiparticle notation which proves to be quite useful throughout this paper. The average energy $\langle E \rangle$ is then calculated through second order in V (see end of Sec. 2). Basing it on the results for the average energy $\langle E \rangle$, we propose a phenomenological model for He II in Sec. 3. Via the prescriptions (3.15) of the phenomenological theory of Sec. 3, the quasiparticle energies and the chemical potential are calculated in Sec. 4 and compared with earlier work in the literature. Agreement with the earlier results then provides further justification for our phenomenological model. The momentum distribution is calculated in Sec. 5, and an expression for the fraction ξ of particles in the zero-momentum state is derived.

Although our calculations are performed assuming the interactions to be weak, the results can easily be specialized to the case of a dilute hard-sphere Bose gas (DHSBG), as is shown in Appendix F. It is found (see end of Sec. 5) that the explicit expression for ξ at $T = 0$ °K, for the model system of a dilute Bose gas of hard spheres, disagrees with an earlier result of Wu.[1]

2. AVERAGE ENERGY

We begin by writing the many-boson Hamiltonian in Fock space as

$$H = \sum_k \omega(k) a_k^\dagger a_k + \tfrac{1}{2} \sum_{\substack{k_1 k_2 \\ k_3 k_4}} \langle k_1 k_2 | \, V^{(s)} \, | k_3 k_4 \rangle \, a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4}, \tag{2.1}$$

where $\omega(k)$ is the kinetic energy $\hbar^2 k^2/2m$ and

$$\langle k_1 k_2 | \, V^{(s)} \, | k_3 k_4 \rangle = \langle k_1 k_2 | \, V \, | k_3 k_4 \rangle + \langle k_1 k_2 | \, V \, | k_4 k_3 \rangle \tag{2.2}$$

is a symmetrized matrix element of the two-body interaction. We shall not specify the nature of the two-body interaction except to say that it is weak. The operators $a_k^\dagger$ and a_k are the creation and annihilation operators, respectively, of free bosons and these operators obey Bose commutation relations. We assume that the phenomenon of Bose–Einstein condensation occurs in the interacting system, as was first suggested by London.[3] This assumption implies, for a system at rest, that the zero-momentum free particle state will be macroscopically occupied below the Bose–Einstein transition temperature T_λ. Following Bogoliubov,[4] we treat the zero-momentum state separately. One assumes in the first approximation that the operators $a_0, a_0^\dagger \sim N_0^{\frac{1}{2}}$, where N_0 is the number of particles in the zero-momentum state, and that, in the limit $N \to \infty, \Omega \to \infty, N_0/\Omega = \xi n$ is finite (n is the

density and Ω is the volume). With this prescription one can rewrite the Hamiltonian (2.1) as

$$H = H_P + H', \tag{2.3}$$

where, using the notation $k = p$ when $k \neq 0$, we have

$$H_P = H_0 + \tfrac{1}{2}\sum_{p_1p_2} \langle p_1p_2|\, V^{(s)}\,|p_1p_2\rangle\, a^\dagger_{p_1}a^\dagger_{p_2}a_{p_1}a_{p_2} + \tfrac{1}{4}\sum_{p_1p_2} \langle p_1, -p_1|\, V^{(s)}\,|p_2, -p_2\rangle\, a^\dagger_{p_1}a^\dagger_{-p_1}a_{p_2}a_{-p_2}, \tag{2.4}$$

with

$$H_0 = \sum_p \omega(p)a^\dagger_p a_p + \tfrac{1}{4}N_0^2\langle 00|\, V^{(s)}\,|00\rangle + N_0\sum_p a^\dagger_p a_p \langle p0|\, V^{(s)}\,|p0\rangle + \tfrac{1}{4}N_0\sum_p [a^\dagger_p a^\dagger_{-p}\langle p, -p|\, V^{(s)}\,|00\rangle + \langle 00|\, V^{(s)}\,|p, -p\rangle\, a_p a_{-p}] \tag{2.5}$$

and

$$H' = \tfrac{1}{2}N_0^{\frac{1}{2}}\sum_{p_2p_3p_4} a^\dagger_{p_2}\langle 0p_2|\, V^{(s)}\,|p_3p_4\rangle\, a^\dagger_{p_3}a_{p_4} + \tfrac{1}{2}N_0^{\frac{1}{2}}\sum_{p_1p_2p_3} a^\dagger_{p_1}a^\dagger_{p_2}\langle p_1p_2|\, V^{(s)}\,|p_30\rangle\, a_{p_3} + \tfrac{1}{4}\sum_{\substack{p_1p_2p_3p_4\\(p_1,p_2)\neq(p_3,p_4)}} a^\dagger_{p_1}a^\dagger_{p_2}\langle p_1p_2|\, V^{(s)}\,|p_3p_4\rangle\, a_{p_3}a_{p_4}, \tag{2.6}$$

where the inequality $(p_1, p_2 \neq p_3, p_4)$ in the last term of (2.6) means that the diagonal terms and also the pair terms corresponding to $p_1 + p_2 = 0 = p_3 + p_4$, should be excluded. From Eqs. (2.4)–(2.6) we notice immediately that the Hamiltonian does not conserve particle number, i.e., it no longer commutes with the particle-number operator

$$N_{op} = \sum_p a^\dagger_p a_p. \tag{2.7}$$

We can circumvent this difficulty by adding a term

$$-g\sum_p a^\dagger_p a_p$$

to the Hamiltonian (2.3). The introduction of g, the chemical potential, enables us to treat N_0 as a parameter, which is eventually determined by the condition

$$n = \langle N_0\rangle/\Omega + (1/\Omega)\sum_p \langle n(p)\rangle, \tag{2.8}$$

where $\langle n(p)\rangle$ is the momentum distribution. The detailed calculation of $\langle N_0\rangle/\Omega$ in perturbation theory will be outlined in Sec. 5. The chemical potential g is given by the thermodynamic relation

$$g = \left.\frac{\partial\langle E\rangle}{\partial\langle N\rangle}\right|_{S,\Omega,\xi}. \tag{2.9}$$

In accordance with the remark following Eq. (2.7), we next define the Hamiltonian

$$H(g) \equiv H_P(g) + H', \tag{2.10}$$

where

$$H_P(g) \equiv H_P - g\sum_p a^\dagger_p a_p. \tag{2.11}$$

Similarly, we define

$$H_0(g) = H_0 - g\sum_p a^\dagger_p a_p. \tag{2.12}$$

It is well known that the Hamiltonian $H_0(g)$ of (2.12) can be diagonalized by means of a Bogoliubov transformation. As was first shown by Wentzel,[5] the pair-Hamiltonian $H_P(g)$ of (2.11) can also be diagonalized, by first reducing it to a form similar to that of $H_0(g)$ and then applying a Bogoliubov transformation. The diagonalization procedure is summarized briefly in Appendix B. After diagonalization, H_P takes the form, in which a two-component notation is used,

$$H_P(g) = U_P + \sum_p\sum_{i=\pm} if_i(ip)_0\epsilon_i(ip)_0\hat{n}_i(ip), \tag{2.13}$$

where U_P is obtained by substituting Eqs. (B12) into (B6):

$$U_P = (\tfrac{1}{2}N_0)^2\langle 00|\, V^{(s)}\,|00\rangle - \tfrac{1}{2}\sum_{p_1p_2}\langle n(p_1)\rangle_0\langle n(p_2)\rangle_0\langle p_1p_2|\, V^{(s)}\,|p_1p_2\rangle - \tfrac{1}{4}\sum_{p_1p_2}\langle p_1, -p_1|\, V^{(s)}\,|p_2, -p_2\rangle \times \langle a^\dagger_{p_1}a^\dagger_{-p_1}\rangle\langle a_{p_2}a_{-p_2}\rangle. \tag{2.14}$$

The operators $\hat{n}_i(ip)$ in (2.13) are given by

$$\hat{n}_i(p) = i\xi_{-i}(p)\xi_i(p), \tag{2.15}$$

with

$$\xi_i(p) = \xi_p, \quad \text{for} \quad i = +, \qquad = \xi^\dagger_p, \quad \text{for} \quad i = -, \tag{2.16}$$

and the quasiparticle operators ξ_p, $\xi^\dagger_p$ have been defined by the transformation equations (B13). The rest of the quantities in Eq. (2.13) are given by the following set of equations:

$$\epsilon_i(jp)_0 = \epsilon_1(p)_0 + \alpha_{-i}(jp)_0\Delta_2(p)_0 = i\{\epsilon_1^2(p)_0 - \Delta_2^2(p)_0\}^{\frac{1}{2}}, \tag{2.17}$$

$$\epsilon_1(p)_0 = \omega(p) - g + \Delta_1(p)_0 = \omega(p) - g + N_0\langle p0|\, V^{(s)}\,|p0\rangle - \tfrac{1}{2}\langle pp|\, V^{(s)}\,|pp\rangle + \sum_{p_1}\langle pp_1|\, V^{(s)}\,|pp_1\rangle\langle n(p_1)\rangle_0, \tag{2.18}$$

$$\Delta_2(p)_0 = -\tfrac{1}{2}N_0\langle 00|\, V^{(s)}\,|p, -p\rangle - \tfrac{1}{2}\sum_{p_2}\langle a^\dagger_{p_2}a^\dagger_{-p_2}\rangle_c\langle p_2, -p_2|\, V^{(s)}\,|p_1, -p_1\rangle, \tag{2.19}$$

$$\alpha_{-i}(jp)_0 = -\Delta_2(p)_0[\epsilon_i(jp)_0 + \epsilon_1(p)_0]^{-1} = [\alpha_i(jp)_0]^{-1}, \tag{2.20}$$

where the fourth term in Eq. (2.18) vanishes in the infinite volume limit. Finally, the quantities $f_i(ip)_0$ in (2.13) are deduced from the diagonalization condition to be

$$f_+(p)_0 = [1 - \alpha_-^2(p)_0]^{-1},$$
$$f_-(p)_0 = \alpha_-^2(p)_0[1 - \alpha_-^2(p)_0]^{-1},$$
$$f_+(p)_0 - f_-(p)_0 = 1, \tag{2.21}$$

where $\alpha_-(p)_0$ is given by (2.20).

Returning to (2.13), we see that the operator $H_P(g)$ describes a gas of noninteracting quasiparticles whose energy–momentum relations are given by (2.17). The thermodynamics of a nonideal Bose gas in the pair Hamiltonian model has been studied extensively by Luban,[2] and therefore we shall not discuss these details here.

We next consider the eigenstates of $H_P(g)$, for which the operators $\hat{n}_i(ip)$ can be replaced by their eigenvalues which are the (approximate) occupation numbers of the quasiparticles. Since $-n_-(-p) = [1 + n_+(p)]$, we conclude that the eigenstates of $H_P(g)$ can be labeled by the occupation numbers $n_+(p_1), n_+(p_2), \cdots$. For convenience, we shall use the following notation for the normalized eigenstates $|\Psi_0\rangle$:

$$|\Psi_0\rangle = |n_+(p_1), n_+(-p_1), \cdots n_+(p_\alpha), \cdots\rangle$$
$$= \prod_\alpha \mathcal{N}_{p_\alpha}[n_+(p_\alpha), n_+(-p_\alpha)][\xi^\dagger_{p_\alpha}]^{n_+(+p_\alpha)}$$
$$\times [\xi^\dagger_{-p_\alpha}]^{n_+(-p_\alpha)} |0_{p_\alpha}\rangle, \tag{2.22}$$

where $\mathcal{N}_{p_\alpha}$ is a normalization constant and $|0_{p_\alpha}\rangle$ is the quasiparticle vacuum defined by

$$\xi_{p_\alpha} |0_{p_\alpha}\rangle = 0. \tag{2.23}$$

We can now define a single-quasiparticle state in which there is excitation or de-excitation of one quasiparticle relative to $|\Psi_0\rangle$. We label this state by $|n_+(ip) - i\rangle$, where $i = +1$ corresponds to de-excitation and $i = -1$ corresponds to excitation of one quasiparticle. It is given by

$$|n_+(ip) - i\rangle = [in_i(ip)]^{-\frac{1}{2}} \xi_i(ip) |\Psi_0\rangle, \tag{2.24}$$

where $|\Psi_0\rangle$ is the rhs of (2.22). Similarly, we can define states in which more than one quasiparticle is excited or de-excited relative to $|\Psi_0\rangle$.

Second-Order Calculation of the Average Energy

We turn now to the calculation of the average energy in perturbation theory through second order in the perturbation H' of (2.6). The average energy E_0 is given by Eq. (B20). The first- and second-order corrections to E_0 and $|\Psi_0\rangle$ through second order in H' of (2.6), using Rayleigh–Schrödinger perturbation theory,[6] are given by

$$E_{10} = \langle\Psi_0| H' |\Psi_0\rangle, \tag{2.25}$$
$$E_{20} = \langle\Psi_0| H'(1/b)H' |\Psi_0\rangle, \tag{2.26}$$
$$|\Psi_1\rangle = (1/b)H' |\Psi_0\rangle, \tag{2.27}$$
$$|\Psi_2\rangle = (1/b)(H' - E_{10})(1/b)H' |\Psi_0\rangle, \tag{2.28}$$

where

$$(1/b) = (1 - P_0)[E_0 - H_P(g)]^{-1}; \tag{2.29}$$

$(1 - P_0)$ is a projection operator defined by

$$(1 - P_0) |\Psi_0\rangle = 0. \tag{2.30}$$

The perturbed wavefunction $|\Psi\rangle$ is not normalized to unity and its norm is given by

$$\langle\Psi | \Psi\rangle = 1 + \langle\Psi_1 | \Psi_1\rangle + O(V^3). \tag{2.31}$$

For perturbation theory calculations it is necessary to rewrite the perturbation H' of (2.6) in terms of the quasiparticle operators $\xi_i(ip)$. This is easily done by using the important relation, which follows from (B13),

$$a^\dagger_{p_1} a^\dagger_{p_2} a_{p_3} a_{p_4}$$
$$= \sum_{ijlm=\pm} ijlm f_i^{\frac{1}{2}}(ip_1)_0 f_j^{\frac{1}{2}}(jp_2)_0 f_l^{\frac{1}{2}}(lp_3)_0 f_m^{\frac{1}{2}}(mp_4)_0$$
$$\times \xi_{-i}(ip_1)\xi_{-j}(jp_2)\xi_l(lp_3)\xi_m(mp_4). \tag{2.32}$$

Upon using this and a similar relation involving three a and $a^\dagger$ operators, and after a few manipulations involving properties satisfied by $f_i(ip)_0$ and $\alpha_{-i}(ip)_0$ [see Eqs. (2.20) and (2.21)], we can rewrite H' as

$$H' = H_1' + H_2', \tag{2.33}$$
$$H_1' = \tfrac{1}{2}N_0^{\frac{1}{2}} \sum_{p_2p_3p_4} \sum_{ijl} ijl f_i^{\frac{1}{2}}(ip_2)_0 f_j^{\frac{1}{2}}(jp_3)_0 f_l^{\frac{1}{2}}(lp_4)_0$$
$$\times [\langle 0p_2| V^{(s)} |p_3p_4\rangle$$
$$- \alpha_{-j}(jp_3)_0 \langle p_2, -p_3| V^{(s)} |p_40\rangle]$$
$$\times \xi_{-i}(ip_2)\xi_{-j}(jp_3)\xi_l(lp_4), \tag{2.34}$$
$$H_2' = \tfrac{1}{4} \sum_{\substack{p_1p_2p_3p_4 \\ (p_1p_2 \neq p_3,p_4)}} \sum_{ijlm} ijlm f_i^{\frac{1}{2}}(ip_1)_0 f_j^{\frac{1}{2}}(jp_2)_0 f_l^{\frac{1}{2}}(lp_3)_0$$
$$\times f_m^{\frac{1}{2}}(mp_4)_0 \langle p_1p_2| V^{(s)} |p_3p_4\rangle$$
$$\times \xi_{-i}(ip_1)\xi_{-j}(jp_2)\xi_l(lp_3)\xi_m(mp_4). \tag{2.35}$$

One can see from these equations the great simplification which is achieved by the introduction of the two-component notation.

We now turn to the explicit calculation of E_{10} and E_{20}. Since H' of (2.33) does not have any diagonal part, it is easy to see from (2.25) that

$$E_{10} = 0. \tag{2.36}$$

All diagonal terms in the Hamiltonian have, of course, already been included in the pair Hamiltonian (2.4).

The second-order correction to E_0, i.e., E_{20} is derived from (2.26). From the form of H', as presented in Eqs. (2.33)–(2.35), it is clear that the relevant intermediate states for the calculation of the matrix element on the rhs of (2.26) are three- and four-quasiparticle states of the type (2.24). Thus we can write E_{20} as

$$E_{20} = \sum_{ijl} (E_{20})_{ijl} + \sum_{ijlm} (E_{20})_{ijlm}, \tag{2.37}$$

where

$$(E_{20})_{ijl} = \langle \Psi_0 | H_1' S_{ijl}(1/b) H_1' | \Psi_0 \rangle, \tag{2.38}$$

$$(E_{20})_{ijlm} = \langle \Psi_0 | H_2' S_{ijlm}(1/b) H_2' | \Psi_0 \rangle, \tag{2.39}$$

and where S_{ijl} and S_{ijlm} are the orthogonal projectors defined by (C1) and (C2) in Appendix C. Some useful identities needed in the evaluation of $(E_{20})_{ijl}$ and $(E_{20})_{ijlm}$ are listed in Appendix C. The calculation of E_{20} is then straightforward, and the final results are

$$\begin{aligned}(E_{20})_{ijl} = (N_0/3!) \sum_{p_1p_2p_3} & [if_i(ip_1)_0 n_i(ip_1)] \\ & \times [jf_j(jp_2)_0 n_j(jp_2)][lf_l(lp_3)_0 n_l(lp_3)] \\ & \times [\epsilon_i(ip_1)_0 + \epsilon_j(jp_2)_0 + \epsilon_l(lp_3)_0]^{-1} \\ & \times A_{ijl}^{(T)}(p_1p_2p_3) A_{ijl}(p_1p_2p_3),\end{aligned} \tag{2.40}$$

$$\begin{aligned}(E_{20})_{ijlm} = (1/4!) \sum_{p_1p_2p_3p_4} & [if_i(ip_1)_0 n_i(ip_1)][jf_j(jp_2)_0 n_j(jp_2)] \\ & \times [lf_l(lp_3)_0 n_l(lp_3)][mf_m(mp_4)_0 n_m(mp_4)] \\ & \times [\epsilon_i(ip_1)_0 + \epsilon_j(jp_2)_0 + \epsilon_l(lp_3)_0 + \epsilon_m(mp_4)_0]^{-1} \\ & \times A_{ijlm}^{(T)}(p_1p_2p_3p_4) A_{ijlm}(p_1p_2p_3p_4),\end{aligned} \tag{2.41}$$

where the quantities $A_{ijl}(p_1p_2p_3)$ and $A_{ijlm}(p_1p_2p_3p_4)$ are given by (C8) and (C11) and it is understood that principal values of the energy denominators should be taken.

Equations (B20), (2.37), (2.40), and (2.41) taken together give the complete second-order expression for E. The $T \neq 0\,^\circ\mathrm{K}$ expressions are obtained by replacing $n_i(ip)$ in (2.40) and (2.41) by (3.19), with the justification for this procedure being given in Appendix A and also at the end of Appendix B.

A detailed discussion of the various terms in the average energy $\langle E \rangle$ obtained above will be presented in the next section. To our knowledge, no previous microscopic second-order calculation of $\langle E \rangle$ has been reported in the literature. Hence the above expression for $\langle E \rangle$ forms a useful consistency check on any future, more general, microscopic calculations of $\langle E \rangle$. The dilute-hard-sphere-Bose-gas limit of our expression for $\langle E \rangle$ can be deduced by substituting (F9) and (F12) into (2.40) and (2.41). An examination of the DHSBG expression for $\langle E \rangle$ and comparison with the result obtained by Wu at $T = 0\,^\circ\mathrm{K}$ will be given in Appendix F. At the present time, we have not investigated (see Ref. 1) how the "complications arising in the calculation of E_{20} at $T = 0\,^\circ\mathrm{K}$ due to the three-body problem" change with temperature. It is also easy to verify from (F21), as $T \to T_\lambda^-$ where T_λ is the transition temperature, that the DHSBG limit of our expression is in agreement with that of Sikora and Mohling.[7] In the temperature region $T \to T_\lambda^-$, the part of $\langle E \rangle$ given by (2.39) is expected to play an important role and the reasons for this are discussed at the end of Sec. 4.

3. PHENOMENOLOGICAL THEORY OF A BOSE FLUID

In this section we develop a phenomenological theory of the highly degenerate Bose fluid. The starting point of this theory is an energy expression [see Eq. (3.13)] which has a firm basis in microscopic theory. This development is a generalization of the Landau theory of a Fermi liquid,[8] and therefore we first give a brief review[9,10] of the phenomenological model of a normal Bose liquid, which model is a straightforward generalization of the Fermi liquid case. We then present a corresponding model for the degenerate Bose fluid and outline in detail the consequences of such a model.

A. Phenomenological Model of a Normal Bose Fluid

The phenomenological model of a normal Bose fluid is based on the representation of all many-body microscopic degrees of freedom by a set of single-particle states, which are called quasiparticle states in direct analogy with the particle states to which they correspond when the interactions are gradually turned off. Particular attention is devoted to the dependence of the thermodynamic quantities upon the quasiparticle distribution functions labeled $n'(k)$. The quantum numbers k which characterize the quasiparticle states can be identified, for an infinite system, with allowed momentum-state and spin-state degrees of freedom. Thus the energy expression for He I can be written, quite generally, in the form[9,10]

$$\begin{aligned}E = E[n'(k)] = & \sum_k n'(k)\omega(k) \\ & + \tfrac{1}{2} \sum_{k_1k_2} n'(k_1)n'(k_2)U(k_1, k_2),\end{aligned} \tag{3.1}$$

where $\omega(k)$ is the free particle energy $\hbar^2k^2/2m$. The second term in (3.1) represents the interaction energy of the system and it exhibits explicitly the fact that at least two quasiparticles must interact in order for there to be an interaction energy. It is important to emphasize

that $U(k_1, k_2)$ can in turn depend functionally on $n'(k)$. This dependence arises because more than two particles or quasiparticles can interact simultaneously; it may also occur if there are many-body interaction energies.

Quasiparticles in the system are characterized by their quantum numbers k and a distribution function $n'(k)$ which, for an interacting system, does not equal $\langle n(k)\rangle$ even though

$$\sum_k n'(k) = \sum_k \langle n(k)\rangle = N,$$

where N is the total number of particles in the system. Here $\langle n(k)\rangle$ is the momentum distribution of the interacting system. Quasiparticles are also characterized by their energies $\omega'(k)$. We consider the most general functional variation of the energy E with respect to the distribution functions $n'(k)$. The energy $\omega'(k)$ is then defined by

$$\begin{aligned}\delta E &\equiv \sum_k \omega'(k)\delta n'(k)\\ &= \sum_k [\omega'(k) - g]\delta n'(k) + g\delta N, \qquad (3.2)\end{aligned}$$

since, if $\delta n'(k) = \delta(k, k_0)$, then the corresponding change in E must be the quasiparticle energy of the state k_0. The quantity g in the second line of Eq. (3.2) is the chemical potential. Upon solving this equation for $\omega'(k)$ and substituting Eq. (3.1), one finds the general result

$$\begin{aligned}\omega'(k_1) &= \left.\frac{\delta E}{\delta n'(k_1)}\right|_N\\ &= \omega(k_1) + \sum_{k_2} n'(k_2)U(k_1, k_2)\\ &\quad + \tfrac{1}{2}\sum_{k_3k_4} n'(k_3)n'(k_4)\frac{\delta U(k_3, k_4)}{\delta n'(k_1)}, \qquad (3.3)\end{aligned}$$

where, for finite systems, the derivatives are ordinary partial derivatives. The last term in Eq. (3.3) results from a functional dependence of $U(k_1, k_2)$ on $n'(k)$, as discussed above, and this term is called the rearrangement energy. The interaction energy $U(k_1, k_2)$ depends, in general, on $\omega'(k)$, which in turn depends on $n'(k)$. Hence $U(k_1, k_2)$ has an implicit dependence on n' via $\omega'(k)$.

The popular belief is that the Landau theory of a normal Fermi liquid is valid only at low temperatures. With this view one would question the above development for He I, which exists only at temperatures $T > 2\,^\circ\mathrm{K}$, but we believe that the above development is valid for the high-temperature domain of He I. The reason for the earlier belief that the Landau theory is valid only around $T \sim 0\,^\circ\mathrm{K}$ arises, in our opinion, due to a confusion existing in the literature as to what "quasiparticles" mean. We assert that a quasiparticle picture is the one that arises naturally in a microscopic theory from the study of the self-energy problem associated with a (statistically averaged) real system, which is characterized by a real Hermitian Hamiltonian. Such quasiparticles are real by definition. From this point of view, it is obvious that the Landau theory can be extended to finite temperatures. Thermal excitation produces a distribution of the quasiparticle energies

$$n'(p) = \{e^{\beta[\omega'(p)-g]} - 1\}^{-1}, \qquad (3.4)$$

in the same manner as it does for particle energies in a dilute gas. These quasiparticles are not to be confused with the collective modes which one observes experimentally when one excites the liquid by means of an external probe. These latter collective modes decay, even when, as in He II, they may be identified with the quasiparticles, for an experimental excitation always represents a fluctuation away from the equilibrium state with a corresponding lifetime.

B. Double-Quasiparticle Model

It is now appropriate to consider the phenomenological description of He II. Our model will be a generalization of the description of He I presented above. The generalization is not a trivial one, as we have to incorporate the macroscopic occupation of the zero-momentum state and also the depletion of this zero-momentum state, due to interactions. If the depletion is neglected, one can generalize the results of Subsection A with a few modifications, as has been done earlier by Morita and Tanaka.[10] It is believed that the fraction of particles in the zero-momentum state is around 0.1 at $T = 0\,^\circ\mathrm{K}$.[11] Hence, the nonzero-momentum component (in addition to the particles in the zero-momentum state) of the superfluid must be taken into consideration in our development.

The phenomenological theory which we shall now outline is the result of an attempt to understand the physical predictions derived from the quantum-statistical theory of Mohling, RamaRao, and Shea[12] and also from the present perturbation theory. These attempts suggested a double-quasiparticle notation (see Sec. 2 and Appendix B), which we now introduce, and an understanding of this notation is essential for the rest of this paper. We consider He II at rest. The microscopic theory suggests that there are three different types of quasiparticle states available for occupation by the helium atoms: (1) the macroscopically occupied zero-momentum state with energy g; (2) positive-energy quasiparticle states, with energy $\omega_+(p) = g + \epsilon_+(p)$; (3) negative-energy quasiparticle states with energy $\omega_-(p) = \epsilon_-(p) + g$. Here g is the

chemical potential, and we use the convention that p is the momentum of a nonzero-momentum quasiparticle, i.e., $p \neq 0$. We also assume that $\epsilon_+(p) = -\epsilon_-(-p)$.

The $\epsilon_\pm(p)$ are generalizations of the energies $\epsilon_\pm(p)_0$ which we encountered in the perturbation theory of Sec. 2 [see Eq. (2.17)]. Corresponding to the quasiparticle energies $\epsilon_\pm(p)$ are two distribution functions $n_\pm(p)$. We can imagine that these functions $n_\pm(p)$ are associated in the perturbation theory version of the microscopic theory with the quasiparticle operators $\xi_p^\dagger \xi_p$ and $-\xi_{-p}\xi_{-p}^\dagger$, there being one set of quasiparticle operators ξ_p and $\xi_p^\dagger$ for each p value in the perturbation theory. Thus it is reasonable to assume that $n_+(p)$ and $n_-(-p)$ are related by

$$n_-(-p) = -[1 + n_+(+p)], \tag{3.5}$$

where the one minus sign for p in n_- is introduced for later convenience. [Equation (3.5) follows from Eq. (2.15).]

Because the contributions to physical quantities from the two nonzero-momentum states will be expected to be different, in general, we anticipate such a difference by making the replacement

$$\sum_p \rightarrow \sum_p \sum_{\substack{i \\ i=\pm}} i f_i(p) \tag{3.6}$$

for all single-particle-state sums (momentum-state sums for an infinite system). Here the $f_i(p)$ are the weighting factors for the two states, such that

$$\sum_i i f_i(ip) = f_+(p) - f_-(-p) = 1. \tag{3.7}$$

These weighting factors have a natural basis in microscopic theory. In fact, the $f_\pm(p)$ are generalizations of the $f_\pm(p)_0$ defined by Eq. (2.21). Equation (3.7) is essentially the condition that the Bogoliubov transformation be canonical.

The above introduction of the double-quasiparticle notation is admittedly rather ad hoc, and there should be a more physical way, yet to be discovered, for introducing the quantities $\omega_\pm(p)$, $n_\pm(p)$, and $f_\pm(p)$. In what follows, we describe these quantities heuristically.

Consider a degenerate Bose system with N interacting bosons, and consider further how one can generate an $(N+1)$-particle state starting from the N-particle system. The peculiarity of the degenerate Bose system (with $T < T_\lambda$) is that there are two ways of adding a boson with momentum $\mathbf{p}$, each way having its own definite probability. (1) The boson can be added to the N-particle system directly in the plane-wave state $\mathbf{p}$. (2) The added boson can couple with another boson having momentum $-\mathbf{p}$ to form the paired state $(\mathbf{p}, -\mathbf{p})$. The end result in this second case is equivalent to an $(N-1)$-particle system with a boson of momentum $-\mathbf{p}$ removed from the N-particle system. The double-quasiparticle model seems to incorporate, notationally, the occurrence of this second process.

Perhaps one should not take these suggested interpretations too seriously, since it is possible to show for all physical predictions that our double-quasiparticle model reduces to the more usual single-quasiparticle model. Nevertheless, the appearance of both positive- and negative-energy-quasiparticle quantities throughout the microscopic theory, when it is expressed in its most concise form, justifies attempts at interpretation of the model.

Equation (3.7) shows that both $f_\pm(p)$ can be expressed in terms of a single quantity. We therefore define a quantity $\alpha_-(p)$ such that

$$\begin{aligned} f_+(p) &\equiv [1 - \alpha_-^2(p)]^{-1}, \\ f_-(-p) &\equiv \alpha_-^2(p)[1 - \alpha_-^2(p)]^{-1}. \end{aligned} \tag{3.8}$$

It is useful, for later convenience, to define one further quantity $\alpha_+(p)$, which is related to $\alpha_-(p)$ by

$$\alpha_+(p) \equiv [\alpha_-(-p)]^{-1} \tag{3.9}$$

or

$$\alpha_i(p) = \alpha_{-i}^{-1}(-p).$$

We then rewrite $f_+(p)$ in terms of these two quantities by the single equation

$$\begin{aligned} f_i(ip) &= i[1 - \alpha_{-i}^2(ip)]^{-1} \\ &= -\alpha_{-i}^{-1}(ip)[\alpha_+^{-1}(-p) - \alpha_-^{-1}(+p)]^{-1}. \end{aligned} \tag{3.10}$$

It is trivially verified that Eqs. (3.8) and (3.10) for $f_+(p)$ satisfy the condition (3.7). From (3.8)–(3.10) it is also easy to verify the relation

$$f_+(p)\alpha_-(p) = f_-(-p)\alpha_+(-p). \tag{3.11}$$

We now consider expressions for physical quantities using the notation outlined above. For simplicity, we shall continue to use the language of an infinite system in which the single-particle quantum numbers p refer to plane-wave states. Whenever single-particle sums are involved, we shall often use the left-hand side of (3.6) to mean the right-hand side (the use of the notation being easy to determine by context), thereby suppressing the

$$\sum_i i f_i(p)$$

factor in our equations. In order to indicate that a quantity carries a single label i in this notation, we shall attach a prime to it whenever the label is suppressed. Thus the distribution function $n_i(p)$ will be written as $n'(p)$. The notation $\alpha'_{(-)}(p)$ will represent $\alpha_{-i}(p)$.

Particle Density: One might write down the following plausible form for the particle density n of the system

$$n = x + \Omega^{-1}\sum_p n'(p)$$
$$= x + \Omega^{-1}\sum_p\sum_i if_i(p)n_i(p) \quad \text{(incorrect)}. \quad (3.12)$$

This result seems reasonable, because the last term in Eq. (3.12) is the sum over all probabilities for both kinds of quasiparticles to be occupied. Although quite plausible, Eq. (3.12) cannot really be justified without appealing to a microscopic theory. In fact, the microscopic calculation of the momentum distribution shows that Eq. (3.12) is only a first approximation to the exact expression. We shall return to this point at the end of Sec. 5. We note, in passing, that the second line of Eq. (3.12) is hard to interpret with a single-quasiparticle model. Thus, the double-quasiparticle picture brings a simple order into the understanding of the microscopic theory in this case.

C. Phenomenological Expression for Energy

Using the notation developed in Subsection B, we now write a phenomenological expression for the energy, in direct analogy with Eq. (3.1) for He I, as

$$E = \sum_p n'(p)\omega(p)$$
$$+ (\tfrac{1}{2}N_0)^2U + N_0\sum_p n'(p)U'(p)$$
$$+ \tfrac{1}{2}\sum_{p_1p_2} n'(p_1)n'(p_2)U''(p_1, p_2), \quad (3.13)$$

in which three different interaction energies U, $U'(p)$, $U''(p_1, p_2)$ have been introduced. In writing Eq. (3.13) for the energy, we have exhibited separately those interaction terms which have no explicit dependence on n', an explicit dependence on only one $n'(p)$, and an explicit dependence on at least two $n'(p)$. The interaction energies U, $U'(p)$, $U''(p_1, p_2)$ can all have an implicit dependence on n' as explained below Eq. (3.3) for the He I case. The interaction energy $U''(p_1, p_2)$ in Eq. (3.13) actually represents four different energies, as can be seen by exhibiting the sums in Eq. (3.13) explicitly with the aid of Eq. (3.6). The second term in Eq. (3.13) represents the interaction of one zero-momentum boson with another zero-momentum boson, and the third term represents the interaction of one zero-momentum boson with a nonzero-momentum quasiparticle. Finally, the last term in Eq. (3.13) represents the interaction energy of one nonzero-momentum quasiparticle with another nonzero-momentum quasiparticle. The U, $U'(p)$, $U''(p_1, p_2)$ will, in general, also depend functionally on N_0. In the next section we shall show that the average energy $\langle E\rangle$ in perturbation theory has indeed the form indicated in (3.13), and we shall also write down expressions for U, $U'(p)$, and $U''(p_1, p_2)$.

The expression (3.13) is valid not only for a pure state, i.e., one derivable, in principle, from a complete many-body perturbation theory calculation involving the unperturbed occupation quantum numbers $n'(p)$, but it is also valid for a real quantum fluid at $T \neq 0\,^\circ\text{K}$. Thus, to be valid for a real quantum fluid, Eq. (3.13) has only to be averaged over the appropriate ensemble (see Appendix A).

We next consider a generalization of Eq. (3.2), for the He II case. It might seem for the He II case that one has only to add to the first line of Eq. (3.2) a term $g\delta N_0$ to allow for the (virtual) variation in the number of zero-momentum bosons. But because Eq. (3.12) is incorrect, we *must* use the second line of Eq. (3.2) for the He II case, i.e.,

$$\delta E = \sum_p \epsilon'(p)\delta n'(p) + g\delta N. \quad (3.14)$$

To use this expression for δE, we can either treat N_0 as an independent variable or eliminate N_0 in favor of N by substituting Eq. (5.13) into the explicit form of (3.13). From this expression we obtain the following relations for $\epsilon'(p)$ and g:

$$\epsilon'(p) = \frac{\delta E}{\delta n'(p)}\bigg|_{N_0,\alpha'} - g\,\frac{\delta N}{\delta n'(p)}\bigg|_{N_0,\alpha'}$$
$$= \omega(p) + \Delta'(p) - g,$$
$$g = \frac{\partial E}{\partial N}\bigg|_{n',\alpha'}, \quad (3.15)$$

in which the quasiparticle self-energy $\Delta'(p)$ is introduced. The reason for holding the quantities $\alpha_\pm(k)$, and hence also the $f_\pm(k)$, constant in these partial derivatives is discussed below Eq. (4.22).

Upon substituting Eq. (3.13) for the energy into Eq. (3.15), we obtain the following expression for $\epsilon'(p)$:

$$\epsilon'(p) = \omega(p) + N_0U'(p) + \sum_{p_2} n'(p_2)U''(p, p_2)$$
$$+ (\tfrac{1}{2}N_0)^2\,\frac{\delta U}{\delta n'(p)} - g\,\frac{\delta N}{\delta n'(p)}$$
$$+ N_0\sum_{p_2} n'(p_2)\,\frac{\delta U'(p_2)}{\delta n'(p)}$$
$$+ \tfrac{1}{2}\sum_{p_3p_4} n'(p_3)n'(p_4)\,\frac{\delta U''(p_3, p_4)}{\delta n'(p)}$$
$$= \omega(p) + \Delta'(p) - g, \quad (3.16)$$

where the second equality serves to define the average interaction potential $\Delta'(p)$, or self-energy, experienced by a quasiparticle of momentum p. Similarly, we obtain for the chemical potential

$$g = \Big\{\tfrac{1}{2}N_0U + \sum_p n'(p)U'(p) + (\tfrac{1}{2}N_0)^2 \frac{\partial U}{\partial N_0}\Big|_{n',\Omega,\alpha'} + N_0 \sum_p n'(p) \frac{\partial U'(p)}{\partial N_0}\Big|_{n',\Omega,\alpha'} + \tfrac{1}{2}\sum_{p_1p_2} n'(p_1)n'(p_2) \frac{\partial U''(p_1, p_2)}{\partial N_0}\Big|_{n',\Omega,\alpha'}\Big\} \times \left[\left(\frac{\partial N}{\partial N_0}\right)_{n',\Omega,\alpha'}\right]^{-1}. \quad (3.17)$$

We can check Eqs. (3.16) and (3.17), and hence Eqs. (3.14) and (3.15), by comparing them with the expressions for $\epsilon'(p)$ and g obtained in a calculation which does not use the energy expression as a starting point. This question is given further discussion at the end of Sec. 4.

We note here that the intimate mathematical relation between the double- and single-quasiparticle models is linked closely to the simple identity $\epsilon_-(-p) = -\epsilon_+(p)$. This identity, mentioned earlier, is given a firm microscopic basis in Sec. 4. It makes possible the consistency of Eqs. (3.5) and (3.19).

Entropy: We now make the fundamental assumption that the $n'(p)$ enumerate all the single-particle degrees of freedom which can be excited thermally in the system. Using this assumption, we can write down the following expression for the entropy by a simple process of state counting[13]:

$$S = \kappa \sum_p \{[1 + n_+(p)] \ln [1 + n_+(p)] - n_+(p) \ln [n_+(p)]\} \quad (3.18a)$$

$$= \kappa \sum_p \{[1 + n'(p)] \ln |1 + n'(p)| - n'(p) \ln |n'(p)|\}, \quad (3.18b)$$

where κ is Boltzmann's constant. The equivalence of Eqs. (3.18a) and (3.18b) is easily verified by using Eqs. (3.7) and (3.5). Thus, the double-quasiparticle model and the single-quasiparticle model give identical results for the entropy.

We next consider liquid helium moving with a linear velocity v_S such that v_S is the velocity of the bosons in the macroscopically occupied single-quantum state. It is shown in Appendix A, when the entropy is maximized over a statistical ensemble, subject to the constraints of constant total energy, constant total number of particles, and constant total momentum, that $n'(p)$ can be expressed in terms of the quasiparticle energies as

$$n'(p) = \{\exp \beta[\epsilon'(p) - p \cdot u] - 1\}^{-1}, \quad (3.19)$$

where $\beta = 1/\kappa T$, p is measured relative to mv_S, and u is defined by Eq. (A10). The physical interpretation of u as being the drift velocity of the normal fluid relative to the velocity v_S of the condensed state is demonstrated at the end of Appendix A.

It is also shown in Appendix A that the energy expression (3.13) continues to be valid in the frame of reference moving with a velocity v_S relative to the laboratory provided the momenta are all measured relative to the momentum mv_S. To translate to the laboratory frame, one has therefore only to (1) add the quantity

$$\tfrac{1}{2}Nmv_S^2 + v_S \cdot \sum_p pn'(p) \quad (3.20)$$

to the right-hand side of Eq. (3.13) for E and (2) replace the chemical potential g by μ, where

$$\mu = g + \tfrac{1}{2}mv_S^2. \quad (3.21)$$

One could now develop a two-fluid model, using this double-quasiparticle picture, and give operational definitions of the normal and superfluid densities, but we shall not give these details here.[14]

As a final matter for this section we derive a useful expression for the heat capacity at constant volume C_V from Eq. (3.14) for δE. We find

$$C_V = \left(\frac{\partial E}{\partial T}\right)_{\Omega,N} = \sum_p \epsilon'(p) \frac{\partial n'(p)}{\partial T} = \sum_p \epsilon_+(p) \frac{\partial n_+(p)}{\partial T}. \quad (3.22)$$

The second line of (3.22), which is precisely the Landau result, is derived by using Eqs. (3.5), (3.7), and (4.24).

4. QUASIPARTICLE ENERGIES

The phenomenological theory of a Bose fluid developed in Sec. 3 gave definite prescriptions for the calculation of the quasiparticle energies and the chemical potential via the relations (3.15)–(3.17). In this section we calculate the quasiparticle energies and the chemical potential, using these prescriptions as the starting point, and compare the results with other, more direct, calculations of the same quantities.

A. Rearrangement of Average Energy

We first rewrite the perturbation theory expression for the energy (see end of Sec. 2), which is a functional of all the zeroth-order quantities $f_i(p)_0$, $\epsilon_i(p)_0$,

$\alpha_{-i}(p)_0$, etc., in terms of the more general $f_i(p)$ and $\alpha_{-i}(p)$ introduced in Eqs. (3.8)–(3.10).[15] Thus we write in the perturbation theory context

$$f_i(p) = f_i(p)_0 + \delta f_i(p) + O(V^3), \tag{4.1}$$

$$\alpha_{-i}(p) = \alpha_{-i}(p)_0 + \delta\alpha_{-i}(p) + O(V^3), \tag{4.2}$$

where the correction terms are $O(V^2)$. In analogy with definition (2.20) of $\alpha_{-i}(p)_0$, we define

$$\alpha_{-i}(p) \equiv -\Delta_{2,-i}(-p)[\epsilon_i(p) + \epsilon_{1,-i}(-p)]^{-1}, \tag{4.3}$$

where

$$\Delta_{2i}(p) = \Delta_{2i}(p)_0 + \Delta_{2i}(p)_2 + O(V^3), \tag{4.4}$$

$$\epsilon_i(p) \equiv \omega(p) - g + \Delta_i(p), \tag{4.5}$$

$$\Delta_i(p) \equiv \Delta_{1i}(p) + \alpha_{-i}(p)\Delta_{2i}(p), \tag{4.6}$$

$$\begin{aligned}\epsilon_{1i}(p) &\equiv \omega(p) - g + \Delta_{1i}(p) \\ &= \epsilon_1(p)_0 + \Delta_{1i}(p)_2 + O(V^3),\end{aligned} \tag{4.7}$$

and $\Delta_2(p)_0$, $\epsilon_1(p)_0$, $\epsilon_i(p)_0$ are given in Eqs. (2.17)–(2.20). It is important to observe that the second-order corrections introduced in Eqs. (4.1)–(4.7) are all unknowns and have to be determined via the prescriptions (3.15)–(3.17) in Sec. 3. Their explicit expressions are, however, unnecessary for rewriting the expression for the average energy (see Appendix D). Also, to be general, we have included an i dependence with the self-energies $\Delta_1(p)$ and $\Delta_2(p)$. The final rearranged result $\langle E\rangle$ is found to be

$$\begin{aligned}\langle E\rangle &= \tilde{E}_0 + E_2 + O(V^3) \\ &= E_0 + E_{20} + O(V^3),\end{aligned} \tag{4.8}$$

where it is shown in Appendix D that

$$\begin{aligned}\tilde{E}_0 &= (\tfrac{1}{2}N_0)^2\langle 00|\, V^{(s)}\,|00\rangle + \sum_p \sum_i if_i(ip)\tilde{\omega}_i(p)_0 n_i(p) \\ &\quad - \tfrac{1}{2}\sum_{p_1p_2}\sum_{ij}[if_i(ip_1)n_i(p_1)] \\ &\quad \times [jf_j(p_2)n_j(p_2)]\langle p_1p_2|\, V^{(s)}\,|p_1p_2\rangle \\ &\quad - \tfrac{1}{4}\sum_{p_1p_2}\sum_{ij}[if_i(p_1)\alpha_{-i}(p_1)n_i(p_1)] \\ &\quad \times [jf_j(p_2)\alpha_{-j}(p_2)n_j(p_2)] \\ &\quad \times \langle p_1, -p_1|\, V^{(s)}\,|p_2, -p_2\rangle \\ &= E_0 + O(V^3),\end{aligned} \tag{4.9}$$

$$\begin{aligned}E_2 &= \left[\begin{array}{l}E_{20} \text{ with } f_i(p)_0 \text{ and } \alpha_{-i}(p)_0 \text{ replaced} \\ \text{by } f_i(p) \text{ and } \alpha_{-i}(p), \text{ respectively}\end{array}\right] \\ &= E_{20} + O(V^3),\end{aligned} \tag{4.10}$$

$$\begin{aligned}\tilde{\omega}_i(p)_0 &\equiv \omega(p) + \Delta_1(p)_0 + \alpha_{-i}(p)\Delta_2(p)_0 \\ &= \tilde{\epsilon}_i(p)_0 + g.\end{aligned} \tag{4.11}$$

It is now straightforward to verify that the expression for $\langle E\rangle$ given by (4.8)–(4.10) can indeed be written in the form (3.13) if we make the following identifications:

$$U = \langle 00|\, V^{(s)}\,|00\rangle + O(V^3), \tag{4.12}$$

$$\begin{aligned}U'(p) &= \langle p0|\, V^{(s)}\,|p0\rangle \\ &\quad - \tfrac{1}{2}\alpha'_{(-)}(p)\langle 00|\, V^{(s)}\,|p, -p\rangle + O(V^3),\end{aligned} \tag{4.13}$$

$$\begin{aligned}U''(p_1, p_2) &= \langle p_1p_2|\, V^{(s)}\,|p_1p_2\rangle + \tfrac{1}{2}\alpha'_{(-)}(p_1)\alpha'_{(-)}(p_2) \\ &\quad \times \langle p_1, -p_1|\, V^{(s)}\,|p_2, -p_2\rangle \\ &\quad + \frac{N_0}{3}\sum_{p_3} n'(p_3)A^{(T)\prime\prime\prime}(p_1p_2p_3)A'''(p_1p_2p_3) \\ &\quad \times [\epsilon'(p_1) + \epsilon'(p_2) + \epsilon'(p_3)]^{-1} \\ &\quad + \tfrac{1}{12}\sum_{p_3p_4} n'(p_3)n'(p_4) \\ &\quad \times A^{(T)\prime\prime\prime\prime}(p_1p_2p_3p_4)A''''(p_1p_2p_3p_4) \\ &\quad \times [\epsilon'(p_1) + \epsilon'(p_2) + \epsilon'(p_3) + \epsilon'(p_4)]^{-1} \\ &\quad + O(V^3).\end{aligned} \tag{4.14}$$

The interpretations given below (3.13) for U, U_i, and U_{ij} should also be evident from these explicit expressions.

B. Second-Order Calculations of Quasiparticle Self-Energies

We now proceed to the calculation of the quasiparticle self-energies and the chemical potential. One can use either (3.15) or (3.16) and (3.17) as a starting point. We have used (3.15) in the calculations to be presented in this section. It is convenient first to rewrite E_2 of Eq. (4.10) as

$$\begin{aligned}E_2 &= (N_0/6)\sum_{p_1p_2p_3}[\epsilon'(p_1) + \epsilon'(p_2) + \epsilon'(p_3)]^{-1} \\ &\quad \times \{n'(p_1)n'(p_2)n'(p_3)C''(p_1p_2p_3)A^{(T)\prime\prime\prime}(p_1p_2p_3) \\ &\quad - [1 + n'(p_1)][1 + n'(p_2)][1 + n'(p_3)] \\ &\quad \times A'''(p_1p_2p_3)C^{(T)\prime\prime}(p_1p_2p_3)\} \\ &\quad + \tfrac{1}{24}\sum_{p_1p_2p_3p_4}[\epsilon'(p_1) + \epsilon'(p_2) + \epsilon'(p_3) + \epsilon'(p_4)]^{-1} \\ &\quad \times \{n'(p_1)n'(p_2)n'(p_3)n'(p_4)D''''(p_1p_2p_3p_4) \\ &\quad \times A^{(T)\prime\prime\prime\prime}(p_1p_2p_3p_4) - [1 + n'(p_1)][1 + n'(p_2)] \\ &\quad \times [1 + n'(p_3)][1 + n'(p_4)] \\ &\quad \times A''''(p_1p_2p_3p_4)D^{(T)\prime\prime\prime\prime}(p_1p_2p_3p_4)\}.\end{aligned} \tag{4.15}$$

In deriving (4.15) from (4.10) we have used (C12), (C14), (3.9)–(3.11), and (4.24). Also the permutation symmetry among the momenta which existed in (2.40) and (2.41) has been destroyed and preference has been exhibited for the momentum variable p_1. Since the choice of the momentum p_1 is arbitrary, when we take the functional derivative in (3.15), we can perform our differentiation with respect to p_1 only and then multiply the result by 3 for the first term in (4.15) and

by 4 for the second term in (4.15). This arbitrary procedure enables us to avoid terms proportional to $[\alpha'_{(-)}(p)]^2$ in $\Delta'(p)$, thereby simplifying the analysis of the quasiparticle-energy expression.

We can now use (4.9), (4.15), and (5.14) to calculate all the self-energies through second order in V. As the details are straightforward, we simply summarize the final results here:

$$\epsilon'(p) = \omega(p) + \Delta'(p) - g, \tag{4.16}$$

$$\Delta'(p) = \Delta'_1(p) + \alpha'_{(-)}(p)\Delta'_2(p), \tag{4.17}$$

$$\begin{aligned}\Delta'_1(p_1) = {} & N_0 \langle p_1 0| V^{(s)} |p_1 0\rangle \\ & + \sum_{p_2} n'(p_2) \langle p_1 p_2| V^{(s)} |p_1 p_2\rangle \\ & - \tfrac{1}{2} N_0 \sum_{p_2 p_3} [\epsilon'(p_2) + \epsilon'(p_3) + \epsilon'(p_1)]^{-1} \\ & \times [1 + n'(p_2) + n'(p_3)] \\ & \times C''(p_1 p_2 p_3) C^{(T)\prime\prime}(p_1 p_2 p_3) \\ & - \tfrac{1}{6} \sum_{p_2 p_3 p_4} [\epsilon'(p_2) + \epsilon'(p_3) + \epsilon'(p_4) + \epsilon'(p_1)]^{-1} \\ & \times \{[1 + n'(p_2)][1 + n'(p_3)][1 + n'(p_4)] \\ & - n'(p_2) n'(p_3) n'(p_4)\} \\ & \times D'''(p_1 p_2 p_3 p_4) D^{(T)\prime\prime\prime}(p_1 p_2 p_3 p_4) + O(V^3) \\ = {} & \Delta'_1(p_1)_0 + \Delta'_1(p_1)_1 \\ & + \Delta'_1(p_1)_{2A} + \Delta'_1(p_1)_{2B} + O(V^3),\end{aligned} \tag{4.18}$$

$$\begin{aligned}\Delta'_2(p_1)_2 = {} & -\tfrac{1}{2} N_0 \langle 00| V^{(s)} |p_1, -p_1\rangle \\ & + \tfrac{1}{4} \sum_{p_2} n'(p_2) \alpha'_{(-)}(p_2) \\ & \times [\langle p_1, -p_1| V^{(s)} |p_2, -p_2\rangle \\ & + \langle p_2, -p_2| V^{(s)} |p_1, -p_1\rangle] \\ & + \tfrac{1}{2} N_0 \sum_{p_2 p_3} \alpha'_{(-)}(p_2) \alpha'_{(-)}(p_3) \\ & \times [\epsilon'(p_2) + \epsilon'(p_3) + \epsilon'(p_1)]^{-1} \\ & \times \{[1 + n'(p_2)][1 + n'(p_3)] \\ & \times C^{(T)\prime\prime}(p_1 p_2 p_3) C^{(T)(-,-)}(-p_1, -p_2, -p_3) \\ & - n'(p_2) n'(p_3) C''(p_1 p_2 p_3) \\ & \times C^{(-,-)}(-p_1, -p_2, -p_3)\} \\ & - \tfrac{1}{6} \sum_{p_2 p_3 p_4} \alpha'_{(-)}(p_2) \alpha'_{(-)}(p_3) \alpha'_{(-)}(p_4) \\ & \times [\epsilon'(p_2) + \epsilon'(p_3) + \epsilon'(p_4) + \epsilon'(p_1)]^{-1} \\ & \times \{[1 + n'(p_2)][1 + n'(p_3)][1 + n'(p_4)] \\ & \times D^{(T)\prime\prime\prime}(p_1 p_2 p_3 p_4) \\ & \times D^{(T)(-,-,-)}(-p_1, -p_2, -p_3, -p_4) \\ & - n'(p_2) n'(p_3) n'(p_4) D'''(p_1 p_2 p_3 p_4) \\ & \times D^{(-,-,-)}(-p_1, -p_2, -p_3, -p_4)\} \\ = {} & \Delta'_2(p_1)_0 + \Delta'_2(p_1)_1 \\ & + \Delta'_2(p_1)_{2A} + \Delta'_2(p_1)_{2B} + O(V^3),\end{aligned} \tag{4.19}$$

where $C_{ij}(p_1 p_2 p_3)$ and $D_{jkl}(p_1 p_2 p_3 p_4)$ are given by (C13) and (C15), respectively, and the corresponding quantities with $(-)$ superscripts involve subscripts $-i$, $-j$, $-k$, etc. From (4.17) and (4.18) we find that $\Delta_{1i}(p)$ is i dependent, as indicated earlier, and

$$\Delta_{2+}(p) = \Delta_{2-}^{(T)}(-p). \tag{4.20}$$

Finally the chemical potential g, obtained by substituting Eqs. (4.9), (4.15), and (5.14) into the second of Eqs. (3.15) and treating N_0 as an independent variable, is

$$\begin{aligned} g = {} & \tfrac{1}{2} N_0 \langle 00| V^{(s)} |00\rangle \\ & + \sum_p n'(p) \langle p0| V^{(s)} |p0\rangle + g_2 + O(V^3) \\ = {} & g_0 + g_1 + g_2 + O(V^3),\end{aligned} \tag{4.21}$$

where

$$\begin{aligned} g_2 = {} & -\tfrac{1}{2} \sum_p n'(p) \alpha'_{(-)}(p) \langle 00| V^{(s)} |p, -p\rangle \\ & + \tfrac{1}{6} \sum_{p_1 p_2 p_3} [\epsilon'(p_1) + \epsilon'(p_2) + \epsilon'(p_3)]^{-1} \\ & \times \{n'(p_1) n'(p_2) n'(p_3) C''(p_1 p_2 p_3) A^{(T)\prime\prime\prime}(p_1 p_2 p_3) \\ & - [1 + n'(p_1)][1 + n'(p_2)][1 + n'(p_3)] \\ & \times C^{(T)\prime\prime}(p_1 p_2 p_3) A'''(p_1 p_2 p_3)\}.\end{aligned} \tag{4.22}$$

In the derivation of the results (4.18), (4.19), (4.21), and (4.22), it is essential to hold constant the quantities $\alpha_i(p)$, as indicated in the functional derivatives of Eq. (3.15). By means of this somewhat arbitrary convention we are able to achieve agreement, for the DHSBG model, between the quasiparticle energy–momentum relation derived in this section and earlier work in the literature (see Appendix F). Thus, $\alpha_i(p)$ and $f_i(p)$ must be regarded as parameters in the theory, as indeed they are, for example, in the zeroth-order pair Hamiltonian theory before the diagonalization condition is used [see below Eq. (B13)].

The above expressions for $\Delta_i(p)$ and g agree completely with the perturbation-theory limit of the corresponding expressions obtained in quantum statistics.[12,16]

C. Explicit Expressions for $\epsilon_i(p)$

We come next to the calculation of $\epsilon_i(p)$. Upon substitution of (4.18), (4.19), (4.21), and (4.22) into (4.5), we can obtain an expression for $\epsilon_i(p)$ which is valid to second order in V. However, as is readily seen from (4.18) and (4.19), this gives an integral equation for $\epsilon_i(p)$ which we would have to solve to get a complete solution for $\epsilon_i(p)$ [note that Δ_{1i} and $\Delta_{2i}(p)$ are themselves functionals of $\epsilon_i(p)$ internally]. Here, we shall only give a general partial solution to $\epsilon_i(p)$ and then consider the special case of the DHSBG at the end of the section.

The partial solution to the integral equation (4.5) is found, by using (4.3), to be

$$\epsilon_i(p) = \tfrac{1}{2}[\epsilon_{1i}(p) - \epsilon_{1,-i}(-p)] + i\{\tfrac{1}{4}[\epsilon_{1i}(p) + \epsilon_{1,-i}(-p)]^2 - \Delta_{2i}(p)\Delta_{2,-i}(-p)\}^{\frac{1}{2}}. \quad (4.23)$$

From (4.23) we can conclude quite generally that

$$\epsilon_-(-p) = -\epsilon_+(p). \quad (4.24)$$

Moreover, in Appendix E it is shown, provided we neglect $\Delta_1'(p)_{2B}$, $\Delta_2'(p)_{2B}$, and the second term in (4.22), that

$$g = \Delta_1'(0) + \Delta_2'(0) + O(V^3). \quad (4.25)$$

Then, using (4.25) in (4.23), we can verify immediately that

$$\epsilon_i(0) \equiv 0, \quad (4.26)$$

which in turn implies that there is no gap in the excitation spectrum. However, if we include $\Delta_1'(p)_{2B}$ in $\Delta_1'(p)$, $\Delta_2'(p)_{2B}$ in $\Delta_2'(p)$, and the second term of (4.22) in g_2, then we will end up with a gap in the excitation spectrum. Justification for neglecting these terms is given in Appendix E. The result (4.26) is equivalent to assuming, quite generally, that

$$g \equiv \Delta_1'(0) + \Delta_2'(0) \quad (4.27)$$

to all orders in V. This equation can be called the "no gap theorem." A consequence of (4.27) is that

$$\alpha_{-i}(0) \equiv 1, \quad (4.28)$$

as can be established with the aid of (4.3), (4.7), and (4.26).

Returning to (4.23), we expand the rhs of the expression for $\epsilon_i(p)$ through second order in V to obtain the following results (for an isotropic system):

$$\epsilon_i(p) = \epsilon_i(p)_0 + \delta\epsilon_i(p)_2 + O(V^3), \quad (4.29)$$

where $\epsilon_i(p)_0$ is given by (2.17) with g replaced by $(g_0 + g_1)$ and

$$\begin{aligned}\delta\epsilon_i(p)_2 &= i\{\alpha_{-i}(p)_0[\Delta_{2i}(p)_2 + \Delta_{2,-i}(-p)_2]f_i(p)_0 \\ &\quad + f_i(p)_0\Delta_{1i}(p)_2 + f_{-i}(-p)_0\Delta_{1,-i}(-p)_2 \\ &\quad - ig_2[f_i(p)_0 + f_{-i}(-p)_0]\} \\ &= -\delta\epsilon_{-i}(-p)_2. \end{aligned} \quad (4.30)$$

Upon substituting (4.18) and (4.19) for $\Delta_1'(p)_2$ and $\Delta_2'(p)_2$ into (4.30) for $\delta\epsilon_i(p)_2$, we get after a few manipulations using (C12) and (C14), for Hermitian V,

$$\begin{aligned}\delta\epsilon_i(p)_2 &= -\tfrac{1}{2}N_0[if_i(p)_0] \\ &\quad \times \sum_{p_2p_3}\sum_{jl}[\epsilon_i(p)_0 + \epsilon_j(p_2)_0 + \epsilon_l(p_3)_0]^{-1} \\ &\quad \times [jf_j(p_2)_0][lf_l(lp_3)_0][1 + n_j(p_2) + n_l(p_3)] \\ &\quad \times A_{ijl}(pp_2p_3)A_{ijl}^{(T)}(pp_2p_3) \\ &\quad - \tfrac{1}{6}[if_i(p)_0]\sum_{p_2p_3p_4}\sum_{jlm} jlmf_j(p_2)_0f_l(p_3)_0f_m(p_4)_0 \\ &\quad \times [\epsilon_i(p)_0 + \epsilon_j(p_2)_0 + \epsilon_l(p_3)_0 + \epsilon_m(p_4)_0]^{-1} \\ &\quad \times \{[1 + n_j(p_2)][1 + n_l(p_3)][1 + n_m(p_4)] \\ &\quad - n_j(p_2)n_l(p_3)n_m(p_4)\} \\ &\quad \times A_{ijlm}(pp_2p_3p_4)A_{ijlm}^{(T)}(pp_2p_3p_4) \\ &\quad - ig_2[f_+(p)_0 + f_-(p)_0]. \end{aligned} \quad (4.31)$$

We can also derive the results of (4.29)–(4.31) directly, if we observe the following relation:

$$\begin{aligned}\epsilon_i(p) &= \omega(p) - g + \Delta_i(p) \\ &= i\{f_+(p)\omega_+(p) + f_-(-p)\omega_-(-p) \\ &\quad - [f_+(p) + f_-(-p)]g\}, \end{aligned} \quad (4.32)$$

where the second line of (4.32) follows from the first line and the relations $f_+(p) - f_-(-p) = 1$ and $\epsilon_-(-p) = -\epsilon_+(p)$. The second line of (4.32) is useful, because when $i = +$ it provides a useful form for $\epsilon_+(p)$ to use in comparison with other results which have appeared in the literature (see below).

We now consider the special case of the dilute hard-sphere Bose gas which is studied in detail in Appendix F. It is shown in Appendix F that if we neglect the second term of (4.31), then our expression agrees completely with that of Mohling and Morita.[17] In the zero-temperature limit we set $n_+(p) = 0$ and $n_-(-p) = -1$, in which case if we again neglect the second term of (4.31) then our expression for $\epsilon_+(p)$ agrees with that of Mohling and Sirlin.[18] Also, at $T = 0\,^\circ\mathrm{K}$ our expressions for the self-energies $\Delta_1'(p)_2$ and $\Delta_2'(p)_2$ agree completely with Belyaev[19] if we neglect $\Delta_1'(p)_{2B}$ and $\Delta_2'(p)_{2B}$.

The behavior of $\epsilon_+(p)$ in the $p \to 0$ limit has been investigated by Mohling and Morita,[17] who find that the low-momentum excitations are phonons. However, their expression for the velocity of phonons vanishes in the limit $T \to T_\lambda^-$, where T_λ is the transition temperature, whereas one would expect the velocity of phonons to change only slightly with temperature on the basis of experimental evidence. Sikora and Mohling[7] have shown theoretically that the phonon behavior for the DHSBG persists above the transition temperature (i.e., in the region T_λ^+). If we include the term $\Delta_1'(p)_{2B}$, our expression for $\epsilon_+(p)$ readily reduces to theirs at $T = T_\lambda^-$. This suggests that the term

$\Delta_1'(p)_{2B}$ plays an important role in the region of the transition temperature. We note in passing that to our knowledge none of the microscopic theories in the literature except that of Mohling, RamaRao, and Shea[12] seem to have terms in the expression for $\epsilon_i(p)$ which can be meaningful at the transition temperature T_λ.

The fact that our results are in agreement with previous work in the literature suggests that our prescription (3.15) for the calculation of the quasiparticle energies may be true quite generally. If so, then we have achieved considerable insight into the phenomenological theory of the Bose liquid. Certainly, the results in this section provide a microscopic basis for the phenomenological theory as it is presented in Sec. 3.

5. MOMENTUM DISTRIBUTION

In this section we derive an expression for the momentum distribution $\langle n(p)\rangle$ through second order in $V^{(s)}$. We are interested in such a calculation for three reasons: (1) to check the suggestion of the phenomenological theory, as given in Eq. (3.12); (2) to calculate the fraction of particles in the zero-momentum state; and (3) to obtain an expression for $\langle n(p)\rangle$ which is required in the study of correlation functions.

The momentum distribution is defined by

$$\langle n(p)\rangle \equiv \langle \Psi | a_p^\dagger a_p | \Psi\rangle / \langle \Psi \,|\, \Psi\rangle, \tag{5.1}$$

where the wavefunction $|\Psi\rangle$ is given in perturbation theory by

$$|\Psi\rangle = |\Psi_0\rangle + |\Psi_1\rangle + |\Psi_2\rangle + O(V^3), \tag{5.2}$$

with $|\Psi_1\rangle$ and $|\Psi_2\rangle$ defined by Eqs. (2.27) and (2.28). Upon substituting (5.2) into (5.1) and using (2.27) and (2.28), we find for $\langle n(p)\rangle$ the expression

$$\langle n(p)\rangle = \langle n(p)\rangle_0 + \langle n(p)\rangle_2 + O(V^3), \tag{5.3}$$

$$\langle n(p)\rangle_2 = 2A_1(p) + A_2(p), \tag{5.4}$$

where

$$A_1(p) = \langle \Psi_0 | a_p^\dagger a_p (1/b) H' (1/b) H' | \Psi_0\rangle, \tag{5.5}$$

$$A_2(p) = \langle \Psi_0 | (H')^\dagger (1/b)[a_p^\dagger a_p - \langle n(p)\rangle](1/b) H' | \Psi_0\rangle. \tag{5.6}$$

The expression (5.3) for $\langle n(p)\rangle$ can be simplified considerably by substituting the transformation equations (B13) and the zeroth-order expression (B17) for $\langle n(p)\rangle$ into (5.5) and (5.6) and then recombining the terms. The final result, for an isotropic system, is given by (for Hermitian V)

$$\langle n(p)\rangle_2 = 2A_{1a}(p) + A_{2a}(p), \tag{5.7}$$

where

$$A_{1a}(p) = f_+(p)_0 \alpha_-(p)_0 [2\epsilon_+(p)_0]^{-1} \times \sum_i i \langle \Psi_0 | [\xi_i(p)\xi_i(-p), H'](1/b) H' | \Psi_0\rangle, \tag{5.8}$$

$$A_{2a}(p) = [f_+(p)_0 + f_-(p)_0] \times \langle \Psi_0 | (H')^\dagger (1/b)^2 [\xi_p^\dagger \xi_p, H'] | \Psi_0\rangle. \tag{5.9}$$

It is now straightforward to evaluate the matrix elements in Eqs. (5.8) and (5.9), which are quite similar to those encountered in the calculation of the average energy (see Appendix C). We do not need the detailed expressions for $A_{1a}(p)$ and $A_{2a}(p)$ here, for we are interested only in a quantity $A(p)$ defined via

$$\langle n(p)\rangle \equiv \sum_i i f_i(p) n_i(p) + A(p). \tag{5.10}$$

Thus,

$$A(p) = 2A_{1a}(p) + A_{2a}(p) - \sum_i i \delta f_i(p) n_i(p), \tag{5.11}$$

where $\delta f_i(p)$ is defined in Eq. (4.1) and its explicit expression is given in Appendix D [see Eqs. (D1) and (D7)]. We obtain finally the following expression for $A(p)$, when the potential is Hermitian:

$$\begin{aligned} A(p) = {} & -\tfrac{1}{2} N_0 \sum_{ijkl} \sum_{p_2 p_3} [i f_i(p)_0 n_i(p)] \\ & \times [l f_l(p)_0][1 + \alpha_{-l}(p)_0 \alpha_{-i}(p)_0] \\ & \times [j f_j(p_2)_0 n_j(p_2)][k f_k(p_3)_0 n_k(p_3)] \\ & \times A_{ijk}(p p_2 p_3) A_{ijk}^{(T)}(p p_2 p_3) \\ & \times [\epsilon_j(p_2)_0 + \epsilon_k(p_3)_0 + \epsilon_i(p)_0]^{-1} \\ & \times [\epsilon_j(p_2)_0 + \epsilon_k(p_3)_0 + \epsilon_l(p)_0]^{-1} \\ & - \tfrac{1}{6} \sum_{ijklm} \sum_{p_2 p_3 p_4} [i f_i(p)_0 n_i(p)][l f_l(p)_0] \\ & \times [1 + \alpha_{-l}(p)_0 \alpha_{-i}(p)_0][j f_j(p_2)_0 n_j(p_2)] \\ & \times [k f_k(p_3)_0 n_k(p_3)][m f_m(p_4)_0 n_m(p_4)] \\ & \times A_{ijkm}^{(T)}(p p_2 p_3 p_4) A_{ljkm}(p p_2 p_3 p_4) \\ & \times [\epsilon_j(p_2)_0 + \epsilon_k(p_3)_0 + \epsilon_m(p_4)_0 + \epsilon_l(p)_0]^{-1} \\ & \times [\epsilon_j(p_2)_0 + \epsilon_k(p_3)_0 + \epsilon_m(p_4)_0 + \epsilon_i(p)_0]^{-1}, \end{aligned} \tag{5.12}$$

where $(p + p_2 + p_3) = 0$ in the first term and $(p + p_2 + p_3 + p_4) = 0$ in the second term.

The fraction of particles in the zero-momentum state is given by

$$\begin{aligned} \xi &= 1 - (n\Omega)^{-1} \sum_p \langle n(p)\rangle \\ &= 1 - (n\Omega)^{-1} \sum_i \sum_p [i f_i(p) n_i(p)] \\ &\quad - (n\Omega)^{-1} \sum_p A(p), \end{aligned} \tag{5.13}$$

where $A(p)$ is given by (5.12). We note from (5.12) that

$$\sum_p A(p) \neq 0. \tag{5.14}$$

This result contradicts the phenomenological theory prediction (3.12). It is not a surprising result, however, when one realizes that the number of quasiparticles in a degenerate Bose fluid is not conserved, as it is for a normal fluid. Thus, there is no one-to-one correspondence between particles and quasiparticles in a degenerate Bose fluid. Also, we may note that the wavefunction $|\Psi_0\rangle$ of (2.22) is not an eigenstate of the total particle number.

The DHSBG limit of the expression for ξ is obtained from (5.13) by expanding $f_i(p)$ through second order in the hard-sphere-gas parameter $(na^3)^{\frac{1}{2}}$ and using Eqs. (F1), (F6), and (F9)–(F12). The resultant expression specialized to $T = 0\,^\circ\mathrm{K}$, and obtained by setting $n_+ = 0$ and $n_- = -1$, disagrees[20] in part with an earlier result by Wu.[1] The lowest-order expression for ξ is given in Eq. (F8).

6. SUMMARY

The main results obtained in this paper will now be summarized. (1) We have derived an explicit expression, valid for all temperatures below T_λ, through second order in the interaction $V^{(s)}$. This result constitutes a useful check on any realistic calculation of $\langle E\rangle/N$. Since (in most of our calculations) we have not used the hermiticity of $V^{(s)}$, we have also applied it to the dilute hard-sphere Bose gas. (2) Basing it on the form of the average energy obtained in perturbation theory, we have proposed a phenomenological expression for $\langle E\rangle/N$ which is asserted to be valid even for He II. From this expression, useful prescriptions are deduced for the calculation of the quasiparticle energy and the chemical potential. This phenomenology is a generalization of the earlier work of Morita and Tanaka,[10] who neglected the depletion effect, known to play an important role in theoretical studies of He II. (3) The quasiparticle energies and the chemical potential have also been derived for all $T < T_\lambda$ through second order in $V^{(s)}$. The results agree completely with previous zero-temperature calculations. A significant feature is that our quasiparticle energies do not reduce to free-particle values when $T \to T_\lambda^-$ as they do for many of the earlier calculations. The importance of the nonvanishing self-energy terms near $T = T_\lambda^-$ has been emphasized.

APPENDIX A: LINEARLY MOVING SYSTEMS, STATISTICAL AVERAGING

The total energy expression (3.13) may properly be thought of as arising from a perturbation theory calculation (see end of Sec. 2) tediously carried out to all orders. If the degenerate Bose system is moving, then we must add the kinetic energy of bosons in the condensed state to the right-hand side of Eq. (3.13). When this state is one of linear motion with velocity v_S, then this added term is $\frac{1}{2}[N - \sum_p n'(p)]mv_S^2$. We now study the most probable, or equilibrium, state for He II in linear motion.

We find the most probable state for the case of linear motion by maximizing the entropy (3.18b) in the double-quasiparticle formulation, subject to the constraints of constant total energy E, constant total number of particles N, and constant total momentum $\mathbf{P}$. The variation of all of these quantities with respect to the occupation numbers $n'(p)$ and N gives

$$\kappa^{-1}\delta S = \sum_p \ln\left[\frac{1 + n'(p)}{n'(p)}\right]\delta n'(p), \tag{A1}$$

$$\delta E = \sum_p \epsilon'(p, mv_S)\delta n'(p) + \mu\delta N, \tag{A2}$$

$$\delta N = 0, \tag{A3}$$

$$\delta P = \sum_p p\delta n'(p) + mv_S\delta N. \tag{A4}$$

We have defined the single-particle momenta p to be measured relative to mv_S and have used Eqs. (3.14) and (3.21). Then, upon introducing the Lagrangian multipliers α, β, and $\boldsymbol{\gamma}$, we find the condition for the most probable state to be

$$\kappa^{-1}\delta S + \alpha\delta N - \beta\delta E + \gamma\cdot\delta P = 0. \tag{A5}$$

Equating the coefficient of $n'(p)$ to zero, we obtain

$$\ln\{[1 + \langle n'(p)\rangle]/\langle n'(p)\rangle\} = \beta\epsilon'(p, mv_S) - \gamma\cdot p, \tag{A6}$$

where we have denoted the value of $n'(p)$ for the most probable state by using the bracket symbols. [Note that $\langle n'(p)\rangle \neq \langle n(p)\rangle$, the momentum distribution of the system.] Similarly, by equating the coefficient of δN to zero, we obtain

$$\alpha = \beta\mu - \gamma\cdot mv_S. \tag{A7}$$

Upon solving Eq. (A6) for $\langle n'(p)\rangle$, we find

$$\langle n'(p)\rangle = \{e^{\beta[\epsilon'(p, mv_S) - \mathbf{v}_N\cdot p]} - 1\}^{-1}, \tag{A8}$$

where $\mathbf{v}_N \equiv \beta^{-1}\boldsymbol{\gamma}$ and β can be identified as $(\kappa T)^{-1}$ by considering the ideal-Bose-gas limit with $v_S = v_N = 0$.

We now refer back to (3.13), which can be expressed for equilibrium systems in terms of the distribution functions $\langle n'(p)\rangle$ and $N_0 = N - \sum_p \langle n(p)\rangle$, where $\langle n(p)\rangle$ is the momentum distribution. Since the plane-wave matrix elements of the helium-atom interaction potential are invariant under linear translations in

momentum space (Galilean invariance), we may readily conclude that the interaction energy terms in $\langle E \rangle$ can all be written with the momentum sums over p relative to mv_S. For the kinetic energy term, we make the substitution $p \to p + mv_S$ and obtain thereby the extra term in $\langle E \rangle$ indicated by (3.20). We also conclude from Galilean invariance that $\langle n'(p) \rangle$ cannot depend on v_S.

We next conclude from (A2) and (3.13), with (3.20) added, that

$$\epsilon'(p, mv_S) = \epsilon'(p) + p \cdot v_S, \tag{A9}$$

a result which can also be derived using the argument of Galilean invariance. Finally, we define a velocity **u** via

$$V_N \equiv v_S + u. \tag{A10}$$

Upon substituting (A9) into (A8) and using this definition, we obtain (3.19), where $\epsilon'(p) = \omega'(p) - g$. A mathematical justification of (3.21) occurs at this point in the analysis, if $\langle n'(p) \rangle$ is to be independent of v_S. We note with regard to (3.19) for $\langle n_\pm(p) \rangle$ that if $\epsilon_+(p) = -\epsilon_-(-p)$, as is shown in Sec. 4, then

$$\langle n_-(-p) \rangle = -[1 + \langle n_+(p) \rangle]. \tag{A11}$$

We can now deduce the finite-temperature expression for the total energy $\langle E \rangle$ in perturbation theory, by simply replacing the $n_\pm(p)$ in (4.9) and (4.15) by (3.19). Outside of this appendix, we usually drop the bracket symbols on statistically-averaged quantities for convenience, since it can always be determined what is meant in context.

We turn to the physical interpretation of the velocity u. In the limit $\Omega \to \infty$, one can easily verify from (3.19) that

$$\sum_p [\nabla_p \epsilon_+(p) - u] n_+(p) = 0. \tag{A12}$$

Since the distribution function for the thermal excitations of both kinds (+ and −) of quasiparticles is $n_+(p)$, we may conclude that u is the group velocity of the (normal-fluid) quasiparticles relative to the velocity of the bosons in the condensed state [see (A10)]. The relative velocity u can thus be interpreted as the drift velocity of the gas of quasiparticles.

APPENDIX B: PAIR HAMILTONIAN MODEL

In this appendix we summarize briefly the method for diagonalizing the "pair Hamiltonian" H_P, given by Eq. (2.11), in order to establish notation which proves to be quite useful in this paper. To begin, it is well known that $H_0(g)$ of (2.12) can be diagonalized by means of a Bogoliubov transformation.

In order to apply this transformation to diagonalize H_P, we have somehow to reduce H_P to a form which is similar to $H_0(g)$ of Eq. (2.12), i.e., to a form which is quadratic in the operators a_p and $a_p^\dagger$. Wentzel[5] has given a method, which we shall now outline, for accomplishing this objective. We define two new operators B_p and C_p to be

$$B_p \equiv a_p^\dagger a_p - \delta_p, \tag{B1}$$

$$C_p \equiv a_p a_{-p} - \eta_p, \tag{B2}$$

where δ_p and η_p are c-numbers and, at this stage, considered to be trial functions. In terms of these operators we can rewrite H_P of Eq. (2.11) as

$$H_P = H_P^{(0)} + H_P', \tag{B3}$$

where

$$H_P' = \tfrac{1}{2} \sum_{p_1 p_2} B_{p_1} B_{p_2} \langle p_1 p_2 | V^{(s)} | p_1 p_2 \rangle + \tfrac{1}{4} \sum_{p_1 p_2} C_{p_1}^\dagger C_{p_2} \langle p_1, -p_1 | V^{(s)} | p_2, -p_2 \rangle, \tag{B4}$$

$$H_P^{(0)} = U_P + \sum_p [a_p^\dagger a_p \epsilon_1(p)_0 - \tfrac{1}{2} \Delta_2^\dagger(p)_0 a_p^\dagger a_{-p}^\dagger - \tfrac{1}{2} \Delta_2(p)_0 a_p a_{-p}], \tag{B5}$$

and where the c-number quantities U_P, $\epsilon_1(p)_0$, and $\Delta_2(p)_0$ are given by

$$U_P = (\tfrac{1}{2} N_0)^2 \langle 00 | V^{(s)} | 00 \rangle - \tfrac{1}{2} \sum_{p_1 p_2} \delta_{p_1} \delta_{p_2} \langle p_1 p_2 | V^{(s)} | p_1 p_2 \rangle - \tfrac{1}{4} \sum_{p_1 p_2} \langle p_1, -p_1 | V^{(s)} | p_2, -p_2 \rangle \eta_{p_1}^\dagger \eta_{p_2}, \tag{B6}$$

$$\epsilon_1(p)_0 = \omega(p) - g + N_0 \langle p0 | V^{(s)} | p0 \rangle - \tfrac{1}{2} \langle pp | V^{(s)} | pp \rangle + \sum_{p_1} \langle pp_1 | V^{(s)} | pp_1 \rangle \delta_p \equiv \omega(p) - g + \Delta_1(p)_0, \tag{B7}$$

$$\Delta_2(p)_0 = -\tfrac{1}{2} N_0 \langle 00 | V^{(s)} | p, -p \rangle - \tfrac{1}{2} \sum_{p_2} \eta_{p_2}^\dagger \langle p_2, -p_2 | V^{(s)} | p, -p \rangle. \tag{B8}$$

The grand partition functions associated with $H_P^{(0)}$ and H_P are

$$\Omega f_p^{(0)} = \ln \{ \mathrm{Tr} \exp [-\beta H_P^{(0)}] \}, \tag{B9}$$

$$\Omega f_P = \ln \{ \mathrm{Tr} \exp [-\beta H_P] \}. \tag{B10}$$

Wentzel[5] has proved that for the trial functions δ_p and η_p which minimize $\Omega f_P^{(0)}$, i.e., for

$$\frac{\partial(\Omega f_P^{(0)})}{\partial \delta_p} = \frac{\partial(\Omega f_P^{(0)})}{\partial \eta_p} = 0, \tag{B11}$$

H_P' of (B4) does not contribute to Ωf_P in the infinite volume limit, i.e., $f_P = f_P^{(0)}$ in the limit $\Omega \to \infty$. Wentzel has also shown that the proper choices of δ_p and η_p consistent with (B11) are

$$\delta_p = \langle a_p^\dagger a_p \rangle, \quad \eta_p = \langle a_p a_{-p} \rangle, \quad \eta_p^\dagger = \langle a_p^\dagger a_{-p}^\dagger \rangle. \tag{B12}$$

Henceforth we shall neglect H_P' because it does not contribute to the thermodynamics of the system in the infinite volume limit when the choice (B12) of the trial functions is made. The Hamiltonian $H_P^{(0)}$ of (B5) is now formally similar to $H_0(g)$ of Eq. (2.12). We consider an isotropic system at rest; assume that $H_P^{(0)}$ is Hermitian. (This assumption is necessary in order to apply the Bogoliubov transformation.) We can then diagonalize $H_P^{(0)}$ by the Bogoliubov transformation

$$a_p = f_+^{\frac{1}{2}}(p)_0 \xi_p - f_-^{\frac{1}{2}}(-p)_0 \xi_{-p}^\dagger,$$
$$a_p^\dagger = f_+^{\frac{1}{2}}(p)_0 \xi_p^\dagger - f_-^{\frac{1}{2}}(-p)_0 \xi_{-p}, \qquad \text{(B13)}$$

where the operators ξ_p and $\xi_p^\dagger$ must satisfy Bose commutation relations and Eq. (2.21) in order that the transformation be canonical. The unknown quantities $f_\pm(p)_0$ are determined by demanding that the Hamiltonian be diagonal after the transformation (B13) has been made.

We shall not outline the diagonalization procedure, as it has been given at several places in the literature.[2,5] The results are summarized by Eqs. (2.13)–(2.21). We can also rewrite Eq. (2.13) for $H_P^{(0)}$ using (2.21) and the commutation relations for ξ_p and $\xi_p^\dagger$ as

$$H_P^{(0)} = U_P - \sum_p f_-(p)_0 \epsilon_+(p)_0 + \sum_p \epsilon_+(p)_0 \xi_p^\dagger \xi_p. \qquad \text{(B14)}$$

The Hamiltonian $H_P^{(0)}$ of Eq. (B14) can be interpreted as describing a set of noninteracting quasiparticles whose energy–momentum relation is given by (2.17). Thus the thermodynamics in the pair Hamiltonian model is the same as that of an ideal gas of quasiparticles. The grand potential $f_P^{(0)}$ of (B9) can readily be calculated using (B14), and one finds

$$f_P^{(0)} = -\beta U_P + \beta \sum_p f_-(p)_0 \epsilon_+(p)_0 - \sum_p \ln\,[1 - e^{-\beta \epsilon_+(p)_0}]. \qquad \text{(B15)}$$

With the aid of Eq. (B15), all the thermodynamic quantities of interest can be calculated. We quote a few relevant results:

$$n_\pm(p) = \pm \mathrm{Tr}\,[\rho \xi_\mp(p) \xi_\pm(p)] = \{\exp\,[\beta \epsilon_\pm(p)_0] - 1\}^{-1}, \qquad \text{(B16)}$$

$$\langle n(p)\rangle_0 = \sum_{i=\pm} i f_i(ip)_0 n_i(ip), \qquad \text{(B17)}$$

$$\langle a_p^\dagger a_{-p}^\dagger\rangle = \langle a_p a_{-p}\rangle = -\frac{\alpha_-(p)_0}{1 - \alpha_-^2(p)_0}[1 + 2n_+(p)] = -\sum_i i f_i(ip)_0 \alpha_{-i}(ip)_0 n_i(ip). \qquad \text{(B18)}$$

The average energy $\langle E\rangle_0$ is given by

$$\langle E\rangle_0 = \langle E_P\rangle + g \sum_p \langle n(p)\rangle_0. \qquad \text{(B19)}$$

Upon substituting (2.13) and (2.14) into (B19) and using (B17) and (B18), we can rewrite $\langle E\rangle_0$ as

$$E_0 \equiv \langle E\rangle_0 = (\tfrac{1}{2}N_0)^2 \langle 00|\, V^{(s)}\,|00\rangle + \sum_p \sum_i i f_i(ip)_0 n_i(ip)[\epsilon_i(ip)_0 + g] - \tfrac{1}{2}\sum_{p_1 p_2} \sum_{ij} [i f_i(ip_1)_0 n_i(ip_1)][j f_j(jp_2)_0 n_j(jp_2)] \times [\langle p_1 p_2|\, V^{(s)}\,|p_1 p_2\rangle + \tfrac{1}{2}\alpha_{-i}(ip_1)_0 \alpha_{-j}(jp_2)_0 \times \langle p_1, -p_1|\, V^{(s)}\,|p_2, -p_2\rangle]. \qquad \text{(B20)}$$

The chemical potential g can be calculated from the approximate expression

$$g = (\delta\langle E\rangle/\delta N_0)|_S, \qquad \text{(B21)}$$

and one finds

$$g = \tfrac{1}{2}N_0 \langle 00|\, V^{(s)}\,|00\rangle + \sum_p \sum_i i f_i(ip)_0 n_i(ip) \times [\langle p0|\, V^{(s)}\,|p0\rangle - \tfrac{1}{2}\alpha_{-i}(ip)_0 \langle 00|\, V^{(s)}\,|p, -p\rangle]. \qquad \text{(B22)}$$

APPENDIX C: THREE- AND FOUR-QUASIPARTICLE MATRIX ELEMENTS

The operators S_{ijk} and S_{ijkl} of (2.38) and (2.39) are given by

$$S_{ijk} \equiv (1/3!) \times \sum_{p_1 p_2 p_3} |n_+(ip_1) - i,\, n_+(jp_2) - j,\, n_+(kp_3) - k\rangle \times \langle n_+(kp_3) - k,\, n_+(jp_2) - j,\, n_+(ip_1) - i|, \qquad \text{(C1)}$$

$$S_{ijkl} \equiv (1/4!) \times \sum_{p_1 p_2 p_3 p_4} |n_+(ip_1) - i,\, n_+(jp_2) - j,\, n_+(kp_3) - k,\, n_+(lp_4) - l\rangle \times \langle n_+(lp_4) - l,\, n_+(kp_3) - k,\, n_+(jp_2) - j,\, n_+(ip_1) - i|. \qquad \text{(C2)}$$

It is easily verified that S_{ijk} and S_{ijkl} satisfy the following relations:

$$S_{ijk}^\dagger = S_{ijk}, \quad S_{ijkl}^\dagger = S_{ijkl}, \qquad \text{(C3)}$$

$$S_{ijk}^2 = S_{ijk}, \quad S_{ijkl}^2 = S_{ijkl}; \qquad \text{(C4)}$$

hence S_{ijk} and S_{ijkl} are projection operators. They are also orthogonal, S_{ijk} being a projector onto states which differ by three quasiparticles relative to $|\Psi_0\rangle$ and S_{ijkl} being a projector onto states which differ by four quasiparticles relative to $|\Psi_0\rangle$.

We next evaluate typical matrix elements occurring in (2.38) and (2.39). We define a quantity $B_{ijk}(p_1, p_2, p_3)$ by

$$B_{ijk}(p_1, p_2, p_3) \equiv \langle n_+(ip_1) - i,\, n_+(jp_2) - j,\, n_+(kp_3 - k|\, H_1'\,|\Psi_0\rangle, \qquad \text{(C5)}$$

$$
\begin{aligned}
&B_{ijk}(p_1, p_2, p_3) \\
&\quad = \tfrac{1}{2} N_0^{\frac{1}{2}} \sum_{lmn} \sum_{p_4 p_5 p_6} lmn f_i^{\frac{1}{2}}(lp_4)_0 f_m^{\frac{1}{2}}(mp_5)_0 f_n^{\frac{1}{2}}(np_6)_0 \\
&\qquad \times [\langle 0p_4 | V^{(s)} | p_5 p_6\rangle - \alpha_{-m}(mp_5)_0 \\
&\qquad \times \langle p_4, -p_5 | V^{(s)} | p_6 0\rangle] \\
&\qquad \times \langle n_+(ip_1) - i, n_+(jp_2) - j, n_+(kp_3) - k | \\
&\qquad \times \xi_{-l}(lp_4)\xi_m(mp_5)\xi_n(np_6) | \Psi_0\rangle. \qquad \text{(C6)}
\end{aligned}
$$

The matrix element in Eq. (C6) is straightforward to evaluate with the aid of (2.24), and after a few manipulations we obtain (in the infinite volume limit)

$$
\begin{aligned}
B_{ijk}(p_1, p_2, p_3) = &-N_0^{\frac{1}{2}} ijk A_{ijk}(p_1 p_2 p_3) \\
&\times \{[if_i(ip_1)_0 n_i(ip_1)][jf_j(jp_2)_0 n_j(jp_2)] \\
&\times [kf_k(kp_3)_0 n_k(kp_3)]\}^{\frac{1}{2}}, \qquad \text{(C7)}
\end{aligned}
$$

where

$$
\begin{aligned}
&A_{ijk}(p_1 p_2 p_3) \\
&\quad = \alpha_{-i}(ip_1)_0 \langle 0, -p_1 | V^{(s)} | p_2 p_3\rangle \\
&\qquad + \alpha_{-j}(jp_2)_0 \langle 0, -p_2 | V^{(s)} | p_1 p_3\rangle \\
&\qquad + \alpha_{-k}(kp_3)_0 \langle 0, -p_3 | V^{(s)} | p_1 p_2\rangle \\
&\qquad - \alpha_{-i}(ip_1)_0 \alpha_{-j}(jp_2)_0 \langle -p_1, -p_2 | V^{(s)} | p_3 0\rangle \\
&\qquad - \alpha_{-i}(ip_1)_0 \alpha_{-k}(kp_3)_0 \langle -p_1, -p_3 | V^{(s)} | p_2 0\rangle \\
&\qquad - \alpha_{-j}(jp_2)_0 \alpha_{-k}(kp_3)_0 \langle -p_2, -p_3 | V^{(s)} | p_1 0\rangle. \qquad \text{(C8)}
\end{aligned}
$$

Similarly, we need the four-quasiparticle generalization of Eqs. (C7) and (C8) for (2.39). We thus define a quantity $B_{ijkl}(p_1, p_2, p_3, p_4)$ by

$$
\begin{aligned}
&B_{ijkl}(p_1, p_2, p_3, p_4) \\
&\quad \equiv \langle n_+(ip_1) - i, n_+(j - p_2) - j, n_+(kp_3) - k, \\
&\qquad\qquad n_+(lp_4) - l | H_2' | \Psi_0\rangle. \qquad \text{(C9)}
\end{aligned}
$$

The evaluation of this matrix element is done in exactly the same way as above. We obtain (in the infinite volume limit)

$$
\begin{aligned}
&B_{ijkl}(p_1, p_2, p_3, p_4) \\
&\quad = ijkl A_{ijkl}(p_1 p_2 p_3 p_4) \\
&\qquad \times \{[if_i(ip_1)_0 n_i(ip_1)][jf_j(jp_2)_0 n_j(jp_2)] \\
&\qquad \times [kf_k(kp_3)_0 n_k(kp_3)][lf_l(lp_4)_0 n_l(lp_4)]\}^{\frac{1}{2}}, \qquad \text{(C10)}
\end{aligned}
$$

where

$$
\begin{aligned}
&A_{ijkl}(p_1 p_2 p_3 p_4) \\
&\quad = \alpha_{-i}(ip_1)_0 \alpha_{-j}(jp_2)_0 \langle -p_1, -p_2 | V^{(s)} | p_3 p_4\rangle \\
&\qquad + \alpha_{-i}(ip_1)_0 \alpha_{-k}(kp_3)_0 \langle -p_1, -p_3 | V^{(s)} | p_4 p_2\rangle \\
&\qquad + \alpha_{-i}(ip_1)_0 \alpha_{-l}(lp_4)_0 \langle -p_1, -p_4 | V^{(s)} | p_3 p_2\rangle \\
&\qquad + \alpha_{-j}(jp_2)_0 \alpha_{-k}(kp_3)_0 \langle -p_3, -p_2 | V^{(s)} | p_1 p_4\rangle \\
&\qquad + \alpha_{-j}(jp_2)_0 \alpha_{-l}(lp_4)_0 \langle -p_2, -p_4 | V^{(s)} | p_1 p_3\rangle \\
&\qquad + \alpha_{-k}(kp_3)_0 \alpha_{-l}(lp_4)_0 \langle -p_3, -p_4 | V^{(s)} | p_1 p_2\rangle. \\
&\qquad\qquad \text{(C11)}
\end{aligned}
$$

[Note that the excluded terms in the momentum sums of (2.35) give only $O(1)$ contributions to $\langle E\rangle$ in the infinite volume limit.]

Finally, we observe that Eq. (C8) can also be written as

$$
\begin{aligned}
A_{ijk}(p_1 p_2 p_3) = &C_{jk}(p_1 p_2 p_3) - \alpha_{-i}(ip_1)_0 \alpha_{-j}(jp_2)_0 \alpha_{-k}(kp_3)_0 \\
&\times C^{(T)}_{-j,-k}(-p_1, -p_2, -p_3), \qquad \text{(C12)}
\end{aligned}
$$

where

$$
\begin{aligned}
&C_{jk}(p_1 p_2 p_3) \\
&\quad = \alpha_{-j}(jp_2)_0 \langle 0, -p_2 | V^{(s)} | p_1 p_3\rangle \\
&\qquad + \alpha_{-k}(kp_3)_0 \langle 0, -p_3 | V^{(s)} | p_1 p_2\rangle \\
&\qquad - \alpha_{-j}(jp_2)_0 \alpha_{-k}(kp_3)_0 \langle -p_2, -p_3 | V^{(s)} | p_1 0\rangle, \qquad \text{(C13)}
\end{aligned}
$$

and the superscript (T) indicates the transpose of all matrix elements. Similarly,

$$
\begin{aligned}
&A_{ijkl}(p_1 p_2 p_3 p_4) \\
&\quad = D_{jkl}(p_1 p_2 p_3 p_4) \\
&\qquad + \alpha_{-i}(ip_1)_0 \alpha_{-j}(jp_2)_0 \alpha_{-k}(kp_3)_0 \alpha_{-l}(lp_4)_0 \\
&\qquad \times D^{(T)}_{-j,-k,-l}(-p_1, -p_2, -p_3, -p_4), \qquad \text{(C14)}
\end{aligned}
$$

where

$$
\begin{aligned}
&D_{jkl}(p_1 p_2 p_3 p_4) \\
&\quad = \alpha_{-k}(kp_3)_0 \alpha_{-l}(lp_4)_0 \langle -p_3, -p_4 | V^{(s)} | p_1 p_2\rangle \\
&\qquad + \alpha_{-j}(jp_2)_0 \alpha_{-k}(kp_3)_0 \langle -p_3, -p_2 | V^{(s)} | p_1 p_4\rangle \\
&\qquad + \alpha_{-j}(jp_2)_0 \alpha_{-l}(lp_4)_0 \langle -p_4, -p_2 | V^{(s)} | p_1 p_3\rangle. \\
&\qquad\qquad \text{(C15)}
\end{aligned}
$$

APPENDIX D: GENERALIZED WEIGHTING FACTORS

In this appendix we prove the result (4.8). For this purpose we need the general forms of the corrections $\delta f_i(p)$ and $\delta\alpha_{-i}(p)$, defined in Eqs. (4.1) and (4.2). These corrections can be derived by iterating Eqs. (3.8) and the first line of (4.3) and using definitions (4.4)–(4.7). The results are

$$
\delta f_i(p) = 2\alpha_{-i}(p)_0 [1 - \alpha_{-i}^2(p)_0]^{-1} f_i(p)_0 \delta\alpha_{-i}(p), \qquad \text{(D1)}
$$

$$
\begin{aligned}
\delta\alpha_{-i}(p) = &-[1 - \alpha_{-i}^2(p)_0]^{-1} [\epsilon_i(p)_0 + \epsilon_1(p)_0]^{-1} \\
&\times \{\alpha_{-i}(p)_0 [\Delta_{1+}(p)_2 + \Delta_{1-}(-p)_2] \\
&+ [1 + \alpha_{-i}^2(p)_0] \Delta_{2i}(p)_2\}, \qquad \text{(D2)}
\end{aligned}
$$

where $\Delta_{1i}(p)_2$ and $\Delta_{2i}(p)_2$ are the second-order corrections to the self-energies. The corrections $\delta f_i(p)$ and $\delta\alpha_{-i}(p)$ are second order in $V^{(s)}$, and hence the result (4.10) ensues. The result of (4.9) and (4.11) can be proved as follows:

$$
\begin{aligned}
&\sum_i i f_i(p) \tilde{\omega}_i(p)_0 n_i(p) \\
&\quad = \sum_i i f_i(p)_0 [\epsilon_i(p)_0 + g] n_i(p) \\
&\qquad + \sum_i i [\delta f_i(p) \epsilon_i(p)_0 + \delta\alpha_{-i}(p) \Delta_2(p)_0 f_i(p)_0] n_i(p) \\
&\qquad + O(V^3). \qquad \text{(D3)}
\end{aligned}
$$

Using (D1) and also the relation

$$[1 - \alpha_{-i}^2(p)_0] = 2\epsilon_i(p)_0[\epsilon_i(p)_0 + \epsilon_1(p)_0]^{-1} = -2\epsilon_i(p)_0\alpha_{-i}(p)_0[\Delta_2(p)_0]^{-1}, \quad \text{(D4)}$$

we can easily prove that

$$\delta f_i(p)\epsilon_i(p)_0 + \delta\alpha_{-i}(p)\Delta_2(p)_0 f_i(p)_0 \equiv 0. \quad \text{(D5)}$$

Substitution of (D5) into (D3) gives

$$\sum_i i f_i(p)\tilde{\omega}_i(p)_0 n_i(p) = \sum_i i f_i(p)_0[\epsilon_i(p)_0 + g]n_i(p) + O(V^3). \quad \text{(D6)}$$

Finally, substitution of (D6) into (B20) gives (4.9) after we also observe that $f_i(p)_0$ and $\alpha_{-i}(p)_0$ in the third term of (B20) can be replaced by $f_i(p)$ and $\alpha_{-i}(p)$ through second order in $V^{(s)}$. Equation (D4) can also be used to check that

$$\sum_i i f_i(ip) = \sum_i i f_i(ip)_0 = 1.$$

An explicit expression for $\delta\alpha_{-i}(p)$ can be obtained by substituting Eqs. (4.18) and (4.19) into the rhs of (D2). For completeness we list the result below, for Hermitian V, inasmuch as it is required in Sec. 5:

$$\begin{aligned}\delta\alpha_{-i}(p) = {} & \tfrac{1}{2}N_0[2\epsilon_i(p)_0]^{-1}\alpha_{-i}(p)_0 \sum_{p_2p_3}\sum_{jk} jk f_j(p_2)_0 f_k(p_3)_0 \\ & \times [1 + n_j(p_2) + n_k(p_3)] \\ & \times A_{ijk}^{(T)}(pp_2p_3)A_{-i,jk}(pp_2p_3) \\ & \times [\epsilon_j(p_2)_0 + \epsilon_k(p_3)_0 + \epsilon_i(p)_0]^{-1} \\ & + \tfrac{1}{6}[2\epsilon_i(p)_0]^{-1}\alpha_{-i}(p)_0 \\ & \times \sum_{p_2p_3p_4}\sum_{jkl} jkl f_j(p_2)_0 f_k(p_3)_0 f_l(p_4)_0 \\ & \times A_{ijkl}^{(T)}(pp_2p_3p_4)A_{-i,jkl}(pp_2p_3p_4) \\ & \times [\epsilon_i(p)_0 + \epsilon_j(p_2)_0 + \epsilon_k(p_3)_0 + \epsilon_l(p_4)_0]^{-1} \\ & \times \{[1 + n_j(p_2)][1 + n_k(p_3)][1 + n_l(p_4)] \\ & - n_j(p_2)n_k(p_3)n_l(p_4)\}. \end{aligned} \quad \text{(D7)}$$

APPENDIX E: NO-GAP THEOREM

The expression for the quasiparticle energy in the pair-Hamiltonian model possesses a gap in the zero-momentum limit as can be easily verified from (2.17). The reason for this gap can be understood in the following manner. If we examine carefully the expressions (4.18) and (4.19) for $\Delta_1'(p)_{2A}$ and $\Delta_2'(p)_{2A}$, respectively, then we find in the limit $p \to 0$ that these terms have the same form as the last term in (B22) or the first term in (4.22). This discovery leads one to suspect that $\Delta_2(p)_1$ of (4.19) and the last term in (B22) should be considered as being second order in perturbation theory. Thus, using (4.18), (4.19), and (4.22), we can verify, after some manipulations with the help of (C13), that

$$\begin{aligned} g^{(1)} \equiv {} & g_0 + g_1 - \tfrac{1}{2}\sum_p n'(p)\alpha'_{(-)}(p)\langle 00|\, V^{(s)}\,|p, -p\rangle \\ = {} & [\Delta_1'(0)_0 + \Delta_2'(0)_0] \\ & + \{\Delta_1'(0)_1 + \Delta_1'(0)_{2A} + \Delta_2'(0)_1 + \Delta_2'(0)_{2A}\}, \end{aligned} \quad \text{(E1)}$$

whereas

$$g^{(1)} \neq \Delta_1'(0)_0 + \Delta_2'(0)_0 + [\Delta_1'(0)_1 + \Delta_2'(0)_1]. \quad \text{(E2)}$$

A similar difficulty occurs with the second term in (4.22) for g_2, in the sense that if we had included this term along with $\Delta_1(p)_{2B}$ and $\Delta_2(p)_{2B}$ of (4.18) and (4.19), then we would have again ended up with a gap in $\epsilon_i(p)$ to second order. In the same way in which a gap obtained in the first order is eliminated in the second order, we believe that the second-order terms cited above will combine with certain third-order self-energies to eliminate the "second-order gap." In general, we will have to mix different orders in perturbation-theory calculations. This fact, i.e., the cancellation of a gap in any particular "order" by mixing with higher-order terms, has been proved by Hugenholtz and Pines[21] to all orders in perturbation theory at $T = 0\,^\circ\mathrm{K}$. Thus, we shall always truncate the expressions for g and $\Delta_2(p)$ in order to be consistent with the no-gap theorem.

APPENDIX F: DILUTE HARD-SPHERE BOSE GAS

In this appendix we show how to extract the "dilute hard-sphere Bose gas" (DHSBG) results from the perturbation-theory calculations.

The hard-sphere Bose gas was first studied extensively by Lee, Huang, and Yang,[22] who used the pseudopotential method to study the ground-state ($T = 0\,^\circ\mathrm{K}$) properties. The use of the pseudopotential for the DHSBG is equivalent to the following replacement, due to Wu,[1] in the Hamiltonian H of Eq. (2.1):

$$\langle k_1k_2|\, V^{(s)}\,|k_3k_4\rangle \to 16\pi a(\Omega)^{-1}\cos[\epsilon(k_3 - k_4)/p_0] \times \delta_{\mathrm{KR}}(k_1 + k_2 - k_3 - k_4), \quad \text{(F1)}$$

where a is the hard sphere diameter, $p_0 = (16\pi an\xi)^{\frac{1}{2}}$, and $\delta_{\mathrm{KR}}(\ )$ is a Kronecker-δ function. (We have also used units $\hbar = 2m = 1$.) We must set $\epsilon \to 0^+$ at the end of any calculation.

The DHSBG model is characterized by three lengths: (1) the interparticle distance $\ell = n^{-\frac{1}{3}}$, (2) the hard sphere diameter a, and (3) the thermal wavelength $\lambda_T = (4\pi\beta)^{-\frac{1}{2}}$. Three dimensionless parameters of interest in this model are (1) a/λ_T, (2) $(na^3)^{\frac{1}{2}}$, and (3) $na\lambda_T^2$. A dilute hard-sphere gas is characterized by the condition $(na^3)^{\frac{1}{2}} \ll 1$.

Equation (F1) shows that the pseudopotential $V^{(s)}$ is non-Hermitian. We have generally been careful to write down expressions correctly for non-Hermitian potentials. However, we have not been completely consistent, in this respect, in writing down the zeroth-order expressions of Sec. 2 and Appendix B. The difficulty there was that we cannot diagonalize $H_0(g)$ of (2.4) by a canonical transformation for a non-Hermitian potential. Wu[1] introduced the concept of "left" and "right" eigenstates to overcome this difficulty, and we can use the consequences of Wu's procedure whenever we encounter inconsistencies.

As was shown by Wu,[1] we can set $\epsilon \to 0^+$ in most of the first-order calculations from the outset. However, it is not permissible to set $\epsilon \to 0^+$ in second-order expressions before explicit calculations, although it is still permissible to set $\epsilon \to 0^+$ in the zeroth-order quantities $\alpha_{-i}(p)_0$ and $\epsilon_i(p)_0$. Thus, we can extract mostly correct DHSBG expressions from our results by using (F1).

Before we proceed to obtain explicit expressions for $\langle E\rangle$, $\epsilon_+(q)$, and $\langle n(q)\rangle$, we first list DHSBG limits of some important quantities which occur frequently in second-order calculations. The procedure for obtaining the proper DHSBG limits consists of three steps: (i) Use Eq. (F1) for $\langle k_1k_2|\, V^{(s)}\,|k_3k_4\rangle$ everywhere; (ii) expand the pair-Hamiltonian-model results to any desired order in the expansion parameters $(na^3)^{\frac{1}{2}}$ and (a/λ_T); (iii) follow the subtraction procedure described below to eliminate all divergences.

We now illustrate this procedure for the lowest-order DHSBG results. With prescriptions (i) and (ii) we obtain

$$\Delta_1(p) \cong W\xi, \tag{F2}$$

$$\Delta_2(p) \cong -(\tfrac{1}{2}W\xi), \tag{F3}$$

$$g_0 \cong \tfrac{1}{2}(W\xi), \tag{F4}$$

$$\epsilon_i(p)_0 \cong ip(p^2 + 16\pi an\xi)^{\frac{1}{2}} \equiv i\epsilon_p, \tag{F5}$$

$$\alpha_{-i}(p)_0 \cong 1 + 2y^2 - 2iy(y^2+1)^{\frac{1}{2}} \equiv g_{-i}(y), \tag{F6}$$

where $y = p/p_0$ and $W = 16\pi an$, and the fraction of particles in the zero-momentum state at $T = 0\,^\circ\mathrm{K}$ is given (in the lowest approximation) by

$$\begin{aligned}\xi &\cong 1 - (n\Omega)^{-1}\sum_p \langle n(p)\rangle_0 \\ &= 1 - (n\Omega)^{-1}\sum_p g^2(y)[1 - g^2(y)]^{-1},\end{aligned} \tag{F7}$$

with $g(y) \equiv g_-(y)$. The integral in (F7) can be readily evaluated, and one obtains

$$\xi = 1 - \frac{8}{3}\left(\frac{n\xi^3a^3}{\pi}\right)^{\frac{1}{2}} + O((na^3)^{\frac{1}{2}}), \tag{F8}$$

which is a well-known result first derived by Lee, Huang, and Yang.[22]

The quantities $A_{ijk}(p_1p_2p_3)$ and $A_{ijkl}(p_1p_2p_3p_4)$ of (C8) and (C11) occur very frequently in the second-order calculations of this work. Hence we list their DHSBG limits here:

$$\begin{aligned}A_{ijk}(p_1p_2p_3) = \left(\frac{16\pi a}{\Omega}\right)\{&\alpha_{-i}(y_1)_0\cos\epsilon\,|y_2 - y_3| \\ &+ \alpha_{-j}(y_2)_0\cos\epsilon\,|y_3 - y_1| \\ &+ \alpha_{-k}(y_3)_0\cos\epsilon\,|y_2 - y_1| \\ &- \alpha_{-i}(y_1)_0\alpha_{-j}(y_2)_0\cos\epsilon y_3 \\ &- \alpha_{-i}(y_1)_0\alpha_{-k}(y_3)_0\cos\epsilon y_2 \\ &- \alpha_{-j}(y_2)_0\alpha_{-k}(y_3)_0\cos\epsilon y_1\},\end{aligned} \tag{F9}$$

$$\begin{aligned}A^{(T)}_{ijk}(p_1p_2p_3) = \left(\frac{16\pi a}{\Omega}\right)\{&\alpha_{-i}(y_1)_0\cos\epsilon y_1 \\ &+ \alpha_{-j}(y_2)_0\cos\epsilon y_2 + \alpha_{-k}(y_3)_0\cos\epsilon y_3 \\ &- \alpha_{-i}(y_1)_0\alpha_{-j}(y_2)_0\cos\epsilon\,|y_1 - y_2| \\ &- \alpha_{-i}(y_1)_0\alpha_{-k}(y_3)_0\cos\epsilon\,|y_1 - y_3| \\ &- \alpha_{-j}(y_2)_0\alpha_{-k}(y_3)_0\cos\epsilon\,|y_2 - y_3|\}.\end{aligned} \tag{F10}$$

In the limit $\epsilon \to 0^+$, we get, for $A_{ijk}(p_1p_2p_3)$,

$$\begin{aligned}A_{ijk}(p_1p_2p_3) &= A^{(T)}_{ijk}(p_1p_2p_3) \\ &= \left(\frac{16\pi a}{\Omega}\right)\{\alpha_{-i}(y_1)_0 + \alpha_{-j}(y_2)_0 + \alpha_{-k}(y_3)_0 \\ &\quad - \alpha_{-i}(y_1)_0\alpha_{-j}(y_2)_0 - \alpha_{-i}(y_1)_0\alpha_{-k}(y_3)_0 \\ &\quad - \alpha_{-j}(y_2)_0\alpha_{-k}(y_3)_0\}.\end{aligned} \tag{F11}$$

For $A_{ijkl}(p_1p_2p_3p_4)$, we obtain

$$\begin{aligned}A_{ijkl}(p_1p_2p_3p_4) = (16\pi a/\Omega)&\times\{\alpha_{-i}(y_1)_0\alpha_{-j}(y_2)_0\cos\epsilon\,|y_3 - y_4| \\ &+ \alpha_{-k}(y_3)_0\alpha_{-l}(y_4)_0\cos\epsilon\,|y_1 - y_2| \\ &+ \alpha_{-i}(y_1)_0\alpha_{-k}(y_3)_0\cos\epsilon\,|y_2 - y_4| \\ &+ \alpha_{-j}(y_2)_0\alpha_{-l}(y_4)_0\cos\epsilon\,|y_3 - y_1| \\ &+ \alpha_{-i}(y_1)_0\alpha_{-l}(y_4)_0\cos\epsilon\,|y_2 - y_3| \\ &+ \alpha_{-j}(y_2)_0\alpha_{-k}(y_3)_0\cos\epsilon\,|y_4 - y_1|\},\end{aligned} \tag{F12}$$

etc.

We now list the results obtained for the chemical potential, the self-energies, and the average energy $\langle E\rangle$ by following the procedure described above (F2).

Chemical Potential

The DHSBG limit of the chemical potential is derived by referring to Eqs. (4.21) and (4.22). We find

$$g = g_0 + g_1 + g_2 + O(na^3) + O(na\lambda_T^2), \quad \text{(F13)}$$

where

$$g_0 = 8\pi an\xi = \tfrac{1}{2}W\xi, \quad \text{(F14)}$$

$$g_1 = W(n\Omega)^{-1}\sum_p \langle n(p)\rangle = W(1-\xi), \quad \text{(F15)}$$

$$g_2 = -\tfrac{1}{2}W(n\Omega)^{-1}\sum_p \frac{g(p)}{1-g^2(p)}[1+2n_+(p)]. \quad \text{(F16)}$$

A straightforward calculation of Eq. (F16) for g_2 shows that the integral is divergent. This divergence is well known and comes from the $y \to \infty$ limit at $T = 0$. To avoid this divergence, we subtract the $y \to \infty$ term from the rhs of (F16), i.e., according to Wu[1] we write

$$g_2 = -\tfrac{1}{2}W(n\Omega)^{-1}\sum_p \left(\frac{g(p)}{1-g^2(p)}[1+2n_+(p)] - \tfrac{1}{4}W\xi[\omega(p)-g_0]^{-1}\right). \quad \text{(F17)}$$

The real justification for this subtraction procedure is to avoid setting $\epsilon \to 0^+$ until the divergence in Eq. (F16) is apparent and then to take the limit $\epsilon \to 0^+$ with proper care. We adopt the above procedure wherever necessary below.

The results (F13)–(F17) agree with previous results of various authors.[23] The integral in (F17) can be evaluated easily at $T = 0\,^\circ$K. Then upon substituting the expression (F8) for ξ, we obtain for g at $T = 0\,^\circ$K the well-known result

$$g = (\tfrac{1}{2}W\xi)[1 + \tfrac{4}{3}(n\xi^3a^3/\pi)^{\frac{1}{2}} + O(na^3)]. \quad \text{(F18)}$$

The self-energies $\Delta_{1i}(p)$ and $\Delta_{2i}(p)$, for the DHSBG, can be obtained by applying the procedure outlined above (F2) to Eqs. (4.18) and (4.19). The final results are

$$\begin{aligned}\Delta_{1i}(p) &= (W\xi) + W(1-\xi) - \tfrac{1}{2}W^2\xi(n\Omega)^{-1}\\ &\times \sum_{\substack{p_2p_3\\(p+p_2+p_3=0)}}\sum_{jk}[1+n_j(p_2)+n_k(p_3)]\\ &\times [jkf_j(p_2)_0f_k(p_3)_0]\\ &\times [\epsilon_j(p_2)_0+\epsilon_k(p_3)_0+\epsilon_i(p)_0]^{-1}\\ &\times [\alpha_{-j}(p_2)_0+\alpha_{-k}(p_3)_0-\alpha_{-j}(p_2)_0\alpha_{-k}(p_3)_0]^2\\ &+ \tfrac{1}{4}W^2\xi(n\Omega)^{-1}\sum_{p_2}[\omega(p_2)-g_0]^{-1}\\ &+ \Delta_{1i}(p)_{2B}, \end{aligned} \quad \text{(F19)}$$

$$\begin{aligned}\Delta_{2i}(p) &= -(\tfrac{1}{2}W\xi) + \tfrac{1}{2}W(n\Omega)^{-1}\\ &\times \sum_{p_2}\left\{\frac{g(p_2)}{1-g^2(p_2)}[1+2n_+(p_2)]\right.\\ &\left. - (\tfrac{1}{4}W\xi)\cdot(\omega(p_2)-g_0)^{-1}\right\}\\ &+ (\tfrac{1}{2}W^2\xi)(n\Omega)^{-1}\sum_{\substack{p_2p_3\\(p+p_2+p_3=0)}}\sum_{jk}[1+n_j(p_2)+n_k(p_3)]\\ &\times [jf_j(p_2)_0kf_k(p_3)_0]\\ &\times [\alpha_{-j}(p_2)_0+\alpha_{-k}(p_3)_0-\alpha_{-j}(p_2)_0\alpha_{-k}(p_3)_0]\\ &\times [\alpha_{-j}(p_2)_0+\alpha_{-k}(p_3)_0-1]\\ &\times [\epsilon_j(p_2)_0+\epsilon_k(p_3)_0+\epsilon_i(p)_0]^{-1}+\Delta_{2i}(p)_{2B}. \end{aligned} \quad \text{(F20)}$$

If we neglect the terms $\Delta_{1i}(p)_{2B}$ and $\Delta_{2i}(p)_{2B}$ and take the $T = 0\,^\circ$K limit by setting $n_+(p) = 0$ in Eqs. (F19) and (F20), then we find that the above results agree completely with the earlier results of Belyaev.[19] The justification for neglecting the terms $\Delta_{1i}(p)_{2B}$ and $\Delta_{2i}(p)_{2B}$ near $T = 0\,^\circ$K, and their significance at $T \neq 0\,^\circ$K, will be discussed at the end of this appendix.

Average Energy

An expression for the average energy of the DHSBG can be deduced from Eqs. (B20) and (2.37), after expanding the pair-Hamiltonian result (B20) for E_0 through second order in $(na^3)^{\frac{1}{2}}$. We also need to use the lowest-order results given by Eqs. (F2)–(F8) and (F14) in Eqs. (2.37), (2.40), and (2.41). We shall not give the straightforward and tedious intermediate details here but will quote only the final result:

$$\langle E\rangle = E_0 + \sum_{ijk}(E_2)_{ijk} + \sum_{ijkl}(E_2)_{ijkl}, \quad \text{(F21a)}$$

where $(E_2)_{ijk}$ and $(E_2)_{ijkl}$ are obtained from (2.40) and (2.41) by substituting Eqs. (F9)–(F12) without setting $\epsilon \to 0^+$. The quantity E_0 in (F21) is given by

$$\begin{aligned}E_0/N &= \tfrac{1}{4}W[1+(1-\xi)^2] - (\tfrac{1}{2}W\xi)^2[2n\Omega]^{-1}\\ &\times \sum_p\{[\epsilon_p+\epsilon_1(p)_0]^{-1} - \tfrac{1}{2}[\omega(p)-g_0]^{-1}\}\\ &+ (n\Omega)^{-1}\sum_p n_+(p)\epsilon_p\\ &+ (n\Omega)^{-1}(g_1+g_2)\sum_p\langle n(p)\rangle_0\\ &+ \tfrac{1}{4}W\left[(n\Omega)^{-1}\sum_p\left(\frac{g(p)}{1-g^2(p)}[1+2n_+(p)]\right.\right.\\ &\left.\left. - (\tfrac{1}{4}W\xi)[\omega(p)-g_0]^{-1}\right)\right]^2 + E_{21}, \end{aligned} \quad \text{(F21b)}$$

where E_{21} denotes the (small) part[24] of the rhs of (B20) that is not included with the other terms of (F21b). Also $\epsilon_1(p)_0$, in the second term of (F21b), is

the lowest-order contribution in the expansion of (4.7), obtained by making the approximations indicated in (F2) and (F4).

At $T = 0\,^\circ\mathrm{K}$, the term $(E_2)_{ijkl}$ can be neglected for the following reason. The only dimensionless parameter after setting $n_+(p) = 0$ is $(n\xi a^3/\pi)^{\frac{1}{2}}$. Each momentum sum in (F21), when replaced by an integral, gives a factor of p_0^3 after it is converted to dimensionless variables. Each energy denominator gives a factor of $1/p_0^2$ and each matrix element gives p_0^2. With these observations one can easily check that $(E_2)_{ijkl} \sim (p_0)^{11}$ which is indeed of a higher order and can therefore be neglected. The term E_{21} in (F21b) can also be neglected in the zero-temperature limit for the same reasons.[25] In this limit then we find that the result (F21) agrees with Wu,[1] except for the term $(g_1 + g_2) \times (n\Omega)^{-1} \sum_p \langle n(p)\rangle_0$, which is third order in $(na^3)^{\frac{1}{2}}$. As noted by Wu,[1] and also by Hugenholtz and Pines,[21] the evaluation of the third-order terms in the energy is quite uncertain except for a logarithmic term which comes from a careful study of $(E_2)_{ijk}$. On the other hand, near the Bose–Einstein transition temperature T_λ, where ξ is small, the term $(E_2)_{ijkl}$ cannot be neglected, as has already been indicated at the end of Secs. 2 and 4.

Quasiparticle Energies

The quasiparticle energies $\epsilon_i(p)$ for the DHSBG are derived most easily by applying the procedure outlined above (F2) directly to Eqs. (4.29) and (4.31). We need to expand Eq. (2.17) for $\epsilon_i(p)_0$, through second order in $(na^3)^{\frac{1}{2}}$, by using (F2)–(F8) and also (F13)–(F15). The final result is

$$\epsilon_i(p) = i\epsilon_p + \tfrac{1}{2}iW(n\Omega)^{-1}[1 + g(y)]^2[1 - g^2(y)]^{-1} \times \sum_{p_2} \left(\frac{g(p_2)}{1 - g^2(p_2)} [1 + 2n_+(p_2)] - (\tfrac{1}{4}W\xi)[\omega(p_2) - g_0]^{-1} \right) + \delta\epsilon_i(p)_2, \quad \text{(F22)}$$

where $\delta\epsilon_i(p)_2$ is obtained explicitly by substituting Eqs. (F9), (F10), and (F12) into the rhs of Eq. (4.31).

In the temperature region near $T = 0\,^\circ\mathrm{K}$, the second term in (4.31) can be neglected for the same reasons mentioned below (F21b). Then the result (F22) agrees completely with the real part of the corresponding result derived earlier by Mohling and Morita[17] after the following additional observation is made. Mohling and Morita used a parameter X, defined to be the fraction of zero-momentum particles in the unperturbed plane-wave states, instead of ξ, which is the fraction of zero-momentum particles in the perturbed plane-wave states, i.e.,

$$(1 - X)N = \sum_{p \neq 0} n_+(p) \neq \sum_{p \neq 0} \langle n(p)\rangle = (1 - \xi)N. \quad \text{(F23)}$$

We can rewrite (F5) in terms of X as

$$\epsilon_i(p)_0 = ip[p^2 + 16\pi anX]^{\frac{1}{2}} - iW(2n\Omega)^{-1}[1 - g(p)]^2[1 - g^2(p)]^{-1} \times \sum_{p_2} \left(\frac{g^2(p_2)}{1 - g^2(p_2)} [1 + 2n_+(p_2)] - \tfrac{1}{4}W\xi[\omega(p) - g_0]^{-1} \right) + O(Wna^3). \quad \text{(F24)}$$

Equation (F24) is derived from (F5) by taking the difference between the two sides in the inequality (F23) and then using the lowest-order expression for $\langle n(p)\rangle$ given in (F7). Hence when we compare our result (F22) with that of Mohling and Morita, we must make the substitution indicated by the right-hand side of (F24). We need not evaluate the integrals in (F22) any further, because they have already been examined in Ref. 17 for various limiting cases of interest ($T \sim 0\,^\circ\mathrm{K}$ and $T \sim T_\lambda$). For completeness, we quote Mohling and Morita's result here for the case $T \sim 0\,^\circ\mathrm{K}$ and $p \ll p_0$:

$$\epsilon_i(p) = ip(16\pi an)^{\frac{1}{2}} \left[1 + 8\left(\frac{na^3}{\pi}\right)^{\frac{1}{2}} + O(na^3) + O\left(\frac{p^2}{p_0^2}\right) \right]. \quad \text{(F25)}$$

An unphysical feature in the above analysis is that unless care is exercised the phonon velocity vanishes as $T \to T_\lambda^-$. This fact can be verified immediately from (F22), since, if we let $\xi \to 0$ and neglect the second term in (4.31), we obtain $\epsilon_+(p) \sim p^2$ when $p \to 0$. We mention in this connection that, in the high-temperature region $T \sim T_\lambda$, Eq. (F5) for $\epsilon_i(p)_0$ is not a good first approximation because $\xi \to 0$; hence the iteration procedure used to obtain (F22) is no longer justified. In this limit $T \to T_\lambda^-$, the terms $\Delta_1(p)_{2B}$ and $\Delta_2(p)_{2B}$ of Eqs. (4.18) and (4.19), and hence the second term in (4.31), are expected to play an important role. This point is discussed at the end of Sec. 4. We have not pursued the analysis of $\epsilon_i(p)$ for the DHSBG any further. In particular, the detailed study of $\epsilon_i(p)$ in the temperature region $T \to T_\lambda^-$ is left for future investigation.

We now summarize the results of this appendix. (1) In the zero-temperature limit our expressions for the average energy and the quasiparticle energies agree with all previous work in the literature through second order in the hard-sphere gas parameter $(na^3)^{\frac{1}{2}}$.

(2) We have emphasized the importance of some additional terms in the quasiparticle energy and the average energy in the region $T \lesssim T_\lambda$. To our knowledge these terms have not been obtained previously. (3) Agreement with all previous work in the literature for $\epsilon_i(p)$ and $\langle E \rangle$, as mentioned in (1), gives support to the phenomenological theory developed in Sec. 3.

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[15] At this point we make the following sign reversals, for convenience, in the results of Sec. 2: $f_-(-p) \to f_-(p)$, $n_-(-p) \to n_-(p)$, $\epsilon_-(-p) \to \epsilon_-(p)$, and $\alpha_+(-p) \to \alpha_+(p)$. These sign reversals bring the notation of our perturbation-theory calculations into agreement with the conventions established in Sec. 3.

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Coupling of de Sitter Space-Time and Internal Symmetry

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(Received 31 August 1971)

Via Levi's radial splitting theorem for Lie algebras, all possible unifications of the de Sitter algebras with a real, simple, internal symmetry algebra are found.

1. INTRODUCTION

It has been pointed out by several authors[1–4] that, in view of the theorems of O'Raifeartaigh,[5] Jost,[6] and Segal,[7] Poincaré invariance is incompatible with the description of free particles in terms of linear representations of higher symmetry or noninvariance groups and the discreteness of the mass spectrum of the elementary particles. They suggest that the Poincaré group P should be replaced by a group which has P as a limiting case. The de Sitter groups, which are isomorphic to $SO(4, 1)$ and $SO(3, 2)$, are obvious canditates for a geometrical group, for they both contact into P in the limit in which the de Sitter radius goes to infinity; and

$$\lim_{\alpha \to 0} \alpha C_2 = p_\mu p^\mu,$$

where C_2 is the second-order Casimir operator of the de Sitter algebras, α is proportional to the curvature of the Universe, and p_μ is the momentum 4-vector in the Poincaré algebra. If P is a subalgebra of an algebra G, then it is the nilpotency of P in its adjoint action on G which leads to the result of the theorems mentioned above, namely that the spectrum of the mass-squared operator is either continuous or is a single point in an irreducible representation of G. Since this criterion of nilpotency is removed by replacing P by either of the de Sitter algebras,[1–3] it is worthwhile considering all possible unifications[8] $U(D, S)$, over the real field, of the de Sitter algebras $SO(4, 1)$ and $SO(3, 2)$, both denoted by D, with a real, simple, integral symmetry algebra S. A similar analysis for P has been carried out by Flato and Sternheimer.[8]

Let $A_1, \cdots, A_n$ be n finite-dimensional Lie algebras

(2) We have emphasized the importance of some additional terms in the quasiparticle energy and the average energy in the region $T \lesssim T_\lambda$. To our knowledge these terms have not been obtained previously. (3) Agreement with all previous work in the literature for $\epsilon_i(p)$ and $\langle E \rangle$, as mentioned in (1), gives support to the phenomenological theory developed in Sec. 3.

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Via Levi's radial splitting theorem for Lie algebras, all possible unifications of the de Sitter algebras with a real, simple, internal symmetry algebra are found.

1. INTRODUCTION

It has been pointed out by several authors[1–4] that, in view of the theorems of O'Raifeartaigh,[5] Jost,[6] and Segal,[7] Poincaré invariance is incompatible with the description of free particles in terms of linear representations of higher symmetry or noninvariance groups and the discreteness of the mass spectrum of the elementary particles. They suggest that the Poincaré group P should be replaced by a group which has P as a limiting case. The de Sitter groups, which are isomorphic to $SO(4, 1)$ and $SO(3, 2)$, are obvious canditates for a geometrical group, for they both contact into P in the limit in which the de Sitter radius goes to infinity; and

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where C_2 is the second-order Casimir operator of the de Sitter algebras, α is proportional to the curvature of the Universe, and p_μ is the momentum 4-vector in the Poincaré algebra. If P is a subalgebra of an algebra G, then it is the nilpotency of P in its adjoint action on G which leads to the result of the theorems mentioned above, namely that the spectrum of the mass-squared operator is either continuous or is a single point in an irreducible representation of G. Since this criterion of nilpotency is removed by replacing P by either of the de Sitter algebras,[1–3] it is worthwhile considering all possible unifications[8] $U(D, S)$, over the real field, of the de Sitter algebras $SO(4, 1)$ and $SO(3, 2)$, both denoted by D, with a real, simple, integral symmetry algebra S. A similar analysis for P has been carried out by Flato and Sternheimer.[8]

Let $A_1, \cdots, A_n$ be n finite-dimensional Lie algebras

over the same commutative field K. A Lie algebra X over K is defined to be a unification of $A_1, \cdots, A_n$, if there exist isomorphisms λ_k of A_k into X ($k = 1, \cdots, n$) such that

$$X = \lambda_1(A_1) + \cdots + \lambda_n(A_n),$$

where the direct sum of vector spaces is not necessarily implied, so that

$$\dim X \leq \dim A_1 + \cdots + \dim A_n.$$

It is customary to use the notation

$$X = U(A_1, \cdots, A_n).$$

The concept of a unification is useful as a minimality condition in finding a group which combines internal and external symmetries. However, there arises the conceptual difficulty of having a nonzero intersection of the internal and external symmetry groups which would imply, for example, that a space–time transformation could change the internal quantum numbers of a particle state. This conflict, in a higher symmetry scheme, between keeping the number of uninterpreted generators down to a minimum and avoiding a nonzero intersection of D and S, has led Vigier[4] to propose a novel solution to the problem, namely that there should be two de Sitter groups D_L and D_R which are left and right translations of D. D_L commutes with D_R and their Casimir invariants are equal. D_R is a subgroup of the unification, while D_L is taken to be the external space–time symmetry whose representations describe the states of free particles.

Examples of the unifications of P with an internal symmetry which have been considered are $R_9 \dot{+} SL(3, C) = U(P, SL(3, C))$, where R_9 is a nine-dimensional commutative ideal,[8] and

$$SU(2, 2) = U(P, SU(2, 1)).^{9-11}$$

Since the advent of the O'Raifeartaigh theorem, more attention has been paid to the de Sitter groups as space–time symmetries.

$$SU(2, 2) = U(D, SU(2, 1)),^{1,12,13}$$

and

$$SO(6, 1) = U(SO(4, 1), SU(4))^{4}$$

have both been considered, and it is worth noting that, in terms of certain representations of these groups, some progress has been made in finding a discrete mass spectrum for the strongly interacting particles.

As the natural unit of mass-squared in a de Sitter cosmology is very small because of the very large radius of the universe, Roman[2] and Roman and Koh[3] have made the proposal, which they have examined in detail, that the mass-squared operator should be $(R^2/r^2)\alpha C_2$, where R is the radius of the universe and r is the Compton wavelength of an elementary particle. This gives the correct magnitude for the masses under consideration.

2. ANALYSIS

Let $G = U(D, S)$, where S and D are both simple and where, by assumption,

$$\dim G \leq \dim D + \dim S. \tag{1}$$

By Levi's radial splitting theorem,[14] any Lie algebra G may be decomposed into the semidirect sum of its radical R and a semisimple subalgebra F, i.e.,

$$G = R \dot{+} \left(\overset{n}{\underset{i=1}{\oplus}} F_i \right), \tag{2}$$

since F, being semisimple, is a direct sum of a set of simple ideals F_i. This implies that

$$\dim G = \dim R + \sum_{i=1}^{n} \dim F_i.$$

Because of the semidirect sum structure of G, there exist[15] homomorphic mappings of S and D into F, with images that will be denoted by $S(F)$ and $D(F)$, respectively. As S and D are simple, $S(F) \approx O$ or S, and $D(F) \approx O$ or D, where $\approx$ denotes an isomorphic mapping. But, if $S(F) \approx O$, then S is contained in R, which is impossible. Thus $S(F) \approx S$ and similarly $D(F) \approx D$. There also exist homomorphic mappings of S and D into each F_i of (2) with images denoted by $S(F_i)$ and $D(F_i)$, respectively. Again $S(F_i) \approx O$ or S, and $D(F_i) \approx O$ or D. The three possibilities for embedding $S(F)$ and $D(F)$ in F will now be examined in turn.

(a) $\exists$ an F_i with $S(F_i) = O$ and $D(F_i) \approx D$.

Let $S(F_1) = O$, and $D(F_1) \approx D$; then $\dim D \leq \dim F_1$. From (1) and (2),

$$\dim \left(\overset{n}{\underset{i=2}{\oplus}} F_i \right) + \dim R \leq \dim S,$$

and so $\dim F_i \leq \dim S$ for $i \geq 2$. Therefore $\exists$ an F_j such that $F_j = S$. It follows that $F_1 \approx D$, $R \approx O$, and $F_i \approx O$ for $i \neq 1, j$. Thus

$$F = F_1 \oplus F_j = D(F_1) \oplus S(F_j),$$

where the image $D(F_j)$ need not be zero. If D is isomorphic to a subalgebra of S, then either $D(F_j) \approx D$ or $D(F_j) \approx O$. In the first case,

$$G = S \dot{+} D,$$

and, in the second,

$$G = S \oplus D.$$

If D is not isomorphic to a subalgebra of S, then $D(F_j) \approx O$, and only the second case can occur.

(b) $\exists$ an F_i with $D(F_i) = O$ and $S(F_i) \approx S$.

The treatment for case (b) is analogous to that for (a), with the result that either $G = D \overset{\frown}{+} S$ or $G = D \oplus S$. Clearly case (b) is not very restrictive as there are an infinite number of candidates for S.

(c) $\exists$ an F_i with $D(F_i) \approx D$ and $S(F_i) \approx S$. This is the most interesting type of unification.

Let $i = 1$. There are three possibilities, (C1), (C2), and (C3):

(C1) $F_1 \approx D$. Then $D \supseteq \approx S$, and, since dim $F_1 =$ dim D,

$$\sum_{i=2}^{n} \dim F_i + \dim R \leq \dim S. \tag{3}$$

If $\exists$ an F_j, $j \geq 2$, such that $S(F_j) \approx S$, then $R \approx O$, and

$$G = F_1 \oplus F_j, \quad F_1 \approx D, \quad F_j \approx S.$$

Then $G = D \overset{\frown}{+} S$ as in case (b) above. If $\exists$ an F_j $(j \geq 2)$ such that $D(F_j) \approx D$, then $R \approx O$, and so it is necessary that $S \approx D$, and

$$G = F_1 \oplus F_j, \quad F_1 \approx F_j \approx D.$$

The remaining possibility is that for F_j, $j \geq 2$, $S(F_j) \approx D(F_j) \approx O$, implying that

$$G = R \overset{\frown}{+} (F_1 \oplus F_2),$$

where

$$F_1 \approx D, \quad F_2 = \bigoplus_{i=2}^{n} F_i. \tag{4}$$

However, as F_2 commutes with F_1 and S and D have no images in F_2, it follows that F_2 is redundant, and (4) may be rewritten as

$$G = R \overset{\frown}{+} F_1, \quad F_1 \approx D. \tag{5}$$

For $D = SO(3, 2)$, $S = SO(3, 2)$, $SO(3, 1)$, $SO(2, 1)$ or $SO(3)$. From (3), dim $R \leq$ dim S. As R is a real Lie algebra, the elements of R must provide a basis for a real (but not necessarily irreducible) representation of F_1. The five- and ten-dimensional representations of $SO(3, 2)$ are the only real irreducible representations of dimension ≤ 10, so that the semidirect product in (5) survives only if $S = SO(3, 2)$ or $SO(3, 1)$ and the direct product otherwise. In the latter case R becomes redundant and may be discarded.

Similarly for $D = SO(4, 1)$, R need be kept only for $S = SO(4, 1)$ or $SO(3, 1)$. $ISO(4, 1)$ and $ISO(3, 2)$ are examples of such unifications. When $R \approx O$, $G = D \supset S$ and the unification is said to be banal.[8]

(C2) $F_1 \approx S$. Then $S \supseteq \approx D$. An analysis similar to (C1) may be carried out but it is not very restrictive since there are an infinite number of possibilities for S.

(C3) $D \neq F_1 \neq S$, so that

$$\max (10, \dim S) < \dim F_1 \leq \dim S + 10.$$

Since dim $F_1 > 10$, for $i \geq 2$ it follows that dim $F_i <$ dim S, and so the image $S(F_i) \approx S$ cannot be realized. Hence $i = 1$, and F is simple, i.e.

$$G = R \overset{\frown}{+} F, \quad F \text{ simple.}$$

It is now necessary to see if F actually exists, and, to do this, all simple Lie algebras F containing D and S, satisfying

$$\dim F \leq \dim S + \dim D, \tag{6}$$

are examined.

Let $\tilde{F}$, $\tilde{D}$, and $\tilde{S}$ be the complexifications of F, D, and S, respectively. There are two cases: (1) $\tilde{F}$ is simple or (2) $\tilde{F}$ is semisimple, being the direct sum of two isomorphic simple Lie algebras. These will be discussed in turn.

(1) $\tilde{D} \approx B_2$ is simple. $\tilde{S}$ is simple or $\tilde{S} = \tilde{S}_1 \oplus \tilde{S}_1'$, where $\tilde{S}_1 \approx \tilde{S}_1'$ (both simple). The inclusion $\tilde{F} \supset \tilde{S}$ must satisfy

$$10 < \dim \tilde{F} \leq \dim \tilde{S} + 10.$$

The only possible $\tilde{F} \supset \tilde{S}$ are

(i) $A_3 \supset B_2$, (ii) $B_3 \supset D_3$, (iii) $B_4 \supset D_4$,
(vi) $B_5 \supset D_5$, (v) $D_4 \supset B_3$, (vi) $D_5 \supset B_4$,
(vii) $G_2 \supset A_2$, (viii) $A_4 \supset A_3$, (ix) $A_3 \supset A_2$,
(x) $D_3 \supset D_2$.

Examination of the real forms of $\tilde{F}$ and its subalgebras shows that all the above pairs except (vii) $(G_2 \not\supset B_2)$ provide unifications. These are summarized in Table I. The method of Cornwell[16] for determining the real simple subalgebras of real simple lie algebras has been used to show that these are the *only* unifications, i.e., real forms of $\tilde{F}$ which contain none of the real forms of $\tilde{S}$ are omitted. For example, ND_{10}, one of the real forms of D_5, contains none of the real forms of B_4. ND_8 does not appear explicitly as a possible F, since it has been established[16] that it is locally isomorphic to $SO(6, 2)$.

(2) $\tilde{F} = \tilde{F}_1 \oplus \tilde{F}_1'$, $\tilde{F}_1 \approx \tilde{F}_1'$ (both simple); $\tilde{S} = \tilde{S}_1 \oplus \tilde{S}_1'$ or $\tilde{S}$ is simple, i.e., $\tilde{S}_1' = O$. In the mapping of $\tilde{S}$ and $\tilde{D}$ into $\tilde{F}$, let $\tilde{F}_1 \supset \approx \tilde{D}$ and $\tilde{S}_1$. Then, as

$$\dim \tilde{F} (= 2 \dim \tilde{F}_1) \leq 10 + 2 \dim \tilde{S}_1,$$

it is necessary to find all $\tilde{F}_1 \supset \tilde{S}_1$ which satisfy

$$10 \leq \dim \tilde{F}_1 \leq 5 + \dim \tilde{S}_1$$

The only candidates are (i) $\tilde{F}_1 \approx \tilde{S}_1$, (ii) $\tilde{F}_1 = A_3$, $\tilde{S}_1 = B_2$. These will be considered in turn.

TABLE I. Unifications for $\tilde{F}$ simple.

$\tilde{F}$	F	D	Compact S	Noncompact S
(i)	$SO(5,1)$	$SO(4,1)$	$SO(5)$	$SO(4,1)$
	$SO(4,2)$	both	—	$SO(4,1)$, $SO(3,2)$
	$SO(3,3)$	$SO(3,2)$	—	$SO(3,2)$
(ii) to (vi)	$SO(n,1)$ $6 \leq n \leq 10$	$SO(4,1)$	$SO(n)$	$SO(n-1,1)$
	$SO(p,q)$ $p+q=n+1$ $p>q>1$	both	—	$SO(r,s), r+s=n, r \leq p, s \leq q$
(viii)	$SU(4,1)$	$SO(4,1)$	$SU(4)$	$SU(3,1)$
	$SU(3,2)$	both	—	$SU(3,1)$, $SU(2,2)$
	$SL(5,R)$	both	—	$SL(4,R)$
(ix)	$SU(2,2)$	both	—	$SU(2,1)$
	$SL(4,R)$	$SO(3,2)$	—	$SL(3,R)$
(x)	$SO(5,1)$	$SO(4,1)$	—	$SO(3,1)$
	$SO(4,2)$	both	—	$SO(3,1)$
	$SO(3,3)$	$SO(3,2)$	—	$SO(3,1)$

(i) $\tilde{S} = \tilde{S}_1$, as otherwise dim F = dim S, contrary to the assumption that F strictly contains S, so that $2 \dim \tilde{S} = \dim \tilde{F} \leq \dim \tilde{S} + 10$, i.e.,

$$\dim \tilde{S} = \dim \tilde{F}_1 \leq 10.$$

However, $\tilde{F}_1 \supset \approx \tilde{D}$, so that $\dim \tilde{F}_1 = 10$. It follows that $\tilde{F}_1 \approx \tilde{S} \approx B_2$. Thus $F = SO(5, C)$, as this is the only real simple form of $B_2 \oplus B_2$.

(ii) Suppose $\tilde{S} \approx \tilde{S}_1$; then $\dim \tilde{F} \leq \dim B_2 + 10$, i.e., $\dim \tilde{F}_1 \leq 10$, and so, since $\tilde{F}_1 \supset \tilde{S}_1$, $\dim \tilde{F}_1 = 10$. But $\dim A_3 = 15$, so that $\tilde{S}_1' \approx \tilde{S}_1$ is necessary. Therefore, $S = B_2 \oplus B_2$, which only has $SO(5, C)$, considered as a real Lie algebra, as a simple real form.

The possible unifications are shown in Table II.

From Tables I and II, it can be seen that G can have the form $G = R \textcircled{+} F$ only in the case $F = SO(3,3)$, $S = SO(3,2)$, since $SO(3,3)$, being locally isomorphic to $SL(4,R)$, has a four-dimensional real representation. For example $G = ISL(4,R)$. In all other cases $G = R \oplus F$ and R, being redundant, may be discarded.

3. CONCLUSIONS

The unifications (a), (b), (C1), and (C2) are neither illuminating nor restrictive from a physical point of view, since they involve only the banal unifications, and direct or semidirect products of D and S.

The case (C3) provides nontrivial and nonbanal unifications, which, because of the restriction on their dimensions, are more likely to be of physical interest. They are displayed in Tables I and II, where it can be seen that there is no nontrivial unification of D and $SU(3)$. A similar result holds[8] for P and $SU(3)$. To establish the suitability of any of these algebras G, as a higher symmetry or noninvariance algebra, it is first of all necessary to see if the corresponding S has irreducible representations, capable of classifying a subset of the elementary particles. A representation of G can then (if possible) be constructed on these representation spaces of S, so that the spectrum of C_2 may be examined.

TABLE II. Unification for $\tilde{F}$ semisimple.

F	D	Compact S	Noncompact S
$SO(5, C)$	both	$SO(5)$	$SO(4,1)$, $SO(3,2)$
$SL(4, C)$	both	—	$SO(5, C)$

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Analytic Solutions of the Reference Spectrum Equation

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Analytic solutions of the fundamental equation of the reference spectrum method for nuclear matter are obtained in the cases of the square well and exponential potentials with hard cores. In the former case analytic wavefunctions are obtained for every partial wave L. These wavefunctions are expressed in terms of spherical Bessel and Hankel functions or in terms of spherical Bessel, Hankel, and Newmann functions of order L. In the latter case an analytic expression is obtained for the s wavefunction only. This is given in terms of the transcendental functions $G_{\pm\nu}(r)$ and $M_{\pm\nu}(r)$ which are defined as series of well-known functions. Finally an application is made of our results to the calculation of the well depth of a Λ particle in its ground state in nuclear matter.

1. INTRODUCTION

Considerable effort has been made for obtaining analytic solutions of various equations of mathematical physics. In particular, concerning quantum theory and its applications, the Schrödinger and also the Klein-Gordon and the Dirac equations have been studied in detail with the aim of obtaining analytic solutions for various types of potentials. We refer to the classical treatise of Morse and Feshbach[1] and also to the article of Vasudevan, Venkatesan, and Jagannathan.[2]

In the recent years the interest pertaining to the applications of quantum theory to nuclear problems has been shifted to the study of equations governing the motion of a pair of nucleons in a nucleus or in the (infinite) nuclear matter. One of the most popular methods which have been used in nuclear matter calculations is the reference spectrum method,[3–9] in which the radial differential equation for the relative motion of two nucleons in nuclear matter is linear but not homogeneous. In this method the following two approximations are made for the solution of the Brueckner integral equation. First the Pauli principle is neglected, that is, one puts $Q = 1$ in the Brueckner equation for the reaction matrix G. Secondly the actual energy spectrum in intermediate states is replaced by a "reference spectrum" of the form $A + k^2/2m^*$, where the constant A and the dimensionless effective mass $m^* = M^*/M$ are chosen in such a way that the reference spectrum is a good approximation to the actual one in the "important region": $3 \leqslant k \leqslant 5fm^{-1}$.

The reference spectrum method has a number of technical advantages: The Brueckner integral equation reduces to the reference spectrum equation, which, as we already stated, is a differential, linear, inhomogeneous equation. Also the contribution to the reference reaction matrix elements from the hard core can be approximately summed over angular momentum. The contribution from the outer part of the potential is determined by the solutions of the above mentioned differential equation. There is also an iteration expansion for the outer contribution which is analogous to Born series and has been called "modified Born expansion."[3]

The aim of this paper is to give analytic solutions of the fundamental equation of the reference spectrum method for nuclear matter in the cases in which the interparticle potential is of square well or exponential shape with hard core. Although in most calculations methods of numerical analysis are used for obtaining solutions of the reference spectrum equation, it seems desirable to have, whenever possible, analytic solutions as for the other differential equations of mathematical physics. One advantage of analytic solutions is that they are free of the inaccuracies involved in the solutions obtained by numerical integration. These inaccuracies depend on the step length of the integration and also on the large number which is taken as an upper boundary point (when the actual upper boundary point is infinity) and may not be negligible, if, for example, a parameter which appears in the differential equation has values in certain regions. Analytic solutions are therefore useful in making an independent check of the solutions obtained with numerical methods and also in deriving asymptotic behaviors, etc.

In the next section we describe briefly the way in which the (radial) fundamental equation of the reference spectrum method for nuclear matter is derived, and we write this equation in the form which will be used in this paper. In Sec. 3 we obtain analytic solutions of this equation, for any partial wave in the case of the square well potential with hard core. An analytic expression for the s-wave part of the diagonal reference reaction matrix element is also given. In

Sec. 4 we obtain the s-wave solution of the reference spectrum equation for the exponential potential with hard core. Finally in the last section we calculate the s-wave contribution to the "spin average" well depth of a Λ particle in its ground state in nuclear matter, using the analytic expressions obtained in the previous sections.

2. THE FUNDAMENTAL EQUATION OF THE REFERENCE SPECTRUM METHOD FOR NUCLEAR MATTER

We denote by an index R the quantities of the Brueckner theory calculated with the reference spectrum approximations. We follow also Ref. 3 and define all energy quantities such as e and v as the actual ones multiplied by $M \cdot \hbar^{-2}$. Thus these quantities are expressed in units fm^{-2}. In order to convert to MeV, we use the relation

$$1fm^{-2} = 41.467 \text{ MeV}. \tag{1}$$

The equation for the "reference reaction matrix" is

$$G^{\mathrm{R}} = v - ve_{\mathrm{R}}^{-1}G^{\mathrm{R}}, \tag{2}$$

where

$$e_{\mathrm{R}} = 2A + k'^2/m^* + P^2/m^* - H_{(k_0,P)}. \tag{3}$$

In this expression k' is the relative momentum in the intermediate state, $\mathbf{P}$ the "average" momentum ($2\mathbf{P}$ = momentum of the center of mass), $\mathbf{k}_0$ the initial relative momentum, and H the "starting energy."

Using the equations

$$G^{\mathrm{R}} = v\Omega^{\mathrm{R}} \quad \text{and} \quad \psi^{\mathrm{R}} = \Omega^{\mathrm{R}}\phi, \tag{4}$$

we can write Eq. (2), in coordinate space in the following form:

$$(\gamma^2 - \nabla^2)\zeta^{\mathrm{R}} = m^*v\psi^{\mathrm{R}}, \tag{5}$$

where

$$\gamma^2 = P^2 + m^*[2A - H_{(k_0,P)}]. \tag{6}$$

The function ζ is the "distortion of the wavefunction":

$$\zeta = \phi - \psi. \tag{7}$$

In the above equations ϕ is the free-particle wavefunction and ψ the actual one for the relative motion of a pair of particles in nuclear matter.

Equation (5) is the fundamental equation of the reference spectrum method.

Consider now the partial wave expansions

$$\begin{pmatrix} \phi \\ \psi^{\mathrm{R}} \\ \zeta^{\mathrm{R}} \end{pmatrix} = \frac{1}{k_0 r}\sum_{L=0}^{\infty}(2L+1)\cdot i^L \begin{pmatrix} k_0 r j_L(r) \\ u_L^{\mathrm{R}}(r) \\ \chi_L^{\mathrm{R}}(r) \end{pmatrix} P_L(\cos\theta). \tag{8}$$

The functions $k_0 r j_L(k_0 r)$ and $u_L^{\mathrm{R}}(r)$ satisfy the differential equations

$$\left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} + k_0^2\right)k_0 r j_L(k_0 r) = 0, \tag{9}$$

$$\left(\frac{d^2}{dr^2} - \frac{L(L+1)}{r^2} - \gamma^2\right)\chi_L^{\mathrm{R}}(r) = -m^*v(r)u_L^{\mathrm{R}}(r). \tag{10}$$

Substituting into (10) the

$$\chi_L^{\mathrm{R}}(r) = k_0 r j_L(k_0 r) - u_L^{\mathrm{R}}(r), \tag{11}$$

which is derived from Eqs. (7) (corresponding to the reference spectrum) and (8) and taking into consideration Eq. (9), we obtain the radial fundamental equation of the reference spectrum method for nuclear matter in the following form:

$$\frac{d^2u_L^{\mathrm{R}}(r)}{dr^2} - \left(\frac{L(L+1)}{r^2} + m^*v(r) + \gamma^2\right)u_L^{\mathrm{R}}(r) = -(k_0^2 + \gamma^2)k_0 r j_L(k_0 r), \quad c < r < \infty. \tag{12}$$

The $u_L^{\mathrm{R}}(r)$ has to vanish inside and at the hard core radius c and approach the unperturbed wavefunction for large separations. Therefore, the boundary conditions for $u_L^{\mathrm{R}}(r)$ are

$$u_L^{\mathrm{R}}(c) = 0, \quad \lim_{r\to\infty} u_L^{\mathrm{R}}(r) = k_0 r j_L(k_0 r). \tag{13}$$

The parameter γ in Eq. (12) is called the "healing parameter." The larger the value of γ, the more rapidly $u_L^{\mathrm{R}}(r)$ approaches the unperturbed wavefunction $k_0 r j_L(k_0 r)$.

We may finally remark that Eq. (12) can be easily transformed, by using, for example, the transformation

$$w_L^{\mathrm{R}}(r) = u_L^{\mathrm{R}}(r) - \left(k_0 r j_L(k_0 r) - k_0 c j_L(k_0 c)\cdot\frac{i\gamma r h^{(1)}(i\gamma r)}{i\gamma c h^{(1)}(i\gamma c)}\right) \tag{14}$$

into another one which has a different inhomogeneous term, but homogeneous boundary conditions: $w_L^{\mathrm{R}}(c) = 0$, $w_L^{\mathrm{R}}(\infty) = 0$. The conditions for the existence and the uniqueness of the solution for such a boundary value problem are very well known.[10,11]

3. REFERENCE SPECTRUM WAVEFUNCTIONS FOR THE SQUARE WELL WITH HARD CORE POTENTIAL

We consider the case in which the internucleon potential is of square well shape with hard core:

$$v(r)\begin{cases} = \infty, & 0 < r < c \\ = -v_0, & c < r < \alpha \\ = 0, & \alpha < r < \infty \end{cases}. \tag{15}$$

Although potentials of this type are crude approximations to the internucleon potential, they have been used for simplicity in various nuclear structure calculations.[12,13]

In the case of potential (15), Eq. (12) is written

$$\frac{d^2u_L^R(r)}{dr^2} - \left(\frac{L(L+1)}{r^2} - m^*v_0 + \gamma^2\right)u_L^R(r) = -(k_0^2+\gamma^2)k_0 r j_L(k_0 r), \quad c < r < \alpha, \tag{16a}$$

$$\frac{d^2u_L^R(r)}{dr^2} - \left(\frac{L(L+1)}{r^2} + \gamma^2\right)u_L^R(r) = -(k_0^2+\gamma^2)k_0 r j_L(k_0 r), \quad \alpha < r < \infty. \tag{16b}$$

We proceed in finding the $u_L^R(r)$ by distinguishing two cases according to the sign of the constant $-m^*v_0 + \gamma^2$:

(i) $$-m^*v_0 + \gamma^2 = g^2 > 0.$$

We treat first the case of the s waves because this is simpler and will indicate also how to find the solution for arbitrary L. Particular solutions of Eqs. (16a) and (16b) (with $L = 0$) are respectively

$$u_{0,p}^R(r) = [(k_0^2+\gamma^2)/(k_0^2+g^2)]\sin k_0 r, \quad c < r < \alpha, \tag{17a}$$

$$u_{0,p}^R(r) = \sin k_0 r, \quad \alpha < r < \infty. \tag{17b}$$

These particular solutions are very easily found since the differential equations for $L = 0$ are of constant coefficients and their inhomogeneous term of well-known type.

Using particular solutions (17a) and (17b) and the general solutions of the homogeneous equations corresponding to (16a) and (16b) with $L = 0$, we find that the s wave $u_0^R(r)$, which also satisfies the boundary conditions (13), is

$$u_0^R(r) = \begin{cases} A_s \sinh g(r-c) - \dfrac{(k_0^2+\gamma^2)}{(k_0^2+g^2)}(e^{-g(r-c)}\sin k_0 c - \sin k_0 r), & c \le r \le \alpha \quad (18a) \\ B_s e^{-\gamma r} + \sin k_0 r, & \alpha \le r < \infty. \quad (18b) \end{cases}$$

The constants A_s and B_s are determined by matching the $u_0^R(r)$ and du_0^R/dr at the point $r = \alpha$. The result is

$$A_s = [\gamma \sinh g(a-c) + g\cosh g(\alpha - c)]^{-1} \times \left(\frac{(k_0^2+\gamma^2)}{(k_0^2+g^2)}(\gamma - g)e^{-g(\alpha-c)}\sin k_0 c - \frac{m^*v_0}{(k_0^2+g^2)}(\gamma \sin k_0\alpha + k_0 \cos k_0\alpha)\right), \tag{19}$$

$$B_s = e^{\gamma\alpha}\left(A_s \sinh g(\alpha - c) - \frac{(k_0^2+\gamma^2)}{(k_0^2+g^2)}e^{-g(\alpha-c)}\sin k_0 c + \frac{m^*v_0}{(k_0^2+g^2)}\sin k_0\alpha\right). \tag{20}$$

We find now the solutions of (16a) and (16b) for arbitrary L. The fact that for $L = 0$ the particular solution of (16a) is

$$u_{0,p}^R(r) = [(k_0^2+\gamma^2)/(k_0^2+g^2)]\sin k_0 r = C_0'(k_0 r j_0(k_0 r))$$

suggests looking for a particular solution of the form $u_{L,p}^R(r) = C_L' k_0 r j_L(k_0 r)$. Substituting into Eq. (16a), we see that, the C_L' being chosen appropriately, $u_{L,p}^R(r)$ is indeed a particular solution. We find

$$u_{L,p}^R(r) = [(k_0^2+\gamma^2)/(k_0^2+g^2)]k_0 r j_L(k_0 r), \quad c < r < \alpha, \tag{21a}$$

and similarly

$$u_{L,p}^R(r) = k_0 r j_L(k_0 r), \quad \alpha < r < \infty. \tag{21b}$$

We choose as a fundamental set of solutions of the homogeneous equations corresponding to (16a) and (16b) the $(k_0 r h_L^{(1)}(igr),\ k_0 r h_L^{(2)}(igr))$ and $(k_0 r h_L^{(1)}(i\gamma r),\ k_0 r h_L^{(2)}(i\gamma r))$, respectively. Using these and also the particular solutions (21a) and (21b), we find that the $u_L^R(r)$ which satisfies the boundary conditions (13) is

$$u_L^R(r) = \begin{cases} k_0 r \cdot \Big[A_L \cdot [h_L^{(1)}(igc)\cdot h_L^{(2)}(igr) - h_L^{(1)}(igr)h_L^{(2)}(igc)] - \dfrac{(k_0^2+\gamma^2)}{(k_0^2+g^2)}\cdot\left(\dfrac{j_L(k_0 c)}{h_L^{(1)}(igc)}h_L^{(1)}(igr) - j_L(k_0 r)\right)\Big], & c \le r \le \alpha \quad (22a) \\ k_0 r \cdot [B_L \cdot h_L^{(1)}(i\gamma r) + j_L(k_0 r)], & \alpha \le r < \infty. \quad (22b) \end{cases}$$

The constants A_L and B_L are determined by matching $u_L^R(r)$ and $du_L^R(r)/dr$ at $r = \alpha$. The two equations which we obtain in this way contain derivatives of spherical Bessel and Hankel functions. We can eliminate these derivatives by using the relation

$$\frac{dj_L(\rho)}{d\rho} = \frac{L}{\rho}j_L(\rho) - j_{L+1}(\rho), \tag{23}$$

which we obtained by using Eqs. (15.9) and (15.10) of Ref. 14. In this way we find the following formulas

for A_L and B_L:

$$\begin{aligned}A_L = \{&ig\alpha h_L^{(1)}(i\gamma\alpha)[h_{L+1}^{(1)}(ig\alpha)h_L^{(2)}(igc)\\&- h_L^{(1)}(igc)h_{L+1}^{(2)}(ig\alpha)]\\&+ i\gamma\alpha h_{L+1}^{(1)}(i\gamma\alpha)[h_L^{(1)}(igc)h_L^{(2)}(ig\alpha)\\&- h_L^{(1)}(ig\alpha)h_L^{(2)}(igc)]\}^{-1}\\&\times\left(\frac{(k_0^2+\gamma^2)}{(k_0^2+g^2)}\cdot\frac{j_L(k_0c)}{h_L^{(1)}(igc)}[i\gamma\alpha h_{L+1}^{(1)}(i\gamma\alpha)h_L^{(1)}(ig\alpha)\right.\\&- h_L^{(1)}(i\gamma\alpha)ig\alpha h_{L+1}^{(1)}(ig\alpha)]\\&-\frac{m^*v_0}{(k_0^2+g^2)}[j_L(k_0\alpha)i\gamma\alpha h_{L+1}^{(1)}(i\gamma\alpha)\\&\left.- k_0\alpha j_{L+1}(k_0\alpha)h_L^{(1)}(i\gamma\alpha)]\right),\end{aligned}\tag{24}$$

$$\begin{aligned}B_L = [h_L^{(1)}(i\gamma\alpha)]^{-1}&\left(A_L[h_L^{(1)}(igc)h_L^{(2)}(ig\alpha)\right.\\&- h_L^{(1)}(ig\alpha)h_L^{(2)}(igc)]\\&-\frac{(k_0^2+\gamma^2)}{(k_0^2+g^2)}\frac{j_L(k_0c)}{h_L^{(1)}(igc)}h_L^{(1)}(ig\alpha)\\&\left.+\frac{m^*v_0}{(k_0^2+g^2)}j_L(k_0\alpha)\right).\end{aligned}\tag{25}$$

Note that A_0 and B_0 differ from A_s and B_s by a factor. A similar remark holds for C_0 and D_0 in case (ii):

(ii) $$-m^*v_0 + \gamma^2 = -g^2 < 0.$$

We choose in this case as a fundamental set of solutions of the homogeneous equation corresponding to Eq. (16a) the $(k_0rj_L(g_0r),\ k_0rn_L(gr))$, where $n_L(gr)$ is the spherical Neumann function of order L.[14] The results at which we arrive are the following: For the s-wave solution,

$$u_0^{\mathrm{R}}(r) = \begin{cases} C_s\sin g(r-c) \\ \quad -\dfrac{(k_0^2+\gamma^2)}{(k_0^2-g^2)}\left[\dfrac{\sin k_0c}{\sin gc}\sin gr - \sin k_0r\right], \\ \qquad\qquad c \le r \le \alpha, \quad (26a) \\ D_se^{-\gamma r} + \sin k_0r, \quad \alpha \le r < \infty, \quad (26b)\end{cases}$$

where

$$\begin{aligned}C_s = [g\cos g(\alpha-c) &+ \gamma\sin g(\alpha-c)]^{-1}\\&\times\left(\frac{(k_0^2+\gamma^2)}{(k_0^2-g^2)}\frac{\sin k_0c}{\sin gc}(g\cos g\alpha+\gamma\sin g\alpha)\right.\\&\left.-\frac{m^*v_0}{(k_0^2-g^2)}(k_0\cos k_0\alpha+\gamma\sin k_0\alpha)\right),\end{aligned}\tag{27}$$

$$\begin{aligned}D_s = e^{\gamma\alpha}&\left(C_s\sin g(\alpha-c) - \frac{(k_0^2+\gamma^2)}{(k_0^2-g^2)}\frac{\sin k_0c}{\sin gc}\sin g\alpha\right.\\&\left.+\frac{m^*v_0}{(k_0^2-g^2)}\sin k_0\alpha\right),\end{aligned}\tag{28}$$

while, for an arbitrary partial wave,

$$u_L^{\mathrm{R}}(r) = \begin{cases} k_0r\left[C_L[j_L(gc)n_L(gr) - j_L(gr)n_L(gc)]\right. \\ \quad \left. -\dfrac{(k_0^2+\gamma^2)}{(k_0^2-g^2)}\left(\dfrac{j_L(k_0c)}{j_L(gc)}j_L(gr) - j_L(k_0r)\right)\right], \\ \qquad\qquad c \le r \le \alpha, \quad (29a) \\ k_0r[D_L\cdot h_L^{(1)}(i\gamma r) + j_L(k_0r)], \\ \qquad\qquad \alpha \le r < \infty, \quad (29b)\end{cases}$$

where

$$\begin{aligned}C_L = \{&g\alpha h_L^{(1)}(i\gamma\alpha)[j_{L+1}(g\alpha)n_L(gc) - j_L(gc)n_{L+1}(g\alpha)]\\&+ i\gamma\alpha h_{L+1}^{(1)}(i\gamma\alpha)[j_L(gc)n_L(g\alpha) - j_L(g\alpha)n_L(gc)]\}^{-1}\\&\times\left(\frac{(k_0^2+\gamma^2)}{(k_0^2-g^2)}\frac{j_L(k_0c)}{j_L(gc)}[i\gamma\alpha h_{L+1}^{(1)}(i\gamma\alpha)j_L(g\alpha)\right.\\&- h_L^{(1)}(i\gamma\alpha)g\alpha j_{L+1}(g\alpha)]\\&-\frac{m^*v_0}{(k_0^2-g^2)}[j_L(k_0\alpha)i\gamma\alpha h_{L+1}^{(1)}(i\gamma\alpha)\\&\left.- k_0\alpha j_{L+1}(k_0\alpha)h_L^{(1)}(i\gamma\alpha)]\right),\end{aligned}\tag{30}$$

$$\begin{aligned}D_L = [h_L^{(1)}(i\gamma\alpha)]^{-1}&\\&\times\left(C_L[j_L(gc)n_L(g\alpha) - j_L(g\alpha)n_L(gc)]\right.\\&\left.-\frac{(k_0^2+\gamma^2)}{(k_0^2-g^2)}\frac{j_L(k_0c)}{j_L(gc)}j_L(g\alpha) + \frac{m^*v_0}{(k_0^2-g^2)}j_L(k_0\alpha)\right).\end{aligned}\tag{31}$$

We may remark that in the case $-m^*v_0 + \gamma^2 < 0$ the forms of the above reference wavefunctions are similar to those obtained by Razavy and Sprung.[5] These authors applied the reference spectrum method to the boundary condition model of Feshbach and Lomon.[15,16] However, there are differences as far as the determination of the constants is concerned, because the solution they obtained was meant to be used only in connection with the Boundary condition model.

Before ending this section it may be worthwhile to point out that in some cases we can use the analytic reference wavefunctions we have derived in order to obtain analytic expressions of the reference reaction matrix elements. As an example, consider the s-wave part of the "direct" diagonal element of G^{R} for two particles of relative momentum k_0 and distinct (spin-isospin) states. Using expression (5.1) of Ref. 3, we have (for any m^*)

$$\langle k_0|\, G^{\mathrm{R}}\,|k_0\rangle_{L=0} = \frac{4\pi(k_0^2+\gamma^2)}{m^*k_0^2}\int_0^\infty \chi_0^{\mathrm{R}}(r)\sin k_0r\,dr.\tag{32}$$

This can be calculated analytically with our wavefunctions (18a) and (18b). After a rather lengthy calculation we arrive at the following result:

$$\langle k_0|\, G^{\mathrm{R}}\,|k_0\rangle_{L=0} = \frac{4\pi v_0}{k_0^2(k_0^2+g^2)}\Bigg[B_s e^{-\gamma a}(\gamma \sin k_0\alpha + k_0 \cos k_0\alpha) + \frac{(k_0^2+\gamma^2)}{m^* v_0}\sin k_0 c \times \left(\frac{(k_0^2+\gamma^2)}{(k_0^2+g^2)}(g \sin k_0 c + k_0 \cos k_0 c) + gA_s\right) + \frac{(k_0^2+\gamma^2)^2}{2m^* v_0}\left(c - \frac{\sin 2k_0 c}{2k_0}\right) - \frac{(k_0^2+\gamma^2)}{2}\left(\alpha - \frac{\sin 2k_0\alpha}{2k_0}\right)\Bigg], \tag{33}$$

where A_s and B_s are given by expressions (19) and (20). The above result was checked by using the alternative expression for $\langle k_0|\, G^{\mathrm{R}}\,|k_0\rangle_{L=0}$, that is, the expression in terms of u_L^{R} instead of χ_L^{R} (see Sec. 5 of Ref. 3).

4. REFERENCE SPECTRUM s WAVEFUNCTIONS FOR THE EXPONENTIAL WITH HARD CORE POTENTIAL

In this section we obtain the s-wave solution of Eq. (12), when the internucleon potential is of exponential shape with hard core

$$v(r) = \begin{cases} \infty, & r < c \\ -v_0 e^{-\mu(r-c)}, & c < r \end{cases}. \tag{34}$$

Potentials of this shape have been used extensively in various nuclear structure calculations.[17–23] Among the most popular potentials of this type are the "Moszkowski and Scott potential"[17] (sometimes referred as "standard hard core potential") and also the Kállio–Kolltveit potential,[18] which has different strengths and ranges in singlet and triplet spin states.

With potential (34), Eq. (12) for $L = 0$ becomes

$$\frac{d^2u_0^{\mathrm{R}}(r)}{dr^2} + (m^* v_0 e^{\mu c} e^{-\mu r} - \gamma^2)u_0^{\mathrm{R}}(r) = -(k_0^2+\gamma^2)\sin k_0 r, \quad c < r < \infty. \tag{35}$$

The corresponding homogeneous equation can be easily solved using the transformation $z = 2(m^* v_0 e^{\mu c}/\mu^2)^{\frac{1}{2}} e^{-\mu r/2}$ (see p. 1670 of Ref. 1). The result is

$$u_{0,h}^{\mathrm{R}}(r) = C_1 J_\nu((2/\mu)(m^* v_0)^{\frac{1}{2}} e^{-\mu(r-c)/2}) + C_2 J_{-\nu}((2/\mu)(m^* v_0)^{\frac{1}{2}} e^{-\mu(r-c)/2}), \tag{36}$$

where

$$J_\nu((2/\mu)(m^* v_0)^{\frac{1}{2}} e^{-\mu(r-c)/2}) \equiv u_1(r), \qquad J_{-\nu}((2/\mu)(m^* v_0)^{\frac{1}{2}} e^{-\mu(r-c)/2}) \equiv u_2(r) \tag{37}$$

are Bessel functions of the first kind of order ν and $-\nu$, respectively[24] ($\nu = 2\gamma/\mu$, $\nu \neq$ integer). If ν happens to be an integer n, it is well known that J_n and J_{-n} are not linearly independent. In such a case we can use as a fundamental set of solutions, the J_n and Y_n,[24] where Y_n is the Bessel function of the second kind (or Neumann's function). The Green's function which we need for solving Eq. (35) can be constructed in the usual way.[25] We find

$$G(r, r') = \begin{cases} \dfrac{\pi[(u_2(c)/u_1(c))\cdot u_1(r) - u_2(r)]\cdot u_1(r')}{\mu \sin \nu\pi}, \\ \qquad\qquad c \le r < r', \quad (38a) \\ \dfrac{\pi[(u_2(c)/u_1(c))u_1(r') - u_2(r')]\cdot u_1(r)}{\mu \sin \nu\pi}, \\ \qquad\qquad r' \le r < \infty. \quad (38b) \end{cases}$$

In calculating the Wronskian of $W[u_<, u_>]$ where

$$u_<(r') = [u_2(c)/u_1(c)]\cdot u_1(r') - u_2(r'), \qquad u_>(r') = u_1(r'), \tag{39}$$

we used the expression[24]

$$J_\nu(z)\frac{dJ_{-\nu}(z)}{dz} - J_{-\nu}(z)\frac{dJ_\nu(z)}{dz} = -\frac{2\sin\nu\pi}{\pi z}. \tag{40}$$

In terms of the Green's function, the solution of an inhomogeneous second-order differential equation with inhomogeneous boundary condition is given by a quite well-known formula (Ref. 25, Chap. IV, 11.5). Applying this to our case and observing that the surface term is zero, we arrive after some algebra at the following expression for $u_0^{\mathrm{R}}(r)$:

$$\begin{aligned} u_0^{\mathrm{R}}(r) &= \int_c^\infty G(r, r')[-(k_0^2+\gamma^2)\sin k_0 r']\,dr' \\ &= \frac{(k_0^2+\gamma^2)\pi}{\mu \sin\nu\pi}\Bigg[-J_{-\nu}\left(\frac{2}{\mu}(m^* v_0)^{\frac{1}{2}}\right)\Big/ J_\nu\left(\frac{2}{\mu}(m^* v_0)^{\frac{1}{2}}\right) \\ &\quad \times J_\nu\left(\frac{2}{\mu}(m^* v_0)^{\frac{1}{2}} e^{-\mu(r-c)/2}\right) \\ &\quad \times \int_c^\infty J_\nu\left(\frac{2}{\mu}(m^* v_0)^{\frac{1}{2}} e^{-\mu(r'-c)/2}\right)\sin k_0 r'\,dr' \\ &\quad + J_\nu\left(\frac{2}{\mu}(m^* v_0)^{\frac{1}{2}} e^{-\mu(r-c)/2}\right) \\ &\quad \times \int_c^r J_{-\nu}\left(\frac{2}{\mu}(m^* v_0)^{\frac{1}{2}} e^{-\mu(r'-c)/2}\right)\sin k_0 r'\,dr' \\ &\quad + J_{-\nu}\left(\frac{2}{\mu}(m^* v_0)^{\frac{1}{2}} e^{-\mu(r-c)/2}\right) \\ &\quad \times \int_r^\infty J_\nu\left(\frac{2}{\mu}(m^* v_0)^{\frac{1}{2}} e^{-\mu(r'-c)/2}\right)\sin k_0 r'\,dr'\Bigg]. \end{aligned} \tag{41}$$

The integrals can be calculated analytically using the series expression of Bessel function. We have, for example,

$$\int_c^r J_\nu\left(\frac{2}{\mu}(m^*v_0)^{\frac{1}{2}}e^{-\mu(r'-c)/2}\right)\sin k_0r'\,dr'$$
$$=\sum_{n=0}^{\infty}\frac{(-1)^n(m^*v_0e^{\mu c}/\mu^2)^{\frac{1}{2}\nu+n}}{n!\,\Gamma(\nu+n+1)}\int_c^r e^{-\mu(\frac{1}{2}\nu+n)r'}\sin k_0r'\,dr'$$
$$=\left(\frac{m^*v_0}{\mu^2}\right)^{\frac{1}{2}\nu}\left(\sum_{n=0}^{\infty}\frac{(-1)^n(m^*v_0/\mu^2)^n\cdot[k_0\cos k_0c+\mu(\frac{1}{2}\nu+n)\sin k_0c]}{n!\,\Gamma(\nu+n+1)[k_0^2+\mu^2(\frac{1}{2}\nu+n)^2]}\right.$$
$$\left.-e^{-\frac{1}{2}\nu\mu(r-c)}\cdot\sum_{n=0}^{\infty}\frac{(-1)^n(m^*v_0/\mu^2)^ne^{-n\mu(r-c)}\cdot[k_0\cos k_0r+\mu(\frac{1}{2}\nu+n)\sin k_0r]}{n!\,\Gamma(\nu+n+1)\cdot[k_0^2+\mu^2(\frac{1}{2}\nu+n)^2]}\right). \quad (42)$$

Our final result for $u_0^R(r)$ can be put in a rather elegant form if we define the transcendental functions

$$G_{\pm\nu}(r)=\sum_{n=0}^{\infty}\frac{(-1)^n(m^*v_0/\mu^2)^ne^{-n\mu(r-c)}}{n!\,(\pm\nu)(\pm\nu+1)\cdots(\pm\nu+n)}, \quad (43)$$

$$M_{\pm\nu}(r)=\sum_{n=0}^{\infty}\frac{(-1)^n(m^*v_0/\mu^2)^ne^{-n\mu(r-c)}\cdot[k_0\cos k_0r+\mu(\pm\frac{1}{2}\nu+n)\sin k_0r]}{n!\,(\pm\nu)(\pm\nu+1)\cdots(\pm\nu+n)[k_0^2+\mu^2(\pm\frac{1}{2}\nu+n)^2]}. \quad (44)$$

The functions $G_{\pm\nu}(r)$ are closely related to Bessel functions of exponential argument:

$$G_{\pm\nu}(r)=\Gamma_{(\pm\nu)}(m^*v_0/\mu^2)^{\mp\frac{1}{2}\nu}e^{\pm\frac{1}{2}\nu\mu(r-c)}$$
$$\times J_{\pm\nu}([2(m^*v_0)^{\frac{1}{2}}/\mu]e^{-\mu(r-c)/2}). \quad (45)$$

The functions $M_{\pm\nu}(r)$ have their origin to the integrals in expression (41), containing Bessel functions of exponential argument.

The final result for $u_0^R(r)$ in terms of $G_{\pm\nu}(r)$ and $M_{\pm\nu}(r)$ is the following:

$$u_0^R(r)=\frac{2\gamma(k_0^2+\gamma^2)}{\mu^2}\left([G_{-\nu}(c)\cdot M_\nu(c)\right.$$
$$-G_\nu(c)\cdot M_{-\nu}(c)]\frac{G_\nu(r)}{G_\nu(c)}e^{-\gamma(r-c)}$$
$$\left.+G_\nu(r)M_{-\nu}(r)-G_{-\nu}(r)M_\nu(r)\right). \quad (46)$$

As a test we computed the wavefunction $u_0^R(r)$ from expression (46) for values of r in the interval $0.4 < r < 12$F, using the parameters of the Moszkowski and Scott potential[17] ($v_0 = 6.29\text{F}^{-2}$, $c = 0.4$F, and $\mu = 2.083\text{F}^{-1}$) and the values $m^* = 0.88$, $k_0 = 0.822\text{F}^{-1}$, and $\gamma = 1.643\text{F}^{-1}$. The values of the functions $G_{\pm\nu}(r)$ and $M_{\pm\nu}(r)$ were computed to a high degree of accuracy from expressions (43) and (44), using simple subroutines. The results were compared with the numerical solution of Eq. (35), and good agreement was obtained.

We may finally point out that we can very easily check from expression (46) that $u_0^R(r)$ satisfies the required boundary conditions. The boundary condition at the hard core radius is obviously satisfied. The boundary condition at infinity is also satisfied since for large r only the last two terms in (46) survive, due to the contribution of the term with $n = 0$ in the expressions (43) and (44); that is,

$$\lim_{r\to\infty}u_0^R(r)=\frac{2\gamma(k_0^2+\gamma^2)}{\mu^2}\left(-\frac{k_0\cos k_0r-\gamma\sin k_0r}{\nu^2(k_0^2+\gamma^2)}\right.$$
$$\left.+\frac{k_0\cos k_0r+\gamma\sin k_0r}{\nu^2(k_0^2+\gamma^2)}\right)=\sin k_0r. \quad (47)$$

5. APPLICATION TO HYPERNUCLEAR MATTER

In this final section we make an application of the results of the previous sections to the calculation of the well depth D of a Λ-hyperon in its ground state in nuclear matter. This problem aroused considerable interest in the recent years,[26–30] and most potentials which have been used in calculating this well depth are of the type discussed in this paper.

We use spin-average potentials

$$\bar{V}=\tfrac{1}{4}V_s+\tfrac{3}{4}V_t,$$

and therefore the Λ well depth which we obtain is the "spin-average" one, $\bar{D}$.

We consider the s-wave contribution to $\bar{D}$, $\bar{D}_0$. In this case we can use analytic wavefunctions for both square well and exponential potentials with hard cores. Note also that most available Λ-nucleon potentials (which are determined from the analyses of s-shell hypernuclei or low-energy Λ-nucleon scattering data) are s-wave potentials.

TABLE I. Values of $\bar{D}_0$ obtained with the square well with hard core potential (51) of Downs and Ware.

$k_F = 1.366\ \text{fm}^{-1}$			$k_F = 1.4\ \text{fm}^{-1}$		
$M_N^*/M_N = 0.638$	$M_N^*/M_N = 0.735$	$M_N^*/M_N = 1$	$M_N^*/M_N = 0.638$	$M_N^*/M_N = 0.735$	$M_N^*/M_N = 1$
20.9	20.4	19.5	22.1	21.4	20.4

The expression for $\bar{D}_0$ is the following:

$$\bar{D}_0 = -\left(\frac{\hbar^2}{2\mu_{\Lambda N}}\right)\frac{16\pi}{(2\pi)^3}\left(\frac{M_N}{\mu_{\Lambda N}}\right)^3 \times \int_0^{(\mu_{\Lambda N}/M_N)\cdot k_F} \langle k_0|\, G^R\, |k_0\rangle_{L=0} k_0^2\, dk_0, \quad (48)$$

where

$$\langle k_0|\, G^R\, |k_0\rangle_{L=0} = \frac{4\pi}{k_0^2}\int_0^\infty \left(k_0 r j_0(k_0 r) v_{(r)} u^R_{0(r)}\, dr = \frac{4\pi}{k_0^2}\left(\frac{(k_0^2+\gamma^2)}{m^*}\int_0^c (\sin k_0 r)^2\, dr + \frac{1}{m^*}\sin k_0 c(k_0 \cos k_0 c + \gamma \sin k_0 c) + \int_c^\infty (\sin k_0 r - \sin k_0 c \cdot e^{-\gamma(r-c)}) v_{(r)} u^R_{0(r)}\, dr\right). \quad (49)$$

The analytic wavefunctions $u_0^R(r)$ of the previous sections can be used here, provided that we take into account that the reduced mass of the pair is no longer $M_N/2$ but $\mu_{\Lambda N} = M_\Lambda \cdot M_N/(M_\Lambda + M_N)$, where M_N is the mass of the nucleon and M_Λ the mass of the Λ-particle. This has the effect that the energy quantities are now in units $\hbar^2/2\mu_{\Lambda N}$.

We use, as in other similar studies, unmodified kinetic energies (together with a gap) for the *intermediate* states, and therefore we put $m^* = 1$ in our formulas.

The expression for γ^2 can be easily obtained using the original definition and the fact that the momentum of the Λ-particle in its ground state in nuclear matter is zero. This expression is the following:

$$\gamma^2 = \frac{2\mu_{\Lambda N}}{\hbar^2}\Delta + \left(\frac{M_N}{M_\Lambda} - \frac{M_N}{M_N^*}\left(1 + \frac{M_N}{M_\Lambda}\right)\right)k_0^2, \quad (50)$$

where the gap $\Delta = \Delta_N + \Delta_\Lambda$ is given in MeV. We performed first numerical calculations using the square well potential with hard core of Downs and Ware.[26] The parameters are

$$c = 0.4\ \text{fm}, \quad \alpha = 1.5\ \text{fm}, \quad v_0 = 44.24\ \text{MeV}. \quad (51)$$

We have chosen the value of $\Delta = 126$ MeV for the gap, as in Ref. 29, and two values for k_F:

$$k_F = 1.366\ \text{fm}^{-1}, \quad k_F = 1.4\ \text{fm}^{-1}.$$

Several values of M_N^*/M_N were assumed, in order to investigate the sensitivity of $\bar{D}_0$ to the effective mass M_N^*/M_N. The results are given in Table I. We see that the dependence of $\bar{D}_0$ on M_N^*/M_N is quite weak. The value of $\bar{D}_0 = 20.4$ MeV, which was obtained with $M_N^*/M_N = 0.735$ and $k_F = 1.366\ \text{fm}^{-1}$, is close to the value (= 18.7 MeV) obtained by Downs and Ware with the same potential and the same values of M_N^*/M_N and k_F but using instead of the reference spectrum wavefunction an approximate Bethe-Goldstone wavefunction.

Secondly, we performed calculations using the exponential potential with hard core of Herndon and Tang[31] (see potential B of their Table IX). The parameters are

$$c = 0.3\ \text{fm}, \quad \mu = 3.935\ \text{fm}^{-1}, \quad v_0 = 544.6\ \text{MeV}. \quad (52)$$

Choosing again a value of Δ, used also in Ref. 29, namely $\Delta = 48.8$ MeV, we obtain the results given in Table II. The values of $\bar{D}_0$ are considerably larger than those with the square well potential with hard core.

In conclusion we should remark that the feasibility of obtaining analytic solutions of the reference spectrum equation, which was shown in this paper,

TABLE II. Values of $\bar{D}_0$ obtained with the exponential with hard core potential (52) of Herndon and Tang.

$k_F = 1.366\ \text{fm}^{-1}$		$k_F = 1.4\ \text{fm}^{-1}$	
$M_N^*/M_N = 0.65$	$M_N^*/M_N = 1$	$M_N^*/M_N = 0.65$	$M_N^*/M_N = 1$
41.1	38.8	44.2	41.5

emphasizes the computational advantages of this method in comparison with certain other methods as, for example, with the method based on the Bethe–Goldstone equation. As it is well known, an analytic solution of the Bethe–Goldstone equation has been obtained only in the case of the hard core potential alone.[26]

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Collective and Single-Particle Coordinates in Nuclear Physics*

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The Schrödinger equation of A nucleons is transformed to new coordinates. Six of them have collective nature and $3A - 9$ are single-particle coordinates. The connection is given to the conventional collective model in which five collective coordinates are used. The additional sixth collective coordinate of this paper gives a simple description of monopole vibrations. The new coordinates can also be used in the theory of nuclear reactions: By introducing a symmetrized distance vector for reaction partners, the antisymmetrization procedure is simplified considerably.

1. INTRODUCTION

In a recent paper Villars and Cooper have shown how to treat nuclear rotations starting from the Schrödinger equation of A nucleons[1] (for further references, see Ref. 1) and how to include the single-particle motion and the coupling between single-particle motion and rotations. Most of the results of the paper of Villars and Cooper have been known before, but have not been derived in such a unified way. Nuclear vibrations have not been included in Villars and Cooper's paper. How this can be done will be shown in the present paper. In some earlier publications[2–6] the author has shown how special sets of coordinates are of advantage for the three- and four-nucleon problems. For completeness here is a short review.

Three Nucleons

For the three-nucleon problem one has six degrees of freedom in the center of mass system. Any wavefunction of a three-nucleon system has to be antisymmetric with respect to an exchange of two nucleons. In conventional Jacobi coordinates such an antisymmetrization is a rather complicated procedure. In many cases it is therefore worthwhile to chose a coordinate system in which as many coordinates as possible are symmetric with respect to exchange of identical particles. In the case of three particles we have five symmetric coordinates. These are the three Euler angles ψ, ϑ, φ of the three axis of the inertia ellipsoid and two coordinates which are simple functions of the two principal moments of inertia, which are independent (the third principal moment of inertia is simply the sum of the two others). If J_1 and J_2 are the independent moments of inertia, the two symmetric coordinates α and y are defined in the following way:

$$\sin\alpha = |J_1 - J_2|/(J_1 + J_2), \tag{1}$$

$$y^2 = 2(J_1 + J_2)/m; \tag{2}$$

m is the nucleon mass.

The remaining sixth coordinate is the only coordinate which changes when identical particles are exchanged. Its properties can best be seen from its connection with the three interparticle distances r_{12}, r_{23}, r_{31}:

$$\begin{aligned} r_{12} &= y[1 - \sin\alpha \sin\beta]^{\frac{1}{2}}/2^{\frac{1}{2}}, \\ r_{23} &= y[1 - \sin\alpha \sin(\beta - \tfrac{2}{3}\pi)]^{\frac{1}{2}}/2^{\frac{1}{2}}, \\ r_{31} &= y[1 - \sin\alpha \sin(\beta - \tfrac{4}{3}\pi)]^{\frac{1}{2}}/2^{\frac{1}{2}}. \end{aligned} \tag{3}$$

Four Nucleons

In the center of mass system one has nine degrees of freedom. Six of these can be defined as symmetric with respect to exchange of identical particles. They again are, as in the three-particle case, the three Euler angles ψ, ϑ, φ of the inertia ellipsoid and three coordinates which are connected with the three principal moments of inertia (instead of two as in the case of three particles). For the latter coordinates the symbols y_1, y_2, y_3 are used, and their connection with the principal moments of inertia J_1, J_2, J_3 is

$$\begin{aligned} J_1 &= m(y_2^2 + y_3^2), \\ J_2 &= m(y_3^2 + y_1^2), \\ J_3 &= m(y_1^2 + y_2^2). \end{aligned} \tag{4}$$

One could also, instead of y_1, y_2, y_3, take J_1, J_2, J_3 as three coordinates. But they are not very useful because the ranges of the variables J_i are not independent. They obey a triangular condition:

$$|J_1 - J_2| \leq J_3 \leq J_1 + J_2. \tag{5}$$

Also there would be mixed derivatives $\partial^2/\partial J_1 \cdot \partial J_2$ in the Schrödinger equation, which are not convenient. The ranges of the variables y_1 are independent and there are no mixed derivatives like $\partial^2/\partial y_1 \partial y_2$ in the Schrödinger equation.[6] The remaining three coordinates are best chosen as three internal Euler angles (α, β, γ).[6] The whole transformation from the Jacobi coordinates to the new coordinate system can then be written in a very simple way. If $\mathbf{r}_1$, $\mathbf{r}_2$,

$\mathbf{r}_3$, $\mathbf{r}_4$ are the space vectors of the four particles, then a set of convenient Jacobi coordinates (obtained by an orthogonal transformation from $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$, $\mathbf{r}_4$) are

$$\begin{aligned}\mathbf{x}_1 &= (\mathbf{r}_1 + \mathbf{r}_2 - \mathbf{r}_3 - \mathbf{r}_4)/2,\\ \mathbf{x}_2 &= (\mathbf{r}_1 - \mathbf{r}_2 + \mathbf{r}_3 - \mathbf{r}_4)/2,\\ \mathbf{x}_3 &= (\mathbf{r}_1 - \mathbf{r}_2 - \mathbf{r}_3 + \mathbf{r}_4)/2.\end{aligned} \tag{6}$$

The transformation from $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$ to y_1, y_2, y_3, ψ, ϑ, φ, α, β, γ is then in matrix notation (with x_{i1}, x_{i2}, x_{i3} as components of $\mathbf{x}_i$):

$$\begin{pmatrix} x_{11}, x_{12}, x_{13}\\ x_{21}, x_{22}, x_{23}\\ x_{31}, x_{32}, x_{33}\end{pmatrix} = \begin{pmatrix} \cos\gamma\cos\alpha - \sin\gamma\sin\alpha\cos\beta, \cdots\\ -\sin\gamma\cos\alpha - \cos\gamma\sin\alpha\cos\beta, \cdots\\ \sin\alpha\sin\beta, \cdots\end{pmatrix} \times \begin{pmatrix} y_1, 0, 0\\ 0, y_2, 0\\ 0, 0, y_3\end{pmatrix} \times \begin{pmatrix} \cos\varphi\cos\psi - \sin\varphi\sin\psi\cos\vartheta, \cdots\\ -\sin\varphi\cos\psi - \cos\varphi\sin\psi\cos\vartheta, \cdots\\ \sin\psi\sin\vartheta, \cdots\end{pmatrix}. \tag{7}$$

The first and the last matrices in Eq. (7) are 3×3 orthogonal matrices in α, β, γ and ψ, ϑ, φ, respectively. Only the first columns have been written down, because the matrix elements are well known and can either be looked up in mathematics books or derived easily. Any exchange of identical particles is a rotation in the (α, β, γ) space.[6]

2. DEFINITION OF THE COORDINATES FOR THE NUCLEAR MANY-BODY PROBLEM

The generalization of the transformation (7) to A nucleons is straightforward when we look at the new coordinates $y_1, y_2, y_3, \varphi, \vartheta, \psi, \alpha, \beta, \gamma$ in the following way: If the coordinates y_1, y_2, y_3, φ, ϑ, ψ are kept fixed, position and magnitude of the inertia ellipsoid are fixed. α, β, γ can be considered as the remaining single-particle coordinates in a nucleus of fixed orientation and with fixed moments of inertia. From this point of view one can write the transformation (7) also in the following way:

$$\begin{aligned}\mathbf{x}_1 &= a_{11}\mathbf{y}_1 + a_{12}\mathbf{y}_2 + a_{13}\mathbf{y}_3,\\ \mathbf{x}_2 &= a_{21}\mathbf{y}_1 + a_{22}\mathbf{y}_2 + a_{23}\mathbf{y}_3,\\ \mathbf{x}_3 &= a_{31}\mathbf{y}_1 + a_{32}\mathbf{y}_2 + a_{33}\mathbf{y}_3;\end{aligned} \tag{8}$$

the a_{ik} are the components of the vectors $\mathbf{x}_i$ in a coordinate system given by $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$. The vectors $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ are obtained from (7) as the rows of the product matrix

$$\begin{pmatrix} y_1 & 0 & 0\\ 0 & y_2 & 0\\ 0 & 0 & y_3\end{pmatrix} \times \begin{pmatrix} \cos\varphi\cos\psi - \sin\varphi\sin\psi\cos\vartheta, \cdots\\ \vdots\\ \vdots\\ \vdots\end{pmatrix}. \tag{9}$$

The a_{ik} are the elements of the first matrix on the right of Eq. (7). Thus, when writing the transformation in the form of Eq. (8), we find that it is connected with the following constraints:

$$\mathbf{y}_i\mathbf{y}_k = y_i y_k \cdot \delta_{ik}, \quad \sum_{i=1}^{3} a_{ij}a_{ik} = \delta_{jk}. \tag{10}$$

If $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ are fixed vectors, then the a_{ik} give the remaining degrees of freedom in a nucleus of fixed orientation and with fixed moments of inertia. From this point of view one can immediately generalize the coordinates to the nuclear many-body problem. The Jacobi coordinate vectors are called $\mathbf{x}_1, \cdots, \mathbf{x}_{A-1}$ now. Then the transformation is given by the following equation:

$$\mathbf{x}_i = a_{i1}\mathbf{y}_1 + a_{i2}\mathbf{y}_2 + a_{i3}\mathbf{y}_3. \tag{11}$$

The constraints are

$$\mathbf{y}_i\mathbf{y}_k = y_i y_k \delta_{ik}, \tag{12}$$

$$\sum_{i=1}^{A-1} a_{ij}a_{ik} = \delta_{jk}. \tag{13}$$

One can show easily that $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ are in the direction of the axis of the inertia ellipsoid. One can also show what the moments of inertia are. If the space vectors of the particles in the center of mass system are given by $\mathbf{r}_i$, then the moment of inertia with respect to an arbitrary axis through the center of mass is ($\mathbf{e}$ is a unit vector in the direction of the axis chosen)

$$J = m\sum_{i=1}^{A}[r_i^2 - (\mathbf{r}_i\mathbf{e})^2]. \tag{14}$$

The transformation from the $\mathbf{r}_i$-vectors to the Jacobi vectors $\mathbf{x}_i$ is an orthogonal one; for example,

$$\begin{aligned}\mathbf{x}_1 &= [\mathbf{r}_1 - \mathbf{r}_2]/2^{\frac{1}{2}},\\ \mathbf{x}_2 &= [\mathbf{r}_1 + \mathbf{r}_2 - 2\mathbf{r}_3]/6^{\frac{1}{2}},\\ \mathbf{x}_3 &= [\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3 - 3\mathbf{r}_4]/12^{\frac{1}{2}},\\ &\vdots \qquad\qquad \vdots\\ \mathbf{x}_{A-1} &= [\mathbf{r}_1 + \mathbf{r}_2 + \cdots + \mathbf{r}_{A-1} - (A-1)\mathbf{r}_A]\\ &\quad \times [1/A(A-1)]^{\frac{1}{2}}.\end{aligned} \tag{15}$$

From Eq. (14) one finds that J has the same form in $\mathbf{x}_i$ as it had in $\mathbf{r}_i$:

$$J = m \cdot \sum_{i=1}^{A-1} [x_i^2 - (\mathbf{x}_i \mathbf{e})^2]. \tag{16}$$

The transformation (11) with the constraints (12) and (13) yields

$$J = m \sum_{i=1}^{3} [y_i^2 - (\mathbf{y}_i \mathbf{e})^2]. \tag{17}$$

From Eq. (17) it is clear that the directions of the vectors $\mathbf{y}_i$ coincide with the axis of the inertia ellipsoid. For the principal moments of inertia one finds

$$\begin{aligned} J_1 &= m(y_2^2 + y_3^2), \\ J_2 &= m(y_3^2 + y_1^2), \\ J_3 &= m(y_1^2 + y_2^2). \end{aligned} \tag{18}$$

Henceforth, the vectors $\mathbf{y}_i$ or the six quantities y_1, y_2, y_3, φ, ϑ, ψ defining them will be called collective coordinates. The internal coordinates are not independent due to the constraint (13). $3A - 9$ of the a_{ik} can be chosen independently.

The Jacobi coordinates $\mathbf{x}_i$ are not very convenient for a system of identical particles such as we deal with in nuclear physics. Their transformation properties under exchange of identical particles are complicated. The same is true for the internal coordinates a_{ik}. This difficulty is overcome by using the components of the single-particle space vectors (in the center of mass system) in the $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ system instead of the a_{ik}:

$$\mathbf{r}_i = s_{i1}\mathbf{y}_1 + s_{i2}\mathbf{y}_2 + s_{i3}\mathbf{y}_3. \tag{19}$$

The constraints for the s_{ik} are

$$\sum_{i=0}^{A} s_{ij} = 0, \tag{20}$$

$$\sum_{i=1}^{A} s_{ij} \cdot s_{ik} = \delta_{jk}. \tag{21}$$

The vectors $\mathbf{y}_i$ are the same as before. Of the s_{ik} again $3A - 9$ can be chosen independently.

The Schrödinger equation will be given in the following section for the two possible sets of internal coordinates.

3. THE SCHRÖDINGER EQUATION IN THE NEW COORDINATES

The transformation of the kinetic energy operator is straightforward, but tedious. With the Jacobi coordinate vectors $\mathbf{x}_1, \cdots, \mathbf{x}_{A-1}$ [e.g., as defined by Eq. (15)], the kinetic energy operator in the center of mass system is

$$(\hbar^2/2m)(\Delta_1 + \cdots + \Delta_{A-1}), \tag{22}$$

with $\Delta_i = \partial^2/\partial x_{i1}^2 + \partial^2/\partial x_{i2}^2 + \partial^2/\partial x_{i3}^2$.

With the set of coordinates defined by Eqs. (11)–(13), one obtains

$$\begin{aligned} \Delta_1 + \cdots + \Delta_{A-1} &= \frac{\partial^2}{\partial y_1^2} + \left(\frac{A-4}{y_1} + \frac{2y_1}{y_1^2 - y_2^2} + \frac{2y_1}{y_1^2 - y_3^2}\right)\frac{\partial}{\partial y_1} \\ &\quad - \frac{y_2^2 + y_3^2}{(y_2^2 - y_3^2)^2}\frac{1}{\hbar^2}(L_{e1}^2 + L_{i1}^2) \\ &\quad - \frac{4y_2y_3}{(y_2^2 - y_3^2)^2}\frac{1}{\hbar^2} L_{e1} \cdot L_{i1} \\ &\quad + \frac{1}{y_1^2}\left(\sum_{\substack{mm' \\ (\text{ind})}} (\delta_{mm'} - \mathbf{a}_m \cdot \mathbf{a}_{m'}) \frac{d^2}{da_{m1} \cdot da_{m'1}} \right. \\ &\quad \left. - (A-4) \sum_{(\text{ind})} a_{m1} \frac{d}{da_{m1}}\right) \\ &\quad + \text{cyclic permutations.} \end{aligned} \tag{23}$$

The cyclic permutations in this equation are to be taken among 1, 2, 3. The operators L_{e1}, L_{e2}, L_{e3} are the components of the orbital angular momentum with respect to the body fixed axis defined by the directions of the vectors $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$:

$$\begin{aligned} L_{e1} \pm iL_{e2} &= i\hbar e^{\mp i\psi}\left(\frac{1}{\sin\vartheta}\frac{\partial}{\partial\varphi} - \frac{\cos\vartheta}{\sin\vartheta}\cdot\frac{\partial}{\partial\psi} \mp i\frac{\partial}{\partial\vartheta}\right), \\ L_{e3} &= -i\hbar\frac{\partial}{\partial\psi}. \end{aligned} \tag{24}$$

The index e with these operators stands for "external." L_{i1}, L_{i2}, L_{i3} are the components of the internal orbital angular momentum:

$$L_{i1} = i\hbar \sum_{\substack{m \\ (\text{ind})}} \left(a_{m2} \cdot \frac{d}{da_{m3}} - a_{m3} \cdot \frac{d}{da_{m2}}\right). \tag{25}$$

L_{i2} and L_{i3} are obtained by cyclic permutations again.

The sums over m and m' appearing in Eqs. (23) and (25) are to be taken over independent components a_{mi} only. This is indicated by (ind) below the summation sign.

If, instead of a_{mi}, the internal single-particle coordinates s_{mi} are used, Eq. (23) is replaced by

$$\begin{aligned} \Delta_1 + \cdots + \Delta_{A-1} &= \frac{\partial^2}{\partial y_1^2} + \left(\frac{A-4}{y_1} + \frac{2y_1}{y_1^2 - y_2^2} + \frac{2y_1}{y_1^2 - y_3^2}\right)\frac{\partial}{\partial y_1} \\ &\quad - \frac{y_2^2 + y_3^2}{(y_2^2 - y_3^2)^2}\frac{1}{\hbar^2}(L_{e1}^2 + L_{i1}^2) \\ &\quad - \frac{4y_2y_3}{(y_2^2 - y_3^2)^2}\frac{1}{\hbar^2} L_{e1} \cdot L_{i1} \\ &\quad + \frac{1}{y_1^2}\left(\sum_{\substack{m \cdot m' \\ (\text{ind})}} \left(\delta_{mm'} - \frac{1}{A} - \mathbf{s}_m \cdot \mathbf{s}_{m'}\right) \frac{d^2}{ds_{m1} \cdot ds_{m'1}} \right. \\ &\quad \left. - (A-4) \sum_{\substack{m \\ (\text{ind})}} s_{m1} \frac{d}{ds_{m1}}\right) \\ &\quad + \text{cyclic permutations,} \end{aligned} \tag{26}$$

with

$$L_{i1} = i\hbar \sum_{\substack{m \\ (\mathrm{ind})}} \left(s_{m2} \frac{d}{ds_{m3}} - s_{m3} \frac{d}{ds_{m2}} \right), \qquad (27)$$

and L_{i2} and L_{i3}, correspondingly.

Again, all the sums over m are to be taken over independent components only.

Calculations with the new coordinates will be difficult as a consequence of the constraints (20) and (21). To facilitate calculations, one has to use approximations; one could require, for example, that the expectation values of the quantities appearing in (20) and (21) are 0 or δ_{jk}, respectively. A big help in calculations will be a special property of the operators appearing in Eqs. (23) and (26). This property which is shown in the following equations can be derived from the constraints (13) or (20) and (21), and it is true for any function $\Psi(s_{ik})$:

$$\sum_{\substack{m \\ (\mathrm{ind})}} \left(s_{m2} \cdot \frac{d}{ds_{m3}} - s_{m3} \frac{d}{ds_{m2}} \right) \Psi(s_{ik}) = \sum_{m=1}^{A} \left(s_{m2} \frac{\partial}{\partial s_{m3}} - s_{m3} \frac{\partial}{\partial s_{m2}} \right) \Psi(s_{ik}), \qquad (28)$$

$$\left[\sum_{\substack{mm' \\ (\mathrm{ind})}} \left(\delta_{mm'} - \frac{1}{A} - \mathbf{s}_m \cdot \mathbf{s}_{m'} \right) \frac{d^2}{ds_{m1} \cdot ds_{m'1}} - (A-4) \sum_{\substack{m \\ (\mathrm{ind})}} s_{m1} \frac{d}{ds_{m1}} \right] \Psi(s_{ik}) = \left[\sum_{m=1}^{A} \sum_{m'=1}^{A} \left(\delta_{mm'} - \frac{1}{A} - \mathbf{s}_m \cdot \mathbf{s}_{m'} \right) \frac{\partial^2}{\partial s_{m1} \cdot \partial s_{m'1}} - (A-4) \sum_{m=1}^{A} s_{m1} \cdot \frac{\partial}{\partial s_{m1}} \right] \Psi(s_{ik}). \qquad (29)$$

The method of proving (28) and (29) is the same for both equations, and so it will be outlined for (28) only: Of the $3A$ variables s_{ik}, nine are determined from the remaining $3A - 9$ variables by the nine constraints (20) and (21). One could choose as dependent variables, for example (this is rather arbitrary), s_{11}, s_{21}, s_{31}, s_{12}, s_{22}, s_{32}, $s_{A-2,3}$, $s_{A-1,3}$, s_{A3}. Any of these dependent variables appearing in the wavefunction Ψ is to be replaced by the independent ones with the constraints (20) and (21). The operator on the left side of Eq. (28) has the following form now:

$$\sum_{m=1}^{A-3} s_{m2} \frac{d}{ds_{m3}} - \sum_{m=4}^{A} s_{m3} \frac{d}{ds_{m2}}. \qquad (28')$$

The total derivatives in (28′) are (for the case that the dependent variables are appearing explicitly in the wavefunction)

$$\frac{d}{ds_{m3}} = \frac{\partial}{\partial s_{m3}} + \frac{\partial s_{11}}{\partial s_{m3}} \frac{\partial}{\partial s_{11}} + \cdots + \frac{\partial s_{A3}}{\partial s_{m3}} \frac{\partial}{\partial s_{A3}}; \qquad (28'')$$

similarly for d/ds_{m2}. The ellipsis in (28″) is for the terms which contain the other partial derivatives with respect to the dependent variables.

Thus one has

$$\sum_{m=1}^{A-3} s_{m2} \frac{d}{ds_{m3}} - \sum_{m=4}^{A} s_{m3} \frac{d}{ds_{m2}} = \sum_{m=1}^{A-3} s_{m2} \frac{\partial}{\partial s_{m3}} - \sum_{m=4}^{A} s_{m3} \frac{\partial}{\partial s_{m2}} + \left(\sum_{m=1}^{A-3} s_{m2} \frac{\partial s_{11}}{\partial s_{m3}} - \sum_{m=4}^{A} s_{m3} \frac{\partial s_{11}}{\partial s_{m2}} \right) \cdot \frac{\partial}{\partial s_{11}} + \cdots + \left(\sum_{m=1}^{A-3} s_{m2} \frac{\partial s_{A3}}{\partial s_{m3}} - \sum_{m=4}^{A} s_{m3} \frac{\partial s_{A3}}{\partial s_{m2}} \right) \cdot \frac{\partial}{\partial s_{A3}}. \qquad (28''')$$

The derivatives $\partial s_{11}/\partial s_{m3}$, etc., are derived from (20) and (21): Taking the derivatives of (20) and (21) with respect to a special independent variable s_{ik}, one obtains nine equations for the nine derivatives of the dependent variables. One obtains, for example, from (20) for the derivatives $\partial s_{11}/\partial s_{m3}$, etc.,

$$\frac{\partial s_{11}}{\partial s_{m3}} + \frac{\partial s_{21}}{\partial s_{m3}} + \frac{\partial s_{31}}{\partial s_{m3}} = 0,$$
$$\frac{\partial s_{12}}{\partial s_{m3}} + \frac{\partial s_{22}}{\partial s_{m3}} + \frac{\partial s_{32}}{\partial s_{m3}} = 0, \qquad (28'''')$$
$$\frac{\partial s_{A-2,3}}{\partial s_{m3}} + \frac{\partial s_{A-1,3}}{\partial s_{m3}} + \frac{\partial s_{A3}}{\partial s_{m3}} = -1.$$

From (21) one obtains six more equations. Thus all derivatives of the dependent variables appearing in (28‴) can be calculated from the constraints. With the results one obtains Eq. (28) from Eq. (28‴). So, if one is looking for eigenfunctions of the operator L_{i3} for example, one can consider s_{ik} as independent variables. From now on the abbreviations O_{s1}, O_{s2}, O_{s3} will be used for the operators appearing in the last term of Eq. (26) and in Eq. (29):

$$O_{s1} = \sum_{m,m'} \left(\delta_{mm'} - \frac{1}{A} - \mathbf{s}_m \cdot \mathbf{s}_{m'} \right) \frac{\partial^2}{\partial s_{m1} \partial s_{m'1}} - (A-4) \sum_{m} s_{m1} \cdot \frac{\partial}{\partial s_{m1}}. \qquad (30)$$

O_{s2} and O_{s3} are obtained by cyclic permutations. For the sum of these three operators the abbreviation O_s will be used:

$$O_s = O_{s1} + O_{s2} + O_{s3}. \qquad (31)$$

4. JACOBIAN OF THE TRANSFORMATION

As mentioned before, it will be difficult for any real calculations to take into account the constraints

connecting the coordinates s_{ik} (or a_{ik}). By treating the s_{ik} as independent and requiring the constraints (20), (21) for the matrix elements only, things are much simpler. The part of the volume element containing the s_{ik} is then simply

$$(ds_{11}\cdots ds_{A1}),\quad (ds_{12}\cdots ds_{A2}),\quad (ds_{13}\cdots ds_{A3}). \tag{32}$$

The calculation of the Jacobian for the collective coordinates yields

$$(y_1y_2y_3)^{A-4}\,|y_1^2-y_2^2|\cdot|y_2^2-y_3^2|\,|y_3^2-y_1^2|\sin\vartheta. \tag{33}$$

Thus the total volume element in the new coordinates with the approximation of independent s_{ik} is

$$\begin{aligned} d\tau_A = {} & [(y_1y_2y_3)^{A-4}\,|y_1^2-y_2^2| \\ & \times |y_2^2-y_3^2|\,|y_3^2-y_1^2|\,dy_1\,dy_2\,dy_3] \\ & \times (\sin\vartheta\,d\vartheta\,d\varphi) \\ & \times [(ds_{11}\cdots ds_{A1})\cdot(ds_{12}\cdots ds_{A2}) \\ & \times (ds_{13}\cdots ds_{A3})]. \end{aligned} \tag{34}$$

5. COLLECTIVE AND SINGLE-PARTICLE EXCITATIONS

A clear separation between single particle and collective excitations will, in general, not be possible. If tensor forces are not taken into account, the solution of the Schrödinger equation will be an eigenfunction of the orbital angular momentum L_e^2, and will be of the following form:

$$\Psi_{LM}=\sum_K D^L_{MK}(\varphi,\vartheta,\psi)\cdot\Phi_K, \tag{35}$$

with $L_{i3}\Phi_K=\hbar K\Phi_K$. Φ_K depends on y_1, y_2, y_3 and the internal degrees of freedom s_{ik}.

As an approximation, one might try a variational calculation with a single term of the sum in (35). But in general this would lead to useless results because there is a coupling between different values of K due to the operators L_{e1}, L_{e2}, L_{i1}, L_{i2} in the Schrödinger equation.

How such a variational calculation could be improved is shown in the paper of Villars and Cooper.[1]

Conditions are especially simple if the internal part of the wavefunction is an eigenfunction of $\mathbf{L}_i^2$, with eigenvalue zero. This is probably a good approximation for spherical nuclei, or—more generally—nuclei which have a strong maximum in the probability distribution in y_1, y_2, y_3 space at $y_1=y_2=y_3$. One can see this very simply if one assumes that tensor forces are of no great importance. In that case the interaction energy of nucleons i and j would be of the form (no spin and isospin dependence written down)

$$V_{ij}[(s_{i1}-s_{j1})^2y_1^2+(s_{i2}-s_{j2})^2y_2^2+(s_{i3}-s_{j3})^2y_3^2]. \tag{36}$$

For a spherical nucleus one could approximately put $y_1=y_2=y_3$ and then would have $V_{ij}[y_1^2(\mathbf{s}_i-\mathbf{s}_j)^2]$ with

$$\begin{aligned}(\mathbf{s}_i-\mathbf{s}_j)^2 & \\ &=(s_{i1}-s_{j1})^2+(s_{i2}-s_{j2})^2+(s_{i3}-s_{j3})^2.\end{aligned} \tag{37}$$

This approximate V_{ij} in (37) commutes with the internal angular momentum operators L_{i1}, L_{i2}, L_{i3}. Therefore, the ground state of a spherical nucleus will approximately be an eigenfunction of $\mathbf{L}_i^2$ with eigenvalue zero.

The case of internal angular momentum 0 will now be considered in more detail, and it will lead to the well-known equations of the collective model of Bohr and Mottelson.

The Schrödinger equation for the collective part C of the wavefunction is

$$\begin{aligned}\Big\{\frac{\hbar^2}{2m}\Big[\frac{\partial^2}{\partial y_1^2}+\Big(\frac{A-4}{y_1}+\frac{2y_1}{y_1^2-y_2^2}+\frac{2y_1}{y_1^2-y_3^2}\Big)\frac{\partial}{\partial y_1} \\ -\frac{y_2^2+y_3^2}{(y_2^2-y_3^2)^2}\frac{1}{\hbar^2}L_{e1}^2+\text{cyclic permutations}\Big] \\ +E-V_c(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3)\Big\}C(\mathbf{y}_1,\mathbf{y}_2,\mathbf{y}_3)=0.\end{aligned} \tag{38}$$

The "potential" V_c in this last equation does not contain the original potential energy alone. It also contains the matrix elements of the terms $O_{s1}/y_1^2+O_{s2}/y_2^2+O_{s3}/y_3^2$. That means it contains part of the kinetic energy, namely the part from the internal degrees of freedom. Instead of five degrees of freedom, as in the ordinary collective model, we have six now. As will be seen shortly, these six degrees of freedom allow for density vibrations also. One can see this best by introducing three new coordinates instead of the three lengths y_1, y_2, y_3:

$$\begin{aligned} y_1 &= \tfrac{1}{3}y(1+\sin\alpha\cos\gamma)^{\frac{1}{2}}, \\ y_2 &= \tfrac{1}{3}y[1+\sin\alpha\cos(\gamma-\tfrac{2}{3}\pi)]^{\frac{1}{2}}, \\ y_3 &= \tfrac{1}{3}y[1+\sin\alpha\cdot\cos(\gamma-\tfrac{4}{3}\pi)]^{\frac{1}{2}}. \end{aligned} \tag{39}$$

The meaning of the new coordinates is obvious: For $\alpha=0$ one has $y_1=y_2=y_3$ and hence, from Eq. (18), $J_1=J_2=J_3$. All three moments of inertia are equal for $\alpha=0$. In the language of the collective model, this means a spherical nucleus. One concludes that α is related to the coordinate β of the collective

model[7,8] (for further information see Ref. 8). It is

$$\alpha = c \cdot \beta, \tag{40}$$

where c is constant.

For $\gamma = 0$, one finds $y_2 = y_3$. From Eq. (18) one finds $J_2 = J_3$. Similarly, one has, for $\gamma = 2\pi/3$, $J_1 = J_3$ and, for $\gamma = 4\pi/3$, $J_1 = J_2$. This means that the coordinate γ describes the deviation of the nucleus from rotational symmetry. γ is identical with the γ defined by Bohr and Mottelson.[7,8]

The meaning of y becomes clear by considering a nucleus with homogeneous mass distribution and with the form of an ellipsoid. The volume is proportional to $y_1 \cdot y_2 \cdot y_3$. Constant volume, as is assumed for the collective model with an incompressible fluid, means

$$y_1 \cdot y_2 \cdot y_3 = \text{const.}$$

Also, it is assumed for the collective model that the deformation is small, that is, small β. In our notation that means small α. Using this assumption, one obtains

$$\begin{aligned} y_1 y_2 y_3 &= 3^{-\frac{3}{2}} y^3 (1 - \tfrac{3}{4} \sin^2 \alpha - \tfrac{1}{4} \sin^3 \alpha \cos 3\gamma)^{\frac{1}{2}} \\ &\approx 3^{-\frac{3}{2}} y^3. \end{aligned} \tag{41}$$

From this equation we conclude that incompressibility is identical with the assumption of constant y; this means the probability distribution for y takes the form of a delta function.

α- and γ-vibrations are obtained by considering special potentials V_c. With the additional degree of freedom y one can get also vibrations in y. This is the case if V_c is of the form

$$V_c = V_y(y) + y^{-2} V_{\alpha\gamma}(\alpha, \gamma). \tag{42}$$

In that case a separation of the Schrödinger equation is possible. The possibility of separation is, of course, the reason for choosing this special V_c. The collective wavefunction C is now of the form

$$C(y_1, y_2, y_3) = Y(y) \sum_k A_k(\alpha, \gamma) \cdot D^L_{MK}(\varphi, \vartheta, \psi). \tag{43}$$

The separation of α- and γ-vibrations requires additional assumptions which are well known.[7,8] The simple form of C in Eq. (43) rests on the assumption that the internal degrees of freedom are not coupled to the collective degrees of freedom. This is the case if one assumes a very simple form of the potential energy V in the original Schrödinger equation, for example, that V has the same form as V_c in Eq. (42). That means no dependence of V on the single-particle coordinates s_{ik}. In that case, the wavefunction of the A-nucleon system will be of the form

$$\Psi = C(\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3) \cdot S(s_{ik}). \tag{44}$$

Apart from collective excitations in which C alone is changed, one will have single-particle excitations in which S is changed. The S function of the excited states will be orthogonal to that of the ground state. But there is a coupling in the kinetic energy (26) between s_{ik} and the collective coordinates through the factors $1/y_i^2$ before O_{si}. This coupling means a change of C for single-particle excited states compared to that of the ground state, but the change may be negligible.

To start any calculations (for example, Ritz variational calculations), one will need a system of orthogonal functions. If one assumes that there are collective excitations which have a wavefunction $C(\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3)$ as given by Eq. (44), one will start the calculations by using simple functions S for the internal structure. It is, of course, difficult to construct a complete orthogonal system for the S wavefunction, as there are a large number of commutable operators to which the functions of the orthogonal system would have to be eigenfunctions. The wavefunction S has to be antisymmetric with respect to an exchange of nucleons. Therefore, one will chose orthogonal functions which have this antisymmetry already. There are three simple operators which commute and which are convenient to handle. These are the operators

$$\mathbf{L}_i^2, \quad L_{i3}, \quad O_s. \tag{45}$$

Constructing the eigenfunctions of these operators, one will, in general, have a number of degenerate eigenfunctions for fixed eigenvalues of these operators, and one has to orthogonalize them. The wavefunctions have also to be eigenfunctions for total momentum 0, that is,

$$\sum_{i=1}^{A} \frac{\partial S}{\partial s_{ij}} = 0, \quad j = 1, 2, 3. \tag{46}$$

Hence the functions of the orthogonal system must be eigenfunctions of the operator

$$\sum_{i=1}^{A} \frac{\partial}{\partial s_{ij}} \tag{47}$$

with eigenvalue zero.

6. CONNECTION WITH THE WELL-KNOWN EQUATIONS OF THE COLLECTIVE MODEL

In the preceding section it was shown that the transformation (39) defines coordinates α and γ which are closely connected to the coordinates defined in the collective model.[7,8] Here it should be mentioned that the transformation (39) contains an approximation already. The original range of the variables y_1, y_2, y_3 is from $-\infty$ to $+\infty$. By allowing only real

values for the variables y, α, γ, this range is not completely covered by Eq. (39). For example, $y_1 = y_2 = 0$ and $y_3 \neq 0$ is excluded by the transformation. It can be shown that the range of the y_i covered by Eq. (39) is given by the triangular conditions

$$|y_i - y_j| \leq y_k \leq y_i + y_j, \quad i \neq j \neq k. \tag{48}$$

The configuration $y_1 = y_2 = 0$ and $y_3 \neq 0$ would mean that all nucleons are on a straight line. This configuration is excluded by the triangular conditions. Similar configurations are excluded too, for example, a nucleus of extreme prolate shape. As in the collective model, only small deformations are considered; therefore, the restriction (48) introduced by Eq. (39) is of no importance in that case. With the transformation (39) one obtains, for the vibrational part of the kinetic energy,

$$\begin{aligned}
&\left[\frac{\partial^2}{\partial y_1^2} + \left(\frac{A-4}{y_1} + \frac{2y_1}{y_1^2 - y_2^2} + \frac{2y_1}{y_1^2 - y_3^2}\right)\frac{\partial}{\partial y_1}\right. \\
&\qquad \left. + \text{cyclic permutations}\right] \\
&= \frac{\partial^2}{\partial y^2} + \frac{3A-4}{y}\frac{\partial}{\partial y} + \frac{1}{y^2} \\
&\quad \times \left(\frac{4}{\cos^2\alpha}(2 - \sin\alpha \cdot \cos 3\gamma - \sin^2\alpha)\frac{\partial^2}{\partial\alpha^2}\right. \\
&\quad + \frac{4}{\sin^2\alpha}(2 + \sin\alpha \cdot \cos 3\gamma)\frac{\partial^2}{\partial\gamma^2} + 8\frac{\sin 3\gamma}{\cos\alpha}\frac{\partial^2}{\partial\alpha\partial\gamma} \\
&\quad + \frac{2}{\sin\alpha \cdot \cos^3\alpha}[2 - (9A - 43)\cos^2\alpha + (9A - 29) \\
&\qquad \times \cos^4(\alpha + 2)\sin\alpha \cdot \cos 2\alpha \cdot \cos 3\gamma]\frac{\partial}{\partial\alpha} \\
&\quad + \frac{4}{\sin^2\alpha \cdot \sin 3\gamma}(3\sin\alpha - 2\sin\alpha \cdot \sin^2 3\gamma \\
&\qquad \left. + 6\cos 3\gamma)\frac{\partial}{\partial\gamma}\right).
\end{aligned} \tag{49}$$

For small deformations, that is, small α, this expression simplifies very much, and one obtains for the Schrödinger equation (38)

$$\begin{aligned}
&\frac{\hbar^2}{2m}\left\{\frac{\partial^2}{\partial y^2} + \frac{3A-4}{y}\frac{\partial}{\partial y} + \frac{8}{y^2}\left[\frac{\partial^2}{\partial\alpha^2} + \frac{4}{\sin\alpha}\frac{\partial}{\partial\alpha}\right.\right. \\
&\qquad \left. + \frac{1}{\sin^2\alpha}\left(\frac{\partial^2}{\partial\gamma^2} + 3\frac{\cos 3\gamma}{\sin 3\gamma}\frac{\partial}{\partial\gamma}\right)\right] \\
&\quad - \frac{2}{\sin^2\alpha}\left(\frac{L_{e1}^2}{\sin^2\gamma} + \frac{L_{e2}^2}{\sin^2(\gamma - 2\pi/3)}\right. \\
&\qquad \left.\left. + \frac{L_{e2}^2}{\sin^2(\gamma - 4\pi/3)}\right)\right\}C \\
&+ (E - V_c)C = 0.
\end{aligned} \tag{50}$$

This agrees with the well-known Schrödinger equation of the collective model.

7. DENSITY VIBRATIONS

The case of pure y-vibrations will be discussed shortly now, and it will be shown that it corresponds to density vibrations of monopole character. Only the case of a spherical nucleus will be considered, that is, a nucleus for which the wavefunction has a strong maximum for $\alpha = 0$. Let all the internal and the collective degrees of freedom apart from y have fixed values. For a spherical nucleus y is then simply proportional to the radius of the nucleus. This follows from Eq. (41). If the density distribution of the nuclear matter in the nucleus for fixed y is known, one can compute the average density distribution from the probability distribution of y. It will be shown now how that can be done. To make that simple, it will be assumed that the wavefunction of the nucleus gives—for a fixed value of y (which is proportional to the radius R)—constant nucleon density for $r < R$ and zero nucleon density for $r > R$:

$$\rho(r) = \rho_c \quad \text{for} \quad r < R, \quad \rho(r) = 0 \quad \text{for} \quad r > R. \tag{51}$$

The probability distribution of R (which is proportional to y) for the ground state will be assumed to be of the simple form (as an approximation):

$$P_0(R) \propto e^{-b(R-R_0)^2}. \tag{52}$$

R_0 is the nuclear radius. For the first excited monopole vibration one has

$$P_1(R) \propto e^{-b(R-R_0)^2} \cdot (R - R_0)^2. \tag{53}$$

Equation (51) gives the nucleon density for a fixed value of R. As different values of R will appear, due to the probability distributions (52) and (53), one has to compute the average nucleon density (averaged over R). For ρ in Eq. (51) this average is simply

$$\rho_0(r) = \rho_c \cdot \frac{\int_r^\infty e^{-b(R-R_0)^2}\,dR}{\int_0^\infty e^{-b(R-R_0)^2}\,dR} \tag{54}$$

for the ground state (52),

$$\rho_1(r) = \rho_c \cdot \frac{\int_r^\infty e^{-b(R-R_0)^2} \cdot (R - R_0)^2\,dR}{\int_0^\infty e^{-b(R-R_0)^2} \cdot (R - R_0)^2\,dR} \tag{55}$$

for the excited state (53).

In the denominators of Eqs. (54) and (55), one can integrate from $-\infty$ to $+\infty$ as an approximation. After a partial integration in Eq. (55) one obtains, instead of Eqs. (54) and (55),

$$\rho_0(r) = \rho_c(b/\pi)^{\frac{1}{2}} \int_r^\infty e^{-b(R-R_0)^2}\, dR, \tag{56}$$

$$\rho_1(r) = \rho_0(r) + (b/\pi)^{\frac{1}{2}}(r - R_0)e^{-b(r-R_0)^2}. \tag{57}$$

Equation (57) shows that $\rho_1(r)$ is different from $\rho_0(r)$ only in the surface region of the nucleus, because the exponential function has appreciable values only in the surrounding of $r = R_0$. Thus we can conclude that y-vibrations are characterized by changes of the density in the nuclear surface.

Papers on calculations of monopole vibrations have been published recently.[9,10] Perhaps the coordinates defined in this paper will be of help in simplifying future calculations.

8. THE OSCILLATOR POTENTIAL

With respect to the mathematics, the simplest shell model is that in which it is assumed that all the nucleons move in an oscillator well of equal strength. The harmonic oscillator has been studied extensively by Moshinsky *et al.*[11,12] (for further references, see Refs. 11 and 12). In the following the very simplest of the oscillator models will be discussed, namely that in which any spin and isospin dependent parts are neglected. It will be seen that there are excited states which are of collective nature, a fact which one cannot see easily in ordinary single-particle coordinates.

The ith nucleon moves in a potential

$$V_i = b^2 r_i^2 \cdot \hbar^2/2m. \tag{58}$$

The total potential entering the Schrödinger equation is then $\sum_{i=1}^{A} V_i$. With the transformation (19) this is transformed to the new coordinates

$$\frac{2m}{\hbar^2} \cdot V = \sum_{i=1}^{A} b^2(s_{i1}\mathbf{y}_1 + s_{i2}\mathbf{y}_2 + s_{i3}\mathbf{y}_3)^2. \tag{59}$$

Using the constraints (20) and (21) for the coordinates s_{ij}, one obtains simply

$$(2m/\hbar^2) \cdot V = b^2(y_1^2 + y_2^2 + y_3^2). \tag{60}$$

Thus the oscillator potential does not depend on the single-particle coordinates. Hence one would expect excited states for this potential which are of purely collective character, others which are single-particle states. Many of these states are degenerate, but their wavefunctions are completely different showing their different character. The degeneracy is just a peculiarity of the oscillator potential.

In the next section the case of ^{16}O is discussed shortly for the oscillator potential (60).

9. ^{16}O IN THE OSCILLATOR POTENTIAL

The wavefunction for ^{16}O in the oscillator potential (60) has an especially simple form. The groundstate is an eigenstate of the three operators O_{s1}, O_{s2}, O_{s3} [Eq. (30)]. This is an exception because O_{s1}, O_{s2}, O_{s3} do not commute and functions of an orthogonal system will, in general, not be eigenfunctions of all three operators at the same time. The dependence of the ground state wavefunction on the single-particle coordinates s_{ik} will be written in the form of a Slater determinant. The spin functions of the nucleons will be abbreviated by $\uparrow_i$ and $\downarrow_i$, where the index i is numbering the nucleons. The two directions of the arrow indicate the two possible spin states of spin $\frac{1}{2}$. The direction to which the spin is referred may be either space-fixed or body-fixed. As the total spin of ^{16}O is zero, one can choose any axis. For the isospin state the abbreviations $\overset{\uparrow}{\underset{\downarrow}{\}}}_i$ and $\overset{\downarrow}{\underset{\uparrow}{\}}}_i$ will be used. The first row of the Slater determinant has the following form:

$$\uparrow_1 \overset{\uparrow}{\underset{\downarrow}{\}}}_1,\ \downarrow_1 \overset{\uparrow}{\underset{\downarrow}{\}}}_1,\ \uparrow_1 \overset{\downarrow}{\underset{\uparrow}{\}}}_1,\ \downarrow_1 \overset{\downarrow}{\underset{\uparrow}{\}}}_1,\ \uparrow_1 \overset{\uparrow}{\underset{\downarrow}{\}}}_1 s_{11},\ \downarrow_1 \overset{\uparrow}{\underset{\downarrow}{\}}}_1 s_{11},\ \uparrow_1 \overset{\downarrow}{\underset{\uparrow}{\}}}_1 s_{11},$$
$$\downarrow_1 \overset{\downarrow}{\underset{\uparrow}{\}}}_1 s_{11},\ \uparrow_1 \overset{\uparrow}{\underset{\downarrow}{\}}}_1 s_{12},\ \downarrow_1 \overset{\uparrow}{\underset{\downarrow}{\}}}_1 s_{12},\ \uparrow_1 \overset{\downarrow}{\underset{\uparrow}{\}}}_1 s_{12},\ \downarrow_1 \overset{\downarrow}{\underset{\uparrow}{\}}}_1 s_{12},\ \uparrow_1 \overset{\uparrow}{\underset{\downarrow}{\}}}_1 s_{13},$$
$$\downarrow_1 \overset{\uparrow}{\underset{\downarrow}{\}}}_1 s_{13},\ \uparrow_1 \overset{\downarrow}{\underset{\uparrow}{\}}}_1 s_{13},\ \downarrow_1 \overset{\downarrow}{\underset{\uparrow}{\}}}_1 s_{13}. \tag{61}$$

The second row is the same as (61), but for the second nucleon; that means that the indices of the spin and the isospin functions and the first indices of the s_{ik} appearing in (61) are replaced by 2 now. For the total Slater determinant the abbreviation S_0 will be used.

Before continuing the discussion of solving the Schrödinger equation in the new coordinates, it will be shown that the well-known ground state of ^{16}O (written with the space vectors $\mathbf{r}_i$) depends on s_{ik} as given by Eq. (61).

To do this, we will start from the Schrödinger equation in the space vectors $\mathbf{r}_i$, solve it for the ground state with the oscillator potential, and transform the wavefunction to the new coordinates. The Schrödinger equation for a particle moving in the oscillator potential (58) is

$$[(\hbar^2/2m)\Delta_i + E_i - (\hbar^2/2m)b^2 r_i^2]\Psi_i(\mathbf{r}_i) = 0. \tag{61'}$$

For the present purpose the components of $\mathbf{r}_i$ are convenient for the use as coordinates:

$$\mathbf{r}_i = (r_{i1}, r_{i2}, r_{i3}). \tag{61''}$$

The ground state and the first excited states Ψ_i are

$$\Psi_i \propto e^{-br_i^2/2}, \quad \Psi_i \propto e^{-br_i^2/2} r_{ij}, \quad j = 1, 2, 3,$$

respectively. The groundstate of ^{16}O is then ($\mathcal{A}$ means antisymmetrization)

$$\Psi_0 = e^{-b(y_1^2+y_2^2+y_3^2)/2} \times \mathcal{A}\{\uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1, \downarrow_2 \overset{\uparrow}{\underset{\uparrow}{\}}}_2, \uparrow_3 \overset{\downarrow}{\underset{\downarrow}{\}}}_3, \downarrow_4 \overset{\downarrow}{\underset{\downarrow}{\}}}_4, r_{51}\uparrow_5 \overset{\uparrow}{\underset{\uparrow}{\}}}_5, r_{61}\downarrow_6 \overset{\uparrow}{\underset{\uparrow}{\}}}_6, r_{71}\uparrow_7 \overset{\downarrow}{\underset{\downarrow}{\}}}_7, r_{81}\downarrow_8 \overset{\downarrow}{\underset{\downarrow}{\}}}_8, \cdots\}. \quad (61''')$$

To obtain (61‴), the factors $e^{-br_i^2/2}$ were put before the $\mathcal{A}$ sign because the product of the 16 factors $e^{-br_i^2/2}$ is symmetric with respect to particle exchange. In the same way as in Eqs. (59) and (60), one can express the sum $\sum r_i^2$ by $y_1^2 + y_2^2 + y_3^2$. In Eq. (61‴) some of the single-particle wavefunctions have not been written down behind the $\mathcal{A}$ sign because the continuation of the scheme is obvious. The antisymmetric factor in (61‴) can also be written as a Slater determinant. The first row has the same form as (61) with s_{1j} replaced by r_{1j}. Now the transformation (19) is performed:

$$r_{1j} = s_{11}y_{1j} + s_{12}y_{2j} + s_{13}y_{3j}, \quad \text{etc.} \quad (61'''')$$

By combining different columns of the Slater determinant which have the same spin–isospin functions, the final form is obtained. It will be illustrated for the 5th, 9th, and 13th columns which have the spin–isospin function $\uparrow_i \overset{\uparrow}{\underset{\uparrow}{\}}}_i$.

5th column

$$(s_{11}y_{11} + s_{12}y_{21} + s_{13}y_{31})\uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$$
$$(s_{21}y_{11} + s_{22}y_{21} + s_{23}y_{31})\uparrow_2 \overset{\uparrow}{\underset{\uparrow}{\}}}_2$$
$$\cdot$$
$$\cdot$$
$$\cdot$$

9th column

$$(s_{11}y_{12} + s_{12}y_{22} + s_{13}y_{32})\uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$$
$$(s_{21}y_{12} + s_{22}y_{22} + s_{23}y_{32})\uparrow_2 \overset{\uparrow}{\underset{\uparrow}{\}}}_2$$
$$\cdot$$
$$\cdot$$
$$\cdot$$

13th column

$$(s_{11}y_{13} + s_{12}y_{23} + s_{13}y_{33})\uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$$
$$(s_{21}y_{13} + s_{22}y_{23} + s_{23}y_{33})\uparrow_2 \overset{\uparrow}{\underset{\uparrow}{\}}}_2$$
$$\cdot$$
$$\cdot$$
$$\cdot$$

To the 5th column the 9th column times y_{12}/y_{11} and the 13th column times y_{13}/y_{11} is added. Thus the 5th column is (this follows from the properties of the vectors $\mathbf{y}_i$) the following.

$$\frac{s_{11}y_1^2}{y_{11}} \uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$$
$$\frac{s_{21}y_1^2}{y_{11}} \uparrow_2 \overset{\uparrow}{\underset{\uparrow}{\}}}_2$$
$$\cdot$$
$$\cdot$$
$$\cdot$$

By subtracting the 5th column times $y_{11}y_{12}/y_1^2$ from the 9th column and the 5th column times $y_{11}y_{13}/y_1^2$ from the 13th column one obtains the following.

5th column	9th column	13th column
$\frac{s_{11}y_1^2}{y_{11}} \uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$	$(s_{12}y_{22} + s_{13}y_{32})\uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$	$(s_{12}y_{23} + s_{13}y_{33})\uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$
$\frac{s_{21}y_1^2}{y_{11}} \uparrow_2 \overset{\uparrow}{\underset{\uparrow}{\}}}_2$	$(s_{22}y_{22} + s_{23}y_{32})\uparrow_2 \overset{\uparrow}{\underset{\uparrow}{\}}}_2$	$(s_{22}y_{23} + s_{23}y_{33})\uparrow_2 \overset{\uparrow}{\underset{\uparrow}{\}}}_2$
.	.	.
.	.	.
.	.	.

Similarly one can eliminate s_{i3} from the 9th and s_{i2} from the 13th column by suitably combining these columns. The result is

5th column	9th column	13th column
$\frac{s_{11}y_1^2}{y_{11}} \uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$	$s_{12}\left(y_{22} - \frac{y_{32}y_{23}}{y_{33}}\right)\uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$	$s_{13}y_{33} \cdot \uparrow_1 \overset{\uparrow}{\underset{\uparrow}{\}}}_1$.
.	.	.
.	.	.
.	.	.

The factors y_1^2/y_{11}, $y_{22} - y_{32}y_{23}/y_{33}$, y_{33} can be put before the Slater determinant. They yield with Eq. (9)

$$(y_1^2/y_{11})(y_{22}y_{33} - y_{32}y_{23}) = y_1 \cdot y_2 \cdot y_3. \quad (61''''')$$

Similarly, one deals with the other columns, obtaining at the end, the Slater determinant (61).

This way we have found the Slater determinant for the ground state of ^{16}O in the oscillator potential. It is an eigenfunction of O_{s1}, O_{s2}, O_{s3} and of L_i^2 (see below). In general, one will not use this way of constructing the eigenfunctions for the operators (45). It is obvious that the completely antisymmetrized wavefunctions in the oscillator potential are polynomials with respect to s_{ik} (this will be true for any potential which depends on $y^2 = y_1^2 + y_2^2 + y_3^2$ only). The eigenfunctions of O_s, L_i^2, L_{i3} are polynomials too.

Thus one will construct these polynomial eigenfunctions and will use them for expanding the wavefunction, hoping that only a few of them are sufficient.

Operating with the operators O_{s1}, O_{s2}, O_{s3} on S_0, one obtains

$$O_{s1}S_0 = O_{s2}S_0 = O_{s3}S_0 = -60 \cdot S_0. \quad (62)$$

S_0 is an eigenfunction of L_{i1}, L_{i2}, L_{i3} with eigenvalue zero:

$$L_{i1}S_0 = L_{i2}S_0 = L_{i3}S_0 = 0. \quad (63)$$

The ground state wavefunction of ^{16}O in the oscillator potential (60) has the following form:

$$\Psi_0 = f_0(\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3) \cdot S_0. \quad (64)$$

For f_0 one obtains the following differential equation from the Schrödinger equation:

$$\left\{\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial y_1^2} + \left(\frac{12}{y_1} + \frac{2y_1}{y_1^2 - y_2^2} + \frac{2y_1}{y_1^2 - y_3^2}\right)\frac{\partial}{\partial y_1} - \frac{60}{y_1^2} + \text{cyclic permutations}\right] + E - \frac{\hbar^2}{2m} \cdot b^2(y_1^2 + y_2^2 + y_3^2)\right\} f_0 = 0. \quad (65)$$

The solution of Eq. (65) is (not normalized)

$$f_0 = (y_1 y_2 y_3)^4 e^{-\frac{1}{2}b(y_1^2 + y_2^2 + y_3^2)}. \quad (66)$$

Excited states can be of different kinds: Collective states are those for which the Slater determinant is the same as in the ground state. Noncollective states are those in which the dependence on the single-particle coordinates is different from the ground state. Only the first excited collective states will be written down here as examples.

They are a 0^+ and a 2^+ state:

$$\Psi_1^{0+} = (y_1 y_2 y_3)^4 e^{-(b/2)(y_1^2 + y_2^2 + y_3^2)} \times \{1 - \tfrac{2}{69}b(y_1^2 + y_2^2 + y_3^2)\} \cdot S_0, \quad (67)$$

$$\Psi_1^{2+} = (y_1 y_2 y_3)^4 e^{-(b/2)(y_1^2 + y_2^2 + y_3^2)} \times \{(y_1^2 - y_2^2) \cdot [D^2_{M2}(\varphi, \vartheta, \psi) + D^2_{M-2}(\varphi, \vartheta, \psi)] + \tfrac{2}{3}(2y_3^2 - y_1^2 - y_2^2)D^2_{M0}(\varphi, \vartheta, \psi)\} \cdot S_0. \quad (68)$$

The parameter b is usually fitted such that the expectation value of the radius agrees with the experimentally measured radius. If that is done, the excitation energy of the two degenerate states (67) and (68) is several times as high as the experimentally measured excitation energy. This disagreement shows the necessity to include residual two-body forces. As a consequence the wavefunctions will in general not be of the simple form as in (64), (67), and (68).

The collective states (67) and (68) cannot be considered as simple β- or γ-vibrations.

10. EFFECTIVE POTENTIALS BETWEEN COMPOSITE NUCLEI

With the help of the coordinates defined in this paper, one can simplify calculations on nuclear reactions in many cases. As an example for illustrating this, the possibilities for simplification in the elastic scattering of two α particles will be considered. One cannot simply treat the two α particles as bosons because the wavefunction of the system must be antisymmetric with respect to exchange of all the nucleons, including exchange between the nucleons which are in different α particles. This latter part of the antisymmetrization is of no importance as long as the α particles are far apart. But, as soon as they come close to each other, one has to antisymmetrize the wavefunction with respect to all exchanges. One can do this the way it is done by Wildermuth and McClure[13] (for further references, see Ref. 13). Then one starts from the variational principle

$$\delta \int \Psi^* H \Psi \, d\tau = 0. \quad (69)$$

For the wavefunction one uses the ansatz

$$\Psi = \mathcal{A}\{\Phi_\alpha(1) \cdot \Phi_\alpha(2)\chi(\mathbf{R})\}, \quad (70)$$

where Φ_α is the α-particle ground state and χ is the function of the relative motion to be determined by the variational principle. The sign $\mathcal{A}$ before the wavefunction means antisymmetrization. The function χ depends on the distance of the two α particles. If nucleons 1, 2, 3, 4 are in the first α particle, then one has

$$\mathbf{R} = \tfrac{1}{4} \cdot (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3 + \mathbf{r}_4 - \mathbf{r}_5 - \mathbf{r}_6 - \mathbf{r}_7 - \mathbf{r}_8). \quad (71)$$

The antisymmetrization effects $\mathbf{R}$ also. As a consequence, one obtains an integro-differential equation for the function $\chi(\mathbf{R})$.[13]

This method can be simplified by introducing a symmetrized α–α distance. Consider the α particles as spheres of radius R_α for simplicity. The principal moments of inertia are (with R as the distance of the α particles)

$$J_1 = \tfrac{4}{5}MR_\alpha^2, \quad J_2 = J_3 = \tfrac{4}{5}MR_\alpha^2 + MR^2/2 \quad (72)$$

Here M is the total mass of an α particle. The sequence of the moments J_1, J_2, J_3 in Eq. (72) is arbitrary, of course. From Eqs. (4) and (39) we have

$$J_1 + J_2 + J_3 = 2m(y_1^2 + y_2^2 + y_3^2) = 2my^2. \quad (73)$$

Equations (72) and (73) together give (with $M = 4m$ as an approximation)

$$y^2 = \tfrac{24}{5}R_\alpha^2 + 2R^2. \quad (74)$$

The direction of the vector **R** is identical in this approximation with the direction of one of the vectors $\mathbf{y}_i$. Therefore, we can define its direction by the angles ϑ and φ. Instead of describing the relative motion of the α particles by the nonsymmetrical vector **R**, one can simplify the mathematics of the problem by describing the relative motion with a symmetrical vector, the direction and length of which are given by ϑ, φ, and y, respectively. The symbol **y** will be used for this vector in the following.

The ansatz (70) is now replaced by an ansatz

$$\Psi = \chi(\mathbf{y})\mathcal{A}\{\Phi_\alpha(1)\Phi_\alpha(2)\}. \tag{75}$$

From the variational principal (69) one obtains a differential equation for $\chi(\mathbf{y})$. The kinetic energy operator will be somewhat different from the well-known two-particle kinetic energy operator. The potential energy is obtained as

$$V_{\text{eff}}(y) = \int \{[\Phi_\alpha(1)\Phi_\alpha(2)]\}^* \cdot [V_{12}(r_{12}) + \cdots] \times \{[\Phi_\alpha(1)\Phi_\alpha(2)]\}\, d\tau_1\, d\tau_2 \cdots d\tau_8\, d\tau_{\alpha,\gamma}\, d\psi. \tag{76}$$

In Eq. (76) only central interactions have been used giving an effective interaction which depends on y only and not on ϑ and φ.

Naturally it is much easier now to solve the problem mathematically, as one has a differential equation for $\chi(\mathbf{y})$ instead of an integro-differential equation as one would have with Eq. (73). Asymptotically, that is, for large α–α distances, there is no difference between Eq. (73) and Eq. (75):

$$y = 2^{\frac{1}{2}}R. \tag{77}$$

The effect of the antisymmetrization on the relative motion of the two α particles is replaced with this method by a potential.

For illustration, here is a little example. At first the case will be considered in which the wavefunction is not antisymmetrized with respect to the nucleons in different α particles. To simplify the problem, only one nucleon in every α particle is considered; nucleon one is in the first α particle, nucleon five in the second. The "average" interaction between these two nucleons will be calculated. We assume identical nucleons with parallel spins to see the effect of the antisymmetrization of the space function. Spin-dependent potentials will not be considered. The wavefunctions of the nucleons are taken to be those of oscillator potentials in the α particles. The wavefunctions of the two nucleons considered are then

$$e^{-\frac{1}{2}b(\mathbf{r}_1-\frac{1}{2}\mathbf{R})^2} \quad \text{and} \quad e^{-\frac{1}{2}b(\mathbf{r}_5+\frac{1}{2}\mathbf{R})^2}, \tag{78}$$

for the interaction of the two nucleons

$$V(r_{15}) = -V_0 e^{-\kappa(\mathbf{r}_1-\mathbf{r}_5)^2} \tag{79}$$

is used. To compute the average interaction of the two nucleons, one would have to replace the appearing coordinate vectors by the coordinates defined in this paper. The integration is difficult. So a further approximation is used: $\mathbf{r}_1$ and $\mathbf{r}_5$ are simply treated as independent vectors, and the integrations are performed over the whole $\mathbf{r}_1$, $\mathbf{r}_5$-space. With that, the average interaction between the two nucleons is

$$V_{\text{av}}(R) = -V_0 \cdot \int d\mathbf{r}_1 \int d\mathbf{r}_5 \times e^{-b(\mathbf{r}_1-\mathbf{R}/2)^2} e^{-b(\mathbf{r}_5+\mathbf{R}/2)^2} e^{-\kappa(\mathbf{r}_1-\mathbf{r}_5)^2} \times \left\{\int d\mathbf{r}_1 \int d\mathbf{r}_5 e^{-b(\mathbf{r}_1-\mathbf{R}/2)^2} e^{-b(\mathbf{r}_5+\mathbf{R}/2)^2}\right\}^{-1}. \tag{80}$$

The result is:

$$V_{\text{av}}(R) = -V_0 \cdot [b/(b+2\lambda)]^{\frac{3}{2}} e^{-R^2 b\lambda/(b+2\lambda)}. \tag{81}$$

Expressed with the symmetric quantity y, this is, with Eq. (74),

$$V_{\text{av}}(y) = -V_0 \cdot \left(\frac{b}{b+2\lambda}\right)^{\frac{3}{2}} \exp\left(\frac{12}{5} R_\alpha^2 \cdot \frac{b\lambda}{b+2\lambda}\right) \times \exp\left(-y^2 \cdot \frac{1}{2}\frac{b\lambda}{b+2\lambda}\right). \tag{82}$$

If the antisymmetrization between the two α particles is taken into account, then one uses for the internal wavefunction (the symmetric spin–isospin function is assumed here)

$$\exp\{-\tfrac{1}{2}b[(\mathbf{r}_1 - \tfrac{1}{2}\mathbf{R})^2 + (\mathbf{r}_5 + \tfrac{1}{2}\mathbf{R})^2]\} - \exp\{-\tfrac{1}{2}b[(\mathbf{r}_5 - \tfrac{1}{2}\mathbf{R})^2 + (\mathbf{r}_1 + \tfrac{1}{2}\mathbf{R})^2]\}. \tag{83}$$

R is treated as the symmetric quantity $\mathbf{R}(\mathbf{y})$ here, as discussed before. The result for the average potential is now

$$V_{\text{av}}(y) = -V_0\left(\frac{b}{b+2\lambda}\right)^{\frac{3}{2}} \exp\left(\frac{12}{5} R_\alpha^2 \cdot \frac{b\lambda}{b+2\lambda}\right) \times \exp\left(-y^2 \frac{1}{2}\frac{b\lambda}{b+2\lambda}\right) \times \left[1 - \exp\left(\frac{6}{5} R_\alpha^2 \frac{\kappa^2}{\kappa+2\lambda}\right) \times \exp\left(-\frac{1}{4} y^2 \frac{\kappa^2}{\kappa+2\lambda}\right)\right]. \tag{84}$$

In the asymptotic region there is no difference between Eq. (82) and Eq. (84). If the α particles are close to each other, a repulsive force is added to the original

attractive force. This is the effect of the antisymmetrization.

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 8 AUGUST 1971

Bose Gas in One Dimension. I. The Closure Property of the Scattering Wavefunctions*

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(Received 12 February 1971)

We verify the closure relation of a continuum basis of Lieb's wavefunctions, describing the scattering states of identical bosons interacting via a δ-function potential in one dimension.

1. INTRODUCTION

We consider the system of N identical Bose particles on an infinite axis interacting via a two-body repulsive δ-function potential. The Schrödinger equation for the wavefunction is

$$-\sum_{i=1}^{N}\frac{\partial^2\psi}{\partial x_i^2}+2c\sum_{i<j}\delta(x_i-x_j)\psi=E\psi. \tag{1}$$

The symmetrical scattering solution of Eq. (1) has been given by Lieb.[1] In the fundamental region D of R_N defined by the inequalities

$$-\infty<x_1<x_2<\cdots<x_N<\infty \tag{2}$$

such a wavefunction is expressed as a sum over all the permutations P of order N,

$$\psi_{\{k\}}(x)=\sum_P a(P)e^{i(Pk,x)}, \tag{3}$$

with the notation

$$(Pk,x)=\sum_{i=1}^{N}k_{Pi}x_i$$

and the rational form of the coefficients $a(P)$:

$$a(P)=\prod_{i<j}\left(1+\frac{ic}{k_{Pi}-k_{Pj}}\right). \tag{4}$$

The set $\{k\}$ parametrizes the scattering state $\psi_{\{k\}}$ and consists of N arbitrary but distinct real numbers,

$$\{k\}\equiv\{k_1,k_2,\cdots,k_N\}, \tag{5}$$

which are the momenta of the particles in the ingoing or outgoing states. The energy of the state is

$$E=\sum_{i=1}^{N}k_i^2. \tag{6}$$

So far, the wavefunction $\psi_{\{k\}}(x)$ is not normalized. Our aim is to prove the following closure relation:

$$I_N\equiv\int_{R_N}dk^N\frac{1}{G(k)}\psi_{\{k\}}(x)\psi^*_{\{k\}}(y)=N!\,(2\pi)^N\delta(x-y), \tag{7}$$

with

$$x\in D,\quad y\in D. \tag{8}$$

The δ function in D is defined as

$$\delta(x-y)=\delta(x_1-y_1)\delta(x_2-y_2)\cdots\delta(x_N-y_N), \tag{9}$$

and the normalization factor is

$$G(k)=\prod_{i<j}\left(1+\frac{c^2}{(k_i-k_j)^2}\right). \tag{10}$$

By introducing the phases ψ_{ij}

$$\psi_{ij}=2\tan^{-1}\left(\frac{c}{k_i-k_j}\right), \tag{11}$$

we infer from (7) that the normalized wavefunction in

attractive force. This is the effect of the antisymmetrization.

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Bose Gas in One Dimension. I. The Closure Property of the Scattering Wavefunctions*

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We verify the closure relation of a continuum basis of Lieb's wavefunctions, describing the scattering states of identical bosons interacting via a δ-function potential in one dimension.

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So far, the wavefunction $\psi_{\{k\}}(x)$ is not normalized. Our aim is to prove the following closure relation:

$$I_N\equiv\int_{R_N}dk^N\frac{1}{G(k)}\psi_{\{k\}}(x)\psi^*_{\{k\}}(y)=N!\,(2\pi)^N\delta(x-y), \tag{7}$$

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The δ function in D is defined as

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By introducing the phases ψ_{ij}

$$\psi_{ij}=2\tan^{-1}\left(\frac{c}{k_i-k_j}\right), \tag{11}$$

we infer from (7) that the normalized wavefunction in

the continuum would be

$$\phi_{(k)}(x) = [N!\,(2\pi)^N]^{-\frac{1}{2}} \times \sum_P \exp\left(\frac{i}{2}\sum_{i<j}\psi_{Pi,Pj} + i\sum_i k_{Pi}x_i\right) \quad (12)$$

for $x \in D$; and after extension of the ϕ by symmetry, we would have

$$\int_{R_N} \phi^*_{(k)}(x)\phi_{(k')}(x)\,d^N x = \delta(k - k'), \quad (13)$$

with k and $k' \in D$.

2. PROOF

A. Algebraic Part

We set

$$a(i,j) = 1 - \frac{ic}{k_i - k_j}. \quad (14)$$

Substituting the right-hand side of equality (3) for the wavefunctions in the expression (7) for I_N, we have

$$I_N = \int_{R_N} dk^N \sum_{P,Q} \frac{1}{G(k)} \prod_{i<j} a(Pj, Pi)a(Qi, Qj) \times \exp\,[i(Pk, x) - i(Qk, y)] \quad (15)$$

as a sum over independent permutations P and Q.

Substituting the expression (10) for $G(k)$ and summing over P and $R = Q^{-1}P$, we get

$$I_N = \int_{R_N} dk^N \sum_{P,R} \prod_{i<j} \frac{a(PR^{-1}i, PR^{-1}j)}{a(Pi, Pj)} \times \exp\,[i(Pk, (x - Ry))]. \quad (16)$$

Now we consider the double product over all pairs of indices (a pair is defined as a set of two elements) in the integrand of (16). By the following change of indices in the numerator,

$$R^{-1}i = i', \quad (17)$$

we write

$$\prod_{<j} \frac{a(PR^{-1}i, PR^{-1}j)}{a(Pi, Pj)} = \frac{\prod_{Ri'<Rj'} a(Pi', Pj')}{\prod_{i<j} a(Pi, Pj)}. \quad (18)$$

In any double product, the $\frac{1}{2}N(N-1)$ pairs occur. With each pair (i,j) in the denominator of the right-hand side of (18), we associate the corresponding identical pair (i',j') in the numerator. Thus we have two possibilities:

(a) $i' = i, j' = j$, which means

$$i < j, \quad Ri < Rj \quad (19)$$

and that the corresponding terms cancel in (18);

(b) $i' = j, j' = i$, which means

$$i < j, \quad Ri > Rj. \quad (20)$$

We will denote the inversion of the pair (i,j) by R with the notation $(i,j)_R$. For example, with the permutation $R_1 = \left[\begin{smallmatrix}1234\\3142\end{smallmatrix}\right]$, we have the inverted pairs $(1,2)_{R_1}$, $(1,4)_{R_1}$, and $(3,4)_{R_1}$.

In case (b), the corresponding factor in (18) is clearly

$$\frac{a(Pj, Pi)}{a(Pi, Pj)}, \quad i < j, (i,j)_R. \quad (21)$$

Therefore we can write

$$I_N = \int_{R_N} dk^N \sum_{P,R} \prod_{(i,j)_R} \frac{k_{Pi} - k_{Pj} + ic}{k_{Pi} - k_{Pj} - ic} \times \exp\left(i\sum_l k_{Pl}(x_l - y_{Rl})\right). \quad (22)$$

The change of integration variables

$$k_{Pi} \to k_i$$

gives us

$$I_N = \sum_R I(R),$$

with

$$I(R) = N!\int_{R_N} dk^N \prod_{(i,j)_R} \frac{k_i - k_j + ic}{k_i - k_j - ic} \times \exp\left(i\sum_l k_l(x_l - y_{Rl})\right). \quad (23)$$

B. Integration Part

It remains to perform the integrations (23); let us isolate the term $I(1)$ associated with the identical permutation. There is no pair inverted by $R =$ identity, and we have

$$I(1) = N!\,(2\pi)^N \delta(x_1 - y_1)\delta(x_2 - y_2)\cdots\delta(x_N - y_N). \quad (24)$$

Now we prove

$$I(R) = 0, \quad \text{for all } R \neq \text{identity}, x, y \in D. \quad (25)$$

Suppose R is given. For each pair $(i,j)_R$ inverted by R, we have the implications

$$i < j \text{ and } x \in D \Rightarrow x_i < x_j, \quad (26)$$

$$Ri > Rj \text{ and } y \in D \Rightarrow y_{Ri} > y_{Rj}. \quad (27)$$

Therefore, by setting

$$\xi_i = x_i - y_{Ri}, \quad (28)$$

we deduce from (26) and (27)

$$\xi_i < \xi_j \quad \text{for} \quad (i,j)_R, \quad i < j. \quad (29)$$

The quantities ξ_i form a set partially ordered by the relation "inverted by R." Let us introduce the graph Γ, the vertices of which are labeled by the indices i, with a line between i and j, if $(i,j)_R$. Since R is not the

identity, the graph Γ contains at least one line. The integrand of $I(R)$ is clearly constructed by associating one factor with each line of Γ. Thus the integral $I(R)$ is a product of integrals associated with each connected part of Γ. Consider one connected part Γ_c of Γ, with L vertices and at least one line. Call the corresponding integral $I(\Gamma_c)$. Changing the name of the variables k, we have

$$I(\Gamma_c) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dk_1 \cdots dk_L \prod_{(i,j)_R \in \Gamma_c} \frac{k_i - k_j + ic}{k_i - k_j - ic} \times \exp\left(i\sum_{l=1}^{L} k_l \xi_l\right). \quad (30)$$

In the variables ξ, $I(\Gamma_c)$ is a distribution Fourier transform of a rational function translationally invariant; hence its support is the plane

$$\sum_{l=1}^{L} \xi_l = 0, \quad (31)$$

On the other hand, there exists a vertex $m \in \Gamma_c$ such that

$$\xi_m \leq \xi_i, \quad \forall\, i \in \Gamma_c. \quad (32)$$

Call $\{n\}$ the set of vertices of Γ_c connected to m by a line. Since the line (m, n) exists, we have $(m, n)_R$; this means from (39) that

$$m < n \quad \text{and} \quad \xi_m < \xi_n$$

or

$$m > n \quad \text{and} \quad \xi_m > \xi_n.$$

From (32), the second part of the alternative is impossible and we are left with

$$m < n \quad \text{and} \quad \xi_m < \xi_n \quad (33)$$

for the vertices $\{n\}$ connected to m. Now we deduce

$$\xi_m < 0. \quad (34)$$

Assume $\xi_m \geq 0$; from (32) and (33) this would imply

$$\sum_{i \in \Gamma_c} \xi_i > 0,$$

which contradicts Eq. (31).

With the results $\xi_m < 0$ and $n > m$ for the vertices n connected to m by a line of Γ_c, we are able to show that $I(\Gamma_c)$ is zero. According to a theorem (Schwartz[2] and Gel'fand[3]) on the generalized functions, the Fourier transform $I(\Gamma_c)$ can be calculated as limit of the corresponding integral over a box $[-K_i < k_i < K_i]$, $i = (1, L)$ with $\lim K_i = +\infty$. We first integrate over the variable k_m. The corresponding factor J_m in $I(\Gamma_c)$ is

$$J_m = \lim_{K_m \to \infty} \int_{-K_m}^{+K_m} dk_m e^{ik_m \xi_m} \prod_{n>m} \frac{k_m - k_n + ic}{k_m - k_n - ic}. \quad (35)$$

The poles of the integrand (35) are all in the upper half-plane $k_m \doteq k_n + ic$ $(c > 0)$, and at infinity we have

$$\prod_{n>m} = 1 + O\left(\frac{1}{k_m}\right).$$

Thus we deduce $J_m = 2\pi\delta(\xi_m) +$ a function of ξ_m which is zero for $\xi_m < 0$. Therefore, in the open domain $\xi_m < 0$, the distribution J_m is zero. This proves $I(\Gamma_c) = 0$ and $I(R) = 0$ in the open domain D, for $R \neq$ identity. Then the closure property follows from (23) and (24):

$$I_N = I(1) = N!\,(2\pi)^N \delta(x - y) \quad x, y \in D.$$

In the following paper, we will give a direct proof of the orthogonality relation (13).

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Bose Gas in One Dimension. II. Orthogonality of the Scattering States*

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A direct calculation gives the normalization integral for a basis of scattering wavefunctions of interacting bosons in one dimension.

In the preceding, Paper I, we found the closure relation of a basis of scattering wavefunctions for the one-dimensional system of bosons with repulsive δ interaction. Here is given a direct calculation of the normalization integral (I.13). This approach is based on algebraic identities which show once more the interesting structure of Bethe's wavefunctions.

With the notations of Paper I, a convenient basis of scattering states for the system of N repulsive bosons is the following:

$$\psi_{\{k\}}(x) = \sum_P a(P) e^{i(Pk.x)}, \tag{1}$$

with x $(x_1, x_2, \cdots, x_N)$ in the fundamental region D_N of R_N: $x_1 < x_2 < \cdots < x_N$. The k are distinct real momenta in D_N, and the coefficient $a(P)$ is

$$a(P) = \prod_{i<j} \left(1 + \frac{ic}{k_{Pi} - k_{Pj}}\right). \tag{2}$$

So far, the $\psi_{\{k\}}(x)$ are not normalized.

We calculate the normalization integral

$$\mathcal{N}\begin{pmatrix} k_1 k_2 \cdots k_N \\ k'_1 k'_2 \cdots k'_N \end{pmatrix} = \int_{D_N} \psi^*_{\{k\}}(x) \psi_{\{k'\}}(x) d^N x, \tag{3}$$

which is a generalized function, the sum of Fourier transforms of characteristic functions of the domain D_N.

Using the definitions (1) and (2), we have

$$\mathcal{N} = \sum_{P,Q} a^*(P) a'(Q) \int_{D_N} \exp\left[i((Qk' - Pk), x)\right] d^N x. \tag{4}$$

Setting

$$Pk - Qk' = q, \tag{5}$$

we calculate the distribution in q,

$$J_N = \int_{D_N} e^{-i(q \cdot x)}\, d^N x = \int_{-\infty < x_1 < x_2 < \cdots < x_N < \infty} e^{-i(q_1 x_1 + \cdots + q_N x_N)}\, dx_1 \cdots dx_N, \tag{6}$$

and we easily find

$$J_N(q) = 2\pi\delta(q_1 + q_2 + \cdots + q_N) \times \frac{i^{N-1}}{(q_1 + io)(q_1 + q_2 + io)\cdots(q_1 + \cdots + q_{N-1} + io)}. \tag{7}$$

Here we derive an equality which will be useful later. From the definition (6) of $J_N(q)$ we have

$$\sum_P J_N(Pq) = (2\pi)^N \delta(q_1)\delta(q_2)\cdots\delta(q_N). \tag{8}$$

On the other hand, a known algebraic identity gives us from (7) the result

$$\sum_P J_N(Pq) = 2\pi\delta(q_1 + q_2 + \cdots + q_N) \times \sum_{j=1}^{N} \frac{i^{N-1}}{(q_1 + io)\cdots(q_{j-1} + io)(q_{j+1} + io)\cdots(q_N + io)} = (2\pi)^N \delta(q_1)\cdots\delta(q_N). \tag{9}$$

Now, using (5) and (7), we obtain

$$\mathcal{N} = 2\pi i^{N-1} \delta(k_1 + \cdots + k_N - k'_1 - \cdots - k'_N) \times \tilde{\Delta}\begin{pmatrix} k_1 + io, & k_2 + io, & \cdots, & k_N + io \\ k'_1, & k'_2, & \cdots, & k'_N \end{pmatrix}, \tag{10}$$

with the following definition of $\tilde{\Delta}$, a rational function of $\{k\}$ and $\{k'\}$:

$$\tilde{\Delta}\begin{pmatrix} k \\ k' \end{pmatrix} = \sum_{P,Q} a^*(P) a'(Q) \times [(k_{P1} - k'_{Q1})(k_{P1} + k_{P2} - k'_{Q1} - k'_{Q2})\cdots (k_{P1} + \cdots + k_{P(N-1)} - k'_{Q1} - \cdots - k'_{Q(N-1)})]^{-1}. \tag{11}$$

In the expression (10), the norm $\mathcal{N}$ appears as the product of an over-all δ function expressing the conservation of total momentum by the boundary value of an analytic function of $\{k\}$ in $\operatorname{Im} k > 0$.

Now the fundamental identity proved in the Appendix [Eq. (A11)] is used to write $\tilde{\Delta}$ in a form which exhibits its true singularities. We obtain

from (A4)–(A6)

$$\tilde{\Delta}\binom{k}{k'} = \Delta\binom{k}{k'}(k_1 + \cdots + k_N - k'_1 - \cdots - k'_N)$$
$$= \sum_R I(R)\, d(R) \times \frac{(k_1 + \cdots + k_N - k'_1 - \cdots - k'_N)}{(k_1 - k'_{R1})(k_2 - k'_{R2}) \cdots (k_N - k'_{RN})}, \tag{12}$$

with the coefficients $d(R)$ given by

$$d(R) = \frac{1}{\delta_N} \frac{1}{(k_1 - k'_{R1} + ic) \cdots (k_N - k'_{RN} + ic)} \tag{13}$$

and

$$\delta_N = \left| \frac{1}{k_i - k'_j + ic} \right|_N. \tag{14}$$

The only singularities of $\tilde{\Delta}$ are the poles $k_i = k'_{Ri}$.

Using the expansion (12), we write

$$\delta(k_1 + \cdots + k_N - k'_1 - k'_2 - \cdots - k'_N)\tilde{\Delta}\begin{pmatrix} k_1 + io & \cdots & k_N + io \\ k'_1 & \cdots & k'_N \end{pmatrix}$$
$$= \sum_R I(R) d(R) \delta(k_1 + \cdots - k'_1 - \cdots - k'_N) \times \sum_{j=1}^{N} \frac{1}{(k_1 - k'_{R1} + io) \cdots (k_{j-1} - k'_{R(j-1)} + io)(k_{j+1} - k'_{R(j+1)} + io) \cdots}. \tag{15}$$

The equality (9) applied to each term of the sum over R gives for the left-hand side of Eq. (15)

$$\tilde{\Delta}\binom{k + io}{k'} \delta(k_1 + \cdots - k'_N)$$
$$= \left(\frac{2\pi}{i}\right)^{N-1} \sum_R d(R) I(R) \delta(k_1 - k'_{R1}) \cdots \delta(k_N - k'_{RN}). \tag{16}$$

Clearly the function $d(R)$ has to be evaluated at the point $k_i = k'_{Ri}$ for all i. This gives from (13) and (14)

$$d(R) = I(R) \frac{\prod_{i<j} (k_i - k_j)^2}{\prod_{i<j} (k_i - k_j)^2 + c^2}. \tag{17}$$

From (10), (16), and (17), we finally obtain

$$\mathcal{N}\begin{pmatrix} k_1 \cdots k_N \\ k'_1 \cdots k'_N \end{pmatrix} = (2\pi)^N \prod_{i<j} \left(1 + \frac{c^2}{(k_i - k_j)^2}\right) \times \sum_R \delta(k_1 - k'_{R1}) \cdots \delta(k_N - k'_{RN}). \tag{18}$$

Together with the previous result on the closure property, the formula (18) expresses the unitarity of the following transformation function introduced in Paper I:

$$\langle \{k\} \mid \{x\} \rangle = (2\pi)^{-N/2} [G(k)]^{-\frac{1}{2}} \psi_{\{k\}}(x)$$
$$= (2\pi)^{-N/2} \sum_P \exp\left(\frac{i}{2} \sum_{i<j} \psi_{Pi,Pj} + i \sum_j k_{Pj} x_j\right), \tag{19}$$

with both x and k in the domain D_N.

APPENDIX

1. Identity (A4)

Consider the coefficients $a(P)$ of the scattering Bethe's wavefunction as a function of N complex numbers $\{k\}$. We choose the rational form

$$a(P) = \prod_{1 \le i < j \le N} \left(1 + \frac{\gamma}{k_{Pi} - k_{Pj}}\right), \tag{A1}$$

with $\gamma = ic$. We call $a'(Q)$ the coefficient defined with another set $\{k'\}$, for a current permutation Q, and we note $\bar{a}(P)$, the result of reversing the sign of the constant c (or γ) in $a(P)$. When the k are real, we have $\bar{a}(P) = a^*(P)$. From the definition (A1), we have also

$$\bar{a}(P) = a(PT), \tag{A2}$$

where T is the permutation $\left[\begin{smallmatrix} 1 & 2 & \cdots & N \\ N & (N-1) & \cdots & 1 \end{smallmatrix}\right]$.

Let us define the quantity $\Delta_N\binom{k}{k'}$ by the following double sum over permutations P and Q:

$$\Delta_N = \sum_{P,Q} \bar{a}(P) a'(Q) \times [(k_{P1} - k'_{Q1})(k_{P1} + k_{P2} - k'_{Q1} - k'_{Q2}) \cdots (k_{P1} + \cdots + k_{PN} - k'_{Q1} - \cdots - k'_{QN})]^{-1}. \tag{A3}$$

Clearly Δ_N is a rational and completely symmetric function of the k, and separately of the k'. It will be expressed as the quotient of two determinants, in a way reminiscent of the bialternant of the theory of symmetric functions. We have the *identity*

$$\Delta\begin{pmatrix} k_1 & \cdots & k_N \\ k'_1 & \cdots & k'_N \end{pmatrix} = \frac{D_N}{\delta_N}, \tag{A4}$$

with

$$D_N = \left| \frac{1}{(k_i - k'_j)(k_i - k'_j + \gamma)} \right|_N \tag{A5}$$

and Cauchy's determinant

$$\delta_N = \left| \frac{1}{k_i - k'_j + \gamma} \right|_N. \tag{A6}$$

The indices i and j label, respectively, the lines and the columns in (A5) and (A6).

This identity was verified at the lowest order $N = 2$ by noticing that the sum

$$\sum_{P,Q} \bar{a}(P)a'(Q)\frac{1}{k_{P1} - k'_{Q1}}$$

is divisible by $(k_1 + k_2 - k'_1 - k'_2)$. We obtain in a straightforward way

$$\Delta_2\begin{pmatrix} k_1 & k_2 \\ k'_1 & k'_2 \end{pmatrix} = \left(1 + \frac{c^2 - ic(k_1 + k_2 - k'_1 - k'_2)}{(k_1 - k_2)(k'_1 - k'_2)}\right) \times \frac{1}{(k_1 - k'_1)(k_2 - k'_2)} + \left(1 - \frac{c^2 - ic(k_1 + k_2 - k'_1 - k'_2)}{(k_1 - k_2)(k'_1 - k'_2)}\right) \times \frac{1}{(k_1 - k'_2)(k_2 - k'_1)}. \quad \text{(A7)}$$

Subtracting and adding the quantity $[(k_1 - k_2)(k'_1 - k'_2)]^{-1}$, we find a sum of two terms:

$$\Delta_2 = \sum_R I(R)d(R)\frac{1}{(k_1 - k'_{R1})(k_2 - k'_{R2})}, \quad \text{(A8)}$$

with $I(R)$ the sign of the permutation R and

$$d(R) = -\frac{(k_1 - k'_{R2} + ic)(k_2 - k'_{R1} + ic)}{(k_1 - k_2)(k'_1 - k'_2)}. \quad \text{(A9)}$$

In this form the generalization of (A8) and (A9) is almost obvious and leads us to

$$d(R) = \frac{\prod_{i \neq j}(k_i - k'_{Rj} + ic)}{\prod_{i<j}(k_i - k_j)(k'_j - k'_i)} \quad \text{(A10)}$$

and

$$\Delta_N = \sum_R I(R)d(R)\frac{1}{(k_1 - k'_{R1})\cdots(k_N - k'_{RN})}. \quad \text{(A11)}$$

Using Cauchy's identity, one gets (A4).

2. Proof of Identity (A4)

The definition (A3) of Δ_N is equivalent to the following recurrence relation, obtained by multiplying the two sides of Eq. (A3) by $\sum_{i=1}^N (k_i - k'_i)$, setting $PN = r$, $QN = s$, and using the definition of $\bar{a}(P)$ and $a'(Q)$:

$$\sum_{i=1}^N (k_i - k'_i)\Delta_N = \sum_{r=1}^N \sum_{s=1}^N \Delta_{N-1}\begin{pmatrix} \cdots \not{k}_r \cdots \\ \cdots \not{k}'_s \cdots \end{pmatrix} \times \prod_{j(\neq r)}\left(1 - \frac{\gamma}{k_j - k_r}\right)\prod_{i(\neq s)}\left(1 + \frac{\gamma}{k'_i - k'_s}\right). \quad \text{(A12)}$$

The identity (A12) has been proved for $N = 2$ in (A7)–(A11) and now we proceed by induction over N. Assume that (A4) is true to order $N - 1$; then we have

$$\Delta_{N-1}\begin{pmatrix} \cdots \not{k}_r \cdots \\ \cdots \not{k}'_s \cdots \end{pmatrix} = \frac{\text{cofactor } |D_N|_{rs}}{\text{cofactor } |\delta_N|_{rs}} = \frac{\text{cofactor } |D_N|_{r,s}}{\delta_N} \times \frac{(-)^{r+s}\prod_{j(\neq r)}(k_r - k_j)\prod_{i(\neq s)}(k'_s - k'_i)}{(k_r - k'_s + \gamma)\prod_{j(\neq s)}(k_r - k'_j + \gamma)\prod_{i(\neq r)}(k_i - k'_s + \gamma)}. \quad \text{(A13)}$$

We choose the definition

$$|A| = \sum_s (-)^{r+s}a_{rs}\,\text{cofactor } |a_{rs}|.$$

Substituting in (A12) for Δ_{N-1} given by (A13), we reduce the equality to be proved to

$$\sum (k - k')\,|D_N| = \frac{1}{\gamma^2}\sum_{r,s}(-)^{r+s}\text{cofactor } |D_N|_{rs}(k_r - k'_s + \gamma)e_r e'_s, \quad \text{(A14)}$$

with

$$e_r = \prod_{j=1}^N \frac{k_j - k_r - \gamma}{k'_j - k_r - \gamma}, \quad \text{(A15)}$$

$$e'_s = \prod_{i=1}^N \frac{k'_i - k'_s + \gamma}{k_i - k'_s + \gamma}. \quad \text{(A16)}$$

Clearly the right-hand side of (A14) is the sum of three determinants of order $N + 1$ obtained by adding to D_N one line and one column of index 0. Thus we have to prove the identity

$$-\gamma^2 \sum (k - k')D_N = D^{(1)} - D^{(2)} + \gamma D^{(3)}, \quad \text{(A17)}$$

with the definitions

$$\begin{aligned} D^{(\alpha)}_{oo} &= 0, \quad D^{(\alpha)}_{rs} = |D_N|_{rs}, \quad r, s = [1, N], \\ D^{(1)}_{os} &= e'_s, \quad D^{(1)}_{ro} = k_r e_r, \\ D^{(2)}_{os} &= k'_s e'_s, \quad D^{(2)}_{ro} = e_r, \\ D^{(3)}_{os} &= e'_s, \quad D^{(3)}_{ro} = e_r. \end{aligned} \quad \text{(A18)}$$

Now we remark that the new line (or column) is a linear combination of those of D_N. By a partial fraction decomposition of e_r and e'_s in the variable γ, we have

$$e_r = 1 - \sum_{j=1}^N \frac{f_j}{k_r - k'_j + \gamma}, \quad \text{(A19)}$$

$$e'_s = 1 - \sum_{i=1}^N \frac{f'_i}{k_i - k'_s + \gamma}. \quad \text{(A20)}$$

From their definition, (A15) and (A16), these quantities are zero for $\gamma = 0$. Thus we obtain

$$e_r = \gamma \sum_j \frac{f_j}{(k_r - k'_j)(k_r - k'_j + \gamma)}, \quad \text{(A21)}$$

$$e'_s = \gamma \sum_i \frac{f'_i}{(k_i - k'_s)(k_i - k'_s + \gamma)}, \quad \text{(A22)}$$

or in other terms,

$$D^{(3)}_{ro} - \gamma \sum_j f_j D^{(3)}_{rj} = 0. \quad \text{(A23)}$$

Thus, by combining the lines for $D^{(1)}$ and $D^{(3)}$, the columns for $D^{(2)}$ and $D^{(3)}$, we obtain

$$D^{(1)} = -D_N \cdot \gamma \left(\sum_i f'_i k_i e_i \right), \quad \text{(A24)}$$

$$D^{(2)} = -D_N \cdot \gamma \left(\sum_j f_j k'_j e'_j \right), \quad \text{(A25)}$$

$$D^{(3)} = -D_N \cdot \left(\gamma \sum_j f_j e'_j \right) = -D_N \cdot \gamma \left(\sum_i f'_i e_i \right). \quad \text{(A26)}$$

Substituting for the quantities e_i and e'_j the expressions (A19) and (A20), we add (A24), (A25), and (A26) divided by D_N:

$$\begin{aligned} \frac{1}{D_N}(D^{(1)} - D^{(2)} + \gamma D^{(3)}) &= -\gamma \sum_j (k'_j f_j - k_j f'_j) - \gamma^2 \sum_i f'_i \\ &\quad + \gamma \sum_{j,i} \left(\frac{-k'_j f_j f'_i}{k_i - k'_j + \gamma} + \frac{k_j f'_i f_j}{k_i - k'_j + \gamma} + \gamma \frac{f'_i f_j}{k_i - k'_j + \gamma} \right) \\ &= -\gamma^2 \sum f'_i + \gamma \sum_i (k_i f'_i - k'_i f_i) + \gamma \sum_{i,j} f'_i f_j. \end{aligned} \quad \text{(A27)}$$

It remains to use the definitions of the residues f_i and f'_i from (A15) and (A19):

$$\sum_i f'_i = \left(\text{coefficient of } \frac{1}{\gamma} \text{ in } e'_s \right) = \sum_i (k_i - k'_i). \quad \text{(A28)}$$

In the same way, we find

$$\sum_i f_i = \sum_i (k_i - k'_i), \quad \text{(A29)}$$

$$\sum_i k_i f'_i = \tfrac{1}{2} \sum (k'^2 - k^2) - \tfrac{1}{2} \left(\sum (k' - k) \right)^2, \quad \text{(A30)}$$

$$\sum_i k'_i f_i = \tfrac{1}{2} \sum (k'^2 - k^2) + \tfrac{1}{2} \left(\sum (k' - k) \right)^2. \quad \text{(A31)}$$

By using equalities (A28)–(A31), the equality (A27) becomes

$$D^{(1)} - D^{(2)} + \gamma D^{(3)} = -\gamma^2 D_N \cdot \sum (k - k'), \quad \text{(A32)}$$

which is exactly the required identity (A17). This completes the proof of the identity (A4).

3. Limiting Cases

$c \to \infty$: We have for the leading term

$$\tilde{a}(P) a'(Q) \propto I(P) I(Q) \frac{c^{N(N-1)}}{\prod_{i<j} (k_i - k_j)(k'_i - k'_j)}.$$

By summing over P the right-hand side of (A3) at $R = QP^{-1}$ fixed, we deduce from a known identity

$$\lim_{c \to \infty} \frac{\Delta_N}{c^{N(N-1)}} = \frac{1}{\prod_{i<j} (k_i - k_j)(k'_i - k'_j)} \times \sum_R \frac{I(R)}{(k_1 - k'_{R1}) \cdots (k_N - k'_{RN})},$$

which is precisely the limiting form available from (A10) and (A11).

$c \to 0$: $\tilde{a}(P) a'(Q) \to 1$ and we have

$$\Delta_N = \left| \frac{1}{k_i - k'_j} \right|^{+}_{N} \quad \text{(permanent)}.$$

Even in this limit we get a nontrivial identity due to Borchart[1] between this permanent and the quotient of two determinants

$$\left| \frac{1}{k_i - k'_j} \right|^{+}_{N} \cdot \left| \frac{1}{k_i - k'_j} \right|^{+}_{N} = \left| \frac{1}{(k_i - k'_j)^2} \right|_N,$$

which can be proved directly. In a following paper we will show a surprising connection between the bisymmetric $\Delta_N(^k_{k'})$ and Bethe's wavefunction for the spin-$\frac{1}{2}$ fermion system.

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[1] T. Muir, *Theory of Determinants* (Dover, New York), Chap. VI, p. 151.

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Euler Factorization of $SO(p,q)$ and $SU(p,q)$ Groups

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A parametrization scheme for orthogonal and unitary groups is developed. This scheme is broadly similar to one developed earlier by Wigner, but differs from it in some essential details. It is shown that an arbitrary element g of the group $SO(p,q)$, $[SU(p,q)]$, $3 \leq p < \infty, 0 \leq q < \infty, p+q = N$, can be written as a product of three factors, $g = aBc$, such that the extreme factors a and c belong to $SO(p,q-1)$ $[SU(p,q-1)]$ and the middle factor is an element of $SO(p,q)$, $[SU(p,q)]$ depending on at most two parameters and representing a "rotation" (real, complex, unitary or pseudo-unitary, as the case may be) in the $(1-N)$ plane. This parametrization includes the Euler parametrization $R = R_{12}(\varphi_1)R_{13}(\theta)R_{12}(\varphi_2)$ of the group $SO(3)$ as a special case, and is therefore a generalization of the Euler angle concept to more general orthogonal and unitary groups. The present factorization scheme differs from Wigner's, which is of the form $g = [SO(p) \otimes SO(q)]K[SO(p) \otimes SO(q)]$ [and similarly for $SU(p,q)$], in that the extremal factors of this latter scheme are not the next natural subgroup of the original group. Consequently, the middle term K may depend on more than two parameters. Furthermore, the method of proof presented here is entirely different from Wigner's, and may serve as a useful alternative, if further generalization to real Lie groups that preserve some other types of bilinear forms is envisaged. By stepwise factorization, the element g may ultimately be expressed as a product of real, complex, unitary or pseudo-unitary "rotations" in the plane.

1. INTRODUCTION

The expression of the general element of an n-parameter Lie group, as a product of factors depending on fewer than n parameters, usually simplifies the problem of deriving the representation matrices of the group. In fact, in deriving matrices for finite transformations of such groups as $SU(3)$, such a factorization is virtually imperative.[1] Such a factorization in terms of the Euler angles φ and θ is well known for the rotation group $SO(3)$. Thus, if $R \in SO(3)$, then $R = R_{12}(\varphi_1)R_{13}(\theta)R_{12}(\varphi_2)$. Murnaghan[2] has worked out a factorization (and hence a parametrization) scheme for more general orthogonal and unitary groups in terms of the so-called latitude and longitude angles. For $SO(3)$, this factorization differs essentially from the Euler factorization in that there is no repeated $R_{12}(\varphi)$ factor. The Euler angles are useful parameters for the analysis of rigid body motions. It is therefore reasonable to require that when symmetry groups other than $SO(3)$ are used in physics, the factorization (and parametrization) of such groups should be such as to preserve the advantages of the Euler angle parametrization. This can best be achieved by ensuring that the parameters used are simple and direct generalizations of the Euler angles of rigid body mechanics. The latitude and longitude angles do not quite satisfy this criterion. In the book of Murnaghan,[3] there is a statement: "The repetition of the 12-plane in the Euler factorization impedes the extension of this factorization to n-dimensional rotation matrices, where $n > 3$." The results of our present paper indicate that the contrary is rather the case: The Euler factorization $R = R_{12}(\varphi_1)R_{13}(\theta)R_{12}(\varphi_2)$ of the group $SO(3)$ can be generalized in a simple and straightforward way to all $SO(p,q)$ and $SU(p,q)$ groups, for $p \geq 3, q \geq 0$.

We present the problem in the form of the following two theorems:

Theorem 1: Every matrix $g \in SO(p,q)$, $3 \leq p < \infty$, $0 \leq q < \infty$, $p+q = N$, $p \geq q$, may be represented in the form $g = aB(\theta)c$, where $a, c \in SO(p,q-1)$ if $q > 0$ or $a, c \in SO(p-1)$ if $q = 0$, and $B(\theta)$ belongs to a one-parameter subgroup of $SO(p,q)$.

Theorem 2: Every matrix $g \in SU(p,q)$, $3 \leq p < \infty$, $0 \leq q < \infty$, $p+q = N$, $p \geq q$, may be represented in the form $g = uB(\varphi_1, \varphi_2 = 0, \theta)v$, where $u, v \in SU(p,q-1)$ if $q > 0$ or $u, v \in SU(p-1)$ if $q = 0$; and $B(\varphi_1, \varphi_2, \theta)$ is an element of a three-parameter subgroup of $SU(p,q)$.

The factorization scheme which is embodied in the above theorems is somewhat similar to that derived by Wigner[4] as a by-product of his theory of peripheral nuclear reactions. This factorization given in Ref. 4 is of the form

$$g = [SQ(p) \otimes SQ(q)]U'[SQ(p) \otimes SQ(q)],$$
$$g \in SQ(p,q), \quad Q = 0 \text{ or } U,$$

where U' is of the form

$$U' = \begin{pmatrix} C & S \\ -S^{\mathrm{T}} & C' \end{pmatrix}.$$

C and C' are real diagonal matrices, with the last $n-m$ diagonal elements of C being 1, the first m elements being identical with those of C'. S is a real $n \times m$ matrix. The last $n-m$ rows of S are equal to zero, and the relations

$$C^2 - SS^{\mathrm{T}} = 1_p = p \times q \text{ unit matrix},$$
$$C'^2 - S^{\mathrm{T}}S = 1_q = q \times q \text{ unit matrix}$$

hold. (The superscript "T" denotes matrix transposition.) The middle term U' is therefore not as simple as that derived in the present paper. Admittedly either form of factorization can be converted into the other by some similarity transformation of the middle factor. However, the method of proof that leads to our factorization scheme is also different from that of Ref. 4, and may serve as a useful alternative procedure if one contemplates a further generalization of the Euler angle concept to real Lie groups that preserve other types of bilinear forms, e.g., to $Sp(p, q)$.

In proving our Theorems 1 and 2, we have used the general ideas behind Naimark's derivation[5] of the factorization of the general element g of the proper Lorentz group $SO(3, 1)$ into the product ubv, where u and v belong to $SO(3)$ and b is the Lorentz transformation along the x axis.

Since the groups $SU(3)$ and $SU(2, 1)$ are very useful in physics, we have, in Sec. 4, written out their factor matrices explicitly.

With regard to our notation, the following remarks are important: Throughout this paper, the Einstein summation convention is used for lower case subscripts that are repeated; Greek lower case subscripts $\alpha, \beta, \cdots$ take the values $1, 2, \cdots, N$; Latin lower case subscripts $a, b, \cdots$ take the values $1, 2, \cdots, N-1$. Thus if we write $\beta_{ij}\delta_{j\alpha}$ rather than $\beta_{i\alpha}$, it would be because the object β_{ij} is (for convenience) defined *only for* $1 \leq i, j \leq N-1$.

2. FACTORIZATION OF $SO(p, q)$; PROOF OF THEOREM 1

A. The Case $q > 0$

Let the $N \times N$ matrix g be an arbitrary element of $SO(p, q)$, and let $g_{\mu\nu}$ be its matrix elements. The following relations hold:

$$g_{j\alpha}\beta_{ji}g_{i\beta} = \beta_{tm}\delta_{t\alpha}\delta_{m\beta} - \delta_{N\alpha}\delta_{N\beta} + g_{N\alpha}g_{N\beta}, \quad (2.1)$$
$$g_{\alpha i}\beta_{ij}g_{\beta j} = \beta_{tm}\delta_{t\alpha}\delta_{m\beta} - \delta_{\alpha N}\delta_{\beta N} + g_{\alpha N}g_{\beta N}, \quad (2.2)$$

where

$$\begin{aligned}\beta_{ij} &= \delta_{ij} \quad \text{for} \quad 1 \leq i, j \leq p \\ &= -\delta_{ij} \quad \text{for} \quad p < i,\ j \leq N-1. \end{aligned} \quad (2.3)$$

Let

$$\begin{aligned}K^2 &= (g_{NN})^2 - 1, \\ K_p^2 &= (g_{1N})^2 + (g_{2N})^2 + \cdots + (g_{pN})^2, \\ K_q^2 &= K_p^2 - K^2. \end{aligned} \quad (2.4)$$

Let us define $N-1$ real $(N-1)$-component vectors α_i' with components α_{ij}', such that

$$\begin{aligned}\alpha_{1t}' &= g_{tN} \quad \text{for} \quad t \leq p \\ &= -g_{tN} \quad \text{for} \quad p+1 \leq t \leq N-1. \end{aligned}$$

Hence

$$\begin{aligned}\alpha_{1t}'\beta_{ts}g_{sN} &= K_p^2 + K_q^2 \\ &= D^2, \text{ say.} \end{aligned} \quad (2.5)$$

Also let

$$\alpha_{ji}'\beta_{it}\alpha_{kt}' = \alpha_{ij}'\beta_{it}\alpha_{lk}' = D^2\beta_{jk}. \quad (2.6)$$

Thus the general form of (2.5) is

$$\alpha_{ks}'\beta_{st}g_{tN} = D^2\beta_{k1}. \quad (2.7)$$

Now, either $D^2 = 0$, or $D^2 \neq 0$. Suppose $D^2 = 0$. Then $K_q^2 = K_p^2 = 0$. It therefore follows from (2.1) and (2.2) that $g_{Ni} = g_{iN} = 0$, for all $i < N$. Hence $g \in SO(p, q-1)$, and the theorem follows trivially if we put $B = c = E$, the unit matrix, and $g = a$.

Having thus disposed of this trivial case, we shall assume in the following that $D^2 \neq 0$. We may therefore normalize the vectors α_i' by putting

$$\alpha_{ij} = D^{-1}\alpha_{ij}'. \quad (2.8)$$

Hence

$$\alpha_{ks}\beta_{st}g_{tN} = D\beta_{k1} \quad (2.9)$$

and

$$\alpha_{ji}\beta_{it}\alpha_{kt} = \alpha_{ij}\beta_{it}\alpha_{tk} = \beta_{jk}. \quad (2.10)$$

We now define an $N \times N$ matrix R with elements

$$R_{\alpha\beta} = \alpha_{ij}\beta_{jt}\delta_{i\alpha}\delta_{t\beta} + \delta_{N\alpha}\delta_{N\beta}. \quad (2.11)$$

Hence

$$(Rg)_{\alpha\lambda} = \alpha_{ij}\beta_{jt}\delta_{i\alpha}g_{t\lambda} + \delta_{N\alpha}g_{N\lambda}. \quad (2.12)$$

We note that, for $\alpha \neq N$,

$$\begin{aligned}(Rg)_{\alpha N} &= (Rg)_{sN} \quad \text{for some} \quad s \\ &= \alpha_{sj}\beta_{jt}g_{tN} \\ &= D\beta_{s1}, \quad \text{via (2.9)}, \\ &= 0 \quad \text{unless} \quad s = 1. \end{aligned}$$

Furthermore, $(Rg)_{N\beta} = g_{N\beta}$.

If we now consider R as an $(N-1) \times (N-1)$ matrix, that is, if we ignore the unity in the (N, N) position and the zeros in the rest of the Nth row and the Nth column, we find, after some calculation,

using (2.10), that

$$(R^{\mathrm{T}}\beta R)_{ts} = \beta_{ts}.$$

It follows that $R \in SO(p, q-1) \subset SO(p, q)$. Hence $Rg \in SO(p, q)$.

We now define $(N-1)$ real $(N-1)$-component vectors f_i with components[6] f_{ji} given by

$$f_{j1} = D^{-1}g_{Nj}, \quad f_{ji} = (Rg)_{ij}, \quad 1 < i \leq N-1. \tag{2.13}$$

With the aid of (2.2), (2.3), (2.9), and (2.10), one easily verifies the relation

$$f_{ij}\beta_{it}f_{tk} = \beta_{jk}. \tag{2.14}$$

We now construct another $N \times N$ matrix S with elements

$$S_{\alpha\beta} = f_{ij}\beta_{it}\delta_{t\alpha}\delta_{j\beta} + \delta_{N\alpha}\delta_{N\beta}. \tag{2.15}$$

The matrix S satisfies

$$(S^{\mathrm{T}}\beta S)_{st} = \beta_{st},$$

i.e., $S \in SO(p, q-1) \subset SO(p, q)$.

Finally we construct the $N \times N$ matrix

$$B = RgS. \tag{2.16}$$

Using (2.12) and (2.15), we have the elements of B as

$$\begin{aligned} B_{\alpha\mu} = {} & \alpha_{ij}f_{rp}\beta_{jt}\beta_{rs}\delta_{i\alpha}g_{ts}\delta_{p\mu} + D\beta_{i1}\delta_{i\alpha}\delta_{N\mu} \\ & + \delta_{N\alpha}(g_{Ns}f_{rp}\beta_{rs}\delta_{p\mu} + g_{NN}\delta_{N\mu}). \end{aligned} \tag{2.17}$$

From (2.17) we obtain

$$\begin{aligned} B_{\alpha 1} &= g_{NN}\beta_{i1}\delta_{i\alpha} + D\delta_{N\alpha}, \\ B_{\alpha N} &= D\beta_{i1}\delta_{i\alpha} + \delta_{N\alpha}g_{NN}, \\ B_{tk} &= \beta_{tk}, \quad t, k \neq 1. \end{aligned} \tag{2.18}$$

Putting $R^{-1} = a$ and $S^{-1} = c$, we have

$$g = aB(\theta)c, \tag{2.19}$$

where $a, c \in SO(p, q-1)$, and

$$\begin{aligned} & B = B(\theta) \text{ has the form} \\ & B_{11} = B_{NN} = g_{NN} = \cosh\theta, \quad \text{say}, \\ & B_{1N} = B_{N1} = D = \sinh\theta, \\ & B_{jk} = \beta_{jk}, \quad j, k \neq 1. \end{aligned} \tag{2.20}$$

QED

B. The Case $q = 0$

The group is now compact. The preceding analysis holds provided we make the following adjustments. Equations (2.21) and (2.22) replace (2.1) and (2.2):

$$g_{i\alpha}g_{i\beta} = \delta_{\alpha\beta} - g_{N\alpha}g_{N\beta}, \tag{2.21}$$

$$g_{\alpha i}g_{\beta i} = \delta_{\alpha\beta} - g_{\alpha N}g_{\beta N}. \tag{2.22}$$

All β_{ij} are replaced by δ_{ij}. We now put

$$D = [1 - (g_{NN})^2]^{\frac{1}{2}} \neq 0. \tag{2.23}$$

The case $D = 0$ is as trivial as in the case $q > 0$ of this proof, implying in this case that $g \in SO(p-1)$.

With the vector α_i defined by $\alpha_{1t} = D^{-1}g_{tN}$ and $\alpha_{jt}\alpha_{kt} = \alpha_{tj}\alpha_{tk} = \delta_{jk}$, we find that the matrix P, with elements

$$P_{\alpha\beta} = \alpha_{ij}\delta_{i\alpha}\delta_{j\beta} + \delta_{N\alpha}\delta_{N\beta}, \tag{2.24}$$

satisfies $(P^{\mathrm{T}}P)_{st} = \delta_{st}$, i.e., $P \in SO(p-1) \subset SO(p)$. It follows that $Pg \in SO(p)$.

Equation (2.13) is now replaced by[7]

$$f_{j1} = -D^{-1}g_{Nj}, \quad f_{ji} = (Pg)_{ij}, \quad 1 < i \leq N-1. \tag{2.25}$$

Then the $N \times N$ matrix Q defined by

$$Q_{\alpha\beta} = f_{ij}\delta_{i\alpha}\delta_{j\beta} + \delta_{N\alpha}\delta_{N\beta} \tag{2.26}$$

satisfies $(Q^{\mathrm{T}}Q)_{st} = \delta_{st}$, i.e., $Q \in SO(p-1) \subset SO(p)$.

Finally, we construct the matrix $B = PgQ$. Using (2.24) and (2.26), we have

$$\begin{aligned} B_{\alpha\mu} = {} & \alpha_{ij}\delta_{i\alpha}g_{jl}f_{tm}\delta_{m\mu} + D\delta_{\alpha 1}\delta_{N\mu} \\ & + \delta_{N\alpha}(\delta_{N\mu}g_{NN} + g_{Nt}f_{tm}\delta_{m\mu}). \end{aligned} \tag{2.27}$$

From (2.27), we have

$$\begin{aligned} B_{\alpha 1} &= \delta_{1\alpha}g_{NN} - D\delta_{N\alpha}, \\ B_{\alpha N} &= D\delta_{\alpha 1} + \delta_{N\alpha}g_{NN}, \\ B_{jk} &= \delta_{jk}, \quad j, k \neq 1. \end{aligned} \tag{2.28}$$

Hence

$$\begin{aligned} B_{11} = B_{NN} = g_{NN} = \cos\theta, \quad \text{say}, \\ B_{1N} = -B_{N1} = D = \sin\theta. \end{aligned} \tag{2.29}$$

Putting $P^{-1} = a$, $Q^{-1} = c$, we have $g = aB(\theta)c$, where $a, c \in SO(p-1)$ and B is given by (2.28) and (2.29). This completes the proof of Theorem 1.

3. FACTORIZATION OF $SU(p, q)$; PROOF OF THEOREM 2

A. The Case $q > 0$

If g is an arbitrary element of $SU(p, q)$, the following relations hold:

$$g^*_{j\alpha}\beta_{ji}g_{i\beta} = \beta_{tm}\delta_{t\alpha}\delta_{m\beta} - \delta_{N\alpha}\delta_{N\beta} + g^*_{N\alpha}g_{N\beta}, \tag{3.1}$$

$$g^*_{\alpha i}\beta_{ij}g_{\beta j} = \beta_{tm}\delta_{t\alpha}\delta_{m\beta} - \delta_{\alpha N}\delta_{\beta N} + g^*_{\alpha N}g_{\beta N}, \tag{3.2}$$

where

$$\begin{aligned} \beta_{ij} &= \delta_{ij} \quad \text{for} \quad 1 \leq i, j \leq p \\ &= -\delta_{ij} \quad \text{for} \quad p < i, j \leq N-1, \end{aligned} \tag{3.3}$$

and the asterisk denotes complex conjugation.[8]

Let

$$K^2 = |g_{NN}|^2 - 1,$$
$$K_p^2 = |g_{1N}|^2 + |g_{2N}|^2 + \cdots + |g_{pN}|^2, \quad (3.4)$$
$$K_q^2 = K_p^2 - K^2, \quad D^2 = K_p^2 + K_q^2.$$

As in the proof of Theorem 1, we see that $D = 0$ implies $K_p^2 = K_q^2 = 0$, i.e., $g_{Ni} = g_{iN} = 0$ for all $i < N$. Hence $g \in SU(p, q-1)$, and the theorem follows: $B = v = E$, the identity, and $g = u$. Therefore, let $D \neq 0$ in all that follows.

We define $N-1$ complex $(N-1)$-component vectors α_i with components α_{ij} such that

$$\alpha_{1j} = D^{-1}g_{jN} \quad \text{for} \quad j \leq p$$
$$= -D^{-1}g_{jN} \quad \text{for} \quad p+1 \leq j \leq N-1 \quad (3.5)$$

and such that

$$\alpha_{ji}\beta_{it}\alpha_{kt}^* = \alpha_{ij}^*\beta_{it}\alpha_{tk} = \beta_{jk}. \quad (3.6)$$

It follows that

$$\alpha_{ks}^*\beta_{st}g_{tN} = D\beta_{k1}. \quad (3.7)$$

We now construct an $N \times N$ matrix U with elements

$$U_{\alpha\beta} = \alpha_{ij}^*\beta_{jt}\delta_{i\alpha}\delta_{t\beta} + \delta_{N\alpha}\delta_{N\beta}. \quad (3.8)$$

Thus

$$(Ug)_{\alpha\mu} = \alpha_{ij}^*\beta_{jt}\delta_{i\alpha}g_{t\mu} + \delta_{N\alpha}g_{N\mu}. \quad (3.9)$$

Hence $(Ug)_{jN} = D\beta_{j1} = 0$, unless $j = 1$. It follows from (3.9) that $(Ug)_{N\alpha} = g_{N\alpha}$ and that $(U^\dagger\beta U)_{st} = \beta_{st}$, i.e., $U \in SU(p, q-1) \subset SU(p, q)$. Hence $Ug \in SU(p, q)$.

Let us define $N-1$ complex $(N-1)$-component vectors f_i with components f_{ji} given by

$$f_{j1} = D^{-1}g_{Nj}, \quad f_{ji} = (Ug)_{ij}, \quad 1 < i \leq N-1. \quad (3.10)$$

It follows from (3.2), (3.6), and (3.7) that

$$f_{ij}^*\beta_{it}f_{tk} = \beta_{jk}. \quad (3.11)$$

The matrix V defined by

$$V_{\alpha\beta} = f_{ij}^*\beta_{it}\delta_{t\alpha}\delta_{j\beta} + \delta_{N\alpha}\delta_{N\beta} \quad (3.12)$$

satisfies $(V^\dagger\beta V)_{st} = \beta_{st}$. Hence $V \in SU(p, q-1) \subset SU(p, q)$. From (3.9) and (3.12), the matrix $B = UgV$ has elements

$$B_{\alpha\mu} = \alpha_{ij}^*f_{rp}^*\beta_{jt}\beta_{rs}\delta_{i\alpha}g_{ts}\delta_{p\mu} + D\delta_{i\alpha}\beta_{i1}\delta_{N\mu} + \delta_{N\alpha}(g_{Ns}f_{rp}^*\beta_{rs}\delta_{p\mu} + g_{NN}\delta_{N\mu}). \quad (3.13)$$

Equation (3.13) gives

$$B_{\alpha 1} = \delta_{i\alpha}\beta_{i1}g_{NN}^* + D\delta_{N\alpha},$$
$$B_{\alpha N} = D\beta_{i1}\delta_{i\alpha} + \delta_{N\alpha}g_{NN}, \quad (3.14)$$
$$B_{jk} = \beta_{jk}, \quad j, k \neq 1.$$

Thus

$$B_{11} = B_{NN}^* = \exp(-i\varphi_1)\cosh\theta, \quad \text{say},$$
$$B_{1N} = B_{N1} = \sinh\theta$$
$$= \exp(i\varphi_2)\sinh\theta|_{\varphi_2=0}. \quad (3.15)$$

Putting $U^{-1} = u$, $V^{-1} = v$, we have $g = uBv$, where u, $v \in SU(p, q-1)$ and $B = B(\varphi_1, \varphi_2 = 0, \theta)$ is given by (3.14) and (3.15). QED

B. The Case $q = 0$

The analysis is analogous to the immediately preceding one, with the following adjustments: In place of (3.1) and (3.2), we now have

$$g_{i\alpha}^*g_{i\beta} = \delta_{\alpha\beta} - g_{N\alpha}^*g_{N\beta}, \quad (3.16)$$

$$g_{\alpha i}^*g_{\beta i} = \delta_{\alpha\beta} - g_{\alpha N}^*g_{\beta N}. \quad (3.17)$$

We then replace all β_{ij} by δ_{ij} and put

$$D = (1 - |g_{NN}|^2)^{\frac{1}{2}} \neq 0. \quad (3.18)$$

The case $D = 0$ is trivial, as before. Now let

$$\alpha_{1t} = D^{-1}g_{tN}, \quad \alpha_{jt}^*\alpha_{kt} = \alpha_{tj}^*\alpha_{tk} = \delta_{jk},$$
$$f_{j1} = -D^{-1}g_{Nj}, \quad f_{ji} = (Ug)_{ij}, \quad 1 < i, j \leq N-1, \quad (3.19)$$

where U is given by (3.9), with the adjustments indicated above. The matrix $B = UgV$ then has the following entries:

$$B_{\alpha\mu} = \alpha_{ij}^*f_{tm}\delta_{i\alpha}g_{jt}\delta_{m\mu} + D\delta_{\alpha 1}\delta_{N\mu} + \delta_{N\alpha}(g_{Nt}f_{tm}^*\delta_{m\mu} + g_{NN}\delta_{N\mu}). \quad (3.20)$$

Thus

$$B_{\alpha 1} = \delta_{\alpha 1}g_{NN}^* - D\delta_{N\alpha}$$
$$B_{\alpha N} = D\delta_{\alpha 1} + g_{NN}\delta_{N\alpha}, \quad (3.21)$$
$$B_{jk} = \delta_{jk}, \quad j, k \neq 1,$$

i.e.,

$$B_{11} = B_{NN}^* = g_{NN}^* = \exp(-i\varphi_1)\cos\theta, \quad \text{say},$$
$$B_{1N} = -B_{N1} = D = \sin\theta$$
$$= \exp(i\varphi_2)\sin\theta|_{\varphi_2=0}. \quad (3.22)$$

It follows that $g = uBv$, where $u = U^{-1}$, $v = V^{-1}$, and $B = B(\varphi_1, \varphi_2 = 0, \theta)$ is given by (3.21) and (3.22).

This completes the proof of Theorem 2.

4. FACTOR MATRICES FOR $SU(3)$ AND $SU(2, 1)$

It follows from (3.20)–(3.22) that if $g \in SU(3)$, then

$$g = U_{12}(\varphi_1, \varphi_2, \theta_1)U_{13}(\varphi, 0, \theta)U_{12}(\varphi_1', \varphi_2', \theta_2),$$
$$0 \leq \varphi \leq 2\pi, \quad 0 \leq \theta \leq \pi, \quad (4.1)$$

where

$$U_{12}(\varphi_1, \varphi_2, \theta) = \begin{pmatrix} \exp(i\varphi_1)\cos\theta & -\exp(i\varphi_2)\sin\theta & 0 \\ \exp(-i\varphi_2)\sin\theta & \exp(-i\varphi_1)\cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (4.2)$$

$$U_{13}(\varphi_1, \varphi_2, \theta) = \begin{pmatrix} \exp(i\varphi_1)\cos\theta & 0 & -\exp(i\varphi_2)\sin\theta \\ 0 & 1 & 0 \\ \exp(-i\varphi_2)\sin\theta & 0 & \exp(-i\varphi_1)\cos\theta \end{pmatrix}. \quad (4.3)$$

If $g \in SU(2, 1)$, then (3.13)–(3.15) give

$$g = U_{12}(\varphi_1, \varphi_2, \theta_1)U'_{13}(\varphi, 0, \theta)U_{12}(\varphi'_1, \varphi'_2, \theta_2), \quad (4.4)$$

where U_{12} is given by (4.2) and

$$U'_{13}(\varphi_1, \varphi_2, \theta) = \begin{pmatrix} \exp(i\varphi_1)\cosh\theta & 0 & \exp(i\varphi_2)\sinh\theta \\ 0 & 1 & 0 \\ \exp(-i\varphi_1)\sinh\theta & 0 & \exp(-i\varphi_1)\cosh\theta \end{pmatrix},$$
$$0 \le \varphi \le 2\pi, \quad 0 \le \theta < \infty. \quad (4.5)$$

From (4.1)–(4.5), we may obtain the factorization of the group $SU(2, 2)$, which is locally isomorphic to the conformal group of space–time, another group of physical importance.

5. CONCLUSION

We have derived a factorization of arbitrary elements of pseudo-orthogonal and pseudo-unitary groups of any order in terms of parameters that directly generalize the Euler angle parameters of the rotation group. The method of derivation is applicable to a wider class of groups than is considered here. The results obtained are broadly similar to results obtained earlier by Wigner for the same problem, but differ from the latter in the following details. The Wigner factorization displays the group element as a product of three factors, the extremal factors of which belong to the subgroup $SO(p) \otimes SO(q)$ [or $SU(p) \otimes SU(q)$ as the case may be]. The present factorization displays the group element also as a product of three factors, the extremal elements of which, however, belong to the subgroup $SO(p, q-1)$ [or $SU(p, q-1)$ as the case may be]. The middle term then becomes much simpler than the corresponding factor in Wigner's scheme. The factorization of the present paper also seems to have the advantage of directly lending itself to a recursive breakdown into a product (ultimately!) of rotations in the plane. The factorization of $SU(3)$ in terms of Euler angles makes the calculation of matrices for finite transformations of this group directly deducible from the corresponding matrices for $SU(2)$, that is, from the well-known Wigner $d^j_{mm'}$ functions.

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Abnormal Lattice Thermal Conductivity of a One-Dimensional, Harmonic, Isotopically Disordered Crystal

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Energy transport is investigated in a model system for which exact analytic results can be obtained. The system is an infinite, one-dimensional harmonic crystal which is perfect everywhere except in a finite segment which contains N isotopic defects. Initially, the momenta and displacements of all atoms to the left of the defect region are canonically distributed at a temperature T, and the right half of the crystal is at a lower temperature. This initial nonequilibrium state evolves according to the equations of motion, and ultimately a steady state is established in the vicinity of the region containing the defects. The thermal conductivity is calculated from exact expressions for the steady state energy flux and thermal gradient. For a crystal in which the N isotopic defects are distributed at random but in which the overall defect concentration is fixed, we demonstrate that the thermal conductivity approaches infinity as least as fast as $N^{1/2}$. A Monte Carlo evaluation of the thermal conductivity for a given defect-to-host mass ratio and concentration is carried out for a series of random configurations of N defects for N in the range, $25 \leq N \leq 600$. The thermal conductivity is proportional to $N^{1/2}$ within the statistical uncertainty except for slight deviations at the smallest values of N.

1. INTRODUCTION

In this paper we study the thermal conductivity of an isotopically disordered section of atoms in an otherwise-perfect, infinite, one-dimensional harmonic crystal. Since thermal conduction in solids proceeds via phonon transport, it is important to assess the effectiveness of various phonon scattering mechanisms. It is well known that in a perfect harmonic crystal the thermal conductivity is infinite. In a one-dimensional crystal we determine the extent to which this divergence of the thermal conductivity is modified in the presence of isotopic defects. The model and techniques used are similar to those developed by one of us.[1-3]

The model used to evaluate the thermal conductivity K is an infinite harmonic chain with nearest-neighbor forces which is perfect everywhere except in a finite segment of length L containing N isotopic defects distributed at random. Initially, the momenta and displacements of all the atoms to the left of the defect region are canonically distributed at a temperature T, and the momenta and displacements of the remainder of the system are at some lower temperature which, for convenience, is assumed to be zero. This initial nonequilibrium distribution evolves according to the equations of motion of the system. Ultimately, a steady state is established in the vicinity of the region containing the defects. That is, there is a steady-state value for the energy current J_N through the defect-containing region as well as a steady-state temperature drop $\Delta T_N = T_{\text{right}} - T_{\text{left}}$ across the same region. From explicit expressions for J_N and ΔT_N, we determine the value of the thermal conductivity K_N from the definition

$$J_N = -K_N(\Delta T_N/L). \tag{1.1}$$

Our main interest lies in the limiting value of K_N as $N \to \infty$, when the over-all concentration of defects $C = N/L$ remains constant:

$$K = \lim_{\substack{N\to\infty \\ NL^{-1}=C}} K_N = -\lim_{\substack{N\to\infty \\ NL^{-1}=C}} (NJ_N/C\Delta T_N). \tag{1.2}$$

It will be shown that if $N \to \infty$, $NL^{-1} = C$, then $\Delta T_N \to -T$. Therefore, the limiting value K_N can be written as

$$K_N = NJ_N/CT, \quad N \gg 1 \quad \text{and} \quad NL^{-1} = C. \tag{1.3}$$

The principal results obtained are of two kinds. First, we obtain a lower bound for $N\langle J_N\rangle_c$ of the form

$$N\langle J_N\rangle_c \geq AN^{\frac{1}{2}}, \tag{1.4}$$

which implies that

$$\langle K_N\rangle_c \geq AN^{\frac{1}{2}}/CT, \quad \text{for} \quad N \gg 1 \quad \text{and} \quad NL^{-1} = C,$$

where A is a constant and $\langle J_N\rangle_c$ denotes the average of the energy current for all configurations of N defects weighted according to the frequency of their occurrence in a particular ensemble. In the ensemble, the spacings "a" between adjacent defects are independent random variables with the probability distribution

$$\mathcal{P}(a) = C(1 - C)^{a-1}, \quad a = 1, 2, \cdots. \tag{1.5}$$

Second, we obtain Monte Carlo estimates of NJ_N for $25 \leq N \leq 600$. In this range the following relation is approximately valid in the case $Q = 1.0$, $C = 0.5$:

$$NJ_N = 1.15N^{\frac{1}{2}}, \tag{1.6}$$

which indicates that the exponent $\frac{1}{2}$ in the lower bound Eq. (1.4) may be the best possible estimate.

2. MODEL AND FORMAL SOLUTION

Consider a one-dimensional harmonic crystal with nearest-neighbor interactions. The particles are labeled consecutively by the index r, $-\mathcal{N} < r < \mathcal{N}$, and all particles have the mass m, except for N isotopic defect particles at random lattice positions $r = A_j$, $j = 1, \cdots, N$. The mass of each of the defect particles is M. It is assumed that $A_1 = 0$, that all other defects lie to the right of $r = 0$, and that the subscript j on A_j specifies the order of the defects, i.e., $0 = A_1 < \cdots < A_j < \cdots < A_N = L \ll \mathcal{N}$. Thus $L = A_N$ is the length of the defect-containing region, and $C = N/L$ is the overall concentration of defects in that region. The spacings between adjacent pairs of defects, $A_j - A_{j-1}$, are assumed to be independent, identically distributed random variables with a mean value

$$\overline{(A_j - A_{j-1})} = C^{-1}. \tag{2.1}$$

The nearest-neighbor force constant is assumed to be equal to f everywhere in the crystal. The equations of motion of the one-dimensional crystal are

$$m_r\ddot{\chi}(r,\tau) = \begin{cases} \frac{1}{4}m[\chi(\mathcal{N}-1,\tau) - 2\chi(\mathcal{N},\tau)], \\ \quad r = \mathcal{N}, \\ \frac{1}{4}m[\chi(r-1,\tau) - 2\chi(r,\tau) \\ \quad + \chi(r+1,\tau)], \quad -\mathcal{N} < r < \mathcal{N}, \\ \frac{1}{4}m[-2\chi(-\mathcal{N},\tau) + \chi(-\mathcal{N}+1,\tau)], \\ \quad r = -\mathcal{N}, \end{cases} \tag{2.2}$$

where $\chi(r,\tau)$ is the displacement of particle r from its equilibrium position and m_r is the mass of the particle at lattice site r. In Eq. (2.2), each superscript dot denotes differentiation with respect to τ, a dimensionless time such that $\tau = 2(f/m)^{\frac{1}{2}}t$, where f is the nearest-neighbor force constant and $2(f/m)^{\frac{1}{2}}$ is the maximum normal mode frequency of the infinite perfect crystal. The equations of motion (2.2) correspond to fixed boundary conditions, i.e., $\chi(\mathcal{N}+1,\tau) = \chi(-\mathcal{N}-1,\tau) = 0$, and are chosen so that the potential energy matrix V [the negative of the matrix of the coefficients on the right-hand side of Eq. (2.2)] is positive definite. The formal solution of Eq. (2.2) can be written in matrix notation as[3,4]

$$\mathbf{x}(\tau) = \mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\dot{\mathbf{x}}(0) + \mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\mathbf{x}(0) \tag{2.3a}$$

and

$$\dot{\mathbf{x}}(\tau) = \mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\dot{\mathbf{x}}(0) - \mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\mathbf{x}(0), \tag{2.3b}$$

where M is the diagonal mass matrix whose rth diagonal element is the mass of particle r and $\mathsf{W} = \mathsf{M}^{-\frac{1}{2}}\mathsf{V}\mathsf{M}^{-\frac{1}{2}}$. The rth components of the vectors $\mathbf{x}(\tau)$ and $\dot{\mathbf{x}}(\tau)$ are respectively the position and velocity of particle r at time τ.

In the model, the configuration of the array of defects is specified, $\{A_j\}$, $j = 0, \cdots, N$, and we consider the ensemble of initial conditions in which (i) particle $-R < 0$ is held fixed, (ii) the initial conditions in the portion of the crystal $-\mathcal{N} < r < -R$ are specified by a canonical distribution at temperature T, and (iii) the initial conditions in the portion of the crystal $-R < r < \mathcal{N}$ are specified by the temperature $T = 0$. This initial condition can be summarized as

$$\mathcal{W}\left[\begin{pmatrix}\dot{\mathbf{x}}_h(0)\\0\\\dot{\mathbf{x}}_c(0)\end{pmatrix}, \begin{pmatrix}\mathbf{x}_h(0)\\0\\\mathbf{x}_c(0)\end{pmatrix}\right] = Z\exp\left(-\frac{1}{2kT}\dot{\mathbf{x}}_h(0)^T\mathsf{M}_h\dot{\mathbf{x}}_h(0) - \frac{1}{2kT}\mathbf{x}_h(0)^T\mathsf{V}_h\mathbf{x}_h(0)\right) \times \prod_{r=-R+1}^{\mathcal{N}}\{\delta[\dot{\chi}(r,0)]\delta[\chi(r,0)]\}, \tag{2.4}$$

where the vector $\dot{\mathbf{x}}(0)$ is written as a partitioned vector

$$\dot{\mathbf{x}}(0) = \begin{pmatrix}\dot{\mathbf{x}}_h(0)\\0\\\dot{\mathbf{x}}_c(0)\end{pmatrix},$$

in which the components of $\dot{\mathbf{x}}_h(0)$ are the initial velocities of particles in the hot region, the components of $\dot{\mathbf{x}}_c(0)$ are the initial velocities of particles in the cold region, and the single-zero component refers to the initial velocity of the clamped particle R. The matrices M_h and V_h are, respectively, the diagonal mass matrix and potential energy matrix of the initially clamped, hot region. In the ensemble, the velocities of lattice particles at time τ are linear combinations of the initial conditions which have a multivariate Gaussian distribution. Consequently, the probability distribution of the velocity of each lattice particle is a Gaussian distribution with a time-dependent dispersion which we identify with the local time-dependent temperature. Thus in the initial ensemble the average value of $\langle\dot{\chi}(r,0)^2\rangle$ is kTm_r^{-1}, so that

$$T = m_r k^{-1}\langle\dot{\chi}(r,0)^2\rangle. \tag{2.5}$$

It has been shown[3] from the formal calculation of $\langle\dot{\chi}(r,\tau)^2\rangle$ that the time-dependent local temperature is

$$T_N(r,\tau) = m_r k^{-1}\langle\dot{\chi}(r,\tau)^2\rangle = 2T\delta(r,\tau), \tag{2.6}$$

where $\mathcal{E}(r, \tau)$ is the energy content of the initially hot region at time τ in the case of the special initial condition $\mathbf{x}(0) = 0$ and $\dot{\mathbf{x}}(0) = m_r^{-\frac{1}{2}}\boldsymbol{\Delta}_r$. All components of $\boldsymbol{\Delta}_r$ are zero except the rth which is unity. Thus, in order to determine the local kinetic temperature at r, we must evaluate the expression

$$\mathcal{E}(r, \tau) = \frac{1}{2}\left(\frac{m}{m_r}\right)\sum_{r'=-\mathcal{N}}^{-R}\{[\mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r',r}\}^2 + \frac{1}{8}\frac{m}{m_r}\sum_{r'=-\mathcal{N}}^{-R-1}\{[\mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r'+1,r} - [\mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r',r}\}^2. \quad (2.7)$$

The potential energy contributions of the "springs" connecting particles $-\mathcal{N}$ and $\mathcal{N}$ to the fixed boundary particles have been omitted in Eq. (2.7). In the physically interesting limit $\mathcal{N} \to \infty$ with r, R, and N fixed, this error of omission is negligible.

The approach of the local kinetic temperature to its steady-state value can be described easily in a qualitative way by referring to the connection between local temperature and the special initial value problem set forth in Eqs. (2.6) and (2.7) and Fig. 1. Lattice particles r_1, r_2, and r_3 are all located in the initially cold region, so that the initial energy content of the hot region $\mathcal{E}(r_i, 0)$, $i = 1, 2, 3$, is zero. Subsequently, however, the initial localized excitation corresponding to the special initial condition at r_i spreads. In the case of r_1, the portion of the initial disturbance which propagates to the right is partially reflected by the array of defects. This reflected portion and the pulse initially moving to the left contribute to $\mathcal{E}(r_1, \tau)$, the energy content of the initially hot region. In the case of r_3, a fraction of the initial pulse, which propagates to the left toward the initially hot region, is transmitted through the array of defects and constitutes the only contribution to $\mathcal{E}(r_3, \tau)$. In the case of r_2, which is located approximately in the middle of the array of defects, roughly half the initial kinetic energy propagates to the left into the hot region. In the foregoing discussion we implicitly ignored the contribution of reflections from the fixed boundaries at $\pm\mathcal{N}$ to the time-dependent behavior of $\mathcal{E}(r_i, \tau)$ because, as already mentioned, we are interested in the limit $\mathcal{N} \to \infty$ with r_i, R, and N fixed. In the next section we determine the asymptotic steady-state values of the local temperature required in the expression for the thermal conductivity, Eq. (1.2).

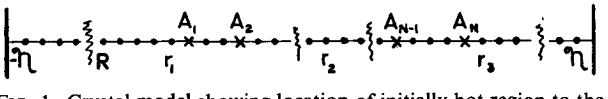

FIG. 1. Crystal model showing location of initially hot region to the left of R and location of segment containing defects.

In the model system, the energy current past particle r' is simply the rate at which work is done on particle r' by particle[5,6] $r' - 1$

$$J_N(r', \tau) = \tfrac{1}{4}m\dot{\chi}(r', \tau)[\chi(r' - 1, \tau) - \chi(r', \tau)]. \quad (2.8)$$

In the nonequilibrium ensemble (2.4), the ensemble average value of the energy current per second past particle $r' > A_N$ is (see Appendix A for details)

$$\langle J_N(r', \tau)\rangle = \tfrac{1}{4}kT\sum_{r=-\mathcal{N}}^{-R}\{[\mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r',r} \times [\mathsf{M}^{\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{-\frac{1}{2}}]_{r,r'-1} - [\mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r',r} \times [\mathsf{M}^{\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{-\frac{1}{2}}]_{r,r'-1}\}. \quad (2.9)$$

The asymptotic, steady-state value of the energy current is obtained in the next section. As in the case of the steady-state local temperature, we set $\mathcal{N} = \infty$ in (2.9) and use the asymptotic formulas for the time-dependent factors which apply in this limiting case.

3. STEADY-STATE VALUES OF LOCAL TEMPERATURE AND ENERGY CURRENT

In this section we outline the evaluation of the local temperature and energy current expressions (2.6), (2.7), and (2.9) in the limit of large τ. Equations (2.7) and (2.9) are quadratic expressions in the time-dependent coefficients which appear in Eqs. (2.3a) and (2.3b). In particular, the coefficients

$$[\mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r',r} \text{ and } [\mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r',r}$$

represent the velocity and position, respectively, of particle r' at time τ for the initial condition in which all particles are at equilibrium positions and at rest, except for particle r whose velocity is one, i.e.,

$$\mathbf{X}_r(\tau) = \mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\boldsymbol{\Delta}_r \quad (3.1a)$$

and

$$\dot{\mathbf{X}}_r(\tau) = \mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\boldsymbol{\Delta}_r, \quad (3.1b)$$

where all components of $\boldsymbol{\Delta}_r$ except the rth are zero and the rth component is one. Explicit expressions have been obtained for these time-dependent response functions[2] in the form of Laplace transforms in the case where the system is infinite ($\mathcal{N} = \infty$). In case $r < 0$, it is shown in R1 that

$$X_r(A_j, \tau) = \frac{1}{2\pi i}\int_{\mathcal{L}}\frac{e^{p\tau}}{p(p^2+1)^{\frac{1}{2}}} \times \frac{[p + (p^2+1)^{\frac{1}{2}}]^{-2[A_j - r]}D_N^{(j)}(p)}{D_N(p)}\,dp \quad (3.2)$$

and, if $r' > A_N$,

$$X_r(r', \tau) = \frac{1}{2\pi i}\int_{\mathfrak{L}} \frac{e^{p\tau}}{p(p^2+1)^{\frac{1}{2}}} \times \frac{[p+(p^2+1)^{\frac{1}{2}}]^{-2[r'-r]}}{D_N(p)}\,dp, \quad (3.3)$$

where $D_N(P)$ is an Nth-order determinant whose (r, s) element is

$$\delta_{r,s} + Qp(p^2+1)^{-\frac{1}{2}}[p+(p^2+1)^{\frac{1}{2}}]^{-2|A_r - A_s|}, \quad (3.4)$$

where $Q = (M-m)/m$, and where $\mathfrak{L}$ is a contour parallel to and to the right of the imaginary p axis. The determinant $D_N^{(j)}(p)$ is identical with $D_N(p)$ except that the elements of the jth column are

$$[p+(p^2+1)^{\frac{1}{2}}]^{-2(A_i - A_j)}, \quad i = 1, \cdots, N. \quad (3.5)$$

The expressions for $\dot{X}_r(A_j, \tau)$ and $\dot{X}_r(r', \tau)$ contain an additional factor of p in the integrand.

It is clear from the form of Eqs. (3.1a) and (3.1b) and the symmetry of W that

$$X_r(r', \tau) = X_{r'}(r, \tau),$$
$$r \neq A_j, \quad j = 1, \cdots, N \quad \text{and} \quad r' \neq A_j,$$
$$X_{A_j}(A_k, \tau) = X_{A_k}(A_j, \tau),$$

and

$$X_{A_j}(r, \tau) = m^{-1}MX_r(A_j, \tau) = (Q+1)X_r(A_j, \tau), \quad r \neq A_k, \quad k = 1, \cdots, N \quad (3.6)$$

Now consider the expression for the energy current past particle $r' > A_N$

$$\langle J_N(r', \tau)\rangle = \tfrac{1}{2}kT\sum_{r=-\infty}^{-R}[\dot{X}_r(r', \tau)X_r(r'-1, \tau) - X_r(r', \tau)\dot{X}_r(r'-1, \tau)]. \quad (3.7)$$

In order to estimate the value of $\langle J_N(r', \tau)\rangle$ as $\tau \to \infty$, we must estimate the asymptotic values of the factors in the sum in Eq. (3.7). It should first be noted that if one excludes the factor $1/D_N(p)$ in the integral representation of $\dot{X}_r(r', \tau)$,

$$\dot{X}_r(r', \tau) = \frac{1}{2\pi i}\int_{\mathfrak{L}} \frac{e^{p\tau}}{(p^2+1)^{\frac{1}{2}}[p+(p^2+1)^{\frac{1}{2}}]^{2(r'-r)}} \frac{dp}{D_N(p)}, \quad (3.8)$$

then one is left with the integral representation of the Bessel function, $J_{2[r'-r]}(\tau)$. Consequently, the asymptotic analysis of $\dot{X}_r(r', \tau)$ in Eq. (3.8) via the method of steepest descents will be identical with the asymptotic analysis of the analogous integral representation for $J_{2[r'-r]}(\tau)$. In particular, when $\beta = 2|r-r'|/\tau < 1$ and $\tau \gg 1$, there are saddle points at

$$p_\pm = \pm i(1-\beta^2)^{\frac{1}{2}}.$$

The integration contour $\mathfrak{L}'$, deformed to pass through the saddle points, is shown in Fig. 2. The only effect of the additional factor $1/D_N(p)$ in Eq. (3.8) on the asymptotic formula for $\dot{X}_r(r', \tau)$ is to multiply the Bessel function contribution from each saddle point by the value of $1/D_N(p)$ at that saddle point. The result is

$$\dot{X}_r(r', \tau) \sim [-i(2\pi\tau)^{-\frac{1}{2}}(1-\beta^2)^{-\frac{1}{4}}\exp\{i\tau[(1-\beta^2)^{\frac{1}{2}} - \beta\cos^{-1}\beta] + \tfrac{1}{4}i\pi\}]/D_N(i(1-\beta^2)^{\frac{1}{2}}) + [i(2\pi\tau)^{-\frac{1}{2}}(1-\beta^2)^{-\frac{1}{4}}\exp\{-i\tau[(1-\beta^2)^{\frac{1}{2}} - \beta\cos^{-1}\beta] - \tfrac{1}{4}i\pi\}]/D_N(-i(1-\beta^2)^{\frac{1}{2}}) \quad (3.9)$$

or

$$\dot{X}_r(r', \tau) \sim \left(\frac{2}{\pi\tau}\right)^{\frac{1}{2}} \times \frac{\sin[\tau(1-\beta^2)^{\frac{1}{2}} - 2(r-r')\cos^{-1}\beta + \frac{1}{4}\pi - \psi_N(\beta)]}{(1-\beta^2)^{\frac{1}{4}}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|}, \quad (3.10)$$

where $D_N(i(1-\beta^2)^{\frac{1}{2}}) = |D_N(i(1-\beta^2)^{\frac{1}{2}})|\exp[i\psi_N(\beta)]$. The asymptotic formula for $X_r(r', \tau)$ is

$$X_r(r', \tau) \sim 1 - \left(\frac{2}{\pi\tau}\right)^{\frac{1}{2}} \times \frac{\cos[\tau(1-\beta^2)^{\frac{1}{2}} - 2(r-r')\cos^{-1}\beta + \frac{1}{4}\pi - \psi_N(\beta)]}{(1-\beta^2)^{\frac{1}{4}}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|}, \quad (3.11)$$

where the leading term, unity, arises when the contour $\mathfrak{L}$ is shifted to $\mathfrak{L}'$, on the other side of the pole of the integrand at $p = 0$.

The asymptotic formulas (3.10) and (3.11) are valid

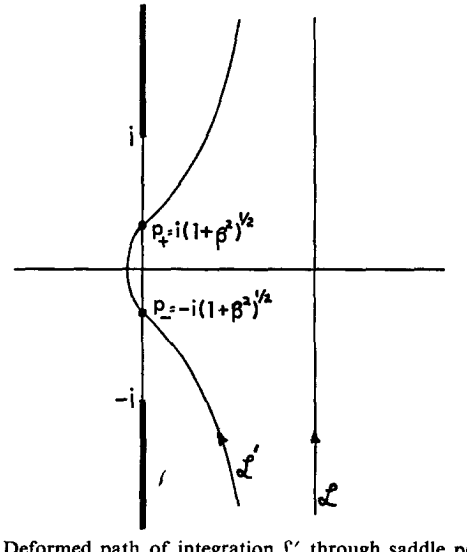

FIG. 2. Deformed path of integration $\mathfrak{L}'$ through saddle points of integrand in Eq. (3.8).

for $\tau \gg N$ and $\beta = 2|r - r'|/\tau$, a constant less than unity. Thus they describe the asymptotic response at r' which arises from an initial disturbance [$\mathbf{X}_r(0) = \mathbf{0}$ and $\dot{\mathbf{X}}_r(0) = \mathbf{\Delta}_r$] at r. As in the case of the Bessel function $J_{\beta\tau}(\tau)$, different asymptotic formulas are obtained for the asymptotic responses, $\dot{X}_r(r', \tau)$ and $X_r(r', \tau)$, in the immediate vicinity of the wavefront $\beta = 1$ and ahead of the wavefront $\beta > 1$. The width of the transition region at the wavefront is of order $\tau^{\frac{1}{3}}$, and the asymptotic responses are exponentially small ahead of the wavefront. Consequently, the expression for the energy current (3.7) is

$$\begin{aligned}\langle J_N(r', \tau)\rangle = \tfrac{1}{4}kT \sum_{r=-[\tau/2]+r'}^{-|R|} \Bigg\{ \left(\frac{2}{\pi\tau}\right)^{\frac{1}{2}} \frac{\sin\left[\tau(1-\beta^2)^{\frac{1}{2}} - 2|r-r'|\cos^{-1}\beta + \frac{1}{4}\pi - \psi_N(\beta)\right]}{(1-\beta^2)^{\frac{1}{4}}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|} \\ \times \left[1 - \left(\frac{2}{\pi\tau}\right)^{\frac{1}{2}} \frac{\cos\left[\tau(1-\beta'^2)^{\frac{1}{2}} - 2|r-r'+1|\cos^{-1}\beta' + \frac{1}{4}\pi - \psi_N(\beta')\right]}{(1-\beta'^2)^{\frac{3}{4}}\,|D_N(i(1-\beta'^2)^{\frac{1}{2}})|}\right] \\ - \left[1 - \left(\frac{2}{\pi\tau}\right)^{\frac{1}{2}} \frac{\cos\left[\tau(1-\beta^2)^{\frac{1}{2}} - 2|r-r'|\cos^{-1}\beta + \frac{1}{4}\pi - \psi_N(\beta)\right]}{(1-\beta^2)^{\frac{3}{4}}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|}\right] \\ \times \left(\frac{2}{\pi\tau}\right)^{\frac{1}{2}} \frac{\sin\left[\tau(1-\beta'^2)^{\frac{1}{2}} - 2|r-r'+1|\cos^{-1}\beta' + \frac{1}{4}\pi - \psi_N(\beta')\right]}{(1-\beta'^2)^{\frac{1}{2}}\,|D_N(i(1-\beta'^2)^{\frac{1}{2}})|}\Bigg\}, \qquad (3.12)\end{aligned}$$

where $\beta' = 2|r - r' - 1|/\tau$ and can be replaced by β in the limit $\tau \to \infty$. The sum in Eq. (3.12) has been truncated because the summand is negligible for $r < -([\tau/2] - r')$, where $[\tau/2]$ denotes the greatest integer less than $\tau/2$. Rearranging the terms in Eq. (3.12), we obtain

$$\begin{aligned}\langle J_N(r', \tau)\rangle &= \tfrac{1}{4}kT \sum_{r=|R|}^{[\tau/2]-r'} \Bigg[\frac{2}{\pi\tau}(1-\beta^2)^{-1}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|^{-2} \\ &\quad \times \{-\sin[\tau(1-\beta^2)^{\frac{1}{2}} - 2(r+r')\cos^{-1}\beta + \tfrac{1}{4}\pi - \psi_N(\beta)] \\ &\quad \times \cos[\tau(1-\beta^2)^{\frac{1}{2}} - 2(r+r'-1)\cos^{-1}\beta + \tfrac{1}{4}\pi - \psi_N(\beta)] \\ &\quad + \cos[\tau(1-\beta^2)^{\frac{1}{2}} - 2(r+r')\cos^{-1}\beta + \tfrac{1}{4}\pi - \psi_N(\beta)] \\ &\quad \times \sin[\tau(1-\beta^2)^{\frac{1}{2}} - 2(r+r'-1)\cos^{-1}\beta + \tfrac{1}{4}\pi - \psi_N(\beta)]\} \\ &\quad + \frac{2}{\pi\tau}(1-\beta^2)^{-\frac{1}{4}}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|^{-1}\{\sin[\tau(1-\beta^2)^{\frac{1}{2}} - 2(r+r')\cos^{-1}\beta + \tfrac{1}{4}\pi - \psi_N(\beta)] \\ &\quad - \sin[\tau(1-\beta^2)^{\frac{1}{2}} - 2(r+r'-1)\cos^{-1}\beta + \tfrac{1}{4}\pi - \psi_N(\beta)]\}\Bigg] \\ &= \tfrac{1}{4}kT \sum_{r=|R|}^{[\tau/2]-r'} \Bigg[\frac{4}{\pi\tau}\beta(1-\beta^2)^{-\frac{1}{2}}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|^{-2} - \left(\frac{2}{\pi\tau}\right)^{\frac{1}{2}} 2(1-\beta^2)^{\frac{1}{4}}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|^{-1} \\ &\quad \times \cos[\tau(1-\beta^2)^{\frac{1}{2}} - (2r+2r'-1)\cos^{-1}\beta + \tfrac{1}{4}\pi - \psi_N(\beta)]\Bigg]. \qquad (3.13)\end{aligned}$$

The sum over r in Eq. (3.13) can be replaced by an integral over β. In the limit $\tau \to \infty$, only the first term in braces contributes to the energy current

$$\begin{aligned}J_N &= \frac{kT}{2\pi}\int_0^1 \beta(1-\beta^2)^{-\frac{1}{2}}\,|D_N(i(1-\beta^2)^{\frac{1}{2}})|^{-2}\,d\beta \\ &= \frac{kT}{2\pi}\int_0^1 |D_N(i\omega)|^{-2}\,d\omega, \qquad (3.14)\end{aligned}$$

where the arguments r' and ∞ of J_N and the brackets associated with the ensemble average have been omitted. The integrand in Eq. (3.14) has been studied extensively in R1 and R2. If a steady wave of unit amplitude and frequency ω is incident on the array of defects, then $|D_N(i\omega)|^{-2} = \mathcal{T}_N^2(\omega)$ is the square of the amplitude of the transmitted wave.

A similar asymptotic evaluation of the local temperature at the right and left sides of the array of defects leads to the expressions (see Appendix B for details)

$$T_N(r, \infty) = \pi^{-1}T\int_0^1 (1-\omega^2)^{-\frac{1}{2}}\,|D_N(i\omega)|^{-2}\,d\omega, \quad r > A_N, \qquad (3.15)$$

$$T_N(A_N, \infty) = (Q+1)T_N(r, \infty), \quad r > A_N, \qquad (3.16)$$

$$T_N(A_1, \infty) = (Q+1)\pi^{-1}T \times \int_0^1 (1-\omega^2)^{-\frac{1}{2}} \left|\frac{D_N^{(1)}(i\omega)}{D_N(i\omega)}\right|^2 d\omega,$$

and

$$T_N(-|r|, \infty) = T\left(1 - \pi^{-1}\int_0^1 (1-\omega^2)^{-\frac{1}{2}} |D_N(i\omega)|^{-2}\, d\omega\right). \quad (3.17)$$

If there are no defects, $Q = 0$, the square of the "transmitted" amplitude is unity, and one obtains the values for energy current and local temperature first obtained by Hemmer,[7]

$$J_0 = kT/2\pi \quad (3.18)$$

and

$$T_0(r, \infty) = T/2. \quad (3.19)$$

Clearly, the maximum value of the energy current is obtained in this case. In the special case of a single defect of mass $M = 2m$ located at $A_1 = 0$, the expressions for energy current and local temperature reduce to values obtained by Kashiwamura and Teramoto,[6]

$$J_1 = kT/3\pi, \quad (3.20)$$

$$T(|r|, \infty) = T/4, \quad (3.21)$$

$$T_1(0, \infty) = T/2, \quad (3.22)$$

and

$$T(-|r|, \infty) = 3T/4. \quad (3.23)$$

4. A LOWER BOUND ON THE ENERGY CURRENT J_N AND MONTE CARLO ESTIMATES OF $C^{-1}NJ_N$

It was noted at the end of Sec. 3 that $kT/2\pi$ is an upper bound on J_N. In this section, in an attempt to evaluate the limiting behavior of J_N for $N \to \infty$, we obtain a lower bound on the configuration average of J_N. In addition, we generate random configurations of defects and compute the values of the integrand and the integral in Eq. (3.14) for each configuration. The number of defects ranges from 25 to 600.

The expression for the thermal conductivity in the model is obtained by combining Eqs. (1.2), (3.14), (3.15), and (3.17):

$$k^{-1}K_N = \frac{N}{2\pi C}\left[1 - \frac{2}{\pi}\int_0^1 (1-\omega^2)^{-\frac{1}{2}} |D_N(i\omega)|^{-2}\, d\omega\right]^{-1} \times \int_0^1 |D_N(i\omega)|^{-2}\, d\omega. \quad (4.1)$$

If this thermal transport coefficient were normal, then one would expect that the limiting value of K_N is independent of the number of defects at constant over-all concentration, or, what is equivalent, one would expect that the limiting value of the energy current,

$$J_N = \frac{kT}{2\pi}\int_0^1 |D_N(i\omega)|^{-2}\, d\omega, \quad (4.2)$$

is proportional to N^{-1}. Such behavior for the energy current, in turn, would imply that the integrand $|D_N(i\omega)|^{-2}$ is small over most of the frequency range. The principal conclusion in earlier investigations[1,2] of the magnitude of $\mathfrak{C}_N^2 = |D_N(i\omega)|^{-2}$ may be summarized as follows:

$$-\lim_{\substack{N\to\infty \\ NA_N^{-1}=C}} \{N^{-1} \ln (\mathfrak{C}_N^2)\} = \alpha(\omega, Q, C) > 0. \quad (4.3)$$

In case $\omega \ll 1$, an explicit expression can be obtained for $\alpha(\omega, Q, C)$

$$-\lim_{\substack{N\to\infty \\ NA_N^{-1}=C}} \{N^{-1} \ln (\mathfrak{C}_N^2)\} = (1-C)(1+QC)^{-1}Q^2\omega^2, \quad \omega \ll 1. \quad (4.4)$$

These conclusions should be approximately valid for large but finite N, provided that $N\alpha(\omega, Q, C)$ is not too small. The estimates[1,2] of $\alpha(\omega, Q, C)$ indicated that $\alpha(\omega, Q, C) \to 0$ as $\omega \to 0$. Thus, the low frequencies make the largest contribution to the energy current (4.2). Our present problem of estimating the value of J_N at fixed N requires, first, the evaluation of $|D_N(i\omega)|^{-2}$ over the entire frequency range including such low frequencies that the associated wavelengths are comparable to or larger than A_N and, second, the determination of the limiting behavior as $N \to \infty$. Thus the order of the limiting processes, $\omega \to 0$, $N \to \infty$, is the reverse of the order implied in (4.3), where $N \to \infty$ at fixed $\omega > 0$.

Before proceeding to the exact calculations, assume that, for N large but finite,

$$\tilde{\mathfrak{C}}_N^2 = \exp\left[-(1-C)(1+QC)^{-1}Q^2\omega^2 N\right], \quad (4.5)$$

and ignore the difficulties involved in reversing the order in which the limits $N \to \infty$, $\omega \to 0$ are taken. Certainly Eq. (4.4) in no way implies (4.5).[8] The value of the energy current obtained by substituting (4.5) in (4.2) is

$$\tilde{J}_N = \frac{kT}{4Q}\left(\frac{1+QC}{\pi(1-C)}\right)^{\frac{1}{2}} N^{-\frac{1}{2}}, \quad (4.6)$$

and the value of the thermal conductivity is

$$k^{-1}\tilde{K}_N = \frac{1}{4CQ}\left[1 - \frac{N^{-\frac{1}{2}}}{Q}\left(\frac{1+QC}{\pi(1-C)}\right)^{\frac{1}{2}}\right]^{-1} \times \left(\frac{1+QC}{\pi(1-C)}\right)^{\frac{1}{2}} N^{\frac{1}{2}}. \quad (4.7)$$

In obtaining Eq. (4.7), we assumed that $\tilde{\mathfrak{C}}_N^2$ decreased so rapidly that the factor $(1-\omega^2)^{-\frac{1}{2}}$ in the integrand of the steady-state temperature difference could be

replaced by unity. The limiting value of $k^{-1}\tilde{K}_N$ is

$$k^{-1}\tilde{K}_N = \frac{1}{4CQ}\left(\frac{1+QC}{\pi(1-C)}\right)^{\frac{1}{2}} N^{\frac{1}{2}}, \tag{4.8}$$

a thermal conductivity coefficient which increases proportional to $N^{\frac{1}{2}}$. The values obtained from (4.8) agree closely with the Monte Carlo estimates described below.

A. Lower Bound on the Average Energy Current

Now consider the problem of determining a lower bound for the configuration average of the energy current in a particular ensemble of configurations. In the ensemble, the spacings between adjacent pairs of defects, $a_n = A_n - A_{n-1}$, are assumed to be independent random variables with the probability distribution (1.5),

$$\mathcal{P}(a_n) = C(1-C)^{a_n-1}. \tag{4.9}$$

The transmitted amplitude, and therefore the energy current through a particular configuration of defects, depend explicitly on the set of nearest-neighbor spacings

$$J_N = J_N(\{a_n\}).$$

The ensemble average of $J_N(\{a_n\})$ is

$$\langle J_N\rangle_c = \sum_{a_2=1}^{\infty}\cdots\sum_{a_N=1}^{\infty}\left\{\prod_{n=2}^{N}[C(1-C)^{a_n-1}]\right\}J_N(\{a_n\})$$
$$= \frac{kT}{2\pi}\int_0^1 \langle|D_N(\{a_n\})|^{-2}\rangle_c\, d\omega. \tag{4.10}$$

Although the configuration average of the reciprocal of $|D_N(\{a_n\})|^2$ cannot be carried out explicitly, the configuration average of $|D_N(\{a_n\})|^2$ can be evaluated.[9] The following inequality between these configuration averages,

$$\langle|D_N(\{a_n\})|^{-2}\rangle_c \geq \langle|D_N(\{a_n\})|^2\rangle_c^{-1}, \tag{4.11}$$

provides an explicit lower bound for $\langle J_N\rangle_c$

$$\langle J_N\rangle_c \geq \frac{kT}{2\pi}\int_0^1 \langle|D_N(\{a_n\})|^2\rangle_c^{-1}\, d\omega. \tag{4.12}$$

The details of the evaluation of $\langle|D_N(\{a_n\})|^2\rangle_c^{-1}$ and $\langle J_N\rangle_c$ are given in Appendix C. In the limit of large N, the lower bound obtained for the ensemble average of the energy current is

$$\langle J_N\rangle_c \geq 0.856[1 + Q^2C^2/4(1+QC)]^{-1}\tilde{J}_N, \tag{4.13}$$

where $\tilde{J}_N$ is defined in Eq. (4.6). Thus the lower bound on $\langle J_N\rangle_c$ is proportional to $N^{-\frac{1}{2}}$ and the corresponding lower bound on $\langle K_N\rangle_c$ increases proportional to $N^{+\frac{1}{2}}$.

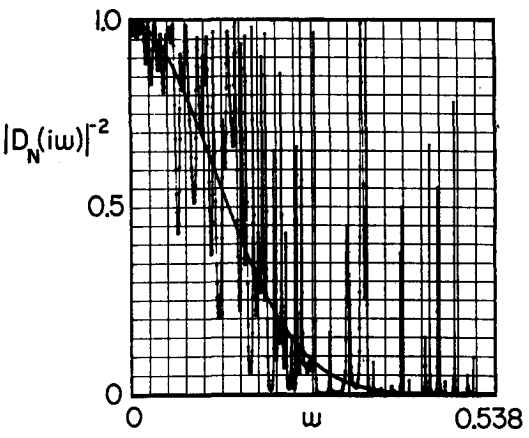

FIG. 3. Computed values of $|D_{100}(i\omega)|^{-2}$ vs ω are indicated by points on the irregular curve. The mass ratio $M/m = 2$, and concentration $C = 0.5$ in this case. The total frequency range covered is $0 \leq \omega \leq 0.538$, and the number of intermediate values at which the calculation is made is 10^3. The smooth curve is a plot of the corresponding value of $\tilde{\mathcal{C}}_N^2$.

B. Numerical Evaluation of J_N in Eq. (4.2) for Different Random Configurations of Defects

The determinantal integrand in the expression for the energy current J_N in Eq. (4.2) can be transformed into a continuant.[1] Since the continuant satisfies a two-term recurrence formula, it is especially well suited for numerical calculations. The computing program, described and used in R1 and R2, was used to generate random configurations of N defects and to evaluate the integrand at a suitable number of points so that the integral, and hence J_N, could be evaluated. In all the calculations, the parameters Q and C were assigned the values 1 and $\frac{1}{2}$, respectively. The results of the calculation of $|D_{100}(i\omega)|^{-2}$ and $|D_{600}(i\omega)|^{-2}$ in typical cases are shown in Figs. 3 and 4. The computed values of $|D_N(i\omega)|^{-2}$ are indicated by the points on the irregular curves. The corresponding values of $\tilde{\mathcal{C}}_{100}^2(\omega)$ and $\tilde{\mathcal{C}}_{600}^2(\omega)$ are plotted for comparison. In all cases, the spikelike appearance of $|D_N(i\omega)|^{-2}$ is enhanced at the higher frequencies where the width of the peaks decreases and the number of large maxima decreases (and, consequently, the interval between maxima increases). The results of all our calculations are summarized in Fig. 5, a log–log plot of $(kTC)^{-1}NJ_N$ vs. N. The lower bound from Eq. (4.13) is plotted as the dashed line, and $(kTC)^{-1}N\tilde{J}_N$ is plotted as the dotted line.

5. SUMMARY AND RELATED INVESTIGATIONS

The expression obtained for the thermal conductivity of the isotopically disordered crystal model

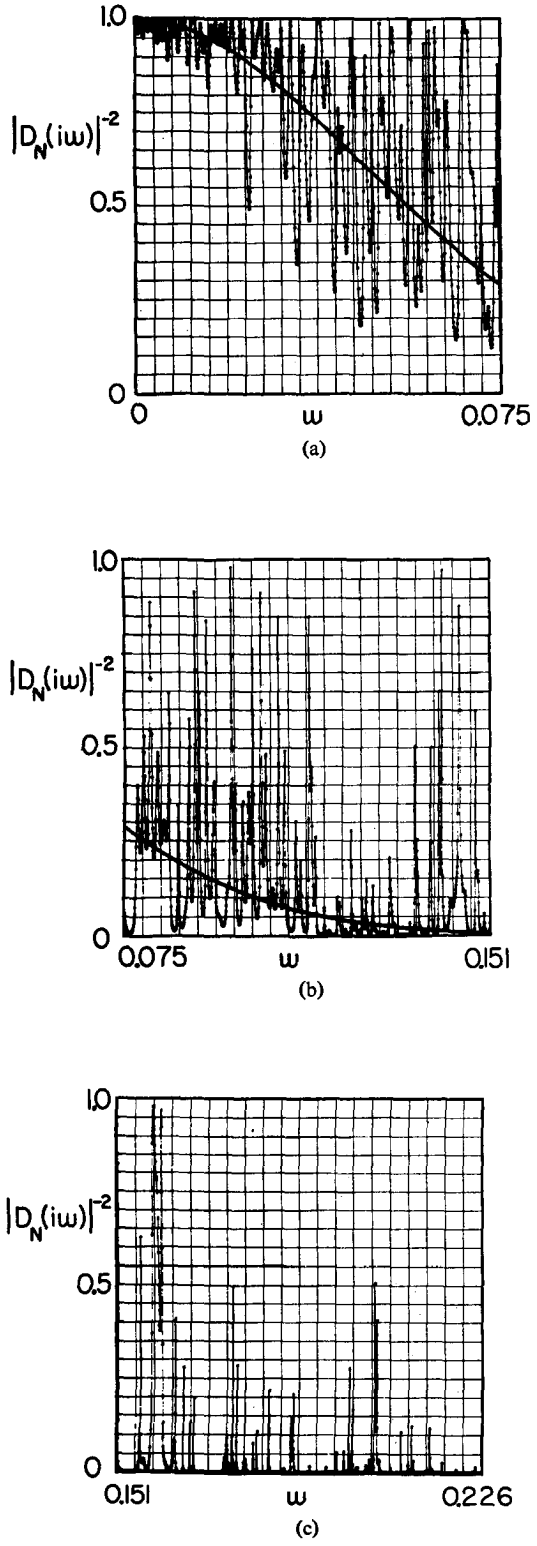

FIG. 4. Computed values of $|D_{600}(i\omega)|^{-2}$ vs ω are indicated by points on the irregular curve. The mass ratio $M/m = 2$, and concentration $C = 0.5$ in this case. The total frequency range covered is $0 \leq \omega \leq 0.226$, and the number of intermediate values at which the calculation is made is 3×10^3. Successive thirds of the frequency range are covered in the three graphs. The smooth curve is a plot of the corresponding values of $\mathfrak{G}_N^2$.

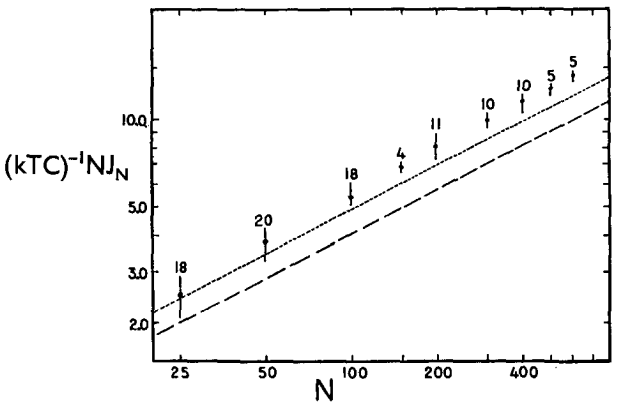

FIG. 5. The averages of the computed values of $(kTC)^{-1}NJ_N$ are plotted vs N. The number of different random configurations on which each average is based is indicated above each plotted point. The range of values entering each average is indicated by the vertical line through each point. The dashed line is a plot of the limiting form of the lower bound, Eq. (4.13), extended to the small N range. The dotted line is a plot of $(kTC)^{-1}N\tilde{J}_N$.

treated in this paper is

$$k^{-1}K_N = N(2\pi C)^{-1} \times \left[1 - 2\pi^{-1}\int_0^1 (1-\omega^2)^{-\frac{1}{2}} |D_N(i\omega)|^{-2}\, d\omega\right]^{-1} \times \int_0^1 |D_N(i\omega)|^{-2}\, d\omega. \tag{4.1}$$

In the limit of large N, the principal contribution to the integrals in (4.1) comes from low frequencies where $|D_N(i\omega)|^{-2}$ approaches unity. If the thermal conductivity coefficient were normal, the energy current integral would approach zero proportional to N^{-1}. It was shown in Sec. 4 that the energy current integral approaches zero no faster than $N^{-\frac{1}{2}}$, thus indicating that the thermal conductivity coefficient of the model is abnormal and depends on the size of the defect array (at constant concentration of defects). The Monte Carlo calculations of the energy current in Sec. 4 cover the range of values of N, $25 \leq N \leq 600$, and in this range the energy current integral is proportional to $N^{-\frac{1}{2}}$ within the statistical uncertainty, except for a small systematic deviation for $25 \leq N \leq 100$.

In the remainder of this section, we summarize some related investigations. The present N-defect model has also been considered by Allen and Ford,[10] who evaluated the Kubo formula for the thermal conductivity and obtained the result [their Eq. (37) in our notation]

$$k^{-1}K_N = \frac{N}{2\pi C}\int_0^1 |D_N(i\omega)|^{-2} \times \frac{(\omega\hbar/kT)^2 \exp(\omega\hbar/kT)}{[\exp(\omega\hbar/kT) - 1]^2}\, d\omega.$$

In the classical limit, their result reduces to

$$k^{-1}K_N = N(2\pi C)^{-1}\int_0^1 |D_N(i\omega)|^{-2}\,d\omega$$
$$= (kTC)^{-1}NJ_N,$$

the limiting form of Eq. (4.1) as $N\to\infty$. Allen and Ford speculated incorrectly that

$$|D_N(i\omega)|^{-2} = \exp(-Nd\omega), \quad \omega \ll 1,$$

where d is a constant, and concluded that the thermal conductivity of the model was independent of N.

As part of an investigation of anharmonic one- and two-dimensional isotopically disordered crystals, Payton, Rich, and Visscher[11] have studied the thermal conductivity of an isotopically disordered harmonic crystal with fixed boundaries in which the end particles of the crystal interact impulsively with perfect-gas thermal reservoirs at different temperatures. For a number of different random configurations of isotopes, these authors integrate the equations of motion which include the random force terms arising from interactions with reservoir particles. The thermal conductivity coefficient of a particular configuration of isotopes is determined when a stable, or steady-state, value of the energy current is established. Payton *et al.* investigated the variation of thermal conductivity with concentration. They did not observe a significant N dependence of the thermal conductivity in their model. However, recently when they repeated their calculations in a few cases with free-end boundary conditions, an N dependence of $k^{-1}K_N$ was observed.[12] The question, does the N dependence in the model change with the boundary conditions and what is the physical explanation of such a change, remains to be answered.

Matsuda, Miyata, and Ishii[13] and Matsuda and Ishii[14] studied the localization of normal mode eigenvectors in isotopically disordered crystals. They obtained an estimate, Eq. (7),[13] for the normal mode amplitude of particle $|n|$ relative to particle zero in the limit $|n|\to\infty$ and $\omega\to 0$, which, in the notation of this paper, is identical with Eq. (4.4), an estimate of $\mathcal{C}_N^2$ obtained in R2 (if N is identified with $|n|$). Using this estimate of the normal mode localization, Matsuda *et al.* reached the conclusion that the thermal conductivity in the Payton–Rich–Visscher model is proportional to $N^{\frac{1}{2}}$. However, their conclusion appears to depend upon having implicitly assumed free boundary conditions for the model.[12]

More recently Casher and Lebowitz[15] have investigated the steady-state energy flux through an isotopically disordered section of harmonic crystal whose end atoms are in contact with reservoirs at different temperatures. This model is one dimensional, and fixed boundary conditions are imposed on the crystal segment. Thus the model is similar to that of Payton *et al.* Except for the introduction of isotopic defects, the model treated by Casher and Lebowitz[15] is identical with the perfect lattice model investigated by Rieder, Lebowitz, and Lieb.[16] Casher and Lebowitz found that the average heat flux approaches zero with probability one as the length of the disordered crystal increases. Their estimate of the rate of approach of the heat flux to zero, which is derived from a lower bound, is consistent with the numerical calculations of Payton, Rich, and Visscher[11] for a crystal model with fixed boundaries.

ACKNOWLEDGMENTS

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APPENDIX A: EVALUATION OF $\langle J_N(r',\tau)\rangle$

Consider the calculation of the ensemble average of

$$J_N(t',\tau) = \tfrac{1}{4}m\dot\chi(r',\tau)[\chi(r'-1,\tau)-\chi(r',\tau)], \quad \text{(A1)}$$

where the initial values of the coordinates and velocities of the lattice particles are specified by the distribution function (2.4)

$$\mathfrak{W}\left[\begin{pmatrix}\dot{\mathbf{x}}_h(0)\\0\\\dot{\mathbf{x}}_c(0)\end{pmatrix},\begin{pmatrix}\mathbf{x}_h(0)\\0\\\mathbf{x}_c(0)\end{pmatrix}\right]$$
$$= Z\exp\left[-\frac{1}{2kT}\dot{\mathbf{x}}_h(0)^{\mathrm{T}}\mathsf{M}_h\dot{\mathbf{x}}_h(0)-\frac{1}{2kT}\mathbf{x}_h(0)^{\mathrm{T}}\mathsf{V}_h\mathbf{x}_h(0)\right]$$
$$\times\prod_{r=-R+1}^{\mathcal{N}}\{\delta[\dot\chi(r,0)]\delta[\chi(r,0)]\}. \quad \text{(A2)}$$

The calculation is identical with that in R3 for $\langle\dot\chi(r,\tau)^2\rangle$. The expressions for the velocity of particle r' and the position of particle s at time τ are, from (2.3a) and (2.3b),

$$\dot\chi(r',\tau) = \Delta_{r'}^{\mathrm{T}}\left[\mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\begin{pmatrix}\dot{\mathbf{x}}_h(0)\\0\\0\end{pmatrix}\right.$$
$$\left.-\mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\begin{pmatrix}\mathbf{x}_h(0)\\0\\0\end{pmatrix}\right] \quad \text{(A3)}$$

and

$$\chi(s,\tau)=\Delta_s^{\mathrm{T}}\left[\mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\begin{pmatrix}\dot{\mathbf{x}}_{\mathrm{h}}(0)\\0\\0\end{pmatrix}+\mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}\begin{pmatrix}\mathbf{x}_{\mathrm{h}}(0)\\0\\0\end{pmatrix}\right], \quad \text{(A4)}$$

or

$$\dot{\chi}(r',\tau)=\Delta_{r'}^{\mathrm{T}}\left[\gamma(\tau)\begin{pmatrix}\dot{\mathbf{x}}_{\mathrm{h}}(0)\\0\\\mathbf{0}\end{pmatrix}+\dot{\gamma}(\tau)\begin{pmatrix}\mathbf{x}_{\mathrm{h}}(0)\\0\\\mathbf{0}\end{pmatrix}\right] \quad \text{(A5)}$$

and

$$\chi(s,\tau)=\Delta_s^{\mathrm{T}}\left[\int_0^\tau\gamma(\sigma)\,d\sigma\begin{pmatrix}\dot{\mathbf{x}}_{\mathrm{h}}(0)\\0\\\mathbf{0}\end{pmatrix}+\gamma(\tau)\begin{pmatrix}\mathbf{x}_{\mathrm{h}}(0)\\0\\\mathbf{0}\end{pmatrix}\right], \quad \text{(A6)}$$

where $\gamma(\tau)=\mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}$. The ensemble average $\langle\dot{\chi}(r',\tau)\chi(s,\tau)\rangle$ is

$$\begin{aligned}\langle\dot{\chi}(r',\tau)\chi(s,\tau)\rangle&=\Delta_{r'}^{\mathrm{T}}\left\{\gamma(\tau)\begin{bmatrix}kT\mathsf{M}_{\mathrm{h}}^{-1}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\end{bmatrix}\left(\int_0^\tau\gamma(\sigma)\,d\sigma\right)^{\mathrm{T}}\right.\\&\left.+\dot{\gamma}(\tau)\begin{bmatrix}kT\mathsf{V}_{\mathrm{h}}^{-1}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\end{bmatrix}\gamma(\tau)^{\mathrm{T}}\right\}\Delta_s\\&=kT\Delta_{r'}^{\mathrm{T}}\left\{\mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\begin{bmatrix}\mathsf{I}_{\mathrm{h}}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\end{bmatrix}\right.\\&\times\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{-\frac{1}{2}}-\mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\\&\left.\times\mathsf{W}\begin{bmatrix}\mathsf{W}_{\mathrm{h}}^{-1}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\end{bmatrix}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{-\frac{1}{2}}\right\}\Delta_s.\end{aligned} \quad \text{(A7)}$$

If we recognize that the matrix W has the form

$$\mathsf{W}=\begin{pmatrix}\mathsf{W}_{\mathrm{h}}&\mathsf{W}_{\mathrm{hb}}&0\\\mathsf{W}_{\mathrm{bh}}&\mathsf{W}_{\mathrm{bb}}&\mathsf{W}_{\mathrm{bc}}\\\mathbf{0}&\mathsf{W}_{\mathrm{cb}}&\mathsf{W}_{\mathrm{c}}\end{pmatrix},$$

then

$$\mathsf{W}\begin{pmatrix}\mathsf{W}_{\mathrm{h}}^{-1}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\end{pmatrix}=\begin{pmatrix}\mathsf{I}_{\mathrm{h}}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\end{pmatrix}+\begin{pmatrix}\mathbf{0}&\mathbf{0}&\mathbf{0}\\\mathsf{W}_{\mathrm{bh}}\mathsf{W}_{\mathrm{h}}^{-1}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\end{pmatrix}.$$

Furthermore, the submatrix (vector) $\mathsf{W}_{\mathrm{bh}}\mathsf{W}_{\mathrm{h}}^{-1}$ contains only one nonzero component. The contribution to $\langle\dot{\chi}(r',\tau)\chi(s,\tau)\rangle$ from this nonzero component is negligible for $\tau\gg1$ and $\mathcal{N}\to\infty$; and, as a result, for $r'>A_N$, $s>A_N$,

$$\begin{aligned}&\langle\dot{\chi}(r',\tau)\chi(s,\tau)\rangle\\&=m^{-1}kT\sum_{r=-\mathcal{N}}^{-R}\left\{[\gamma(\tau)]_{r',r}\left[\left(\int_0^\tau\gamma(\sigma)\,d\sigma\right)^{\mathrm{T}}\right]_{r,s}\right.\\&\left.-\left(\int_0^\tau\gamma(\sigma)\,d\sigma\right)_{r',r}[\gamma(\tau)^{\mathrm{T}}]_{r,s}\right\}.\end{aligned} \quad \text{(A8)}$$

From the form of Eq. (A8), it follows that

$$\langle\dot{\chi}(r',\tau)\chi(r',\tau)=0.$$

Therefore, the final expression for $\langle J_N(r',\tau)\rangle$ is

$$\begin{aligned}&\langle J_N(r',\tau)\rangle\\&=\tfrac{1}{4}kT\sum_{r=-\mathcal{N}}^{-R}\{[\mathsf{M}^{-\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r',r}\\&\times[\mathsf{M}^{\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{-\frac{1}{2}}]_{r,r'-1}\\&-[\mathsf{M}^{-\frac{1}{2}}\mathsf{W}^{-\frac{1}{2}}\sin(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{\frac{1}{2}}]_{r',r}\\&\times[\mathsf{M}^{\frac{1}{2}}\cos(\mathsf{W}^{\frac{1}{2}}\tau)\mathsf{M}^{-\frac{1}{2}}]_{r,r'-1}\}.\end{aligned} \quad \text{(A9)}$$

APPENDIX B: ASYMPTOTIC FORMULAS FOR THE LOCAL STEADY-STATE TEMPERATURE

The expression for the local temperature, as measured by the velocity dispersion of a defect particle, in Eqs. (2.6) and (2.7) can be written with the aid of (3.1) and (3.6) as

$$\begin{aligned}&T^{-1}T_N(A_j,\tau)\\&=(Q+1)^{-1}\left(\sum_{r'=-\infty}^{-R}\dot{X}_{A_j}^2(r',\tau)\right.\\&\left.+\tfrac{1}{4}\sum_{r'=-\infty}^{-R}[X_{A_j}(r'+1,\tau)-X_{A_j}(r',\tau)]^2\right)\\&=(Q+1)\left(\sum_{r'=-\infty}^{-R}\dot{X}_{r'}^2(A_j,\tau)\right.\\&\left.+\tfrac{1}{4}\sum_{r'=-\infty}^{-R}[X_{r'+1}(A_j,\tau)-X_{r'}(A_j,\tau)]^2\right).\end{aligned} \quad \text{(B1)}$$

The difference in the second sum of Eq. (B1) is simplified after substituting Eq. (3.2),

$$\begin{aligned}&X_{r'+1}(A_j,\tau)-X_{r'}(A_j,\tau)\\&=\frac{2}{2\pi i}\int_{\mathfrak{L}}\frac{e^{p\tau}}{(p^2+1)^{\frac{1}{2}}}\frac{[p+(p^2+1)^{\frac{1}{2}}]^{-2A_j+2r+1}D_N^{(j)}(p)}{D_N(p)}\,dp,\end{aligned} \quad \text{(B2)}$$

and this expression in turn leads to simplification of Eq. (B1),

$$\begin{aligned}&T^{-1}T_N(A_j,\tau)\\&=(Q+1)\sum_{s=-\infty}^{-2R+1}\left(\frac{1}{2\pi i}\int_{\mathfrak{L}}\frac{e^{p\tau}}{(p^2+1)^{\frac{1}{2}}}\right.\\&\left.\times\frac{[p+(p^2+1)^{\frac{1}{2}}]^{-2A_j+s}D_N^{(j)}(p)}{D_N(p)}\,dp\right)^2.\end{aligned} \quad \text{(B3)}$$

In the limit in which $\tau \gg A_N$, the procedure for the asymptotic evaluation of the terms in Eq. (B3) is identical with the procedure used in treating Eq. (3.8). The result is

$$\frac{1}{2\pi i}\int_{\mathcal{L}} \frac{\exp\{p\tau - (2A_j + |s|)\ln[p + (p^2+1)^{\frac{1}{2}}]\}}{(p^2+1)^{\frac{1}{2}}} \frac{D_N^{(j)}(p)}{D_N(p)}\,dp$$
$$\sim \left(\frac{2}{\pi\tau}\right)^{\frac{1}{2}} \frac{\sin[\tau(1-\beta^2)^{\frac{1}{2}} - (2A_j + |s|)\cos^{-1}\beta + \frac{1}{4}\pi - \psi_N(\beta) + \psi_N^{(j)}(\beta)]}{(1-\beta^2)^{\frac{1}{4}}} \left|\frac{D_N^{(j)}(i(1-\beta^2)^{\frac{1}{2}})}{D_N(i(1-\beta^2)^{\frac{1}{2}})}\right|, \quad \text{(B4)}$$

where $\beta = (2A_j + |s|)/\tau$. Substituting (B4) in (B3), we obtain

$$T^{-1}T_N(A_j,\tau) = \pi^{-1}(Q+1)\sum_{l=2\tau+2A_j-1}^{[\tau]} \frac{\tau^{-1}}{(1-\beta^2)^{\frac{1}{2}}} \left|\frac{D_N^{(j)}(i(1-\beta^2)^{\frac{1}{2}})}{D_N(i(1-\beta^2)^{\frac{1}{2}})}\right|^2 \{1 - \cos[2\tau(1-\beta^2)^{\frac{1}{2}} - 2l\cos^{-1}\beta$$
$$+ \tfrac{1}{2}\pi - 2\psi_N(\beta) + 2\psi_N^{(j)}(\beta)]\}. \quad \text{(B5)}$$

As in Eq. (3.12), the upper limit on the sum in Eq. (B5) can be truncated and the sum over l can be replaced by an integral over β (from 0 to 1):

$$T^{-1}T_N(A_j,\infty) = \pi^{-1}(Q+1)\int_0^1 \left|\frac{D_N^{(j)}(i(1-\beta^2)^{\frac{1}{2}})}{D_N(i(1-\beta^2)^{\frac{1}{2}})}\right|^2 \frac{d\beta}{(1-\beta^2)^{\frac{1}{2}}} = \pi^{-1}(Q+1)\int_0^1 \left|\frac{D_N^{(j)}(i\omega)}{D_N(i\omega)}\right|^2 \frac{d\omega}{(1-\omega^2)^{\frac{1}{2}}}. \quad \text{(B6)}$$

In Eq. (B6) the oscillatory cosine term makes a negligible contribution in the limit $\tau \to \infty$, and has been omitted.

It is shown in R1 that the determinant $D_N(i\omega)$ can be transformed into an $N \times N$ continuant

$$D_N(i\omega) = \begin{vmatrix} 1+i\Delta & -e^{-2|A_1-A_2|i\sin^{-1}\omega} & 0 & \cdots \\ -e^{-2|A_2-A_1|i\sin^{-1}\omega} & 1+i\Delta+(1-i\Delta)e^{-4|A_2-A_1|i\sin^{-1}\omega} & -e^{-2|A_3-A_2|i\sin^{-1}\omega} & \\ 0 & -e^{-2|A_3-A_2|i\sin^{-1}\omega} & 1+i\Delta+(1-i\Delta)e^{-4|A_3-A_2|i\sin^{-1}\omega} & \\ & & & \ddots \end{vmatrix}_{(N\times N)} \quad \text{(B7)}$$

and, further, that the determinant $D_N^{(j)}(i\omega)$ can be transformed into an $(N-j+1)\times(N-j+1)$ continuant differing from Eq. (B.7) only in the upper left-hand corner element

$$D_N^{(j)}(i\omega) = \begin{vmatrix} 1 & -e^{-2|A_{j+1}-A_j|i\sin^{-1}\omega} & & \\ -e^{-2|A_{j+1}-A_j|i\sin^{-1}\omega} & 1+i\Delta+(1-i\Delta)e^{-4|A_{j+1}-A_j|i\sin^{-1}\omega} & & \\ & & \ddots & \\ & & & 1+i\Delta+(1-i\Delta)e^{-4|A_N-A_{N-1}|i\sin^{-1}\omega} \end{vmatrix}_{(N-j+1)\times(N-j+1)}, \quad \text{(B8)}$$

where $\Delta = Q\omega(1-\omega^2)^{-\frac{1}{2}}$. Consequently, the expression for $T^{-1}T_N(A_N,\infty)$ is somewhat simpler than the one for $T^{-1}T_N(A_1,\infty)$:

$$T^{-1}T(A_N,\infty) = \pi^{-1}(Q+1)\int_0^1 (1-\omega^2)^{-\frac{1}{2}}\,|D_N(i\omega)|^{-\frac{1}{2}}\,d\omega. \quad \text{(B9)}$$

Up to this point, we have dealt with the kinetic temperature of defect particles. We now obtain a simpler expression for $T^{-1}T(A_1,\infty)$ and, in addition, obtain values for $T^{-1}T(r,\infty)$ when $r > A_N$ and when $r < A_1$. In order to proceed, we quote a useful result from R2. In the stationary state transmission problem where a wave of unit amplitude and frequency ω is incident on the array of defects from the left, the transmitted wave amplitude $\mathfrak{T}_N$ and the reflected wave

amplitude $\mathcal{R}_N$ satisfy the following relations:

$$\mathcal{C}_N = |D_N(i\omega)|^{-1}, \tag{B10}$$

$$\mathcal{R}_N = |-1 + \hat{D}_N(i\omega)/D_N(i\omega)|, \tag{B11}$$

and

$$\mathcal{R}_N^2 + \mathcal{C}_N^2 = 1, \tag{B12}$$

where $\hat{D}_N(i\omega) \equiv D_N^{(N)}(i\omega)$. Substituting (B10) and (B11) in (B12), we obtain

$$\frac{\hat{D}_N(i\omega)}{D_N(i\omega)} + \left[\frac{\hat{D}_N(i\omega)}{D_N(i\omega)}\right]^* = \left|\frac{1}{D_N(i\omega)}\right|^2 + \left|\frac{\hat{D}_N(i\omega)}{D_N(i\omega)}\right|^2. \tag{B13}$$

Leave Eq. (B13) for the moment and consider the problem of obtaining an integral representation for $\dot{X}_{A_j}(A_j, \tau)$ analogous to the one quoted for $X_r(A_j, \tau)$ in Eq. (3.2). The procedure by which Eq. (3.2) was obtained in R1 can be repeated step for step in the case of $\dot{X}_{A_j}(A_j, \tau)$. The result is

$$\dot{X}_{A_j}(A_j, \tau) = \frac{Q+1}{2\pi i}\int_{\mathcal{L}} \frac{e^{p\tau}}{(p^2+1)^{\frac{1}{2}}} \frac{\bar{D}_N^{(j)}(p)}{D_N(p)}\, dp, \tag{B14}$$

where the elements of $\bar{D}_N^{(j)}(p)$ are the same as those of $D_N(p)$ except that the jth column of $\bar{D}_N^{(j)}(p)$ is

$$[p + (p^2+1)^{\frac{1}{2}}]^{-2|A_j - A_j|}, \quad i = 1, \cdots, N. \tag{B15}$$

In case $j = 1$,

$$\dot{X}_{A_1}(A_1, \tau) = \frac{Q+1}{2\pi i}\int_{\mathcal{L}} \frac{e^{p\tau}}{(p^2+1)^{\frac{1}{2}}} \frac{\bar{D}_N^{(1)}(p)}{D_N(p)}\, dp \tag{B16}$$

and $\bar{D}_N^{(1)}(p) = D_N^{(1)}(p) \equiv \hat{D}_N(p)$. Since (B16) is an explicit solution of the initial value problem

$$\mathbf{X}(0) = \mathbf{0}, \quad \dot{\mathbf{X}}(0) = \mathbf{\Delta}_{A_1}$$

which gives the velocity of particle A_1 at time τ, we have the following identity from Eq. (B16):

$$1 = \frac{Q+1}{2\pi i}\int_{\mathcal{L}} \frac{\hat{D}_N(p)}{D_N(p)} \frac{dp}{(p^2+1)^{\frac{1}{2}}}. \tag{B17}$$

The elements of $D_N(p)$ and $\hat{D}_N(p)$, given in (3.4) and (B15), have branch points at $p = \pm i$. If we define the functions involved by connecting the branch points with a cut drawn between them along the imaginary p axis and if we deform the path of integration so that it encircles the cut from $-i$ to $+i$ on the right and from $+i$ to $-i$ on the left of the cut, then we obtain

$$\begin{aligned} 1 &= \frac{Q+1}{2\pi i}\left[\int_{-1}^{1} \frac{\hat{D}_N(i\omega)}{D_N(i\omega)} \frac{di\omega}{(1-\omega^2)^{\frac{1}{2}}} - \int_{1}^{-1} \left(\frac{\hat{D}_N(i\omega)}{D_N(i\omega)}\right)^* \frac{di\omega}{(1-\omega^2)^{\frac{1}{2}}}\right] \\ &= \frac{Q+1}{\pi}\int_0^1 \left[\frac{\hat{D}_N(i\omega)}{D_N(i\omega)} + \left(\frac{\hat{D}_N(i\omega)}{D_N(i\omega)}\right)^*\right] \frac{d\omega}{(1-\omega^2)^{\frac{1}{2}}}. \end{aligned} \tag{B18}$$

Now Eq. (B6) in the case $j = 1$ can be combined with Eqs. (B13) and (B18) to give

$$\begin{aligned} T^{-1}T_N(A_1, \infty) &= 1 - \pi^{-1}(Q+1)\int_0^1 (1-\omega^2)^{-\frac{1}{2}} |D_N(i\omega)|^{-2}\, d\omega \\ &= 1 - T^{-1}T_N(A_N, \infty) \end{aligned} \tag{B19}$$

or

$$\begin{aligned} &\pi^{-1}(Q+1)\int_0^1 \left|\frac{\hat{D}_N(i\omega)}{D_N(i\omega)}\right|^2 \frac{d\omega}{(1-\omega^2)^{\frac{1}{2}}} \\ &\quad = 1 - \pi^{-1}(Q+1)\int_0^1 \left|\frac{1}{D_N(i\omega)}\right|^2 \frac{d\omega}{(1-\omega^2)^{\frac{1}{2}}}. \end{aligned} \tag{B20}$$

Thus far, we have obtained a relatively simple expression for the steady-state kinetic temperature of the right-most defect, $T(A_N, \infty)$ in Eq. (B9), and we have expressed the kinetic temperature of the left-most defect, $T(A_1, \infty)$ in Eq. (B19) in terms of $T(A_N, \infty)$.

For the sake of completeness, we now obtain expressions for the kinetic temperatures to the right of A_N and the left of A_1. In case $r > A_N$,

$$\begin{aligned} T^{-1}T(r, \tau) &= \sum_{r'=-\infty}^{-R} \dot{X}_r(r', \tau) \\ &\quad + \tfrac{1}{4}\sum_{r'=-\infty}^{-R} [X_r(r'+1, \tau) - X_r(r', \tau)]^2. \end{aligned} \tag{B21}$$

The asymptotic evaluation of (B21) is identical with that of (B1) for the case $j = N$. The final result is

$$\begin{aligned} T^{-1}T(r, \infty) &= (Q+1)^{-1}T^{-1}T(A_N, \infty) \\ &= \pi^{-1}\int_0^1 (1-\omega^2)^{-\frac{1}{2}} |D_N(i\omega)|^{-2}\, d\omega, \\ &\qquad r > A_N. \end{aligned} \tag{B22}$$

Rather than deal with determinantal expressions in evaluating $T^{-1}T(-|r|, \infty)$, we use a simple physical argument. Equation (B22) is the fraction of the initial kinetic energy [for the initial condition $\mathbf{X}(0) = \mathbf{0}$, $\dot{\mathbf{X}}(0) = m^{-\frac{1}{2}}\mathbf{\Delta}_r$] which crosses the array of defects and enters region h (Fig. 1). Equation (B22) also represents the fraction of the initial kinetic energy [for the initial condition $\mathbf{X}(0) = \mathbf{0}$, $\dot{\mathbf{X}}(0) = m^{-\frac{1}{2}}\mathbf{\Delta}_{-|r|}$] which crosses the array of defects from left to right. Consequently, the fraction of the initial kinetic energy (in this latter case) which enters region h gives the steady-state temperature at $-|r|$,

$$\begin{aligned} T^{-1}T(-|r|, \infty) &= 1 - \pi^{-1}\int_0^1 (1-\omega^2)^{-\frac{1}{2}} |D_N(i\omega)|^{-2}\, d\omega. \end{aligned} \tag{B23}$$

APPENDIX C: EVALUATION OF $\langle|D_N|^2\rangle_c$ AND LOWER BOUND OF $\langle J_N\rangle_c$

In this appendix we evaluate $\langle|D_N|^2\rangle_c$ exactly and express it as the coefficient of z^N in the power series expansion of a generating function $F(z)$ which we obtain in closed form. Our method is based on an idea due to Bellman.[17] Solutions valid for $\omega \ll 1$ are used to obtain an upper bound on the ensemble average transmission coefficient $\langle \mathcal{C}_N^2(\omega)\rangle_c = \langle 1/|D_N|^2\rangle_c$.

As shown in R1, the determinant D_N satisfies the two-term recursion relation [see also Eq. (B7)]

$$D_N = [1 + i\Delta + (1 - i\Delta)e^{-2i\kappa a_N}]D_{N-1} - e^{-2i\kappa a_N}D_{N-2}, \quad \text{(C1)}$$

where $\Delta = Q\omega(1-\omega^2)^{-\frac{1}{2}}$, $\kappa = 2\sin^{-1}\omega$, and $a_N = A_N - A_{N-1}$ and where $D_0 = 1$ and $D_1 = 1 + i\Delta$. Rewrite Eq. (C1) using the method of transfer matrices:

$$\begin{bmatrix} D_N \\ D_{N-1}\end{bmatrix} = \begin{bmatrix} \tilde{A}_N & \tilde{B}_N \\ 1 & 0\end{bmatrix}\begin{bmatrix} D_{N-1} \\ D_{N-2}\end{bmatrix} = \begin{bmatrix} \tilde{A}_N & \tilde{B}_N \\ 1 & 0\end{bmatrix}\begin{bmatrix} \tilde{A}_{N-1} & \tilde{B}_{N-1} \\ 1 & 0\end{bmatrix}\cdots\begin{bmatrix} \tilde{A}_2 & \tilde{B}_2 \\ 1 & 0\end{bmatrix} \times \begin{bmatrix} 1 + i\Delta \\ 1\end{bmatrix}, \quad \text{(C2)}$$

where $\tilde{A}_N$ and $\tilde{B}_N$ are defined to be

$$\tilde{A}_N = 1 + i\Delta + (1 - i\Delta)e^{-2i\kappa a_N}, \quad \tilde{B}_N = -e^{-2i\kappa a_N}. \quad \text{(C3)}$$

D_N is extracted by

$$\begin{pmatrix} D_N \\ 0\end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0\end{pmatrix}\begin{pmatrix} D_N \\ D_{N-1}\end{pmatrix}. \quad \text{(C4)}$$

Combining Eqs. (C2) and (C4), we write $|D_N|^2$ as

$$|D_N|^2 = \begin{pmatrix} D_N^* \\ 0\end{pmatrix}^{\mathrm{T}}\begin{pmatrix} D_N \\ 0\end{pmatrix} = \begin{pmatrix} 1 - i\Delta \\ 1\end{pmatrix}^{\mathrm{T}}\begin{pmatrix} \tilde{A}_2^* & 1 \\ \tilde{B}_2^* & 0\end{pmatrix}\cdots\begin{pmatrix} \tilde{A}_N^* & 0 \\ \tilde{B}_N^* & 1\end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0\end{pmatrix}^2 \times \begin{pmatrix} \tilde{A}_N & \tilde{B}_N \\ 1 & 0\end{pmatrix}\cdots\begin{pmatrix} \tilde{A}_2 & \tilde{B} \\ 1 & 0\end{pmatrix}\begin{pmatrix} 1 + i\Delta \\ 1\end{pmatrix}, \quad \text{(C5)}$$

which simplifies to

$$|D_N|^2 = \begin{pmatrix} 1 - i\Delta \\ 1\end{pmatrix}^{\mathrm{T}}\begin{pmatrix} \Lambda_N & \Sigma_N^* \\ \Sigma_N & \Omega_N\end{pmatrix}\begin{pmatrix} 1 + i\Delta \\ 1\end{pmatrix} \quad \text{(C6)}$$

$$= (1 + \Delta^2)\Lambda_N + (1 - i\Delta)\Sigma_N^* + (1 + i\Delta)\Sigma_N + \Omega_N. \quad \text{(C7)}$$

In Eq. (C6), the elements of the Hermitian matrix are defined by the relations

$$\Lambda_N = |\tilde{A}_N|^2\Lambda_{N-1} + \tilde{A}_N^*\Sigma_{N-1}^* + \tilde{A}_N\Sigma_{N-1} + \Omega_{N-1},$$
$$\Sigma_N = \tilde{A}_N\tilde{B}_N^*\Lambda_{N-1}^* + \tilde{B}_N^*\Sigma_{N-1}^*, \quad \Omega_N = |\tilde{B}_N|^2\Lambda_{N-1}, \quad \text{(C8)}$$

with

$$\Delta_1 = 1, \quad \Sigma_1 = 0, \quad \Omega_1 = 0. \quad \text{(C9)}$$

The elements Λ_N, Σ_N, and Ω_N have been decomposed into the functions Λ_{N-1}, Σ_{N-1}, and Ω_{N-1} which do not depend on the defect spacing a_N and into coefficients which depend only on a_N. This separation is useful in forming the average of $|D_N|^2$ over all a_j, $j = 1, 2, \cdots, N$, because the distribution function $(a_1, a_2, \cdots, a_N)$ is a product of independent distribution functions, each of which depends on only one spacing [see Eq. (4.10)].

Perform the indicated averages over defect spacings and introduce the definitions

$$R \equiv \langle|\tilde{A}_N|^2\rangle_c = 2(1 + \Delta^2) + (1 - i\Delta)\alpha^* + (1 + i\Delta)\alpha,$$
$$S \equiv \langle\tilde{A}_N\rangle_c = 1 + i\Delta + (1 - i\Delta)\alpha, \quad \text{(C10)}$$
$$\alpha \equiv \langle e^{-2i\kappa a_N}\rangle_c = C[e^{4i\sin^{-1}\omega} - 1 + C]^{-1}$$

and the identities

$$\langle|\tilde{B}_N|^2\rangle_c = 1,$$
$$\langle\tilde{A}_N^*\tilde{B}_N\rangle_c = -\langle\tilde{A}_N\rangle_c. \quad \text{(C11)}$$

The average value of $|D_N|^2$ thereby becomes, from Eq. (C7),

$$\langle|D_N|^2\rangle_c = (1 + \Delta^2)\langle\Lambda_N\rangle_c + (1 - i\Delta)\langle\Sigma_N^*\rangle_c + (1 + i\Delta)\langle\Sigma_N\rangle_c + \langle\Omega_N\rangle_c. \quad \text{(C12)}$$

From Eq. (C8) we find

$$\langle\Lambda_N\rangle_c = R\langle\Lambda_{N-1}\rangle_c + S^*\langle\Sigma_{N-1}\rangle_c + S\langle\Sigma_{N-1}^*\rangle_c + \langle\Omega_{N-1}\rangle_c,$$
$$\langle\Sigma_N\rangle_c = -S^*\langle\Lambda_{N-1}\rangle_c - \alpha^*\langle\Sigma_{N-1}^*\rangle_c, \quad \text{(C13)}$$
$$\langle\Sigma_N^*\rangle_c = -S\langle\Lambda_{N-1}\rangle_c - \alpha\langle\Sigma_{N-1}\rangle_c,$$
$$\langle\Omega_N\rangle_c = \langle\Lambda_{N-1}\rangle_c.$$

Because the average values $\langle\Lambda_N\rangle_c$, $\langle\Sigma_N\rangle_c$, and $\langle\Omega_N\rangle_c$ of the N-defect lattice are constructed in a linear fashion from $\langle\Lambda_{N-1}\rangle_c$, $\langle\Sigma_{N-1}\rangle_c$, and $\langle\Omega_{N-1}\rangle_c$, we introduce the generating function $f(z)$ defined by

$$F(z) = \sum_{N=1}^{\infty} z^N\langle|D_N|^2\rangle_c \quad \text{(C14)}$$

and the auxiliary generating functions $L(z)$, $V(z)$, and

$U(z)$ defined by

$$L(z) = \sum_{N=1}^{\infty} z^N \langle \Lambda_N \rangle_c,$$
$$V(z) = \sum_{N=1}^{\infty} z^N \langle \Sigma_N \rangle_c, \tag{C15}$$
$$U(z) = \sum_{N=1}^{\infty} z^N \langle \Omega_N \rangle_c.$$

From Eqs. (C13) and (C15), the following four equations in four unknowns appear:

$$\begin{aligned} L(z) - z &= RzL(z) + S^* z V^*(z) + SzV(z) + zU(z), \\ V^*(z) &= -SzL(z) - \alpha z V(z), \\ V(z) &= -S^* z L(z) - \alpha^* z V^*(z), \\ U(z) &= zL(z), \end{aligned} \tag{C16}$$

for which the solutions are

$$L(z) = z\left[1 - z^2 - Rz - z\left(\frac{S^{*2}\alpha z^2 - |S|^2 z}{1 - |\alpha|^2 z^2}\right) - z\left(\frac{S^2\alpha^* z^2 - |S|^2 z}{1 - |\alpha|^2 z^2}\right)\right]^{-1},$$
$$V(z) = \left(\frac{S\alpha^* z^2 - S^* z}{1 - |\alpha|^2 z^2}\right) L(z),$$

and

$$U(z) = zL(z). \tag{C17}$$

The generating function for $\langle |D_N|^2 \rangle_c$ is

$$F(z) = (1 + \Delta^2)L(z) + (1 - i\Delta)V^*(z) + (1 + i\Delta)V(z) + U(z). \tag{C18}$$

By some algebraic rearrangement and from the definitions of R and S in Eq. (C10), the generating function becomes

$$F(z) = \frac{z}{1 - z}\left(1 - \frac{\Delta^2(1 - |\alpha|^2 z^2)}{|\alpha|^2 G(z)}\right), \tag{C19}$$

in which $G(z)$ is a third order polynomial in z,

$$G(z) = z^3 - [w + |\alpha|^2(2\Delta^2 + 1)]|\alpha|^{-2} z^2 + (w + 2\Delta^2 + 1)|\alpha|^{-2} z - |\alpha|^{-2}. \tag{C20}$$

In Eq. (C20) w is defined to be

$$w = (1 + i\Delta)^2 \alpha^* + (1 - i\Delta)^2 \alpha. \tag{C21}$$

In terms of the roots z_1, z_2, and z_3 of $G(z)$, we write

$$G(z) = (z - z_1)(z - z_2)(z - z_3), \tag{C22}$$

and we resolve $F(z)$ into partial fractions

$$F(z) = z\left(\frac{1 + A_0}{1 - z} + \sum_{j=1}^{3} \frac{A_j}{z - z_j}\right). \tag{C23}$$

The numerators of each fraction, A_j, $j = 0, 1, 2, 3$, are dependent, in general, on Q and ω. The simultaneous equations generated in the process are

$$\begin{aligned} &A_0 = A_1 + A_2 + A_3, \\ &A_0(z_1 + z_2 + z_3) - (1 + z_2 + z_3)A_1 - (1 + z_1 + z_3)A_2 - (1 + z_1 + z_2)A_3 = \Delta^2, \\ &A_0(z_1 z_2 + z_2 z_3 + z_1 z_3) - A_1(z_2 z_3 + z_2 + z_3) - A_2(z_1 z_3 + z_1 + z_3) - A_3(z_1 z_2 + z_1 + z_2) = 0, \\ &A_0 z_1 z_2 z_3 - A_1 z_2 z_3 - A_2 z_1 z_3 - A_3 z_1 z_2 = -\Delta^2 |\alpha|^{-2}, \end{aligned} \tag{C24}$$

and their solution is

$$\begin{aligned} A_0 &= -\tfrac{1}{2}, \\ A_1 &= \frac{(1 + z_1)[\Delta^2 + \tfrac{1}{2}(1 + 2\Delta^2)(|\alpha|^{-2} - 1)]}{z_1(z_2 + z_3 - z_1) - z_2 z_3}, \\ A_2 &= \frac{(1 + z_2)[\Delta^2 + \tfrac{1}{2}(1 + 2\Delta^2)(|\alpha|^{-2} - 1)]}{z_2(z_1 + z_3 - z_2) - z_1 z_3}, \\ A_3 &= \frac{(1 + z_3)[\Delta^2 + \tfrac{1}{2}(1 + 2\Delta^2)(|\alpha|^{-2} - 1)]}{z_3(z_1 + z_2 - z_3) - z_1 z_2}. \end{aligned} \tag{C25}$$

The average value of $|D_N|^2$ is the coefficient of z^N in the power series representation of $F(z)$. Therefore, in terms of z_1, z_2, and z_3 and the four partial fraction numerators A_0, A_1, A_2, and A_3, we find

$$\langle |D_N|^2 \rangle_c = \tfrac{1}{2} + \sum_{j=1}^{3} A_j z_j^{-N}. \tag{C26}$$

At this point we could obtain explicit expressions for the three roots of $G(z)$ by solving the cubic equation $G(z) = 0$ analytically. These roots could be inserted in Eqs. (C25) and (C26) to obtain an explicit solution for $\langle |D_N|^2 \rangle_c$ for arbitrary Q, C, and ω. However, it is sufficient to seek a solution which is valid for very low frequencies.

We solve for the roots of $G(z)$ by rewriting Eq. (C20),

$$G(z) = (z - 1)^3 + pz^2 + qz + r = 0, \tag{C27}$$

where

$$\begin{aligned} p &= 2 - w|\alpha|^{-2} - 2\Delta^2, \\ q &= -2 + w|\alpha|^{-2} + 2\Delta^2, \end{aligned}$$

and

$$r = |\alpha|^{-2}. \tag{C28}$$

Substitution of y for $(z - 1)$ in the preceding expression and use of the identity

$$p + q + r = -2r\Delta^2 \tag{C29}$$

yields

$$G(1 + y) = y^3 + py^2 + (2p + q)y + 2\Delta^2 r = 0. \tag{C30}$$

At this point we introduce power series in frequency

for all frequency-dependent terms in $G(z)$:

$$\begin{aligned} p &= \sum_{n=1}^{\infty} p_{2n}\omega^{2n} = 16C^{-1}(Q+1)\omega^2 + \cdots, \\ q &= \sum_{n=1}^{\infty} q_{2n}\omega^{2n} \\ &= -16C^{-1}[Q+1-C^{-1}(1-C)]\omega^2 + \cdots, \\ r &= \sum_{n=1}^{\infty} r_{2n}\omega^{2n} = -16C^{-2}(1-C)\omega^2 + \cdots. \end{aligned} \tag{C31}$$

Because p, q, and r are even functions of ω, only even powers appear in their Taylor expansions.

Now expand the variable $y = z - 1$ in a power series in ω,

$$y = \sum_{n=1}^{\infty} y_n \omega^n, \tag{C32}$$

and determine the unknown coefficients y_n by substituting Eqs. (C31) and (C32) in $G(y+1) = 0$. By equating coefficients of like powers of ω, we obtain the following series expansions for the roots z_1, z_2, and z_3:

$$\begin{aligned} z_1 &= 1 - 2Q^2(1-C)(1+QC)^{-1}\omega^2 + \cdots, \\ z_2 &= 1 + 4iC^{-1}(1+QC)^{\frac{1}{2}}\omega - [8C^{-1}(Q+1) \\ &\qquad - Q^2(1-C)(1+QC)]\omega^2 + \cdots, \\ z_3 &= z_2^*. \end{aligned} \tag{C33}$$

From these z_j the partial fraction numerators may be computed from Eq. (C25). To lowest order, they are

$$\begin{aligned} A_0 &= -\tfrac{1}{2} \quad \text{(exact to all orders)}, \\ A_1 &= \frac{1}{2} + \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right), \\ A_2 &= A_3 = -\frac{1}{16}\left(\frac{Q^2C^2}{1+QC}\right). \end{aligned} \tag{C34}$$

Assembling all the results, we have the following for a low frequency approximation to $\langle |D_N|^2 \rangle_c$:

$$\begin{aligned} \langle |D_N|^2 \rangle_c &= \frac{1}{2} + \left[\frac{1}{2} + \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right)\right] z_1^{-N} \\ &\quad - \frac{1}{16}\left(\frac{Q^2C^2}{1+QC}\right)(z_2^{-N} + z_2^{*-N}) \\ &= \frac{1}{2} + \left[\frac{1}{2} + \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right)\right] \\ &\quad \times \left[1 - 2\left(\frac{Q^2(1-C)}{1+QC}\right)\omega^2\right]^{-N} \\ &\quad - \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right) \\ &\quad \times \left[1 + 2(1-C)\left(\frac{8}{C^2} + \frac{Q^2}{1+QC}\right)\omega^2\right]^{-N} \\ &\quad \times \cos\left[4NC^{-1}\omega(1+QC)^{\frac{1}{2}}\right]. \end{aligned} \tag{C35}$$

Note that $\langle |D_N|^2 \rangle_c = 1$ if $Q = 0$, $c = 0$, or $\omega = 0$.

The configuration average value of $|D_N|^2$ having been explicitly determined in the frequency interval $0 < \omega < \tilde{\omega} \ll 1$, the lower bound of the configuration average of the energy current from Eq. (4.12) is

$$\begin{aligned} \langle J_N \rangle_c \geq \frac{kT}{2\pi} N^{-\frac{1}{2}} \int_0^{\tilde{\omega}N^{\frac{1}{2}}} d\chi \Bigg\{ &\frac{1}{2} + \left[\frac{1}{2} + \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right)\right] \\ &\times \left[1 - 2\left(\frac{Q^2(1-C)}{1+QC}\right)\frac{\chi^2}{N}\right]^{-N} \\ &- \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right) \\ &\times \left[1 + 2(1-C)\left(\frac{8}{C^2} + \frac{Q^2}{1+QC}\right)\frac{\chi^2}{N}\right]^{-N} \\ &\times \cos\left[4N^{\frac{1}{2}}C^{-1}\chi(1+QC)^{\frac{1}{2}}\right] \Bigg\}^{-1}, \end{aligned} \tag{C36}$$

where the substitution $\omega^2 = N^{-1}\chi^2$ has been made. The integral in Eq. (C36) can be simplified, in the limit of large N, to

$$\begin{aligned} \langle J_N \rangle_c &= \frac{kT}{2\pi N^{\frac{1}{2}}} \int_0^{\infty} \Bigg\{ \frac{1}{2} + \left[\frac{1}{2} + \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right)\right] \\ &\quad \times \exp\left(2\frac{Q^2(1-C)}{1+QC}\chi^2\right) - \frac{1}{8}\frac{Q^2C^2}{1+QC} \\ &\quad \times \exp\left[-2(1-C)\left(\frac{8}{C^2} + \frac{Q^2}{1+QC}\right)\chi^2\right] \\ &\quad \times \cos\left[4N^{\frac{1}{2}}C^{-1}\chi(1+QC)^{\frac{1}{2}}\right] \Bigg\}^{-1} d\chi \\ &\geq \frac{kT}{2\pi N^{\frac{1}{2}}}\left[\frac{1}{2} + \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right)\right]^{-1} \\ &\quad \times \int_0^{\infty} \left[1 + \exp\left(2\frac{Q^2(1-C)}{1+QC}\chi^2\right)\right]^{-1} d\chi. \end{aligned} \tag{C37}$$

Finally, the value of the integral in (C37) is given in terms of the Riemann zeta function,[18] and

$$\begin{aligned} \langle J_N \rangle_c &\geq \frac{kT}{2\pi N^{\frac{1}{2}}}\left[\frac{1}{2} + \frac{1}{8}\left(\frac{Q^2C^2}{1+QC}\right)\right]^{-1} \\ &\quad \times \left(\frac{1+QC}{2Q^2(1-C)}\right)^{\frac{1}{2}} \frac{\pi^{\frac{1}{2}}}{2}\zeta\left(\frac{1}{2}\right)(1-2^{\frac{1}{2}}) \\ &\geq \left(1 + \frac{1}{4}\frac{Q^2C^2}{1+QC}\right)^{-1}\zeta\left(\frac{1}{2}\right)(2^{\frac{1}{2}}-2)\tilde{J}_N \\ &\geq 0.856\left(1 + \frac{1}{4}\frac{Q^2C^2}{1+QC}\right)^{-1}\tilde{J}_N. \end{aligned} \tag{C38}$$

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[8] For example, the value of the configuration average $\langle|D_N(i\omega)|^2\rangle_c$ obtained in Appendix C is

$$\langle|D_N(i\omega)|^2\rangle_c = \frac{1}{2} + \left(\frac{1}{2} + \frac{1}{8}\frac{Q^2C^2}{1+QC}\right)\left(1 - 2\frac{Q^2(1-C)}{1+QC}\omega^2\right)^{-N}$$
$$- \frac{1}{8}\frac{Q^2C^2}{1+QC}\left[1 + 2(1-C)\left(\frac{8}{C^2} + \frac{Q^2}{1+QC}\right)\omega^2\right]^{-N}$$
$$\times \cos\left[4NC^{-1}\omega(1+QC)^{\frac{1}{2}}\right]$$

and

$$\lim_{N\to\infty} N^{-1}\ln\left[\langle|D_N(i\omega)|^2\rangle_c\right] = -\ln\left(1 - 2\frac{Q^2(1-C)}{1+QC}\omega^2\right)$$
$$\cong 2\frac{Q^2(1-C)}{1+QC}\omega^2, \quad \omega \ll 1,$$

a result which, incidentally, differs from Eq. (4.4) by a factor of 2.

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Heat Flow in Regular and Disordered Harmonic Chains*

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(Received 18 January 1971)

We investigate the steady state heat flux J in a large harmonic crystal containing different masses whose ends are in contact with heat baths at different temperatures. Calling ΔT the temperature difference and $\mathfrak{L}$ the distance between the ends, we are interested in the behavior of $J/\Delta T$ as $\mathfrak{L} \to \infty$. For a perfectly periodic harmonic crystal, $J/\Delta T$ approaches a fixed positive value as $\mathfrak{L} \to \infty$ corresponding to an infinite heat conductivity. We show that this will be true also for a general one-dimensional harmonic chain (arbitrary distribution of different masses) if the spectral measure of the infinite chain contains an absolutely continuous part. We also show that for an infinite chain containing two different masses, the cumulative frequency distribution is continuous and that the spectrum is not exhausted by a denumerable number of points, i.e., the spectrum cannot consist entirely of point eigenvalues with a denumerable number of limit points. Using a theorem of Matsuda and Ishii, we show that for a random chain, corresponding to the mass at each site being an independent random variable, the heat flux approaches zero as $\mathfrak{L} \to \infty$, with probability one. This implies that the spectrum of a disordered chain has, with probability one, no absolutely continuous part.

1. INTRODUCTION

Equilibrium statistical mechanics as developed by Gibbs gives a prescription for calculating the free energy of an arbitrary physical system from its microscopic Hamiltonian. It is natural to ask whether this prescription really yields, for systems containing very many particles, free energy densities with the properties required of them by macroscopic thermodynamic theory? While this question can be readily answered in the affirmative for idealized systems such as "ideal" gases and "ideal" harmonic crystals, it is only more recently that this and more was proven rigorously for systems with realistic interactions between their microscopic constituents.[1] This puts equilibrium statistical mechanics in a sound mathematical position, notwithstanding the fact that actual computations on complex real systems can still only be done in approximate ways. At least we know that the quantities we are trying to compute really exist.

The situation in nonequilibrium statistical mechanics is much less satisfactory. Results comparable to those obtained for equilibrium statistical mechanics are not yet in sight. In particular, there is no proof at present that it is possible, even in principle, to compute transport coefficients, e.g., heat conductivity, viscosity, etc., from the microscopic Hamiltonian of a system. (We are speaking here of a "proof" not of faith followed, or preceded, by approximate computations.

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$$\langle|D_N(i\omega)|^2\rangle_c = \frac{1}{2} + \left(\frac{1}{2} + \frac{1}{8}\frac{Q^2C^2}{1+QC}\right)\left(1 - 2\frac{Q^2(1-C)}{1+QC}\omega^2\right)^{-N}$$
$$- \frac{1}{8}\frac{Q^2C^2}{1+QC}\left[1 + 2(1-C)\left(\frac{8}{C^2} + \frac{Q^2}{1+QC}\right)\omega^2\right]^{-N}$$
$$\times \cos\left[4NC^{-1}\omega(1+QC)^{\frac{1}{2}}\right]$$

and

$$\lim_{N\to\infty} N^{-1}\ln\left[\langle|D_N(i\omega)|^2\rangle_c\right] = -\ln\left(1 - 2\frac{Q^2(1-C)}{1+QC}\omega^2\right)$$
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1. INTRODUCTION

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The situation in nonequilibrium statistical mechanics is much less satisfactory. Results comparable to those obtained for equilibrium statistical mechanics are not yet in sight. In particular, there is no proof at present that it is possible, even in principle, to compute transport coefficients, e.g., heat conductivity, viscosity, etc., from the microscopic Hamiltonian of a system. (We are speaking here of a "proof" not of faith followed, or preceded, by approximate computations.

Such computations are very important, perhaps the most important thing to do, but they do not constitute a proof and might just be wrong.) These coefficients play the same role in macroscopic transport theory as the pressure, specific heat, etc., do in macroscopic equilibrium theory. All we can do rigorously at present is to study the nonequilibrium behavior of model systems with well-defined Hamiltonians. Even here we are, however, in a worse situation than in the equilibrium case. It was discovered quite early that the nonequilibrium properties (unlike the equilibrium properties) of the ideal gas and the ideal harmonic, crystal differ qualitatively from those of real systems. In particular, it is impossible to define transport coefficients for these systems. We are therefore forced, in studying transport processes, to use more complex models than the ideal systems mentioned earlier. One such model system, which *may* have well-defined transport coefficients, is the random harmonic crystal which we shall study in this paper.[2]

To be more specific, we wish to find the "steady state" energy flux in a system in contact with heat reservoirs at different temperatures T_α. Following the general principles of statistical mechanics,[3] we identify the observable properties of such a system with averages over a "suitable" phase space ensemble. To obtain such a Gibbs ensemble, we use a formalism developed in earlier papers[4,5] and look for the stationary solution of a generalized Liouville equation having the form

$$\frac{\partial \mu(x,t)}{\partial t} + (\mu, H) = \sum_\alpha \int [\mathcal{K}_\alpha(x,x')\mu(x',t) - \mathcal{K}_\alpha(x',x)\mu(x,t)]\,dx'. \tag{1.1}$$

Here x is a point in the phase space of the system, $H(x)$ is the Hamiltonian of the system, (μ, H) is the Poisson bracket describing the motion of the isolated system, and $\mathcal{K}_\alpha(x,x')\,dx\,dt$ is the conditional probability that when the system is at the point x' in its phase space it will, due to its interaction with the αth reservoir, make a transition to the volume element dx, about x, in the time interval dt. It is assumed here that the reservoirs are "stationary" so that the $\mathcal{K}_\alpha$ are independent of the time. Multiplying (1.1) by H and integrating over x, we obtain

$$\frac{\partial \langle H\rangle}{\partial t} = \sum_\alpha \int \mathcal{K}_\alpha(x,x') \times [H(x) - H(x')]\mu(x',t)\,dx\,dx' = \sum_\alpha J_\alpha, \tag{1.2}$$

where J_α is the energy flux from the αth reservoir. (We refer the reader to Refs. 4 and 5 for a detailed discussion.)

The stationary ensemble density is obtained from (1.1) by setting the time derivative there equal to zero. When all the reservoirs have the same temperature, this will be an equilibrium canonical ensemble while for reservoirs at different temperatures this ensemble will represent a system in a steady nonequilibrium state through which heat is flowing. In the steady state we have, of course, $\sum J_\alpha = 0$. Thus, if the geometry is set up in such a way that the system is in contact with only two reservoirs, one "on the left" at a temperature T_L and "one on the right" at a temperature T_R with $T_L > T_R$, and if the system has a uniform "cross section" S and "length" $\mathfrak{L}$, then we expect that in the stationary state the heat flux $J = J_L = -J_R$ should, for macroscopic size systems, be related via Fourier's law to the average temperature gradient $(T_L - T_R)/\mathfrak{L}$. More precisely, J should have the property that the quantity $\kappa(\mathfrak{L}) \equiv (J/S)/[(T_L - T_R)/\mathfrak{L}]$ should approach a well-defined limit κ when $\mathfrak{L} \to \infty$. If this κ exists, we would identify it with the heat conductivity of the system at temperature T when $T_L \to T_R \to T$.

This formalism was applied in I to a harmonic crystal with some particular forms of interaction with the heat reservoirs. The stationary nonequilibrium ensemble density for such a harmonic system was found to be a generalized Gaussian. The covariance matrix of this Gaussian was obtained there explicitly for a one-dimensional chain of equal masses with nearest neighbor interactions whose end atoms are in contact with heat reservoirs at temperature T_L and T_R. Identifying the number of particles in the chain with its length $\mathfrak{L}$, it was found there that, in the stationary nonequilibrium state, $\kappa(\mathfrak{L}) \sim \mathfrak{L}$, i.e., the heat flux achieves a constant value, for fixed $T_L - T_R$, independent of the length of the chain $\mathfrak{L}$. A similar result obtains for any perfectly periodic harmonic crystal corresponding to an "infinite" heat conductivity if one can speak of a heat conductivity in this case.[6] We therefore thought it of interest to investigate the case of a random harmonic crystal, i.e., what happens, in the same situation, to a crystal whose atoms are not all of the same mass, with the different masses distributed at "random." There seems to be no *a priori* way of deciding on what should happen in this case. On the one hand, it seems reasonable, and in apparent agreement with some machine computations,[7] that such a system would have, even in only one dimension, a well-defined heat conductivity; the reasoning is that the normal modes are scattered by the impurities inhibiting the flow of energy. On the

other hand, one can argue for a behavior similar to that found in the regular chain since the system is still harmonic. A computation by Matsuda and Ishii[8] suggests a compromise giving a $\kappa(\mathfrak{L}) \sim \sqrt{\mathfrak{L}}$, i.e., $J \sim \mathfrak{L}^{-\frac{1}{2}}$ for fixed $T_L - T_R$ (cf. also Ref. 9).

In this paper we describe our work on this problem. Unfortunately, we do not have a definite result for the asymptotic behavior of $\kappa(\mathfrak{L})$ but can show rigorously only that the heat flux J will not vanish as $\mathfrak{L} \to \infty$ if the spectral measure of the infinite chain has an absolutely continuous part. We also show, using a theorem of Matsuda and Ishii,[8] that, for a random chain, $J \to 0$ as $\mathfrak{L} \to \infty$ with probability one with $\langle J \rangle \geq O(\mathfrak{L}^{-\frac{3}{2}})$. This may suggest that the eigenfrequencies of a disordered chain are all isolated, but this is not so, as we show that the spectrum of an infinite chain in which the masses can have only two different values contains a nondenumerable infinity of points and is thus, in particular, not exhausted by a set of discrete eigenvalues having a denumerable number of accumulation points. This result is based on a proof that the cumulative frequency distribution of such a chain is continuous. These results suggest that the spectrum of a disordered chain may be of the singular continuous type, i.e., its continuous spectrum may have its support in a kind of Cantor set. They also raise the possibility that in more realistic systems, too, the existence of transport coefficients may require the absence of an absolutely continuous spectrum, while the irreversible decay of local disturbances requires the absence of localized bound states (corresponding to a point spectrum). Our results are based on a new general formalism for expressing J which brings out its relation to the normal mode spectrum. This also yields some new results for periodic chains showing explicitly how their infinite heat conductivity arises from their having an absolutely continuous spectrum.

2. FORMAL EXPRESSION FOR HEAT FLUX IN GENERAL HARMONIC SYSTEM

We consider a harmonic crystal made up of particles of masses $m_j, j = 1, \cdots, A$. (In I we assumed that all particles have the same mass.) Some of these particles are coupled to external heat reservoirs which are labeled by the same index as the particles. The particles of the jth reservoir, which interact via impulsive collisions with the jth crystal atom, have (prior to each collision) a Maxwellian velocity distribution with temperature T_j. Assuming that the masses of the jth reservoir particles are very small compared to m_j, the integral operators on the right side of (1.1) become Fokker–Planck type differential operators[4,5] and the generalized Liouville equation for $\mu(x, t)$ assumes the form, cf. Eq. (I.2.2),

$$\frac{\partial \mu(x,t)}{\partial t} = \sum_{i,j=1}^{2N} \left\{ \frac{\partial}{\partial x_i} (a_{ij} x_j \mu) + \tfrac{1}{2} d_{ij} \frac{\partial^2 \mu}{\partial x_i \partial x_j} \right\}. \quad (2.1)$$

Here x_i, $i = 1, \cdots, N$, $N \equiv sA$ (s the dimensionality of the space) are the Cartesian coordinates of the particles relative to their equilibrium positions. x_1, x_2, x_s are the coordinates of particle one, etc., while x_j, $j = i + N$, is the momentum conjugate to x_i, a and d are $2N \times 2N$ matrices made up of $N \times N$ matrices

$$\mathsf{a} = \begin{pmatrix} 0 & -\mathsf{M}^{-1} \\ \mathbf{\Phi} & \mathsf{L} \end{pmatrix}, \quad \mathsf{d} = \begin{pmatrix} 0 & 0 \\ 0 & 2\mathsf{MLT} \end{pmatrix}. \quad (2.2)$$

Here $\mathbf{\Phi}$ is the positive-definite symmetric force matrix of the system, M is the diagonal mass matrix of the system (with $M_{11} = M_1, \cdots, M_{ss} = M_s$, etc.), T is the diagonal temperature matrix of the reservoirs (with $T_{11} = T_1, \cdots, T_{ss} = T_s$, etc., and we have set Boltzmann's constant equal to 1), and L is a diagonal matrix with positive or zero elements which describes the reservoir system coupling; $L_{11} = \lambda_1, \cdots, L_{ss} = \lambda_s$, etc., with the λ_i the Fokker–Planck friction constant between the ith crystal atom and the ith reservoir, λ_i being zero if the ith particle is not coupled to any reservoir (cf. I, Sec. 2).

The fundamental solution of Eq. (1.1) can be shown[5] to be a generalized Gaussian. The time evolution of the moments of the distribution function μ may be obtained directly from (1.1) and are seen to satisfy the equations

$$\frac{d\langle x \rangle}{dt} = -\mathsf{a}\langle x \rangle, \quad \langle x_i \rangle \equiv \int x_i \mu(x,t)\, dx, \quad (2.3)$$

$$\frac{d\langle xx \rangle}{dt} = \mathsf{d} - \mathsf{a}\langle xx \rangle - \langle xx \rangle \mathsf{a},$$

$$\langle x_i x_j \rangle = \int x_i x_j \mu(x,t)\, dx. \quad (2.4)$$

The solutions of (2.3) and (2.4) are

$$\langle x(t) \rangle = \exp[-\mathsf{a}t]\langle x(0) \rangle, \quad (2.5)$$

$$\langle x(t)x(t) \rangle = \exp[-\mathsf{a}t]\langle x(0)x(0) \rangle \exp[-\tilde{\mathsf{a}}t] + \int_0^t ds \exp[-\mathsf{a}s]\mathsf{d} \exp[-\tilde{\mathsf{a}}s] \quad (2.6)$$

where $\tilde{\mathsf{a}}$ denotes the transpose of a.

The requirement that $\mathbf{\Phi}$ be positive definite ensures that none of the eigenvalues of $\mathbf{\Phi}$ vanishes. The further requirement that if Q is an eigenvector of $\mathbf{\Phi}$, then $\mathsf{LMQ} \neq 0$ (i.e., there are no normal modes of the isolated system for which *all* the particles which are in contact with the external reservoirs are always

at their equilibrium positions[10]) insures that all eigenvalues of a have positive real parts. This can be readily seen by noting that if $\boldsymbol{\xi} = (\mathbf{Q}; \mathbf{P})$ is an eigenvector of a with eigenvalue α, i.e., $\xi_i = Q_i$ for $i \leq N$, $\xi_{i+N} = P_i$, then we have

$$\tilde{\mathbf{Q}}\boldsymbol{\Phi}\mathbf{Q} - \alpha\tilde{\mathbf{Q}}\mathsf{LM}\mathbf{Q} + \alpha^2\tilde{\mathbf{Q}}\mathsf{M}\mathbf{Q} = 0. \tag{2.7}$$

Since LM is a positive (diagonal) matrix, we see that if α is real, it has to be positive while, if $\operatorname{Im}\alpha \neq 0$, we find by taking the imaginary part of (2.7) that

$$\operatorname{Re}\alpha = \tfrac{1}{2}(\tilde{\mathbf{Q}}\mathsf{LM}\mathbf{Q})/(\tilde{\mathbf{Q}}\mathsf{M}\mathbf{Q}) > 0. \tag{2.8}$$

Returning now to (2.5) and (2.6), we see that $\langle x(t)\rangle$ vanishes as $t \to \infty$ and

$$\lim_{t\to\infty}\langle x(t)x(t)\rangle = \int_0^\infty ds \exp[-\mathsf{a}s]\mathsf{d}\exp[-\tilde{\mathsf{a}}s]. \tag{2.9}$$

Hence the suitable stationary Gibbsian ensemble describing our harmonic system is a Gaussian with the covariance matrix (2.9) which thus contains all the information about the macroscopic properties of the stationary state. In order to obtain this covariance matrix in a more convenient form, we define the two $N \times N$ matrices

$$\begin{aligned}[\mathsf{F}(t)]_{ij} &= [\exp(-\mathsf{a}t)]_{i,N+j},\\ [\mathsf{G}(t)]_{ij} &= [\exp(-\mathsf{a}t)]_{N+i,N+j},\\ &\qquad i,j = 1,\cdots,N.\end{aligned} \tag{2.10}$$

Using the explicit form of a in (2.2), we find that $\mathsf{F}(t)$ and $\mathsf{G}(t)$ satisfy the equations

$$\mathsf{M}\dot{\mathsf{F}}(t) = \mathsf{G}(t); \quad \mathsf{M}\ddot{\mathsf{F}}(t) + \mathsf{ML}\dot{\mathsf{F}}(t) + \boldsymbol{\Phi}\mathsf{F} = 0, \tag{2.11}$$

with the initial conditions $\mathsf{F}(0) = 0$, $\mathsf{G}(0) = 1$ (the unit matrix).

It is now readily seen that

$$(2\pi)^{-1}\int_{-\infty}^{\infty} d\omega e^{-i\omega t}\mathsf{Z}^{-1}(\omega) = \begin{cases}\mathsf{F}(t) & \text{for } t \geq 0\\ 0 & \text{for } t < 0\end{cases}, \tag{2.12}$$

where $\mathsf{Z}(\omega)$ is an $N \times N$ matrix

$$\mathsf{Z}(\omega) = \boldsymbol{\Phi} - i\omega\mathsf{ML} - \omega^2\mathsf{M}. \tag{2.13}$$

Use has been made here of (2.7) and (2.8), which show that all the zeros of $\mathsf{Z}(\omega)$ are in the lower half of the complex ω plane occurring at values of $\omega = -i\alpha$, α an eigenvalue of a. We may now express the stationary correlations (2.9) in terms of the impedance matrix $\mathsf{Z}(\omega)$. Decomposing $\langle x(\infty)x(\infty)\rangle$ into four $N \times N$ matrices, we find

$$\langle q(\infty)q(\infty)\rangle = \pi^{-1}\int_{-\infty}^{\infty} d\omega\mathsf{Z}^{-1}(\omega)\mathsf{LMTZ}^{-1}(-\omega), \tag{2.14a}$$

$$\langle q(\infty)p(\infty)\rangle\mathsf{M}^{-1} = \pi^{-1}\int_{-\infty}^{\infty} d\omega\mathsf{Z}^{-1}(\omega)[i\omega\mathsf{LMT}]\mathsf{Z}^{-1}, \tag{2.14b}$$

$$\mathsf{M}^{-1}\langle p(\infty)p(\infty)\rangle\mathsf{M}^{-1} = \pi^{-1}\int_{-\infty}^{\infty} d\omega\mathsf{Z}^{-1}(\omega)[\omega^2\mathsf{LMT}]\mathsf{Z}^{-1}(-\omega). \tag{2.14c}$$

Equations (2.14) may be evaluated explicitly for the case when all the reservoirs have the same temperature $T_i = T$. We expect that in this case the stationary ensemble will be the canonical equilibrium ensemble with temperature T. This can be readily confirmed for (2.14c), for example. Noting that the matrix $-\omega\mathsf{LM}$ is just the imaginary part of $\mathsf{Z}(\omega)$, we find

$$\begin{aligned}\mathsf{M}^{-1}\langle p(\infty)p(\infty)\rangle\mathsf{M}^{-1} &= T(2\pi i)^{-1}\int_{-\infty}^{\infty} d\omega[\mathsf{Z}^{-1}(\omega) - \mathsf{Z}^{-1}(-\omega)]\omega\\ &= 2T\operatorname{Re}\left\{(2\pi i)^{-1}\int_{-\infty}^{\infty} d\omega[\omega\mathsf{Z}^{-1}(\omega)]\right\}.\end{aligned} \tag{2.15}$$

Closing the contour of integration in (2.15) along an infinite semicircle in the upper half-plane yields the expected result

$$\langle p(\infty)p(\infty)\rangle = \mathsf{M}T, \quad \text{when } T_l = T \text{ for all } l. \tag{2.16}$$

Incidentally we have found the sum rule

$$\pi^{-1}\int_{-\infty}^{\infty} d\omega\mathsf{Z}^{-1}(\omega)[\omega^2\mathsf{ML}]\mathsf{Z}^{-1}(-\omega) = \mathsf{M}^{-1}. \tag{2.17}$$

When the temperatures are not all the same, heat flows into the system from the different reservoirs. Applying (1.2) to our system, we find at all times

$$\langle\dot{H}(t)\rangle = \sum_j \lambda_j[T_j - m_j^{-1}\langle p_j^2(t)\rangle] = \sum_j J_j(t). \tag{2.18}$$

For the heat flux in the steady state, we have, using (2.14) and (2.17),

$$J_l = \sum_j (T_l - T_j)\lambda_l m_l m_j\lambda_j(\pi^{-1})\int_{-\infty}^{\infty} d\omega\omega^2\,|[\mathsf{Z}^{-1}(\omega)]_{lj}|^2. \tag{2.19}$$

Note that due to the symmetry of $\mathsf{Z}(\omega)$ the sum over all J_l vanishes as it should in a steady state.

Henceforth we shall specialize to the case of two heat reservoirs of temperatures T_L and T_R, coupled with equal strength λ to the first and last particles of a one-dimensional chain which consists of A particles, i.e., $T_1 = T_L$, $T_A = T_R$, $\lambda_1 = \lambda_A = \lambda$, $\lambda_j = 0$ for $j \neq 1, A$. Designating $\det[\boldsymbol{\Phi} - \omega^2\mathsf{M}]$ by K, we note that the cofactor C_{1A} of Z_{1A} is equal to that of $(\boldsymbol{\Phi} - \omega^2\mathsf{M})_{1A}$ and that $\det\mathsf{Z}$ may be expressed as a

quadratic function of λ. We are thus led to

$$J = (T_L - T_R)\lambda^2 m_1 m_A \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\omega^2 |C_{1A}(\omega)|^2}{(K_{1,A} - \lambda^2\omega^2 m_1 m_A K_{2,A-1})^2 + \lambda^2\omega^2(m_A K_{1,A-1} + m_1 K_{2,A})^2}, \quad (2.20)$$

where $K_{l,m}(\omega^2)$ is det $(\Phi - \omega^2 \mathsf{M})$ for a chain which starts from the lth particle and ends with the mth one.

Restricting the system further by assuming nearest neighbor forces of unit strength with particles 1 and A tied by springs to fixed positions

$$\Phi_{ij} = 2\delta_{ij} - \delta_{i+1,j} - \delta_{i,j+1}, \quad i, j = 1, \cdots, A, \quad (2.21)$$

leads to $|C_{1A}|^2 = 1$. Moreover, both $K_{1,A}$ and $K_{2,A}$ now satisfy the same recursion relation, namely

$$K_{j,A} = (2 - m_A\omega^2)K_{j,A-1} - K_{j,A-2}, \quad j = 1, 2, \cdots. \quad (2.22)$$

Using Eq. (2.22) for A and $A - 1$ leads to

$$K_{1,A}K_{2,A-1} - K_{1,A-1}K_{2,A} = \text{const independent of } A. \quad (2.23)$$

Evaluating (2.23) for $A = 2$ yields

$$K_{1,A}K_{2,A-1} - K_{1,A-1}K_{2,A} = -1. \quad (2.24)$$

This enables us to eliminate the cross terms in the denominator of Eq. (2.20) with the result

$$\begin{aligned} J_A &= (T_L - T_R)m_1 m_A \frac{\lambda^2}{\pi} \int_{-\infty}^{\infty} d\omega\omega^2/[2m_1 m_A\lambda^2\omega^2 \\ &\quad + (K_{1,A}^2 + \lambda^2\omega^2 m_A^2 K_{1,A-1}^2) \\ &\quad + \lambda^2\omega^2 m_1^2(K_{2,A}^2 + \lambda^2\omega^2 m_A^2 K_{2,A-1}^2)] \\ &\equiv (T_L - T_R)\int_0^{\infty} d\omega j_A(\omega). \end{aligned} \quad (2.25)$$

Equation (2.25) is an expression for the steady state heat flux in a harmonic chain containing A particles with masses $m_1, m_2, \cdots, m_A$. We shall be interested from now on in the behavior of the right side of (2.25) as $A \to \infty$.

3. PERIODIC CHAINS

We shall now specialize the analysis of the last section to the case of a periodic chain with a unit cell containing C particles of masses $m_1, \cdots, m_C$, $m_{C+1} = m_1$, etc. The chain contains N such cells, $A = NC$. It will be shown that for this system the heat flux in (2.25) does not vanish when $N \to \infty$ (i.e., the "heat conductivity" grows proportionally to the length of the chain as discussed in Sec. 1).

To proceed we note that the recursion relation (2.22) may be written as a 2×2 matrix equation[8]

$$\begin{aligned} Q_A &\equiv \begin{pmatrix} K_{1,A} & -K_{2,A} \\ K_{1,A-1} & -K_{2,A-1} \end{pmatrix} \\ &= \begin{pmatrix} 2 - m_A\omega^2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} K_{1,A-1} & -K_{2,A-1} \\ K_{1,A-2} & -K_{2,A-2} \end{pmatrix} \\ &= Q_1 Q_{A-1}, \end{aligned} \quad (3.1)$$

where $K_{1,1} = 2 - m_1\omega^2$, $K_{1,0} = K_{2,1} = 1$, $K_{2,0} = 0$. This leads immediately for $A = NC$ to

$$Q_A = (Q_C)^N. \quad (3.2)$$

The behavior of the integrand in (2.25) depends on the eigenvalues of Q_C. Since Q_C is unimodular and real its eigenvalues have the form $\exp(\pm iq)$ with q real or pure imaginary. In fact q is real whenever ω is such that

$$-2 \leq \text{tr } Q_C \equiv K_{1,C} - K_{2,C-1} = 2\cos q \leq 2. \quad (3.3)$$

This corresponds to wave vectors q with which waves will propagate through the lattice with one of the frequencies in the band $\omega_j(q)$, $j = 1, \cdots, C$. The $\omega_j^2(q)$ are the C roots of the polynomial equation tr $Q_C(\omega^2) = 2\cos q$, tr Q_C being a polynomial of order C in ω^2 and the $\omega_j^2(q)$ are positive for q real. To see that there is always some range of ω for which q is real we note that, for $\omega = 0$, Q_C has the form

$$Q_C(0) = \begin{pmatrix} C + 1 & -C \\ C & -C + 1 \end{pmatrix} \quad (3.4)$$

so that tr $Q_C(0) = 2$. The first-order correction to the trace is negative:

$$\text{tr } Q_C = 2 - \omega^2 C \sum_{\nu=1}^{C} m_\nu + O(\omega^2). \quad (3.5)$$

There will thus always be some $\omega_0 > 0$ such that $|\text{tr } Q_C| \leq 2$ for $0 \leq \omega \leq \omega_0$.

Returning now to (3.2),we may verify that

$$\begin{aligned} Q_A = [Q_C]^N &= [\cos Nq]\,\mathbb{1} \\ &\quad + [(\sin Nq)/\sin q][Q_C - (\cos q)\,\mathbb{1}], \end{aligned} \quad (3.6)$$

where $\mathbb{1}$ is the 2×2 unit matrix. We now note that the denominator of the integrand in (2.25) can be written as $|z_A|^2$, where z_A is the matrix element

$$z_A = (1, -i\lambda m_A\omega)Q_A \begin{pmatrix} 1 \\ i\lambda m_2\omega \end{pmatrix}. \quad (3.7)$$

Using (3.5), we find

$$z_A = (1 + \lambda^2\omega^2 m_1 m_C)\cos Nq + (\sin Nq/\sin q) \times [z_C - (1 + \lambda^2\omega^2 m_1 m_C)\cos q], \quad (3.8)$$

where

$$z_C = [K_{1,C} - \lambda^2 m_1 m_C \omega^2 K_{2,C-1}] - i\lambda\omega[m_1 K_{2,C} + m_C K_{1,C-1}]. \quad (3.9)$$

By writing $J(N, C)$ for J_A, Eq. (2.25) now assumes the form

$$J(N, C) = [(T_L - T_R)m_1 m_C \lambda^2 \pi^{-1}] \times \int_{-\infty}^{\infty} d\omega\omega^2 |(1 + \lambda^2\omega^2 m_1 m_C)\cos Nq + (\sin Nq/\sin q) \times [z_C - (1 + \lambda^2\omega^2 m_1 m_C)\cos q]|^{-2}. \quad (3.10)$$

The dependence of the heat flux on N, the number of cells of the chain, is entirely explicit in (3.10), z_C depending on ω (or q) but is independent of N. We note that as $N \to \infty$ only values of ω (more properly intervals of ω) for which q is real $|K_{1,C} - K_{2,C-1}| \leq 2$ will make a finite contribution to $J(N, C)$, since for imaginary q the integrand will decrease exponentially with N. Hence, to obtain $J(N, C)$ as $N \to \infty$, we may change variables from ω to q and restrict the range over q to the interval $[0, 2\pi]$. For large N the terms in the integrand of (3.10) which do not involve Nq may be regarded as constant while Nq changes by 2π. Calling the integrand in (3.10) $F(q, Nq)$, we may write

$$\int_0^{2\pi} dqF(q, Nq) = \sum_{j=0}^{N-1} \int_{2\pi j/N}^{2\pi(j+1)/N} dqF(q, Nq) = \frac{1}{2\pi} \sum_{j=0}^{N-1} \frac{2\pi}{N} \int_{2\pi j}^{2\pi(j+1)} dxF\left(\frac{x}{N}, x\right) \xrightarrow[N\to\infty]{} \frac{1}{2\pi} \int_0^{2\pi} dq \int_0^{2\pi} F(q, \theta)\, d\theta. \quad (3.11)$$

Carrying out the indicated integration over Nq in (3.10) and going back to the variable ω, we obtain, using also (3.9),

$$\lim_{N\to\infty} J(N, C) = (T_L - T_R)m_1 m_C \lambda\pi^{-1} \int d\omega\, |\omega \sin q| \times |(1 + \lambda^2\omega^2 m_1 m_C)[m_C K_{1,C-1} + m_1 K_{2,C}]|^{-1}, \quad (3.12)$$

the integration being over the region $|K_{1,C} - K_{2,C-1}| \leq 2$ [i.e., over the frequency bands of ω^2: $\min \omega_j^2(k) \leq \omega^2 \leq \max \omega_j^2(k), j = 1, \cdots, C$, which are the solutions of (3.3), $0 \leq k \leq 2\pi$; cf. discussion after Eq. (3.3)]. It is seen from (3.12) that $J \sim \lambda$ for $\lambda \to 0$ and $J \sim \lambda^{-1}$ when $\lambda \to \infty$. This was noted in I, where J was computed for the case of a chain with equal masses, which corresponds to a special case of (3.12) where $C = 1$. In that case, setting $m_1 = m$, we have, $2\cos q = 2 - m\omega^2$, $K_{1,0} = K_{2,1} = 1$, and the integration is over the interval $0 \leq \omega^2 \leq 4/m$. Changing the integration variable to q, we obtain, for the heat flow in an infinite chain with all masses $m_j = m$,

$$J = (T_L - T_R)\lambda(2\pi)^{-1} \times \int_0^{2\pi} dq \sin^2 q[1 + 2m\lambda^2(1 - \cos q)]^{-1} = \tfrac{1}{2}(m^2\lambda^3)^{-1}[T_L - T_R] \times [1 + 2m\lambda^2 - (1 + 4m\lambda^2)^{-\frac{1}{2}}], \quad (3.13)$$

the same result as was obtained in (I.4.6).

4. ASYMPTOTIC HEAT FLUX AND THE SPECTRUM

In this section we shall return to the general formula (2.25) and investigate the connection between the behavior of J_A as $A \to \infty$ and the nature of the spectrum of the semi-infinite chain. [For the periodic chain we have seen in (3.12) that $J_\infty > 0$ is given by an integral over the spectrum of the chain.]

To this end, consider the semi-infinite diagonal matrix M, whose entries are the masses $\{m_\nu\}$, $\nu = 1, 2, \cdots$. The proper frequencies squared of the associated harmonic chain are the eigenvalues of the semi-infinite Hermitian matrix

$$H = \mathsf{M}^{-\frac{1}{2}}\mathbf{\Phi}\mathsf{M}^{-\frac{1}{2}}, \quad (4.1)$$

where $\mathbf{\Phi}$ is the force matrix given in (2.21) with $A = \infty$. Regarded as an operator acting on the Hilbert space of sequences with the L_2 norm, H is bounded, nonnegative, and self-adjoint. In the usual Dirac notation,

$$\langle\nu|\, H\, |\Psi\rangle = -(m_{\nu-1}m_\nu)^{-\frac{1}{2}}\psi_{\nu-1} + 2m_\nu^{-1}\psi_\nu - (m_\nu m_{\nu+1})^{-\frac{1}{2}}\psi_{\nu+1}, \quad \psi_0 \equiv 0. \quad (4.2)$$

$$0 \leq \langle\Psi|\, H\, |\Psi\rangle \leq 4\, \|\Psi\|^2/m', \quad m' = \min\{m_\nu\} = 1, \quad (4.3)$$

and we are assuming that the $\{m_\nu\}$ have a lower bound which we set equal to unity. We see from Eq. (4.3) that the spectral support of H is contained in the interval $[0, 4]$. The spectrum is characterized by the family of spectral projections $E(\lambda)$ satisfying[11]

$$H = \int_0^4 dE(\lambda)\lambda, \quad (4.4)$$

$$E(0) = 0, \quad E(4) = 1. \quad (4.5)$$

Let H operate on the sequence Ψ:

$$\psi_\nu = \sqrt{m_\nu} \cdot K_{\nu-1}(\omega^2), \quad \psi_0 = 0, \tag{4.6}$$

where $K_\nu(\omega^2)$ is the determinant $K_{1,\nu}$ defined in Sec. 2 which satisfies the recurrence relation (2.22), $K_0 = 1$. It is seen from (4.2) that

$$H\Psi = \omega^2\Psi. \tag{4.7}$$

It follows from this that the matrix elements of $E(\lambda)$ can be written in the form[11]

$$\langle \nu | E(\lambda) | \nu' \rangle = (m_\nu m_{\nu'})^{\frac{1}{2}} \int_0^\lambda d\rho(x) K_{\nu-1}(x) K_{\nu'-1}(x), \qquad K_0 = 1, \tag{4.8}$$

where $\rho(x)$ is the spectral measure of H with respect to the vector $|1\rangle$. Since for cyclic vectors the different spectral measures of H are "equivalent," we shall refer to ρ simply as the spectral measure of H. The spectrum of H is the support of the measure $\rho(x)$. It follows from (4.5) and (4.8) that

$$\rho(x) = 0 \text{ for } x < 0, \quad \rho(x) = m_1^{-1} \text{ for } x > 4, \tag{4.9}$$

$$\int_0^4 d\rho(x) K_\nu^2(x) = m_{\nu+1}^{-1} \leq 1. \tag{4.10}$$

[For a chain with all $m_\nu = m$, $\rho'(x) = \pi^{-1}(x/m)^{\frac{1}{2}}(1 - x/4)^{\frac{1}{2}}$ for $0 \leq x \leq 4$].

It is seen from (4.10) that if $\rho(x)$ has an absolutely continuous part with support in a set X of Lebesgue measure $\delta > 0$, then $\exists\, B, B < \infty$, such that $d\rho(x)/dx > B^{-1}$ for $x \in X$ and thus

$$\int_X dx K_\nu^2(x) < B. \tag{4.11}$$

Furthermore, the determinants $K_{2,\nu}(\omega^2)$ which also occur in Eq. (2.25) play the same role with respect to an identical chain except for the first mass which is set equal to ∞. The operator H associated with this chain differs from H in (4.1) by a 2×2 matrix. Hence the absolutely continuous parts of their spectra coincide.[11] We now find, on assuming that the masses m_ν have also an upper bound, that the integral of the reciprocal of the integrand in (2.25) over a set $X' \subset X$

$$\int_{X'} d\omega j_A^{-1}(\omega) \leq B' < \infty, \tag{4.12}$$

where X' is the set $X - [0, \delta/2]$ and B' is a constant independent of A. It therefore follows by the Schwartz inequality that J_A is bounded below, i.e., $\exists \epsilon > 0$ such that

$$J_A \geq \epsilon(T_L - T_R) \quad \text{for all} \quad A \tag{4.13}$$

for fixed $\lambda \neq 0$. Hence we conclude that if the spectrum of the infinite chain with bounded masses $\{m_\nu\}$ has an absolutely continuous part, then the heat conductivity of a segment containing $\mathfrak{L}$ particles has a lower bound $\kappa(\mathfrak{L}) \geq \epsilon(\mathfrak{L})$ and thus *a priori* goes to infinity as $\mathfrak{L} \to \infty$.

We shall now use a theorem of Matsuda and Ishii,[8] which they derived on the basis of a theorem by Furstenberg, to show that for almost all random chains the heat flux $J_A \to 0$ as $A \to \infty$. By a random chain we mean a chain whose masses $m_1, m_2, \cdots$ are a sequence of independent positive random variables with a common distribution $p(m)$ which gives a nonvanishing probability for at least two different masses. A weak form of the Matsuda–Ishii theorem states that for such a chain

$$K_N^2(\eta) \to \infty \quad \text{as} \quad N \to \infty \quad \text{for all} \quad \eta \neq 0, \tag{4.14}$$

with probability one.

It follows from our previous discussion that when $m_\nu \geq 1$ for all possible chains, only the interval $0 \leq \omega \leq 2$ can make a finite contribution to the integral in (2.25). We therefore have

$$J_A = (T_L - T_R) \int_0^2 d\omega j_A(\omega). \tag{4.15}$$

Taking the average of J_A over the probability distribution of the masses m_ν, we have

$$\langle J_A \rangle = (T_L - T_R) \int_0^2 d\omega \langle j_A(\omega) \rangle. \tag{4.16}$$

It follows from (4.14) that

$$\langle j_A(\omega) \rangle \to 0 \quad \text{for} \quad 0 < \omega \leq 2. \tag{4.17}$$

We also have from (2.25) that

$$j_A(\omega) \leq (2\pi)^{-1} \quad \text{for all} \quad \omega; \tag{4.18}$$

hence, by the Lebesgue theorem,[12]

$$\lim_{A \to \infty} \langle J_A \rangle = 0. \tag{4.19}$$

Since $J_A \geq 0$, it follows from (4.19) that for any $\delta > 0$

$$\text{Prob}\,(J_A \geq \delta, \text{ for all } A) = 0. \tag{4.20}$$

Combining (4.20) with our previous result (4.13), we find that the probability that the spectrum of an infinite random chain has an absolutely continuous part is zero.

It will be shown in the next section that the spectrum of a chain containing two different masses cannot consist entirely of a denumerable number of points. Since it will also with probability one not contain an absolutely continuous part, it will "generally" either contain a singular continuous part or have a point

spectrum with a nondenumerable number of limit points.

5. FREQUENCY DISTRIBUTION FUNCTION AND SPECTRUM OF A BINARY CHAIN

We shall be concerned in this section with the simplest type of chain containing unequal masses, i.e., the mass of the νth atom m_ν can take on only two values,

$$m_\nu = 1 \text{ or } M, \quad M > 1, \quad \nu = 1, 2, \cdots, \infty. \tag{5.1}$$

The "average" properties of this system when the $\{m_\nu\}$ are assumed to be a set of independent random variables have, as mentioned earlier, been extensively investigated.[2] We recall this here only to emphasize that the main discussion in this section is *not* concerned with any probability distributions or averages but pertains to a specific chain with specified $\{m_\nu\}$ for *all* positive integer ν.

As was done in the last section, we let H denote the semi-infinite matrix $\mathsf{M}^{-\frac{1}{2}}\Phi\mathsf{M}^{-\frac{1}{2}}$. We also let H_A denote the $A \times A$ matrix consisting of the first A rows and columns of H. The eigenvalues of H_A, which are the squares of the normal frequencies of the chain containing A atoms with masses m_ν, $\nu = 1, \cdots, A$, are the zeros of the equation $K_A(\eta) = 0$ and will be designated by η_A^i, $i = 1, \cdots, A$. As is well known, $0 < \eta_A^i < 4$ and all the η_A^i are distinct for M finite. Let $AG_A(\eta)$ be the number of eigenvalues of H_A which are smaller than η. $G_A(\eta)$ is a monotonic step function,

$$G_A(\eta) = A^{-1} \sum_{\eta_A^i < \eta} 1, \quad G_A(0) = 0, \quad G_A(4) = 1, \tag{5.2}$$

i.e., $G_A(\eta)$ is the integrated normalized density of states. Since a set of uniformly bounded monotonic positive functions is compact, it is always possible to choose a subsequence of $G_A(\eta)$ which will converge to a function $G(\eta)$ as $A \to \infty$.

$G(\eta)$ need not be unique as may be seen by considering a chain for which $m_\nu = 1$, $\nu \leq N$, $m_\nu = M$, $N < \nu \leq N^2$, $m_\nu = 1$, $N^2 < \nu \leq N^4$, etc., with $N > 1$. Lederman's theorem [cf. Ref. 2(a)] asserts that the change in the number of eigenvalues of H_A in a given interval $[\eta_1, \eta_2]$ when a given number, say T, of the masses m_ν are changed is bounded by T. It is thus readily seen that we may choose sequences $G_A(\eta)$ which will converge to either $G^{(1)}(\eta)$ or $G^{(m)}(\eta)$, where $G^{(m)}(\eta)$ is the frequency distribution of the infinite chain, all of whose masses are equal to m.

We shall now show that

$$G(\eta) \text{ is continuous,} \tag{5.3}$$

the spectrum of the infinite chain, i.e., of H, contains a nondenumerable infinity of points. (5.4)

Following Rubin,[7] let $A_1, A_2, \cdots$ designate the positions of the heavy mass particles, $m_{A_\nu} = M$, and let $a_\nu = A_\nu - A_{\nu-1}$ with $A_0 \equiv 0$. Define the variable k and the quantity Δ by

$$\omega = 2 \sin (k/2), \quad \Delta(k) = (M - 1) \tan (k/2), \tag{5.5}$$

and note that $0 \leq \omega \leq 2$ corresponds to $0 \leq k \leq \pi$. It may now be verified that the determinants K_N satisfying the recurrence relation (2.22) can be expressed, for $A_\nu \leq N < A_{\nu+1}$, as

$$K_N = |R_\nu| \, (\sin k)^{-1} \sin [\tfrac{1}{2}\theta(N)], \tag{5.6}$$

where (suppressing the dependence on ω or k whenever possible)

$$R_0 = 1, \quad R_\nu = r_\nu R_{\nu-1},$$
$$r_\nu = 1 - i\Delta + i\Delta e^{i\theta_\nu}, \quad \nu \geq 1, \tag{5.7}$$
$$\theta(N) = \theta_{\nu+1} - 2k(A_{\nu+1} - N - 1),$$
$$A_\nu \leq N < A_{\nu+1}. \tag{5.8}$$

The $\theta_\nu(k)$ are continuous functions of k with $\theta(0) = 0$ and satisfy the recurrence relations

$$\exp [i(\theta_{\nu+1} - \theta_\nu)] = \exp [2ika_{\nu+1}](\bar{r}_\nu/r_\nu)$$
$$\text{for} \quad \nu \geq 1, \quad \theta_1 = 2kA_1, \tag{5.9}$$

with $\bar{r}_\nu$ denoting the complex conjugate of r_ν. It can be verified that these $\theta_\nu(k)$ and the $\theta(N, k)$ are monotonic functions of k for real k whose derivative with respect to k is given by

$$\frac{d\theta_{\nu+1}}{dk} - 2(A_{\nu+1} - N - 1)$$
$$= \frac{d}{dk}\theta(N)$$
$$= 2\Big((N + 1 - A_\nu) + |R_\nu|^{-2} \times \sum_{l=1}^{\nu} (a_l |R_{l-1}^2| + 2\Delta' \sin^2 k \, |K_{A_l-1}^2|)\Big),$$
$$A_\nu \leq N < A_{\nu+1}, \tag{5.10}$$

where

$$\Delta'(k) = (M - 1)/[2 \cos^2 (k/2)]. \tag{5.11}$$

Using the recurrence relation (5.7) yields the bounds

$$0 < C^{-\nu} \leq |R_\nu| \leq [(1 + \Delta^2)^{\frac{1}{2}} + \Delta]^\nu \equiv C^\nu \tag{5.12}$$

so that the zeros of K_N, i.e., the eigenvalues of H_N, occur at those values of k for which $\theta(N, k) = 2\pi j$, with j a positive integer. Since there are altogether N such zeros in the interval $0 < k < \pi$, we must have

$\theta(N, \pi) = 2\pi(N+1)$ [we have here $(N+1)$ rather than N to take care of the zeros of $\sin k$ in the denominator of (5.6)]. In general $G_N(\eta) = j/N$ in the interval $2j\pi < k \leq 2(j+1)\pi$, $j = 0, \cdots, N$ (with the relation $\eta = 4\sin^2 k/2$).

To prove (5.3), we write $K_N(\eta)$ in (5.6) as a product over its zeros

$$K_N = M^{\nu} \prod_{i=1}^{N} (\eta_N^i - \eta), \quad 0 < \eta_N^i < 4, \qquad A_\nu \leq N < A_{\nu+1}. \quad (5.13)$$

A discontinuity at the point $\eta_0 \neq 0$ or 4 ($\eta_0 = 0$ or 4 is excluded by Rayleigh's theorem) in the integrated density of states $G(\eta)$ means that η_0 is an accumulation point for a finite fraction of the zeros η_N^i, i.e., if $f(N, \epsilon)$ is the fraction of zeros of K_N in the interval $I = [\eta_0 - \frac{1}{2}\epsilon, \eta_0 + \frac{1}{2}\epsilon]$, then $N \to \infty$, followed by $\epsilon \to 0, f(N, \epsilon) \to p > 0$. We thus have

$$|K_N|^{1/N} \leq M[4^{(1-f)}\epsilon^f] \quad \text{for} \quad \eta \text{ in } I, \quad (5.14)$$

where $f = f(N, \epsilon)$. On the other hand, $|\sin[\frac{1}{2}\theta(N)]|$ must, according to (5.10), take on the value 1 at Nf points η_N^i inside I. At those points

$$|K_N|^{1/N} = (|R_\nu|/|\sin k|)^{1/N} \geq C^{-\nu/N} \geq C^{-1} \quad (5.15)$$

by (5.12). It is clear that (5.14) and (5.15) cannot be satisfied simultaneously for arbitrary ϵ and $M < \infty$ if $f(N, \epsilon) \to p > 0$ independent of ϵ. We thus conclude that

$$G_N(\eta + \epsilon/2) - G_N(\eta - \epsilon/2) = f(N, \epsilon) \to 0$$

as

$$N \to \infty \quad \text{and} \quad \epsilon \to 0, \quad (5.16)$$

for all η, and thus that $G(\eta)$ is continuous. This will be true for each limiting frequency distribution $G(\eta)$ if there is more than one for the infinite chain in question.

A similar analysis can also be applied to the average cumulative frequency distribution of a random chain[2]

$$\langle G(\eta) \rangle = \lim_{N \to \infty} \langle G_N(\eta) \rangle. \quad (5.17)$$

Taking the logarithms of Eqs. (5.14) and (5.15), we again find that

$$\lim_{\epsilon \to 0} \lim_{N \to \infty} \langle f(N, \epsilon) \rangle = 0 \quad (5.18)$$

and hence $\langle G(\eta) \rangle$ is continuous. The average frequency distribution $\langle G(\eta) \rangle$ determines all the equilibrium thermodynamic properties of the random chain[2] and has been shown elsewhere to be unique.[13,14]

It follows that since $G(\eta)$ increases continuously from 0 to 1 as η goes from 0 to 4 that the points of increase of $G(\eta)$ in the interval $[0, 4]$ are nondenumerable. Indeed it follows from Rayleigh's theorem that the number of normal frequencies in the interval $[(1-\delta)2\pi^{-1}M^{-\frac{1}{2}}\omega, \omega] = [\omega', \omega]$ for a chain containing A atoms of masses 1 and M has a lower bound which may be put in the form

$$G_A(\eta) - G_A(\eta') \geq \delta/\pi \quad \text{for} \quad \eta = \omega^2 < 4, \qquad 0 \leq \delta \leq 1. \quad (5.19)$$

Eq. (5.4) now follows if we can show that every point of increase of $G(\eta)$ for $0 < \eta \leq \eta_0$, $\eta_0 > 0$, is in the spectrum of H.

To prove this, assume that the point $\bar{\eta}$ is not in the spectrum of H. Then $\exists\, \epsilon > 0$ such that, for any sequence of normalized vectors[11] $\phi^{(n)}$,

$$\|(H - \eta)\phi^{(n)}\| \geq \epsilon, \quad \|\phi^{(n)}\| = 1 \quad (5.20)$$

whenever $\eta \in I = [\bar{\eta} - \epsilon/2, \bar{\eta} + \epsilon/2]$. The norm here is the L_2 norm in the space of sequences. Let $\phi^{(n)}$ be the sequence obtained by cutting off the sequence Ψ in (4.6) after n terms and normalizing it

$$\phi_j^{(n)} = \begin{cases} m_j^{\frac{1}{2}} K_{j-1}(\eta)/C_n, \\ \qquad 1 \leq j \leq n, \quad C_n = \left(\sum_{l=0}^{n-1} K_l^2 m_{l+1}\right)^{\frac{1}{2}}, \\ 0, \qquad j > n. \end{cases} \quad (5.21)$$

Substitution of the explicit matrix elements of H given in (4.2) into (5.20) yields

$$\|(H - \eta)\phi^{(n)}\| = (m_n^{-1}K_n^2 + m_{n+1}^{-1}K_{n-1}^2) \Big/ \sum_{l=0}^{n-1} K_l^2 m_{l+1} \geq \epsilon, \quad (5.22)$$

or, since $m_\nu \geq 1$, we have for $A_\nu \leq N < A_{\nu+1}$

$$\sum_{l=1}^{N} K_l^2 \leq (1 + \epsilon^{-1})[K_N^2 + K_{N-1}^2] \leq 2C^2(\sin k)^{-2}(1 + \epsilon^{-1})\,|R_\nu|^2, \quad (5.23)$$

where the last inequality follows from (5.6) and (5.12).

On the other hand, it follows from Eqs. (5.6)–(5.9) that

$$|R_\nu|^2 = \{\sin^2 k/\sin^2 \tfrac{1}{2}[\theta(N) - \theta(N-1)]\} \times |K_N - \exp\{\tfrac{1}{2}i[\theta(N) - \theta(N-1)]\}\rho_N K_{N-1}|^2, \quad (5.24)$$

where $A_\nu \leq N < A_{\nu+1}$ and

$$\rho_N = \begin{cases} 1, & \text{if } A_\nu < N, \\ |r_\nu|, & \text{if } A_\nu = N. \end{cases} \quad (5.25)$$

Moreover, we find from (5.6)–(5.9) that, for any mass M, $\exists\, k_0(M) > 0$ such that, for $k \leq k_0(M)$, $\{\sin^2 k/\sin^2 \frac{1}{2}[\theta(N) - \theta(N-1)]\} < M$. Hence, we have, using (5.11), that

$$\frac{d\theta(N)}{dk} \leq 2(N + 1 - A_\nu) + \sigma \sum_{l=0}^{N} \frac{K_l^2}{|R_\nu|^2}, \qquad k < k_0, \quad A_\nu \leq N < A_{\nu+1}, \quad (5.26)$$

where $\sigma < \infty$ is independent of N. Combining (5.26) with (5.23), we obtain an upper bound on the number of η_N^i in the interval I whenever $\bar{\eta} \leq \eta_0 < 4 \sin^2 (k_0/2)$. This upper bound shows that $\bar{\eta}$ cannot be a point of increase of $G(\eta)$ if, in the sequence of chains of length N for which $G_N(\eta) \to G(\eta)$, we can find a subsequence in which the distance from the end of the chain to the nearest atom with mass M, $(N - A_\nu)$ is of $o(N)$. For such chains then (5.4) is true. It seems clear that we can always choose our first sequence H_N so that this is true unless all the masses m_ν for $\nu > A_l$, $l < \infty$ are equal to unity, in which case $G(\eta)$ will equal $G^{(1)}(\eta)$, corresponding to a chain all of whose masses are unity, and the spectrum of H will have the same[11] absolutely continuous part as the chain whose $m_\nu = 1$ for all ν, i.e., its support will be the interval $[0, 4]$.

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APPENDIX: LOWER BOUND ON THE AVERAGE HEAT FLUX

Although we have no way of directly averaging the expression (2.25), a crude lower bound on J_A may be obtained when the m's are independent random variables by averaging the denominator of the integrand in (2.25).

To this end, we note that $K_{1,A}^2$ is the (11) entry of the (4×4) matrix obtained by taking the direct product of the (2×2) matrix Q_A with itself. It is readily established that

$$Q_A \times Q_A = \begin{bmatrix} f_A^2 & -f_A & -f_A & 1 \\ f_A & 0 & -1 & 0 \\ f_A & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \cdots \begin{bmatrix} f_1^2 & -f_1 & -f_1 & 1 \\ f_1 & 0 & -1 & 0 \\ f_1 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \tag{A1}$$

where $f_\nu \equiv 2 - m_\nu \omega^2$. Averaging $Q_A \times Q_A$ thus reduces to taking the average of a 4×4 matrix and raising it to the Ath power:

$$\langle (Q_A \times Q_A) \rangle = \begin{bmatrix} f^2 + g^2 & -f & -f & 1 \\ f & 0 & -1 & 0 \\ f & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}^A \equiv (\mathsf{F})^A, \tag{A2}$$

where $f = 2 - \langle m \rangle \omega^2$, $g^2 = \langle (m - \langle m \rangle)^2 \rangle \omega^4$. A direct check of the characteristic equation associated with the matrix F shows that its eigenvalues are of the form

$$\lambda_1 = \lambda, \quad \lambda_2 = \lambda^{-\frac{1}{2}} e^{i\alpha}, \quad \lambda_3 = \lambda^{-\frac{1}{2}} e^{-i\alpha}, \quad \lambda_4 = 1, \tag{A3}$$

where $\lambda > 1$. Evidently the dominant term in $\langle K_{1,A}^2 \rangle$ is the one associated with λ_1. An explicit calculation involving the solution of the third-order characteristic equation as $\omega^2 \to 0$ leads to the result

$$\langle K_{1,A}^2 \rangle \simeq e^{cA\sigma\omega^2}, \tag{A4}$$

where $\sigma \equiv \langle (m - \langle m \rangle)^2 \rangle$ and c is a numerical coefficient. Using the estimate (A4) in (2.25) gives[9]

$$\frac{\langle J_A \rangle}{(T_L - T_R)} \geq O[(A\sigma)^{-\frac{3}{2}}]. \tag{A5}$$

* Supported by the U.S.A.F.O.S.R.

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always sufficient, that there be no part of the crystal which is "isolated" from all the atoms which are in contact with the reservoirs.

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[14] The continuity of $\langle G(\eta)\rangle$ for a random chain was proven already by H. Schmidt, Phys. Rev. **105**, 425 (1957).

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Mathematics of the Measurement Problem in Quantum Mechanics

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The mathematical structure of the simplest nontrivial hidden variable theory is derived. The core of the resulting theory is an essentially unique nonlinear differential equation which gives a causal description of the continuous collapse of the wavefunction during a measurement. It is shown that the simplest collapse equation is the same as the equation given ad hoc by Bohm and Bub.

INTRODUCTION

The many papers written since von Neumann's initial paper on the subject of the possible existence of hidden variable theories of quantum mechanics have been thoroughly reviewed and criticized by several authors.[1] In this paper I do not intend to either attack or defend ideas expressed by previous authors on the subject of hidden variables. Instead I will derive the explicit mathematical structure of what I believe is the simplest nontrivial hidden variable theory. The core of the resulting theory is an essentially unique nonlinear differential equation which gives a causal description of the continuous collapse of the wavefunction during a measurement. The simplest collapse equation turns out to be the same as the equation given ad hoc by Bohm and Bub.[2]

DERIVATION OF THE FORM OF THE SIMPLEST HIDDEN VARIABLE THEORY

In my previous papers on this subject[3,4] I have tried to explore the mathematical consequences of the Bohm–Bub theory with the intent of helping to bring it to an experimental test. Due to the complexity of the equations I was not entirely successful. I feel that no real experimental tests of the theory have been conducted or proposed for the following three reasons.[5] First the nonlinearity of the collapse equation makes the theory very difficult to analyze. Secondly the theory is not fully interpreted by Bohm and Bub. The main collapse parameter γ is left practically arbitrary, as are the hidden variables themselves. Since the theory was introduced primarily as a counterexample to various theorems claiming that such a theory could not exist, this lack of completeness is understandable.[6] The third, and perhaps most significant, reason for the lack of experimental tests is the ad hoc and artificial way in which the theory was originally introduced. I will show that a combination of very general and reasonable requirements concerning quantum mechanics, physical measurement, and mathematical simplicity leads inescapably to an equation of the Bohm–Bub type and to a corresponding set of hidden variables. I had previously hoped that a simpler hidden variable theory might exist, but it seems that this hope was false.

If quantum mechanics is interpreted as a statistical theory of quantum ensembles and not as a physical theory concerning individual quanta, then there is no need to introduce the idea of the collapse of the wavefunction during measurement. However, individual quanta do exist experimentally; thus many physicists would like to believe, lacking any other theory, that quantum mechanics applies to the individual. The problem one then faces is that of explaining how the probabilities are changed to certainties by the process of measurement. The so-called projection postulate, first introduced by von Neumann, is the standard explanation of this process; yet, due to its almost metaphysical character, its validity cannot be taken seriously by most physicists.

In classical physics, probabilities enter due to our lack of knowledge of a large number of classical parameters, and not as intrinsic properties of the real world. Furthermore, the probabilities are generally

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In classical physics, probabilities enter due to our lack of knowledge of a large number of classical parameters, and not as intrinsic properties of the real world. Furthermore, the probabilities are generally

arrived at by averaging over the "hidden" parameters. A similar scheme can be made to work in quantum mechanics if the collapse process is given a realistic and physical description. There are, however, important differences in the averaging methods.[7]

In the standard presentation of the quantum theory the individual and the ensemble are mathematically indistinguishable. To facilitate the understanding of my results, I will try to carefully explain my view of the relationship of the individual and the ensemble to each other and to the act of measurement. Consider a pure ensemble of quanta at $t = t_0$, each individual described by the ensemble wavefunction $|\varphi(t_0)\rangle$. Suppose there are N quanta. Then, as long as properties of the individual quanta are not being measured, the wavefunction of the jth quanta will be assumed to be $|\varphi^j(t)\rangle = |\varphi(t_0)\rangle \exp[-iE(t - t_0)/\hbar]$, where $j = 1, 2, \cdots, N$. If a measurement of A is made at $t_1 > t_0$, then $|\varphi^j(t > t_1)\rangle \neq |\varphi(t_0)\rangle \exp[-iE(t - t_0)/\hbar]$. (As usual, assume, without loss of generality, that A is represented by a Hermitian operator with a discrete finite spectrum and that A is nondegenerate with eigenvectors $\{|A_i\rangle\}_1^n$.) The measurement changes the pure state into a mixed state. The original wavefunction of the ensemble can be expanded as $|\varphi(t_0)\rangle = \sum_1^n c_i |A_i\rangle$. The c_i are not changed by the measurement, but instead are *determined* by the measurement. For each j we can also expand $|\varphi^j(t)\rangle = \sum_1^n \varphi_i^j(t) |A_i\rangle$, where $\varphi_i^j(t_0) = \varphi_i^k(t_0)$ for all $j, k \leq N$. During the individual measurements the $\varphi_i^j(t)$ change, and

$$|c_i|^2 = \sum_1^N |\varphi_i^k(\infty)|^2/N = |\varphi_i^j(t_0)|^2$$

for all $j \leq N$. Ordinary quantum mechanics is confusing because it is an incomplete description of the individual. In fact, there is no way to distinguish the individual quanta. There is no "j." I claim the j should be determined by the values of the hidden variables. In the ordinary theory c_i is confused with $\varphi_i^j(t)$. The former must be constant during the measurement on the *ensemble* while the latter must change during the individual measurements. I will, in deference to the usual notation, drop the superscript j and suppress the dependence of the individual's complete state on the hidden variables. Instead of writing $|\varphi^j(t)\rangle$, I will write $|\varphi\rangle$ and, instead of writing $\varphi_i^j(t)$, just φ_i. Unless otherwise stated, one may assume I am discussing measurements made on *individual* quanta. If the components of the wavefunction of the individual quanta actually change in time during a measurement, then the relevant variables are

$$x_i(t) = |\varphi_i(t)|^2, \quad i = 1, \cdots, n,$$

where

$$|\varphi\rangle = \sum_1^n \varphi_i |A_i\rangle \quad \text{and} \quad \sum_1^n x_i = 1$$

for all t. I assume, of course, that the apparatus is insensitive to the relative phase differences between components of the wavefunction. I now assume that the collapse is described by a law which takes the form of a nonautonomous system of differential equations. It seems reasonable to suppose that *any* causal description of the collapse process must take such a form. The simplest such system of equations would be a first-order system. Let $X = (x_1, \cdots, x_n)$. So, for each t, $X \in R^n$. The collapse law, in normal form, is then

$$\dot{X} = f(t, X, \alpha, A).$$

It should be noted that since a particular observable A is being measured, f will depend on A. The equation can be written in a representation-free form, by using projection operators,[4] but it is easiest to use the form given. Also, as we will see later, f depends on some other parameters, represented by α. For the sake of simplicity, I will use the notation $f(t, X)$ instead of $f(t, X, \alpha, A)$. Since X is a vector, f must be a vector also. Furthermore, I assume that the nature of the interaction of the individual system with the particular measurement apparatus can be represented by a separate factor which must involve t and A and that f is a polynomial function of the x_i. The second assumption is justified purely on grounds of mathematical simplicity while the first may be justified on both physical and mathematical grounds as follows. If we write

$$f(t, X) = \gamma(t)G(X),$$

then $\gamma(t)$ is the factor which describes the turning on of the measurement apparatus. It is the interaction term. $\gamma(t)$ should involve neither the individual quanta nor the ensemble (i.e., neither the hidden variables nor the x_i) but should involve the observable A, which is being measured, and the time t. It is assumed that, during the measurement, $\gamma(t)$ is large enough to allow $\dot{X}$ to be nonzero but that $\gamma(t)$ is zero when no measurement is being made. Again, to simplify the notation, I write $G(X)$ rather than $G(X, \alpha, A)$.

If a measurement theory is to be realistic, the $x_i(t)$ should, in some sense, be irreversible. That is, during a measurement one of the x_i should always increase toward one while the rest decrease toward zero. The measured value of the observable being measured should not depend on when the experimenter turned off the apparatus, and results should be reproducible. Consequently, I will assume that the collapse process

is irreversible, in that at least one of the x_i must be a monotonic increasing function of t. The following assumptions have been made so far.

(1) $\sum_1^n x_i(t) = 1$, $x_i \geq 0$ for all t.
(2) The experiment has n distinct outcomes.
(3) The collapse law satisfies:
  (i) $\dot{X} = f(t, X)$, where $\dot{X} = dX/dt$;
  (ii) $f(t, X) = \gamma(t)G(X)$;
  (iii) $G(X)$ is a polynomial function of the x_i.
(4) The collapse is irreversible.
(5) None of the x_i or hidden variables are distinguished by the form of the theory.

As X changes during the measurement, it describes a path in R^n. Let the possible paths in R^n, described by $X(t)$, be called orbits. Assumption (1) implies that the orbits lie in a hyperplane in the positive region of R^n. Call this finite hyperplane the probability plane. The combination of assumptions (2) and (4) implies that for each i it must be possible, for some initial conditions, that $x_i(t) \uparrow 1$ while $x_j(t) \downarrow 0$ for all $j \neq i$ as $t \uparrow$ during a measurement. Given assumption (3), this means that the points of intersection of the coordinate axes with the probability plane,

$$\{(x_1, \cdots, x_n) \mid x_i = 1, x_j = 0 \text{ for all } j \neq i, \quad i = 1, \cdots, n\},$$

must be asymptotically stable critical points of the system of differential equations.[8] Furthermore, by assumption (4), it is easy to see that the $n(n-1)/2$ straight lines between these n points must be orbits. Now, because the end points of these straight line orbits are stable points, there must be a point on each of these lines that is an unstable critical point. Finally, assumption (5) reflects the fact that physically none of the x_i or hidden variables are distinguished. Mathematically this assumption serves to limit the possible collapse equations.

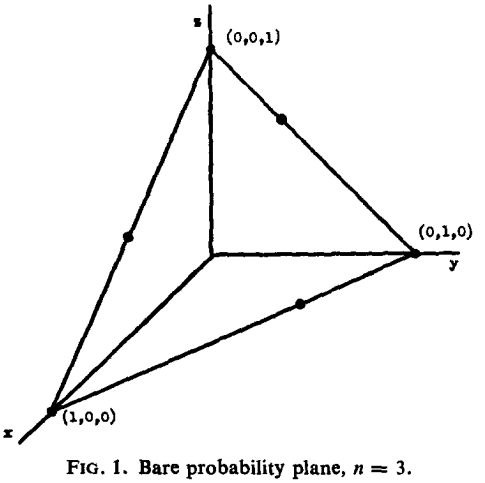

FIG. 1. Bare probability plane, $n = 3$.

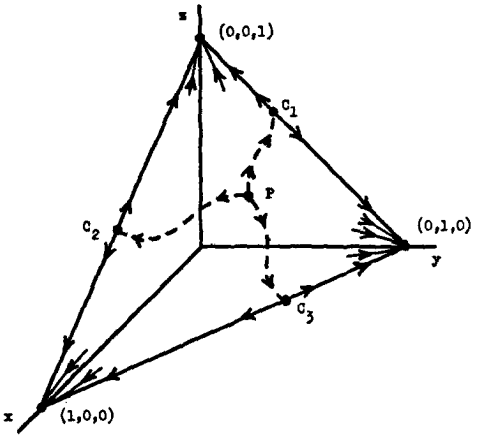

FIG. 2. A possible partition for $n = 3$.

The necessary topological characteristics of the simplest possible flow field described by $\dot{X} = \gamma(t)G(X)$ are difficult to envision in the general case. Hence, at this point, I will particularize the discussion to $n = 3$. The appropriate generalization to the higher dimension cases will become obvious after the following discussion. Figure 1 is the probability plane for $n = 3$. I have let $x_1 = x$, $x_2 = y$, and $x_3 = z$. The six critical points discussed above are shown. Assumptions (2), (3), and (4) imply that the probability plane must be partitioned, in this case, into three regions of asymptotic stability. A possible partition, along with some possible orbits, is shown in Fig. 2. Since there is no reason to suppose otherwise, we can assume that the flow field is a continuous one with singularities but no holes. Now consider a simple closed curve just inside the boundary of the probability plane. The index of the flow field on this curve is $+1$ so that the interior of the probability plane contains at least one unstable critical point. By simplicity, assume that it contains exactly one. (The next simplest case would be the case of two unstable critical points, each of index $+1$, and a saddle point of index -1.[9]) Let the one unstable critical point be called P.

The next question is: What is the simplest possible partition which will not conflict with assumptions (1)–(5)? A "simple" partition should easily be described both geometrically and analytically, and should involve the smallest number of new parameters in its description. Consider Fig. 2. It is clear that we need two independent parameters to locate the point P. If the curves connecting P to C_1, C_2, and C_3 are not straight lines, we will need additional parameters to describe these curves. Furthermore, since the locations of C_1, C_2, and C_3 are arbitrary at this point, we will need more than two independent new parameters even if the boundaries of the three regions are straight lines, unless the points (1, 0, 0), (0, 1, 0),

(0, 0, 1) and P serve to locate C_1, C_2, and C_3. Suppose this last condition is true and that the curves are straight lines. If P has coordinates $(1/\alpha_1, 1/\alpha_2, 1/\alpha_3)$, where $1/\alpha_1 + 1/\alpha_2 + 1/\alpha_3 = 1$, let

$$C_1 = (0, K_1/\alpha_2, K_1/\alpha_3), \quad C_2 = (K_2/\alpha_1, 0, K_2/\alpha_3),$$
$$C_3 = (K_3/\alpha_1, K_3/\alpha_2, 0),$$

where

$$K_i = \alpha_i/(\alpha_i - 1), \quad i = 1, 2, 3.$$

More independent parameters would be needed only if there were an asymmetric treatment of x, y, or z. Consequently, two seems to be the smallest possible number of new parameters involved in the simplest partition if $n = 3$. The three regions of asymptotic stability, called R_1, R_2, and R_3, are given by the following sets:

$$R_1 = \{(x, y, z) \,|\alpha_1 x\rangle\, \alpha_2 y, \alpha_3 z, x + y + z = 1\},$$
$$R_2 = \{(x, y, z) \,|\alpha_2 y\rangle\, \alpha_1 x, \alpha_3 z, x + y + z = 1\},$$
$$R_3 = \{(x, y, z) \,|\alpha_3 z\rangle\, \alpha_1 x, \alpha_2 y, x + y + z = 1\}.$$

The generalization of these regions is obvious. I now make assumption (6):

(6) The ith region of asymptotic stability is given by

$$R_i = \left\{(x_1, \cdots, x_n) \,|\alpha_i x_i\rangle \alpha_j x_j, \right.$$
$$\left. j = 1, \cdots, i-1, i+1, \cdots, n, \sum_1^n x_i = 1\right\},$$

where $i = 1, \cdots, n$. It is clear that these regions form an open partition of the probability plane and furthermore that the boundaries are straight line orbits.

Definition: A collapse equation is said to be *simple* if it leads to no conflicts with assumptions (1)–(6).

The relationship between the ensemble and the individual must be dealt with again at this point. The hidden variables must at least individualize the quanta, explain the outcomes of the individual measurements in a causal fashion, and explain the statistics of the ensemble. If the hidden variables are $1/\alpha_i$, $i = 1, \cdots, n$, then by assumption (6) they serve to partition the probability plane into n regions of asymptotic stability. This really means that G depends on $(\alpha_1, \cdots, \alpha_n)$ as well as on $(x_1, \cdots, x_n)$ as noted earlier. In this sense G is a family of transformations. Each individual quanta, characterized at time t_0 by the ensemble state $X(t_0)$, will ultimately end up in the state e_i, where $\{e_i\}_1^n$ is the standard basis in R^n, if and only if $X(t_0) \in R_i$. Each individual starts out represented by the same point in the probability plane, $X(t_0)$, but due to the fact that the partition may be different for each individual, that is, for each choice of $(\alpha_1, \cdots, \alpha_n,)$ the individuals belong to various regions of asymptotic stability. To explain the quantum statistics, we must require:

(7) The standard measure of the part of the hidden variable space corresponding to the ith outcome, normalized by the standard measure of the entire hidden variable space, must equal $x_i(t_0)$.

The choice of the standard measure on the hidden variable space is made in accordance with assumption (5) and for reasons of simplicity.

It should be noted that assumptions (1), (2), (4), and (5) are rather minimal conditions concerning quantum mechanics and measurement, and are quite general. These should be easy to accept. Assumptions (3) and (6) are related and are also easy to accept provided that one believes that physical processes can be described by differential equations. Acceptance of assumption (7) depends on what one expects of a hidden variable theory. The term "hidden variable theory" means different things to different people, of course. By a hidden variable theory I will mean a theory which at least does not conflict with assumptions (1)–(7).

I will now derive the precise form of what I believe is the simplest collapse equation. The problem essentially is to determine the lowest possible degree of $G(X)$ and the corresponding coefficients.

Theorem 1: Given assumptions (1)–(4), $G(X)$ must be nonlinear.

Proof: The n stable critical points in R^n are just the standard basis vectors in R^n, $e_1, \cdots, e_n$. Suppose G is linear; then, since $G(e_i) = 0$ for $i = 1, \cdots, n$, we have $G(X) \equiv 0$.

The standard form of nonrelativistic quantum mechanics is a linear theory. It is simply postulated that while the system is *not* subjected to any observation the linear superposition of states is preserved in the course of time.[10,11] In other words, the evolution operator must be linear if no measurement is involved. Consequently, we should expect that the idea of measurement is closely tied with nonlinearity as shown by Theorem 1. A nonlinear theory of measurement will not violate the presently held superposition principle since this principle is only required to hold while no single observations are being made.

Although the nonlinearity of G is a rather obvious consequence of the requirement of dynamic stability, few physicists seem to have realized this. Many theories of measurement proceed as follows. It is assumed that the apparatus can be described by a wavefunction $|a\rangle$ and the system by another wavefunction $|s\rangle$. Assume further that there is a finite orthonormal basis in each space, and suppose that the total situation is represented by a vector in the tensor product space. Then the measurement process is characterized by a unitary operator which carries $|a_0\rangle\,|s_\mu\rangle \to |a_\mu\rangle\,|s_\mu\rangle$ and has the form $\exp(-iHt/\hbar)$, where H is the Hermitian interaction Hamiltonian. Now it should be noted that, even though theorem one was proven for the state vector of the quanta, it can be applied to the state vector of the apparatus if one chooses to describe a measurement as a change in the latter rather than the former. Assumptions (1)–(4) apply to the apparatus state. Theorem 1 then says that such a linear operator as $\exp(-iHt/\hbar)$ cannot describe the desired stability of the outcomes. Generally it is not realized that such theories cannot work because the actual construction of H is not attempted. Furthermore, no one has ever written down an actual $|a_0\rangle$ or $|a_\mu\rangle$. Such explanations of the measurement process serve only to assure one that the standard interpretation of quantum mechanics is sufficient and that there is nothing really mysterious or nonquantum mechanical about measurement. We are led to believe that measurement is just complicated, since macrosystems are involved, but basically understandable within the framework of the present theory. I think Theorem 1 shows this belief to be a false one. Requiring the operator which characterizes the measurement to be unitary is too much. We need only require [assumption (1)] that it be norm preserving. (A unitary operator is a norm preserving *linear operator.*)

In the n-dimensional case the Schrödinger equation is $i\hbar\,|\dot{\varphi}\rangle = H\,|\varphi\rangle$, and the associated equation for the evolution operator is $i\hbar\dot{U}(t, t_0) = HU(t, t_0)$, where $|\varphi(t)\rangle = U(t, t_0)|\varphi(t_0)\rangle$. Here $U(t, t_0)$ is a linear transformation from C^n to C^n. Also $U(s, t_0) = U(s, t)U(t, t_0)$, where the product is simply matrix multiplication. This is called the group property. If H is Hermitian, then $U(t, t_0)$ is unitary, and hence preserves the probability sum $\sum_1^n x_i = 1$. Now, if the collapse equation has the form $\dot{X} = \gamma(t)G(X)$, then the associated equation for the evolution operator is $\dot{F}(t, t_0) = \gamma(t)G \circ F(t, t_0)$, where $X(t) = F(t, t_0) \times [X(t_0)]$. If G is nonlinear, then $F(t, t_0)$ must be nonlinear also and, if we require that solutions to the collapse equation be unique, by requiring $\gamma(t)G(X)$ to be continuous, bounded, and Lipschitzian[12] in some appropriate region of R^{n+1}, then $F(t, t_0)$ will possess the group property, with composition replacing matrix multiplication. That is, $F(s, t_0) = F(s, t) \circ F(t, t_0)$. The collapse process could be thought of algebraically as well as analytically.

Theorem 2: Given assumptions (1)–(4), the degree of $G(X)$ is greater than or equal to 3.

Proof: By assumption (4) the line given by $x_i + x_j = 1$ is an orbit. $X \to e_i$ near e_i and $X \to e_j$ near e_j; therefore, there exists at least one saddle point on $x_i + x_j = 1$ between e_i and e_j. On the line, $G(X) = G(x_i)$. Hence each component of G has at least three zeros on $x_i + x_j = 1$. Therefore, $G(X)$ is at least cubic.

Theorem 3: Given assumptions (1)–(7), the degree of $G(X)$ is equal to 3.

Proof: If the hidden variables are to describe the ensemble statistically, then the position of P must be allowed to vary randomly corresponding to the random collection of individuals. The monotonicity involved in assumption (4) implies that the straight line between P and e_i given by $\alpha_j x_j = K_i(1 - x_i)$, for all $j \neq i$, is an orbit. Now, on this line G can be written as a function of x_i only, and it is equal to zero at the three points $x_i = 1/\alpha_i$, 1, 0. Since this line must be allowed to sweep out the entire probability plane, G must be cubic everywhere in the probability plane. G should be thought of as a family of transformations indexed by $(\alpha_1, \cdots, \alpha_n)$. As a family, G is cubic.

The next thing to consider is the explicit form of $G(X)$, together with its possible uniqueness. Again, I will do the derivation for the $n = 3$ case and then generalize. The simplest partition of the probability plane is pictured in Fig. 3. Consider the following theorem.

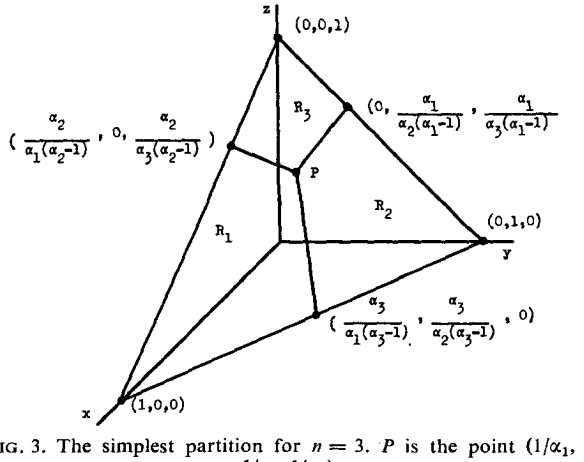

FIG. 3. The simplest partition for $n = 3$. P is the point $(1/\alpha_1, 1/\alpha_2, 1/\alpha_3)$.

Theorem 4: Given assumptions (1)–(7), the collapse equation, in the $n = 3$ case, is unique up to a multiplication factor.

Proof: Since $x + y + z = 1$ for all t, it is enough to consider $\dot{x} = \gamma G_1(x, y)$ and $\dot{y} = \gamma G_2(x, y)$, where, by Theorem 3, G_1 and G_2 are cubic. Let

$$G_1(x, y) = a_0 + a_1x + a_2y + a_3x^2 + a_4xy + a_5y^2 + a_6x^3 + a_7x^2y + a_8xy^2 + a_9y^3,$$

$$G_2(x, y) = b_0 + b_1y + b_2x + b_3y^2 + b_4xy + b_5x^2 + b_6y^3 + b_7y^2x + b_8yx^2 + b_9x^3.$$

The lines $y + z = 1$ and $x + z = 1$ are orbits, so that $G_1(0, y) \equiv 0 \Rightarrow a_0 = a_2 = a_5 = a_9 = 0$ and $G_2(x, 0) \equiv 0 \Rightarrow b_0 = b_2 = b_5 = b_9 = 0$. The line $\alpha_1x = \alpha_2y$ is also an orbit so that $\alpha_1G_1(x, \alpha_1x/\alpha_2) \equiv \alpha_2G_2(x, \alpha_1x/\alpha_2)$ or $(a_1 - b_1)x +$ higher order terms $\equiv 0$. Therefore, $a_1 = b_1$.

Now $G_2 = 0$ at $(0, K_1/\alpha_2, K_1/\alpha_3)$ and $(0, 1, 0)$ implies

$$b_1 + b_3 + b_6 = 0, \tag{1}$$

$$b_1 + b_3K_1/\alpha_2 + b_6(K_1/\alpha_2)^2 = 0, \tag{2}$$

while $G_1 = 0$ at $(K_2/\alpha_1, 0, K_2/\alpha_3)$ and $(1, 0, 0)$ implies

$$a_1 + a_3 + a_6 = 0, \tag{3}$$

$$a_1 + a_3K_2/\alpha_1 + a_6(K_2/\alpha_1)^2 = 0, \tag{4}$$

$$G_1 = G_2 = 0 \quad \text{at} \quad (1/\alpha_1, 1/\alpha_2, 1/\alpha_3)$$

so that

$$a_1/\alpha_1 + a_3/\alpha_1^2 + a_4/(\alpha_1\alpha_2) + a_6/\alpha_1^3 + a_7/(\alpha_1^2\alpha_2) + a_8/(\alpha_1\alpha_2^2) = 0, \tag{5}$$

$$b_1/\alpha_2 + b_3/\alpha_2^2 + b_4/(\alpha_2\alpha_1) + b_6/\alpha_2^3 + b_7/(\alpha_2^2\alpha_1) + b_8/(\alpha_2\alpha_1^2) = 0, \tag{6}$$

$$G_1 = 0 \quad \text{at} \quad (K_3/\alpha_1, K_3/\alpha_2, 0)$$

so that

$$a_1/\alpha_1 + a_3K_3/\alpha_1^2 + a_4K_3/(\alpha_1\alpha_2) + a_6K_3^2/\alpha_1^3 + a_7K_3^2/(\alpha_1^2\alpha_2) + a_8K_3^2/(\alpha_1\alpha_2^2) = 0. \tag{7}$$

The line $x + y = 1$ is an orbit so $G_1(x, 1 - x) + G_2(x, 1 - x) \equiv 0$. This gives

$$b_1 + b_3 + b_6 = 0 \quad \text{(which is not new)},$$

$$a_4 + a_8 - 2b_3 + b_4 - 3b_6 + b_7 = 0, \tag{8}$$

$$a_3 - a_4 + a_7 - 2a_8 + b_3 - b_4 + 3b_6 - 2b_7 + b_8 = 0, \tag{9}$$

$$a_6 - a_7 + a_8 - b_6 + b_7 - b_8 = 0. \tag{10}$$

Now change variables. Let $A_m = a_m/a_1$ and $B_m = b_m/a_1$, $m = 1, 3, 4, 6, 7, 8$. (Recall that $a_1 = b_1$.) We then have ten independent conditions and ten unknowns. Writing equations (1)–(10) in matrix form, we have

$$\begin{pmatrix}
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
K_2/\alpha_1 & 0 & (K_2/\alpha_1)^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & K_1/\alpha_2 & 0 & (K_1/\alpha_2)^2 & 0 & 0 \\
1/\alpha_1^2 & 1/\alpha_1\alpha_2 & 1/\alpha_1^3 & 1/\alpha_1^2\alpha_2 & 1/\alpha_1\alpha_2^2 & 0 & 0 & 0 & 0 & 0 \\
K_3/\alpha_1^2 & K_3/\alpha_1\alpha_2 & K_3^2/\alpha_1^3 & K_3^2/\alpha_1^2\alpha_2 & K_3^2/\alpha_1\alpha_2^2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1/\alpha_2^2 & 1/\alpha_2\alpha_1 & 1/\alpha_2^3 & 1/\alpha_2^2\alpha_1 & 1/\alpha_2\alpha_1^2 \\
0 & 1 & 0 & 0 & 1 & -2 & 1 & -3 & 1 & 0 \\
1 & -1 & 0 & 1 & -2 & 1 & -1 & 3 & -2 & 1 \\
0 & 0 & 1 & -1 & 1 & 0 & 0 & -1 & 1 & -1
\end{pmatrix}
\begin{pmatrix} A_3 \\ A_4 \\ A_6 \\ A_7 \\ A_8 \\ B_3 \\ B_4 \\ B_6 \\ B_7 \\ B_8 \end{pmatrix}
=
\begin{pmatrix} -1 \\ -1 \\ -1 \\ -1 \\ -1/\alpha_1 \\ -1/\alpha_1 \\ -1/\alpha_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

A particular solution to this nonhomogenous linear system of equation is

$$\begin{pmatrix}
-(2 + \alpha_1/\alpha_3) \\
-2 \\
1 + \alpha_1/\alpha_3 \\
2 \\
1 + \alpha_2/\alpha_3 \\
-(2 + \alpha_2/\alpha_3) \\
-2 \\
1 + \alpha_2/\alpha_3 \\
2 \\
1 + \alpha_1/\alpha_3
\end{pmatrix} = v_p.$$

Now v_p is unique if and only if the row vectors of the matrix are linearly independent. By inspection, one can see, without too much difficulty, that no row is a linear combination of the preceding. Hence the rows are independent and v_p is unique.

Initially we had twenty unknowns. Eight are necessarily zero, two are equal and arbitrary, while the other ten are uniquely determined. Substituting the above values for a_i and b_i, $i = 0, \cdots, 9$, into the expressions for G_1 and G_2 gives

$$G_1(x, y) = -(a_1x/\alpha_3)[y(\alpha_1x - \alpha_2y) + z(\alpha_1x - \alpha_3z)], \tag{11}$$

$$G_2(x, y) = -(a_1y/\alpha_3)[x(\alpha_2y - \alpha_1x) + z(\alpha_2y - \alpha_3z)]. \tag{12}$$

It is easy to see, from Eqs. (11) and (12), that

$$\alpha_1 G_1(x, \alpha_1 x/\alpha_2) \equiv \alpha_2 G_2(x, \alpha_1 x/\alpha_2)$$

so that the conditions which would be imposed by setting the coefficients of the x, x^2, and x^3 terms equal to zero are automatically met. Furthermore, these coefficients do not involve a_1 so that it is still left arbitrary. Finally, it is also easy to see that $\alpha_1 x = \alpha_3 z$ and $\alpha_2 y = \alpha_3 z$ will automatically be orbits and that the corresponding equations will not determine a_1 either.

Corollary: If $n = 3$ and $f(t, X)$ is a cubic polynomial in the x_i, then $f(t, X)$ is *necessarily* separable in t.

Proof: Consider $f_i(t, X)$ to be given by $G_i(x, y)$, $i = 1, 2$, where the coefficients $a_0, \cdots, a_9, b_0, \cdots, b_9$ are functions of t. The argument leading to Eqs. (11) and (12) goes through as before and all of the nonzero coefficients are proportional to $a_1(t)$; hence $f(t, X)$ is separable in t.

If one starts with $G_2(x, z)$ and $G_3(x, z)$, then the coefficient corresponding to a_1/α_3 would be $\tilde{a}_1/\alpha$, but, by assumption (5), the final result would have to be the same. Hence we can assume a_1 is proportional to α_3. If γ is assumed to be positive, then we must take $a_1 = -K\alpha_3$ with $K > 0$ since near $(1, 0, 0)$ we must have $\dot{x} > 0$. A natural choice for K is $K = 2$ because K is then eliminated from the equation for $\dot{\varphi}_i$. This choice turns the collapse equation into the one given by Bohm and Bub.

The obvious generalization of Eqs. (11) and (12) (with $a_1 = -2\alpha_n$) is

$$\dot{x}_i = 2\gamma x_i \sum_{k=1}^{n} x_k(\alpha_i x_i - \alpha_k x_k), \quad i = 1, \cdots, n.$$

These are just the Bohm–Bub equations. Consequently, the following theorem has been proven:

Theorem 5: The simplest collapse equations are those given by Bohm and Bub.

Theorem 5 is more general than it seems. It has been proven assuming the regions of asymptotic stability are given by the R_i. More general regions are homeomorphically equivalent to these (i.e., continuously deformable into the R_i) so that more general collapse equations must reduce to the Bohm–Bub equations under an invertable change of variable. Hence the Bohm–Bub equations are the simplest in a very general sense.

Though assumption (7) has gone into the proof of Theorem 4, it is not obvious how the hidden variables are related to the statistics. If the hidden variables are $1/\alpha_i$, $i = 1, \cdots, n$, then the condition $\sum_1^n 1/\alpha_i = 1$ means that they form a plane isomorphic to the probability plane. Call this plane the hidden variable plane. The partition used in the probability plane induces a corresponding partition on the hidden variable plane given by

$$\mathcal{A}_i = \left\{ \left(\frac{1}{\alpha_1}, \cdots, \frac{1}{\alpha_n} \right) \middle| \frac{1}{\alpha_i} < \frac{x_i(t_0)}{[\alpha_j x_j(t_0)]}, \right.$$
$$\left. j = 1, \cdots, i-1, i+1, \cdots, n, \sum_1^n \frac{1}{\alpha_i} = 1 \right\}.$$

Now the area of $\mathcal{A}_i$ is the standard measure of the part of the hidden variable space corresponding to the ith outcome. When this area is normalized by the area of the entire hidden variable plane, it is equal to $x_i(t_0)$ as required by assumption seven.[13] In other words, the partition given by the R_i induces a partition of the hidden variable space which implies the usual statistical results if the distribution of the hidden variables is the simplest one possible.

For example, consider the $n = 3$ case. In Fig. 4 we have the probability plane where P is chosen so that $(x(t_0), y(t_0), z(t_0)) \to (1, 0, 0)$. It is clear that if P is any point in the shaded triangle labeled $\mathcal{A}_1$, then $(1, 0, 0)$ will be the outcome. Now it is easy to see that the area of $\mathcal{A}_1$ is proportional to $x(t_0)$, the area of $\mathcal{A}_2$ is proportional to $y(t_0)$, and the area of $\mathcal{A}_3$ is proportional to $z(t_0)$. By assumption (5) the constant of proportionality must be the same in each case. Call it S. Then $x(t_0) + y(t_0) + z(t_0) = 1 \Rightarrow \mathcal{A}_1 + \mathcal{A}_2 + \mathcal{A}_3 = S$ so that S is just the total area of the probability plane, $\frac{1}{2}\sqrt{3}$. Hence $\mathcal{A}_1/S = x(t_0)$, $\mathcal{A}_2/S = y(t_0)$, and $\mathcal{A}_3/S = z(t_0)$, as desired.

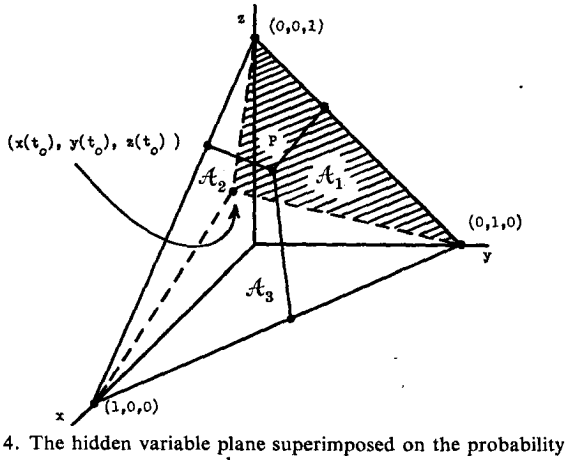

FIG. 4. The hidden variable plane superimposed on the probability plane.

It should be noted that there are a few mathematical restrictions imposed on the hidden variables by assumptions (1)–(7) but that the physical interpretation of these variables is rather arbitrary at this point. In order that the condition of irreversibility is met, we must assume that the hidden variables are constant at least during the measurement. If we are to use the simplest theory, that is, where there is only one point of unstable equilibrium in the interior of the probability plane, then there must be n hidden variables and they must satisfy the normalization condition. Furthermore, since the probability plane lies in the first quadrant, the hidden variables must all be positive. Possible physical interpretations of these new variables will be discussed in future papers.

CONCLUSIONS

It is clear that if the collapse process in quantum mechanics is to be described by differential equations, then the form of these equations is quite well determined by very general considerations. The description of the collapse leads, in a general and natural way, to the necessary introduction of new variables, at present hidden from observation. These new variables must be given a physical interpretation before their existence can be tested by experiments.

ACKNOWLEDGMENTS

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[1] Some of the most recent review articles are: F. J. Belinfante, "A Survey of Hidden Variable Theories," (Purdue University, 1970) (unpublished); V. Capasso, D. Fortunato, and F. Selleri, "Von Neumann's Theorem and Hidden Variable Models," (Istituto di Fisica, Dell' Universitá, Bari, Italy, 1970) (unpublished). These two contain references to most of the previous articles on the subject.

[2] D. Bohm and J. Bub, Rev. Mod. Phys. **38**, 453 (1966).

[3] J. H. Tutsch, Rev. Mod. Phys. **40**, 232 (1968).

[4] J. H. Tutsch, Phys. Rev. **183**, 1116 (1969).

[5] The only experiment to date which attempts to deal with the Bohm–Bub theory is the one reported in Phys. Rev. Letters **18**, 622 (1967) and carried out by Dr. C. Papaliolios. The meaning of the experimental result is difficult to determine due to the lack of a well-formulated physical interpretation of the hidden variables by Bohm and Bub. The outcome, which agreed with the prediction of quantum mechanics, could be explained by assuming the hidden variables to be local properties of the individual photons. The absorption and reemission, which take place in the polarizer, then serves as the necessary randomization mechanism. A better test of the theory would involve an experiment in which the identity of an individual quantum could be preserved during the course of successive measurements.

[6] In my two papers, Refs. 3 and 4, I have given γ a physical interpretation in order that some mathematical results of the theory could be derived. I have taken γ to be the absolute value of the energy change of the system, as a function of time during the measurement, divided by $\hbar$. I assume that every measurement involves some change in energy for the system being measured. This means of course that I do not call theoretical inferences measurements. The hidden variables, however, still lack a physical interpretation.

[7] The main difference is that the probability measures which are involved in this case are relative probability measures. They depend on *what* is being measured. This point is discussed by J. Bub in his recent article in Int. J. Theoret. Phys. [**2**, 101 (1969)] entitled "What Is a Hidden Variable Theory of Quantum Phenomena?"

[8] For more information concerning the stability of solutions to systems of nonlinear differential equations, see E. Coddington and N. Levinson, *Theory of Ordinary Differential Equations* (McGraw-Hill, New York, 1965), D. Kreider, R. Kuller, and D. Ostberg, *Elementary Differential Equations* (Addison-Wesley, Reading, Mass., 1968), W. Leighton, *Ordinary Differential Equations* (Wadsworth, Belmont, Calif., 1963), or any of the numerous textbooks on this subject.

[9] For a general discussion of the relationship of the critical points of a system of nonlinear differential equations to the index of the flow field, see M. S. Berger and M. S. Berger, *Perspectives in Nonlinearity; An Introduction to Nonlinear Analysis* (Benjamin, New York, 1968).

[10] A. Messiah, *Quantum Mechanics* (Wiley, New York, 1958), Vol. 1, p. 310.

[11] E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1960), p. 330.

[12] This means that there exists some positive constant C such that whenever (t, X_1) and (t, X_2) are in the region R, then

$$\|\gamma(t)G(X_1) - \gamma(t)G(X_2)\| \leq C\,\|X_1 - X_2\|.$$

[13] This fact is demonstrated in Ref. 4, p. 1124.

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Properties of Some Connected Kernels in Multiparticle Systems*

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Connectivity of products of many-particle operators is investigated. Connected products of compact and Hilbert–Schmidt operators are in the same class as their factors. However, even in the simplest case of rank-one many-particle factors, the connected products are not necessarily in the trace class, but simple sufficiency conditions are established.

INTRODUCTION

Connectivity of a product of operators is mainly a concept of the nonrelativistic quantum theory of many-body systems. It has appeared in the equations proposed for their study, such as those of Weinberg,[1] or in the analysis of their iterations, as is done, for instance, in Ref. 2 for those of Faddeev and Yakubovsky. In the Dirac bra and ket formalism, many-particle operators such as potentials, transition amplitudes, or Green's functions for subsystems are expressed as singular kernels involving Dirac measures associated with noninteracting particles or conserved quantities; a product of such operators is said to be connected if its kernel does not contain any δ functions except those associated with dynamical variables of the center of mass of the system. It is then often conjectured and sometimes proved (see, for example, Refs. 1 and 3) that such a product inherits some properties of its factors such as compactness and analyticity. Our aim is to supply the basis of this hope by studying connected products of compact, Hilbert–Schmidt, and trace-class operators in a more general context. The theorems concerning Hilbert–Schmidt and compact operators are shown to be true (Theorem 5). For trace-class operators, explicit counter-examples show that even in the simplest case of rank-one factors the connected product is not necessarily a trace-class operator; however, rather simple sufficient conditions can be found ensuring that it is (Theorem 6).

We shall use for this study the so-called "twisted-convolution" formalism, which has been introduced[4] for the description of the free boson field; its particular relevance for systems with a finite number of degrees of freedom has been stressed in Refs. 5 and 6. This formalism does not depend on any particular representation of canonical commutation relations. It associates a tempered distribution on phase space with any bounded linear operator on the irreducible representation space of the system. Various simple analytic characterizations of classes of distributions associated with ideals of compact operators or with dense subsets of them are given in Refs. 5 and 6; this is, in fact, one of our main reasons for choosing this framework described in Sec. 1 rather than the kernel formalism, where apparently the knowledge of such analytic features is rather poor. Section 2 contains elementary results of sympletic geometry needed for later computations. In Secs. 3 and 4 we first state our theorems in their most general form. In Sec. 5 we return to the usual framework of quantum mechanics and apply the results to some common situations found, for example, in the study of the Weinberg equations[7,3] or in a time-dependent treatment of multichannel scattering.[8] We do not know whether a possible version of results of Secs. 3 and 4 in the Fock representation of a free boson field presents some physical interest, and we shall not state it here.

1. THE TWISTED CONVOLUTION FORMALISM

All results of this section are derived from theorems stated in Refs. 4–6. Let E be an Euclidean $2n$-dimensional vector space. Let σ be a regular, bilinear, and antisymmetric (in short, symplectic) form on E. Let F be a $2p$-dimensional, $p \leq n$, subspace of E. It will be said to be regular if, for each η in F, there exists an η' in F such that $\sigma(\eta, \eta') = 1$. If F' is the σ-orthogonal complement of F, that is, the regular subspace of E consisting of vectors η with $\sigma(\eta, F) = 0$, then E can be decomposed in a direct sum

$$E = F \oplus^{\sigma} F'. \tag{1}$$

We shall again denote by σ the restriction of σ to F or F'. Let $\mathcal{H}_F$ be an irreducible representation space of the canonical commutation relations on F [in short, CCR's on (F, σ)]:

$$\mathfrak{U}_F(\eta)\mathfrak{U}_F(\eta') = e^{-i\sigma(\eta,\eta')}\mathfrak{U}_F(\eta + \eta'), \quad \eta, \eta' \in F, \tag{2}$$

where $\mathfrak{U}_F(\eta)$ is a unitary operator on $\mathcal{H}_F$. Up to a unitary equivalence, this representation is unique.[4] Let us consider then the $*$-algebra $\mathcal{F}(F)$ of bounded finite-rank operators on $\mathcal{H}_F$ and the $*$-algebra $\mathcal{F}(F, \sigma)$ of complex-valued functions on F consisting of the

$$\varphi^{(A)}(\eta) = a_F^{-1} \operatorname{Tr}[A\mathfrak{U}_F(\eta)], \quad A \in \mathcal{F}(\mathcal{H}_F),$$
$$a_F^{-1} = \Pi \frac{\dim F}{2}, \tag{3}$$

with

$$\mathrm{Tr}\,(A) = \sum_n (h_n^F |\, A\, | h_n^F), \tag{4}$$

(h_n^F) being an orthonormal basis in $\mathcal{H}_F$.

In particular, if A is a rank-one projection operator $|h)(h|$, $h \in \mathcal{H}_F$, then

$$\varphi^{|h)(h|}(\eta) = a_F^{-1}(h|\, \mathcal{U}_F(\eta)\, |h).$$

The algebraic law on $\mathcal{F}(F, \sigma)$ is given by

$$\varphi^*(\eta) = \bar{\varphi}(-\eta), \tag{5}$$

where the bar stands for complex conjugation, and

$$(\varphi_1 \times \varphi_2)(\eta) = \int_F e^{-i\sigma(\eta,\xi)} \varphi_1(\eta - \xi)\varphi_2(\xi)\, d\xi, \tag{6}$$

where $d\xi$ is the Lebesgue measure on F. One has then

$$\varphi^{(A)^*}(\eta) = \varphi^{(A^*)}(\eta), \tag{7}$$

where A^* is the adjoint of A,

$$(\varphi^{(A_1)} \times \varphi^{(A_2)})(\eta) = \varphi^{(A_1 A_2)}(\eta). \tag{8}$$

Property (8) results from the orthogonality relations satisfied by the coefficients $\omega_{h,g}(\eta) = (h|\, \mathcal{U}_F(\eta)\, |g)$, $h, g \in \mathcal{H}_F$, of the representation $\mathcal{U}_F$ (Ref. 5):

$$\int_F \omega_{h,g}(\eta)\omega_{h',g'}(\eta)\, d\eta = a_F(h \mid h')(g \mid g'). \tag{9}$$

Then the correspondence between $\mathcal{F}(F)$ and $\mathcal{F}(F, \sigma)$ is a $*$-isomorphism. Furthermore, (9) indicates that $\mathcal{F}(F, \sigma)$ consists of square-integrable functions on F and that the relation

$$\|\varphi^{(A)}\|_2^F = \|A\|_{\mathcal{HS}(F)} \tag{10}$$

holds, where

$$\|\varphi\|_2^F = \left(a_F \int_F |\varphi(\eta)|^2\, d\eta\right)^{\frac{1}{2}} \tag{11}$$

and the Hilbert–Schmidt norm $\|A\|_{\mathcal{HS}(F)}$ is given by

$$\|A\|^2_{\mathcal{HS}(F)} = \sum_n \|Ah_n^F\|^2, \tag{12}$$

(h_n^F) being an orthonormal basis in $\mathcal{H}_F$.

In fact, the above isomorphism can be extended as follows[5]:

Theorem 1: The closure of $\mathcal{F}(F, \sigma)$ with respect to the norm (11) is a Banach $*$-algebra $L^2(F, \sigma)$ consisting of the space of square-integrable functions on F equipped with the involution (5) and the product law (6). There exists a $*$-isomorphism Π_F from $L^2(F, \sigma)$ to the algebra $\mathcal{HS}(F)$ of Hilbert–Schmidt operators on $\mathcal{H}_F$, and one has

$$\|\Pi_F(\varphi)\|_{\mathcal{HS}(F)} = \|\varphi\|_2^F. \tag{13}$$

Π_F is given on the dense sub-$*$-algebra $\mathcal{K}(F, \sigma)$ of $L^2(F, \sigma)$, consisting of infinitely differentiable functions on F with compact support, by

$$\Pi_F(\varphi) = \int_F \varphi(\eta)\mathcal{U}_F(\eta)\, d\eta. \tag{14}$$

The inverse of Π_F is given on $\mathcal{F}(F)$ by (3).

By the well-known fact that the algebra $\mathcal{C}(F)$ of trace-class operators on $\mathcal{H}_F$ consists of products of two Hilbert–Schmidt, Π_F is also a $*$-isomorphism between the algebra of square-integrable functions of the form $\varphi_1 \times \varphi_2$, with $\varphi_1, \varphi_2 \in L^2(F, \sigma)$, and $\mathcal{C}(F)$. Owing to (3), one has

$$\mathrm{Tr}\,[\Pi_F(\varphi_1 \times \varphi_2)] = a_F(\varphi_1 \times \varphi_2)(0). \tag{15}$$

With the norm $\|\ \|_{\mathcal{C}(F)}$ induced by $\mathcal{C}(F)$, this set of functions is a Banach $*$-algebra denoted by $\mathcal{C}(F, \sigma)$; the elements of $\mathcal{C}(F, \sigma)$ which can be written as $\Phi = \varphi \times \varphi^*$, $\varphi \in L^2(F, \sigma)$ are called σ-positive-type functions on F. Their image by Π_F is positive trace-class operators. For any set (c_i) of complex constants and any set (η_i) of vectors in F_i, they satisfy the relation

$$\sum_{i,j} c_i c_j e^{-i\sigma(\eta_i,\eta_j)} \Phi(\eta_i - \eta_j) \geq 0.$$

Conversely, any continuous function having this property is a σ-positive-type function. The set of σ-positive-type functions on F with $a_F\Phi(0) = 1$ constitutes a closed convex subset in $\mathcal{C}(F, \sigma)$ whose extremal points consist of the functions $\varphi^{|h)(h|}$, $h \in \mathcal{H}_F$. The functions $\varphi^{|h)(g|}$ will be said to be elementary; each element Φ in $\mathcal{C}(F, \sigma)$ admits a "spectral decomposition" into a sum of elementary functions which corresponds to the spectral decomposition of $\Pi_F(\Phi)$.

A remarkable fact proved in Ref. 6 is the dense topological inclusion of $S(F, \sigma)$ in $\mathcal{C}(F, \sigma)$, the algebra of Schwartz's test functions on F. As a result, the dual space of $\mathcal{C}(F, \sigma)$ is a Banach space of tempered distributions on F. Then, from the fact that the dual space of $\mathcal{C}(\mathcal{H}_F)$ is $\mathcal{B}(\mathcal{H}_F)$, the von Neumann algebra of bounded operators on $\mathcal{H}_F$, this Banach space turns out to be an abstract von Neumann algebra whose elements are the tempered distributions

$$d^{(A)}(\Phi) = a_F^{-1}\,\mathrm{Tr}\,[A\Pi_F(\Phi)], \quad \Phi \in \mathcal{C}(F, \sigma), \quad A \in B(F).$$

The algebraic law on $\mathcal{C}'(F, \sigma)$ is defined by

$$d^{(A)^*} = d^{(A^*)}, \tag{5'}$$

$$d^{(A)} \times d^{(B)} = d^{(AB)}. \tag{6'}$$

The absolute value and the square root of a distribution in $\mathcal{C}'(F, \sigma)$ are defined by $|d^{(A)}| = d^{(|A|)}$ and

$|d^{(A)}|^{\frac{1}{2}} = d^{(|A|^{\frac{1}{2}})}$. Owing to Theorem 1 and (14), one has $d^{(\Pi_F(\varphi))} = \varphi$, if $\varphi \in L^2(F, \sigma)$. Hence $\mathcal{C}'(F, \sigma)$ contains $L^2(F, \sigma)$ as a weakly dense sub-$*$-algebra on which (6') coincides with (6), so that we shall again denote by Π_F the representation of $\mathcal{C}'(F, \sigma)$ as $\mathcal{B}(\mathcal{H}_F)$. From $d^{(\mathcal{U}(\eta))}(\Phi) = \Phi(\eta)$, $\Phi \in S(F, \sigma)$, it results that $d^{(\mathcal{U}_F(\eta))} = \delta^F\eta$, the Dirac measure on F concentrated at η, and from (2) and (6) that

$$(\delta^F\eta \times \varphi)(\xi) = e^{-i\sigma(\eta,\xi)}\varphi(\xi - \eta), \quad \varphi \in L^2(F, \sigma). \quad (16)$$

The norm on $\mathcal{C}'(F, \sigma)$ is defined by

$$\|d^{(A)}\|^F = \sup_{\Phi \in \mathcal{C}(F,\sigma)} \frac{|\mathrm{Tr}\,[A\Pi_F(\Phi)]|}{\|\Phi\|_{\mathcal{C}(F)}}.$$

Since $\mathcal{C}(F, \sigma)$ consists of bounded continuous functions and $a_F|\Phi(0)| \leq \|\Phi\|_{\mathcal{C}(F)}$, it can be shown that the algebra [for the product law (6)] of absolutely integrable functions on F is contained in $\mathcal{C}'(F, \sigma)$ and that its closure with respect to the above norm is a C^*-algebra $C(F, \sigma)$ mapped by Π_F onto the compact operators on $\mathcal{H}_F$.

Let us now consider the irreducible representation $\mathcal{U}_F \otimes \mathcal{U}_{F'}$ of CCR's on (E, σ) in $\mathcal{H}_E = \mathcal{H}_F \otimes \mathcal{H}_{F'}$ and the representation Π_E of $\mathcal{C}'(E, \sigma)$ in this space. We define $\Pi_F^{(E)}(d_F) = \Pi_F(d_F) \otimes I_{\mathcal{H}_{F'}}$, $d_F \in \mathcal{C}'(F, \sigma)$, and $D_E^{(F)} = \Pi_E^{-1}\Pi_F^{(E)}$. Since $\mathcal{C}(\mathcal{H}_E)$ contains product operators $\Pi_F(\Phi_F) \otimes \Pi_{F'}(\Phi_{F'})$, $\Phi_F \in \mathcal{C}(F, \sigma)$, and $\Phi_{F'} \in \mathcal{C}(F', \sigma)$, as a total set, the mapping $D_E^{(F)}$ can be shown to be simply the natural extension to E of distributions in $\mathcal{C}'(F, \sigma)$ obtained by taking their tensor product with $\delta_0^{F'}$. In fact, $D_E^{(F)}(\mathcal{C}'(F, \sigma))$ consists of all distributions in $\mathcal{C}'(E, \sigma)$ having the form of a tensor product $d_F \otimes \delta_0^{F'}$, where d_F has support in F. Hence all the mappings $D_E^{(F)}$, when F varies over all regular subspaces of E, are compatible in the sense that if d_{F_1} and d_{F_2} denote the extensions to F_1 and F_2 of some distribution in $\mathcal{C}'(F_1 \cap F_2, \sigma)$ (this is an equivalence relation), then $D_E^{(F_1)}(d_{F_1}) = D_E^{(F_2)}(d_{F_2})$; we shall then write $D_E(d)$ to denote the extension to E of a member d of an equivalence class. As a result, if d and d' have supports contained in σ-orthogonal regular subspaces of E, then the product $D_E(d) \times D_E(d')$ is commutative. As a simple example of a possible explicit calculation of a twisted convolution product of two distributions in $\mathcal{C}'(E, \sigma)$, we consider two elementary functions on the regular subspaces F and F', respectively. Then, owing to (3), (6'), and definition of $D_E^{(F)}$, we have

$$D_E(\varphi^{|h)(h|}) \times D_E(\varphi^{|h')(h'|}) = \varphi^{|h\otimes h')(h\otimes h'|} = \varphi^{|h)(h|} \cdot \varphi^{|h')(h'|}.$$

By linearity and continuity we also get this product form for arbitrary distributions in $\mathcal{C}'(F, \sigma)$ and $\mathcal{C}'(F', \sigma)$.

2. CONNECTED REGULAR SUBSPACES OF E; GEOMETRICAL STUDY

Let F_1 and F_2 be regular subspaces of E. We shall say that the pair (F_1, F_2) is E-connected if E is spanned by linear combinations of elements of this pair; in general, E is not a direct sum like (2). Let $D = F_1 \cap F_2$, which is regular if nonreduced to zero; let us denote by P_F the projection operator on the regular subspace F along the σ-orthogonal complement F' of F in E. We consider then the linear operators on E,

$$M_j^i = P_{F_j}P_{F_i} - P_D, \quad (17)$$

$$M_{j'}^i = P_{F_{j'}}P_{F_i} \ominus^\sigma D, \quad (18)$$

where $F_i \ominus^\sigma D$ is the σ-orthogonal complement of D in F_i. The linear operators M_2^1 and $M_{2'}^1$ can be considered as some of the matrix elements of the transformation which give the components η_2 and $\eta_{2'}$, along $F_2 \ominus D$ of a vector $\eta \in E$, as linear functions of its components η_1 and $\eta_{1'}$ along $F_1 \ominus D$ and F_1'. All results stated in the following lemmas remain valid by exchanging indices 1 and 2.

Lemma 1: Let the pair (F_1, F_2) be connected. Then $M_{2'}^1$ is a bijective linear map from $F_1 \ominus^\sigma D$ on F_2'.

Proof: If $\eta_{2'} \in F_2'$, there exists a ξ in E with $\sigma(\eta_{2'}, \xi) = 1$. Let us write $\xi = \xi_1 + \xi_2$, where $\xi_1 \in F_1 \ominus^\sigma D$ and $\xi_2 \in F_2$. This is allowed by the E-connectedness of (F_1, F_2); then $\sigma(\eta_{2'}, \xi_1) = 1$. On the other hand, one has $\xi_1 = M_2^1\xi_1 + M_{2'}^1\xi_1$, so that $\sigma(\eta_{2'}, M_{2'}^1\xi_1) = 1$. This implies on the one hand that the range of $M_{2'}^1$ in F_2' is regular and on the other hand that its σ-orthogonal complement is empty; hence this range is all of F_2'. Now by the relation

$$\dim (F_1 \cap F_2) = \dim F_1 + \dim F_2 - \dim (F_1 + F_2),$$

we have $\dim (F_1 \ominus^\sigma D) = \dim F_2'$, so that $M_{2'}^1$ is bijective.

Let us now define the following linear transformations on E for $i \neq j$:

$$\mathcal{M}_i^{i'} = (M_{j'}^i)^{-1}M_{j'}^{i'}, \quad \text{where} \quad M_{j'}^{i'} = P_{F_{i'}}P_{F_{j'}}, \quad (19)$$

$$\mathcal{M}_j^{i'} = -M_j^i\mathcal{M}_i^{i'} + M_j^{i'}, \quad \text{where} \quad M_2^{1'} = P_{F_2}P_{F_{1'}}. \quad (20)$$

Lemma 2: $\mathcal{M}_2^{1'}$ is a bijective linear map from F_1' to $F_2 \ominus^\sigma D$.

Proof: Since $\mathcal{M}_1^{1'} = (M_2^1 + M_{2'}^{1'})\mathcal{M}_1^{1'}$, a simple calculation shows that

$$\mathcal{M}_2^{1'} = -\mathcal{M}_1^{1'} \oplus^\sigma P_{F_{1'}}. \tag{21}$$

The operators on the right of (21) have σ-orthogonal ranges so that $\mathcal{M}_2^{1'}\eta_{1'} = 0$ if and only if $\eta_{1'} = 0$, $\eta_{1'} \in F_1'$. Since, on the other hand, F_1' and $F_2 \ominus^\sigma D$ have the same dimension, the lemma is proved.

We shall denote by K_j the kernel of $\mathcal{M}_i^{j'}$, $(i,j) = (1,2)$. Owing to definition (19), one has $K_j = F_i' \cap F_j$ and also the following.

Lemma 3: K_1 is the σ-orthogonal complement in $F_1 \ominus D$ of the range of $\mathcal{M}_1^{1'}$.

The proof results easily from (21).

Finally, one has the following decomposition of E:

$$E = D \oplus^\sigma K_1 \oplus^\sigma K_2 \oplus^\sigma C(F_1, F_2). \tag{22}$$

$C(F_1, F_2)$ reduces all operators defined above, and these have bijective restrictions to $C(F_1, F_2)$. If D, K_1, and K_2 are empty, we shall say that (F_1, F_2) is an irreducible E-connected pair.

We shall say that a linear mapping S between two subspaces is σ-symplectic, if it is bijective and satisfies $\sigma(S\eta, S\xi) = \sigma(\eta, \xi)$. We observe that the inverse of a σ-symplectic transformation also is σ-symplectic.

Lemma 4: Let (F_1, F_2) be an irreducible E-connected pair. Let $\tilde{\sigma}$ be another symplectic form on E obtained from σ by $\tilde{\sigma} = -\sigma$ on F_1, $\tilde{\sigma} = \sigma$ on F_1', and $\tilde{\sigma}(F_1, F_1') = 0$. Let $S_{2'}^1$ and $S_{1'}^2$ be two symplectic mappings from F_1 to F_2' and F_2 to F_1', respectively. Then the linear mappings on F_1 and F_1', respectively defined by

$$S_1\eta_1 = \mathcal{M}_1^{2'}S_{2'}^1\eta_1 + S_{1'}^2\mathcal{M}_2^{2'}S_{2'}^1\eta_1, \quad \eta_1 \in F_1, \tag{23}$$

$$S_1'\eta_{1'} = \mathcal{M}_1^{1'}\eta_{1'} + S_{1'}^2\mathcal{M}_2^{1'}\eta_{1'}, \quad \eta_{1'} \in F_1', \tag{24}$$

are $\tilde{\sigma}$-symplectic. Their ranges are subspaces H_1 and H_1', regular with respect to $\tilde{\sigma}$ and $\tilde{\sigma}$-orthogonal to each other. They satisfy $H_1 \oplus^{\tilde{\sigma}} H_1' = E$. Furthermore, (F_1, H_1), (F_1, H_1'), (F_1', H_1), and (F_1', H_1') are irreducible E-connected pairs.

Proof: Simple calculations using (20) lead to the three first assertions. Let us prove that $H_1 \oplus^\sigma H_1' = E$; for this, we show, for instance, that $F_1' \subset H_1 \oplus^\sigma H_1'$. Let $\eta_1 \in F_1$ and $\eta_{1'} = (M_{2'}^{1'})^{-1}S_{2'}^1\eta_1$. Then addition of (22) and (23) yields

$$S_1\eta_1 + S_1'\eta_{1'} = S_{1'}^2M_2^{1'}(M_{2'}^{1'})^{-1}S_{2'}^1\eta_1.$$

Since the operator on the right of this equality is a bijective mapping from F_1 to F_1', we obtain the desired inclusion. One can find in the same way that $F_1 \subset H_1 \oplus^\sigma H_1'$, which completes this result.

As to the last assertion, it is an immediate consequence of the fact that each of the operators involved in definitions (23) and (24) is bijective.

3. CONNECTED PRODUCTS OF DISTRIBUTIONS IN $L^2(F, \sigma)$ AND $C(F, \sigma)$

We shall say that a product of distributions on E is connected if it has the form $D_E(\varphi_1) \times D_E(\varphi_2)$, where $\varphi_i \in \mathcal{C}'(F_i, \sigma)$ and (F_1, F_2) is E-connected.

Theorem 2: Let (F_1, F_2) be an E-connected pair and $D_E(\varphi_1)$ and $D_E(\varphi_2)$ be two distributions concentrated on F_1 and F_2, respectively, whose restrictions to their associated subspace are square-integrable functions φ_1 and φ_2. Then the twisted convolution product $D_E(\varphi_1) \times D_E(\varphi_2)$ is a square-integrable function on E, and one has

$$\begin{aligned}\|D_E(\varphi_1) \times D_E(\varphi_2)\|_2^E \\ \leq (a_{F_1}a_{F_2})^{-1}a_E(\det M_2^{1'})^{\frac{1}{2}}(\det M_{2'}^1)^{-1}\,\|\varphi_1\|_2^{F_1}\,\|\varphi_2\|_2^{F_2},\end{aligned} \tag{25}$$

where the equality holds if $D = F_1 \cap F_2$ is empty.

Proof: Let $\eta = (\eta_i, \eta_{i'}, \eta_D)$ be the decomposition of η along the σ-orthogonal subspaces $F_i \ominus^\sigma D$, F_i', and D. Then one has

$$\begin{aligned}[D_E(\varphi_1) \times D_E(\varphi_2)](\eta) \\ = \int \exp\{-i[\sigma(\eta_1, \xi_1) + \sigma(\eta_{1'}, \xi_{1'}) + \sigma(\eta_D, \xi_D)]\} \\ \times \varphi_1(\eta_1 - \xi_1; \eta_D - \xi_D) \\ \times \delta_0^{F_1'}(\eta_{1'} - \xi_{1'})\delta_0^{F_2'}(\xi_{2'})\varphi_2(\xi_2; \xi_D)\,d\xi_1\,d\xi_{1'}\,d\xi_D.\end{aligned}$$

If we define, together with M_2^1 and $M_{2'}^1$, the operators $M_{2'}^{1'} = P_{F_{2'}}P_{F_{1'}}$ and $M_2^{1'} = P_{F_2}P_{F_{1'}}$, we get the transformation formulas

$$\xi_2 = M_2^1\xi_1 + M_2^{1'}\xi_{1'}, \quad \xi_{2'}' = M_{2'}^1\xi_1 + M_{2'}^{1'}\xi_1,$$

whence

$$\begin{aligned}[D_E(\varphi_1) \times D_E(\varphi_2)](\eta) \\ = \int \exp[-i\sigma(\eta_D, \xi_D)] \exp[-i\sigma(\eta_1, \xi_1)] \\ \times \varphi_1(\eta_1 - \xi_1; \eta_D - \xi_D)\delta(M_{2'}^1\xi_1 + M_{2'}^{1'}\xi_{1'}) \\ \times \varphi_2(M_2^1\xi_1 + M_2^{1'}\eta_{1'}; \xi_D)\,d\xi_1\,d\xi_D.\end{aligned}$$

Now by Lemma 1, $M^{1}_{2'}$ can be inverted so that the change of variable $\xi_1 \to M^{1}_{2'}\xi_1$ gives

$$[D_E(\varphi_1) \times D_E(\varphi_2)](\eta) = (\det M^{1}_{2'})^{-1} \exp[-i\sigma(\eta_1, \mathcal{M}_1^{1'}\eta_{1'})] \times \int \exp[-i\sigma(\eta_D, \xi_D)] \times \varphi_1(\eta_1 + \mathcal{M}_1^{1'}\eta_1; \eta_D - \xi_D) \cdot \varphi_2(\mathcal{M}_2^{1'}\eta_{1'}; \xi_D)\, d\xi_D. \tag{26}$$

In order to estimate the L_2-norm of this function, we remember that square-integrable functions on D form a Banach $*$-algebra for the twisted convolution product. Hence

$$\int |[D_E(\varphi_1) \times D_E(\varphi_2)](\eta)|^2\, d\eta \leq (\det M^{1}_{2'})^{-2}(a_D)^{-2} \times \int d\eta_1\, d\eta_{1'} [\|\varphi_1(\psi_1 + \mathcal{M}_1^{1'}\psi_{1'}; \cdot)\|_2^D]^2 \times [\|\varphi_2(\mathcal{M}_2^{1'}\psi_{1'}; \cdot)\|_2^D]^2.$$

Another change of variable $\eta_{1'} \to \mathcal{M}_2^{1'}\eta_{1'}$, which is allowed by Lemma 2, together with (11) gives (25).

Corollary 1: Let $\varphi_1 \in \mathbb{C}(F_1, \sigma)$ and $\varphi_2 \in \mathbb{C}(F_2, \sigma)$. If (F_1, F_2) is an E-connected pair, then $D_E(\varphi_1) \times D_E(\varphi_2)$ is in $\mathbb{C}(E, \sigma)$, and one has

$$\|D_E(\varphi_1) \times D_E(\varphi_2)\|^E \leq \|\varphi_1\|^{F_1} \|\varphi_2\|^{F_2}. \tag{27}$$

Proof: It results immediately from the norm density of $L^2(F, \sigma)$ into $\mathbb{C}(F, \sigma)$ and from Theorem 2. As to (26), it is a consequence of the isometry of D_E and of

$$\|D_E(\varphi_1) \times D_E(\varphi_2)\|^E \leq \|D_E(\varphi_1)\|^E \|D_E(\varphi_2)\|^E.$$

4. CONNECTED PRODUCT OF DISTRIBUTIONS IN $\mathcal{C}(F, \sigma)$

One could hope at the sight of the preceding results that if (F_1, F_2) is an E-connected pair and $\varphi_i \in \mathcal{C}(F_i, \sigma)$, $i = 1, 2$, then $D_E(\varphi_1) \times D_E(\varphi_2) \in \mathcal{C}(E, \sigma)$. This is, unfortunately, not the case, as we shall see, in the simplest situation, where φ_1 and φ_2 are elementary σ-positive-type functions on F_1 and F_2, respectively. Our counterexample is based on the fact that elementary σ-positive-type functions on F are not necessarily absolutely integrable on F, a fact stated in Ref. 6 of Ref. 6. It will be possible, however, to get sufficient conditions ensuring that a connected product of σ-positive-type functions is in $\mathcal{C}(E, \sigma)$.

We begin with some auxiliary results.

Lemma 5: Let $\tilde{\sigma}$ be a symplectic form on E and F a subspace of E regular with respect to $\tilde{\sigma}$. Let $\mathfrak{U}_F$ (resp. $\mathfrak{U}_{F'}$) be an irreducible representation of CCR's on $(F, \tilde{\sigma})$ [resp. $(F', \tilde{\sigma})$] in a Hilbert space $\mathcal{H}_F$ (resp. $\mathcal{H}_{F'}$). Let $\mathfrak{U}_E = \mathfrak{U}_F \otimes \mathfrak{U}_{F'}$ be the irreducible representation of CCR's on $(E, \tilde{\sigma})$ in $\mathcal{H}_E = \mathcal{H}_F \otimes \mathcal{H}_{F'}$. Let $\varphi^{|h\rangle\langle h|}(\eta)$, $\eta \in E$, $h \in \mathcal{H}_E$, be an elementary $\tilde{\sigma}$-positive-type function on E. Denote by Φ_F (resp. $\Phi_{F'}$) the $\tilde{\sigma}$-positive restriction of Φ to F (resp. F'). Then h can be written as a sum

$$a_E^{\frac{1}{2}} \sum_n \lambda_n h_n^F \otimes h_n^{F'}, \quad \lambda_n \geq 0, \quad h_n^F \in \mathcal{H}_F, \quad h_n^{F'} \in \mathcal{H}_{F'},$$

such that

$$\Phi_F = a_F \sum_n |\lambda_n|^2\, \varphi^{|h_n^F\rangle\langle h_n^F|} \tag{28}$$

and

$$\Phi_{F'} = a_{F'} \sum_n |\lambda_n|^2\, \varphi^{|h_n^{F'}\rangle\langle h_n^{F'}|} \tag{28'}$$

are the respective spectral decompositions of Φ_F and $\Phi_{F'}$.

Proof: Let us write the spectral decomposition of Φ_F in the form (28) and let P_n^F be the projection operator in $\mathcal{H}_E$ given by $|h_n^F\rangle\langle h_n^F| \otimes I_{\mathcal{H}_{F'}}$, where $I_{\mathcal{H}_{F'}}$ is the identity operator on $\mathcal{H}_{F'}$. Then

$$P_n^F h = \|P_n^F h\|\, h_n^F \otimes h_n^{F'},$$

where $h_n^{F'}$ is a vector in $\mathcal{H}_{F'}$ with norm equal to 1. We then have

$$\Phi_F(\eta_F) = (a_E)^{-1} \sum_{n,m} (P_n^F h|\, \mathfrak{U}_F(\eta_F) \otimes I_{\mathcal{H}_{F'}}\, |P_m^F h) = (a_E)^{-1} \sum_{n,m} \|P_n^F h\|\, \|P_m^F h\| \times (h_n^{F'} \mid h_n^{F'}) (h_n^F|\, \mathfrak{U}_F(\eta_F)\, |h_m^F).$$

Comparison with (28) gives

$$(a_E)^{-1}(h_n^{F'} \mid h_m^{F'})\, \|P_n^F h\|\, \|P_m^F h\| = \delta_{n,m} |\lambda_n|^2.$$

Hence the set $(h_n^{F'})$ is orthonormal, and

$$(a_E)^{-1}\, \|P_n^F h\|^2 = |\lambda_n|^2.$$

We then have

$$\Phi_{F'}(\eta_{F'}) = (a_E)^{-1} \sum_n (P_n^F h|\, I_{\mathcal{H}_F} \otimes \mathfrak{U}_{F'}(\eta_{F'})\, |P_n^F h)$$

since the P_n^F commute with $\mathfrak{U}_{F'}$. Hence

$$\Phi_{F'}(\eta_{F'}) = \sum_n a_{F'} |\lambda_n|^2 (a_{F'})^{-1} (h_n^{F'}|\, \mathfrak{U}_{F'}(\eta_{F'})\, |h_n^{F'}),$$

and this is the spectral decomposition of $\Phi_{F'}$ owing to the orthonormality of the $h_n^{F'}$.

Lemma 6: Let $\mathfrak{U}_F(\eta)$ be a representation of CCR's on (F, σ) in the Hilbert space $\mathcal{H}_F$. Let J be some anti-unitary operator on $\mathcal{H}_F$ [that is, satisfying

$(Jh \mid Jh') = (h' \mid h)$]. Then $(J^{-1}\mathfrak{U}_F(\eta)J)^*$ is a representation of CCR's on $(F, -\sigma)$ in $\mathcal{H}_F$.

The proof is obvious and will be omitted.

Theorem 3: Let (F_1, F_2) be an irreducible E-connected pair. Let Φ_1 and Φ_2 be elementary σ-positive-type functions on F_1 and F_2, respectively. Then one has

$$[D_E(\Phi_1) \times D_E(\Phi_2)] \times [D_E(\Phi_1) \times D_E(\Phi_2)]^*(\eta) = (\det M_{2'}^1)^{-2}\Phi_1(\eta_1) \cdot \Phi_{F_1'}(\eta_{1'}), \quad (29)$$

where $\Phi_{F_1'}$ is the σ-positive-type function on F_1' given by

$$\Phi_{F_1'}(\eta_{1'}) = \Phi_1(\mathcal{M}_1^{1'}\eta_{1'}) \cdot \Phi_2(\mathcal{M}_2^{1'}\eta_{1'}), \quad \eta_{1'} \in F_1'. \quad (30)$$

As a result, $D_E(\Phi_1) \times D_E(\Phi_2)$ is in $\mathcal{C}(E, \sigma)$ if and only if the square root of $\Phi_{F_1'}$ is in $\mathcal{C}(F_1', \sigma)$.

Proof: Under the conditions of the theorem, formula (26) reads

$$[D_E(\Phi_1) \times D_E(\Phi_2)](\eta) = (\det M_{2'}^1)^{-1} \exp[-i\sigma(\eta_1, \mathcal{M}_1^{1'}\eta_{1'})] \times \Phi_1(\eta_1 + \mathcal{M}_1^{1'}\eta_{1'}) \cdot \Phi_2(\mathcal{M}_2^{1'}\eta_{1'}). \quad (26')$$

Since $D_E(\Phi_{F_1})$ is idempotent, the distribution on the left of (29) is equal to $D_E(\Phi_1) \times D_E(\Phi_2) \times D_E(\Phi_1)$, so that equality (29) follows from an easy calculation.

The fact that $\Phi_{F_1'}(\eta_{1'})$ is a σ-positive-type function on F_1' results from the property of the left member of (28) being a σ-positive-type function on E, owing to the fact that, by Theorem 2, $D_E(\Phi_1) \times D_E(\Phi_2)$ is in $L^2(F, \sigma)$. Hence its restriction to F_1', which is proportional to $\Phi_{F_1'}(\eta_{1'})$, is also a σ-positive-type function on F_1'.

Now according to (29) and owing to the fact that Φ_1 is a σ-elementary positive-type function on F_1, which implies $\Phi_1 \times \Phi_1 = \Phi_1$ [in $\mathcal{C}'(F_1, \sigma)$], one sees, using (6) and $F_1 \oplus^\sigma F_1' = E$, that

$$|D_E(\Phi_1) \times D_E(\Phi_2)|(\eta) = (\det M_2^1)^{-1}\Phi_1(\eta_1) \cdot \Phi_{F_1'}^{\frac{1}{2}}(\eta_{1'}),$$

where $\Phi_{F_1'}^{\frac{1}{2}}$ is the square root of $\Phi_{F_1'}$, that is, the square-integrable function on F_1' such that $\Phi_{F_1'}^{\frac{1}{2}} \times \Phi_{F_1'}^{\frac{1}{2}} = \Phi_{F_1'}$ [in $\mathcal{C}'(F_1', \sigma)$]. Now $D_E(\Phi_1) \times D_E(\Phi_2)$ is in $\mathcal{C}(E, \sigma)$ if and only if its absolute value $|D_E(\Phi_1) \times D_E(\Phi_2)|$ is in $\mathcal{C}(E, \sigma)$, or equivalently if it is a σ-positive-type function on E. But this obviously holds if and only if $\Phi_{F_1'}^{\frac{1}{2}}$ is a σ-positive-type function on F_1'.

Corollary 2: Let (F_1, F_2) be an irreducible E-connected pair. Let Φ_1 and Φ_2 be elementary σ-positive-type functions on F_1 and F_2, respectively. If $\Phi_1 \notin L^1(F_1, \sigma)$ or if $\Phi_2 \notin L_1(F_2, \sigma)$, then

$$[D_E(\Phi_1) \times D_E(\Phi_2)] \notin \mathcal{C}(E, \sigma).$$

Proof: Let J_1 be some anti-unitary operator on $\mathcal{H}_{F_1}$ and $\tilde{\sigma}$ the symplectic form on E defined in Lemma 4. Let $\mathfrak{U}_{F_1}$ (resp. $\mathfrak{U}_{F_1'}$) be some irreducible representation of CCR's on (F_1, σ) [resp. (F_1', σ)] in the Hilbert space $\mathcal{H}_{F_1}$ (resp. $\mathcal{H}_{F_1'}$). Then we define in $\mathcal{H}_{F_1} \otimes \mathcal{H}_{F_1'}$ an irreducible representation $\tilde{\mathfrak{U}}_E$ of CCR's on $(E, \tilde{\sigma})$ by

$$\tilde{\mathfrak{U}}_E(\eta_1) = (J_1^{-1}\mathfrak{U}_{F_1}(\eta_1)J_1)^* \otimes I_{\mathcal{H}_{F_1'}}, \quad \eta_1 \in F_1,$$
$$\tilde{\mathfrak{U}}_E(\eta_{1'}) = I_{\mathcal{H}_{F_1}} \otimes \mathfrak{U}_{F_1}(\eta_{1'}), \quad \eta_{1'} \in F_1'.$$

On the other hand, if $S_{1'}^2$ is a σ-symplectic transformation from F_2 to F_1', then $\Phi_2((S_{1'}^2)^{-1}\eta_{1'})$ is an elementary σ-positive-type function on F_1'; then one can write

$$\Phi_2(\mathcal{M}_2^{1'}\eta_{1'}) = (a_{F_1'})^{-1}(h^{1'} \mid \mathfrak{U}_{F_1'}(S_{1'}^2\mathcal{M}_2^{1'}\eta_{1'}) \mid h^{1'})$$

where $h^{1'} \in \mathcal{H}_{F_1'}$. We then get with the notations of Lemma 4 and, using $a_F a_{F'} = a_E$,

$$\Phi_{F_1'}(\eta_{1'}) = (a_E)^{-1}(h^1 \otimes h^{1'} \mid \mathfrak{U}_{F_1}(\mathcal{M}_1^{1'}\eta_{1'}) \otimes \mathfrak{U}_{F_1'}(S_{1'}^2\mathcal{M}_2^{1'}\eta_{1'}) \mid h^1 \otimes h^{1'}) = (a_E)^{-1}(\tilde{h}^1 \otimes h^{1'} \mid \tilde{\mathfrak{U}}_E(S_1'\eta_{1'}) \mid \tilde{h}^1 \otimes h^{1'}),$$

where $\tilde{h}^1 = J_1^{-1}h^1$. Let $\eta = \eta_1 + \eta_{1'}$, $\eta_1 \in F_1$, and $\eta_{1'} \in F_1'$, and let us define on E the $\tilde{\sigma}$-symplectic transformation

$$S\eta = S_1\eta_1 + S_1'\eta_{1'}.$$

Then

$$\Phi(\eta) = (a_E)^{-1}(\tilde{h}^1 \otimes h^{1'} \mid \tilde{\mathfrak{U}}_E(S\eta) \mid \tilde{h}^1 \otimes h^{1'}), \quad \eta \in E,$$

is an elementary $\tilde{\sigma}$-positive-type function on E, whose restriction to F_1' is precisely $\Phi_{F_1'}$. We can now apply Lemma 5 with $F = F_1$. Writing $\Phi(\eta) = \varphi^{|h\rangle\langle h|}(\eta)$ with $h \in \mathcal{H}_E$, we see that a necessary and sufficient condition in order that $\Phi_{F_1'}^{\frac{1}{2}} \in \mathcal{C}(F_1', \tilde{\sigma})$ [$= \mathcal{C}(F_1', \sigma)$] is that the coefficients λ_n of the decomposition of h satisfy $\sum_n \lambda_n < \infty$. Let us show that this implies absolute integrability of Φ_{F_1} on F_1. One has

$$a_E\Phi_1(\eta_1) = (\tilde{h}^1 \otimes h^{1'} \mid \tilde{\mathfrak{U}}_E(SS^{-1}\eta_1) \mid \tilde{h}^1 \otimes h^{1'}), \quad \eta_1 \in F_1,$$
$$= (h \mid \tilde{\mathfrak{U}}_E(S^{-1}\eta_1) \mid h)$$
$$= (h \mid \tilde{\mathfrak{U}}_E(P_{F_1}S^{-1}\eta_1)\tilde{\mathfrak{U}}_E(P_{F_1'}S^{-1}\eta_1) \mid h)$$
$$\times \sum_{n,m} \lambda_n\lambda_m(\tilde{h}_m^1 \mid \mathfrak{U}_{F_1}(P_{F_1}S^{-1}\eta_1) \mid \tilde{h}_n^1)$$
$$\times (h_m^{1'} \mid \mathfrak{U}_{F_1'}(P_{F_1'}S^{-1}\eta_1) \mid h_n^{1'})$$

with $\tilde{h}_m^1 = J_1h_m^1$. Now, owing to the last assertion of the Lemma 4, the linear mappings $\eta_1 \to P_{F_1}S^{-1}\eta_1$ and $\eta_1 \to P_{F_1'}S^{-1}\eta_1$ are regular. Then, by Theorem 1

and Schwartz inequality,

$$\int_{F_1} (\tilde{h}_m^1 | \mathfrak{U}_{F_1}(P_{F_1}S^{-1}\eta_1) | \tilde{h}_n^1) \times (h_m^{1'} | \mathfrak{U}_{F_1'}(P_{F_1'}S^{-1}\eta_1) | h_n^{1'}) \, d\eta_1 = C < \infty,$$

and we get

$$\int_{F_1} |\Phi_1(\eta_1)| \, d\eta_1 \leq C \sum_{n,m} \lambda_n \lambda_m < \infty.$$

This corollary provides the counterexample announced above since there exists nonabsolutely integrable elementary σ-positive-type functions on F_1 and F_2. It will then be necessary to look for additional conditions ensuring that

$$[D_E(\Phi_1) \times D_E(\Phi_2)] \in \mathcal{C}(E, \sigma).$$

We shall see (Theorem 4) that a kind of absolute integrability on the irreducibly connected subspaces [(33)] is, in fact, a sufficient condition. We now turn to a description of the general situation where (F_1, F_2) is an arbitrary E-connected pair. The regular subspaces D, K_1, and K_2 are defined in Sec. 2; we introduce the regular subspace $\bar{F}_i$ of E by the relation

$$F_i = \bar{F}_i \oplus D \oplus K_i. \tag{31}$$

To simplify the notation, we shall write C for $C(F_1, F_2)$; then

$$C = \bar{F}_1 + \bar{F}_2.$$

Lemma 7: Let (F_1, F_2) be an E-connected pair. There exists an elementary σ-positive-type function $\Omega_{F_i} = \varphi^{|\omega^i)(\omega^i|}$, $\omega^i \in \mathcal{K}_{F_i}$ on F_i, such that if $\eta_{F_i} = (\eta_i, \eta_D, \kappa_i)$ is the decomposition of $\eta_{F_i} \in F_i$ along the σ-orthogonal subspaces $\bar{F}_i$, D, and K_i, then one has

$$\Omega_{F_i}(\eta_{F_i}) = \Omega_i(\eta_i) \cdot \Omega_D(\eta_D) \cdot \Omega_{K_i}(\kappa_i), \tag{32}$$

where Ω_i, Ω_D, and Ω_{K_i} are σ-elementary positive-type functions in $\mathcal{S}(\bar{F}_i, \sigma)$, $\mathcal{S}(D, \sigma)$, and $\mathcal{S}(K_i, \sigma)$, respectively.

Proof: It is sufficient to prove separately the existence of Ω_i, Ω_D, and Ω_{K_i} since a tensor product of rank-one projection operators on $\mathcal{K}_{\bar{F}_i}$, $\mathcal{K}_D$, and $\mathcal{K}_{K_i}$, respectively, is a rank-one projection operator on the representation space $\mathcal{K}_{\bar{F}_i} \otimes \mathcal{K}_D \otimes \mathcal{K}_{K_i}$ of CCR's on (F_i, σ). In order to construct Ω_i, we choose a linear operator I_i on $\bar{F}_i$ satisfying $I_i^2 = -1$ and

$$\sigma(I_i\eta_i, I_i\xi_i) = \sigma(\eta_i, \xi_i);$$

let s_i be the real bilinear symmetric form on F_i defined by $s_i(\eta_i, \xi_i) = \sigma(\eta_i, J\xi_i)$. Then $\Omega_i(\eta_i) = (a_{\bar{F}_i})^{-1} \exp[-\frac{1}{2}s_i(\eta_i, \eta_i)]$ is in $\mathcal{S}(F_i, \sigma)$ and is easily shown to be idempotent; since, in addition, it satisfies $a_{\bar{F}_i}\Omega_i(0) = 1$, Ω_i is an elementary σ-positive-type function on $\bar{F}_i$. Choosing in the same way forms s_D and s_{K_i} on D and K_i provides us with Ω_D and Ω_{K_i}. The function

$$\Omega_{F_i}(\eta_{F_i}) = (a_{F_i})^{-1} \exp[-\tfrac{1}{2}s(\eta_{F_i}, \eta_{F_i})],$$

$s(\eta_{F_i}, \eta_{F_i}) = s_i(\eta_i, \eta_i) + s_D(\eta_D, \eta_D) + s_{K_i}(\kappa_i, \kappa_i)$, enjoys all properties requested.

Theorem 4: Let (F_1, F_2) be an E-connected pair. Let $\Phi_i = \varphi^{|f^i)(h^i|}$, $f^i, h^i \in \mathcal{K}_{F_i}$, be an elementary function on F_i, $i = 1, 2$, such that

$$\int_{F_i} d\eta_i \left(\int_{D \times K_i} d\eta_D \, d\kappa_i \, |\Phi_i(\eta_i, \eta_D, \kappa_i)|^2 \right)^{\frac{1}{2}} < \infty. \tag{33}$$

Then, for any $g^i \in \mathcal{K}_{F_i}$, the distribution $D_E(\varphi^{|g^1)(h^1|}) \times D_E(\varphi^{|h^2)(g^2|}) \in \mathcal{C}(E, \sigma)$.

Proof: Let Ω_{F_i}, $i = 1, 2$, be an elementary σ-positive-type function $\varphi^{|\omega^i)(\omega^i|}$ on F_i satisfying the conditions of Lemma 7. We first show that if (33) holds for some $f^i \in \mathcal{K}_{F_i}$, it also holds for $f^i = \omega^i$. In fact, one has, owing to (8),

$$\Omega_{F_i} \times \varphi^{|f^i)(h^i|} = (\omega^i \,|\, f^i)\varphi^{|\omega^i)(h^i|}, \quad \text{in } \mathcal{C}'(F_i, \sigma).$$

Since there always exists an $\eta_{F_i} \in F_i$ such that $(\omega^i | \mathfrak{U}_{F_i}(\eta_{F_i}) | f^i) \neq 0$, owing to the irreducibility of the representation $\mathfrak{U}_{F_i}$, we can suppose, without restricting, the generality that $(\omega^i \,|\, f^i) \neq 0$. It is then sufficient to prove that twisted convolution by Ω_{F_i} leaves the property (33) invariant, and this results easily from (32) and Schwartz inequality.

Let us now prove that $D_E(\Phi_1) \times D_E(\Phi_2^*) \in \mathcal{C}(E, \sigma)$ if $\Phi_i = \varphi^{|\omega^i)(h^i|}$. Owing to (8) and (16), one has

$$\Phi_1(\xi_{F_i}) = \int_{F_i} d\eta_{F_i} \Phi_1(\eta_{F_i}) \times \exp[-i\sigma(\eta_{F_i}, \xi_{F_i})]\Omega_{F_i}(\eta_{F_i} - \xi_{F_i}),$$

whence

$$D_E(\Phi_1) = \int_{F_i} d\eta_{F_i} \Phi_1(\eta_{F_i}) D_E(\Omega_{F_i}) \times \delta^E_{F_i}.$$

We get then

$$D_E(\Phi_1) \times D_E(\Phi_2^*) = \int_{F_1 \times F_2} d\eta_{F_1} \, d\eta_{F_2} \, \Phi_1(\eta_{F_1}) \Phi_2^*(\eta_{F_2}) \times D_E(\Omega_{F_1}) \times \delta^E \eta_{F_1} \times \delta^E \eta_{F_2} \times D_E(\Omega_{F_2}).$$

As is observed at the end of the first section, one has

$$D_E(\Omega_{F_i}) = D_E(\Omega_i) \times D_E(\Omega_D) \times D_E(\Omega_{K_i}).$$

Let us define

$$T_{K_1}(\eta_1, \eta_D) = \int_{K_1} d\kappa_1 \Phi_1(\eta_1, \eta_D, \kappa_1) \Omega_{K_1} \times \delta_{\kappa_1}.$$

Then, owing to the relation

$$\|\Omega_{K_1} \times \Phi_{K_1}\|_{\mathcal{C}(K_1,\sigma)} \leq \|\Omega_{K_1}\|_{\mathcal{C}(K_1,\sigma)} \|\Phi_{K_1}\|_2^{K_1},$$

$T_{K_1}(\eta_1, \eta_D)$ is in $\mathcal{C}(K_1, \sigma)$ for almost all (η_1, η_D) and

$$\|T_{K_1}(\eta_1, \eta_D)\|_{\mathcal{C}(K_1,\sigma)} \leq \left(a_{K_1} \int_{K_1} d\kappa_1 |\Phi_1(\eta_1, \eta_D, \kappa_1)|^2\right)^{\frac{1}{2}}.$$

We define in the same way $T_{K_2}(\eta_2, \xi_D)$.

Finally, observing the identity $\Omega_D + \delta\eta_D \times \Omega_D = \exp[-\frac{1}{2}s(\eta_D, \eta_D)]\Omega_D$ and remembering the last remark of Sec. 1 concerning distributions with σ-orthogonal complementary supports, we get

$$\begin{aligned} D_E(\Phi_1) \times D_E(\Phi_2^*) &= \int_{F_1 \times F_2} d\eta_1\, d\eta_2 \int_{D \times D} d\eta_D\, d\xi_D \exp[-i\sigma(\eta_D, \xi_D)] \\ &\quad \times \exp[-\tfrac{1}{2}s(\eta_D + \xi_D, \eta_D + \xi_D)] \\ &\quad \times \Omega_D \cdot T_{K_1}(\eta_1, \eta_D) \cdot T_{K_2}^*(\eta_2, \xi_D) \\ &\quad \times D_C(\Omega_1 \times \delta^C\eta_1 \times \delta^C\eta_2 \times \Omega_2). \end{aligned} \tag{34}$$

Let $\overline{F_i'}$ be the σ-orthogonal complement in C of $\overline{F_i}$. Then since $\bar{F}_i \cap \bar{F}_2$ is empty, $(\overline{F_1'}, \overline{F_2'})$ is C-connected, so that

$$\begin{aligned} \delta_{\eta_1}^C \times \delta_{\eta_2}^C &= \exp[-i\sigma(\eta_1, \eta_2)] \\ &\quad \times \exp[i\sigma(\eta_{1'}, \eta_{2'})] \delta_{\eta_{1'}}^C \times \delta_{\eta_{2'}}^C, \end{aligned}$$

with $\eta_{1'} \in \overline{F_1'}$, $\eta_{2'} \in \overline{F_2'}$, and $\eta_1 + \eta_2 = \eta_{1'} + \eta_{2'}$. Then

$$\begin{aligned} D_C(\Omega_1) \times \delta_{\eta_1}^C \times \delta_{\eta_2}^C \times D_C(\Omega_2) \\ = \delta_{\eta_{1'}}^C \times D_C(\Omega_1) \times D_C(\Omega_2) \times \delta_{\eta_{2'}}^C. \end{aligned} \tag{35}$$

Owing to the fact that $S(C, \sigma) \subset \mathcal{C}(C, \sigma)$ and to formula (26'), one has $D_C(\Omega_1) \times D_C(\Omega_2) \in \mathcal{C}(C, \sigma)$ and

$$\begin{aligned} \|D_C(\Omega_1) \times \delta_{\eta_1}^C \times \delta_{\eta_2}^C \times D_C(\Omega_2)\|_{\mathcal{C}(C,\sigma)} \\ = \|D_C(\Omega_1) \times D_C(\Omega_2)\|_{\mathcal{C}(C,\sigma)} = b. \end{aligned}$$

Returning then to (34), we see that $D_E(\Phi_1) \times D_E(\Phi_2)$ is an integral over $\bar{F}_1 \times \bar{F}_2 \times D \times D$ of elements in $\mathcal{C}(E, \sigma)$ whose $\mathcal{C}(E, \sigma)$-norm is equal to

$$\begin{aligned} b \exp[-\tfrac{1}{2}s(\eta_D + \xi_D, \eta_D + \xi)] \|T_{K_1}(\eta_1, \eta_D^D)\|_{\mathcal{C}(K_1,\sigma)} \\ \times \|T_{K_2}^*(\eta_2, \xi_D)\|_{\mathcal{C}(K_2,\sigma)}. \end{aligned}$$

Since a norm-convergent integral of a Banach-space-valued function is in this Banach space, we get that, under condition (33), $D_E(\Phi_1) \times D_E(\Phi_2) \in \mathcal{C}(E, \sigma)$ and

$$\begin{aligned} \|D_E(\Phi_1) \times D_E(\Phi_2^*)\|_{\mathcal{C}(E,\sigma)} \\ \leq b \int d\eta_1\, d\eta_2 \int d\eta_D\, d\xi_D \\ \times \exp[-\tfrac{1}{2}s(\eta_D + \xi_D, \eta_D + \xi_D)] \\ \times \|T_{K_1}(\eta_1, \eta_D)\|_{\mathcal{C}(K_1,\sigma)} \|T_{K_2}(\eta_2, \xi_D)\|_{\mathcal{C}(K_2,\sigma)}. \end{aligned}$$

Using the above estimate of $\|T_{K_i}(\eta_i, \eta_D)\|_{\mathcal{C}(K_i,\sigma)}$, together with the fact that ordinary convolution by the function $\exp[-\frac{1}{2}s(\eta_D, \eta_D)]$ is a bounded linear mapping in $L^2(D, \sigma)$ and with Schwartz's inequality, we get

$$\begin{aligned} \|D_E(\Phi_1) \times D_E(\Phi_2)\|_{\mathcal{C}(E,\sigma)} \\ \leq b \prod_{i=1}^{2} (a_{K_i}) \int_{F_i} d\eta_i \left(\int_{D_i \times K_i} d\eta_D\, d\kappa_i |\Phi_i(\eta_i, \eta_D, \kappa_i)|^2\right)^{\frac{1}{2}}. \end{aligned}$$

To conclude the proof of Theorem 4, we use

$$D_E(\varphi^{|g^i)(\omega^i|}) \times D_E(\varphi^{|\omega^i)(h^i|}) = D_E(\varphi^{|g^i)(h^i|})$$

and the fact that $\mathcal{C}(E, \sigma)$ is a two-sided ideal in $\mathcal{C}'(E, \sigma)$. Hence $D_E(^{|g^1)(h^1|}) \times D_E(\varphi^{|h^2)(g^2|})$, being obtained by left convolution of $D_E(\Phi_1) \times D_E(\Phi_2)$ by $D_E(\varphi^{|g^1)(\omega^1|})$ and right convolution of the result by $D_E(\varphi^{|\omega^2)(g^2|})$, is in $\mathcal{C}(E, \sigma)$.

Corollary 3: Let (F_1, F_2) be an E-connected pair. Let

$$\Phi_i = \sum_{n=1}^{N} \lambda_n \varphi^{|f_n^i)(h_n^i|},$$

where (f_n^i) and (h_n^i) are orthogonal sets of vectors in $\mathcal{K}_{F_i}$, be the spectral decomposition of $\Phi_i \in \mathcal{F}(F_i, \sigma)$. Then, if Φ_i satisfies condition (33), the distribution

$$D_E\left(\sum_{n=1}^{N} \mu_n \varphi^{|g_n^1)(h_n^1|}\right) D_E\left(\sum_{m=1}^{N} \gamma_m \varphi^{|h_m^2)(g_m^2|}\right) \in \mathcal{C}(E, \sigma)$$

for any sets (μ_n), (λ_m) of complex constants and any sets (g_n^1), (g_m^2) of vectors in $\mathcal{K}_{F_1}$ and $\mathcal{K}_{F_2}$, respectively.

Proof: It is sufficient to prove that each $\varphi^{|\omega^i)(h_n^i|}$ satisfies (33) if Φ_i does, since in this case Theorem 4 can be applied to each of these elementary functions separately. One has

$$\sum_{n=1}^{N} \lambda_n \varphi^{|\omega^i)(f_n^i|}(\eta_i) \cdot \varphi^{|\omega^i)(h_n^i|} = \Omega_{F_i} \times \delta\eta_i \times \Phi_i. \tag{36}$$

As was observed in the proof of Theorem 4, the left member of (36) satisfies (33). Since the set $(\lambda_n f_n^i)$ is linearly independent and the set $(\mathfrak{U}_{F_i}(\eta_i)\omega^i)$ spans $\mathcal{H}_{F_i}$ when η_i spans F_i (owing to the irreducibility of $\mathfrak{U}_{F_i}$), there exist N possible choices for η_i giving independent linear combinations (36). Hence this set of equations can be solved and $\varphi^{|\omega^i)(h_n{}^i|}$ expressed as a linear combination of functions satisfying (33). Using the triangle inequality, one then shows that $\varphi^{|\omega^i)(h_n{}^i|}$ also satisfies (33).

In order to obtain results for arbitrary elements in $\mathcal{C}(F, \sigma)$, we observe that any function in $\mathcal{C}(F, \sigma)$ is the restriction to F of an elementary function in some $\mathcal{C}(\hat{F}, \hat{\sigma})$, where $\hat{F}$ is any finite-dimensional space containing F and equipped with simplectic form $\hat{\sigma}$ whose restriction to $\hat{\sigma}$ is σ. In fact, let $\hat{F} = F \oplus^{\delta} G$ satisfy these conditions; let us write the spectral decomposition of $\Phi_F \in \mathcal{C}(F, \sigma)$:

$$\Phi_F(\eta_F) = \sum_n \lambda_n a_F^{-1}(h_n^F|\, \mathfrak{U}_F(\eta_F)\, |f_n^F), \qquad \eta_F \in F, \quad \lambda_n \geq 0,$$

where (f_n^F) and (h_n^F) form an orthonormal basis in $\mathcal{H}_F$. Let $\mathfrak{U}_G$ be an irreducible representation of CCR's on $(G, \hat{\sigma})$ in $\mathcal{H}_G$; let h_n^G be an arbitrary orthonormal basis in $\mathcal{H}_G$. Then defining

$$h^{\hat{F}} = \sum_n |\lambda_n|^{\frac{1}{2}} (a_F)^{-\frac{1}{2}} h_n^F \otimes h_n^G,$$

$$f^{\hat{F}} = \sum_n |\lambda_n|^{\frac{1}{2}} (a_F)^{-\frac{1}{2}} f_n^F \otimes h_n^G,$$

which are vectors in $\mathcal{H}_F \otimes \mathcal{H}_G$, we see that the restriction of $\varphi^{|f^{\hat{F}})(h^{\hat{F}}|}$ to F is Φ_F. Now let (F_1, F_2) be an E-connected pair and E' an arbitrary finite-dimensional space equipped with a symplectic form σ'; then, if (G_1, G_2) is an E'-connected pair, the pair $(F_1 \oplus^{\delta} G_1,\ F_2 \oplus^{\delta} G_2)$ is $\hat{E}$-connected, where $\hat{E} = E \oplus^{\delta} E'$, $\hat{\sigma} = \sigma'$ on E'. If Φ_i is some elementary extension of $\Phi_{F_i} \in \mathcal{C}(F_i, \sigma)$ to $F_i \oplus^{\delta} G_i$, then Theorem 4 gives conditions on Φ_1 and Φ_2 ensuring that $D_{\hat{E}}(\Phi_1) \times D_{\hat{E}}(\Phi_2) \in \mathcal{C}(\hat{E}, \hat{\sigma})$. If these conditions are satisfied, then the restriction of $D_{\hat{E}}(\Phi_1) \times D_{\hat{E}}(\Phi_2)$ to E is in $\mathcal{C}(E, \sigma)$ since it can easily be shown to be a finite linear combination of σ-positive functions on E. But, returning to formula (26), we see that if $G_1 \cap G_2$ is empty, this restriction is proportional to $D_E(\Phi_{F_1}) \times D_E(\Phi_{F_2})$. This provides us with various corollaries to Theorem 4, owing to all possible choices of spaces $(\hat{E}, \hat{\sigma})$ and of $\hat{E}$-connected pairs having the restriction (F_1, F_2) to E. As examples, we consider the two simplest cases for a given E', that is, either (G_1, G_2) is an irreducible E'-connected pair or $G_1 \oplus^{\sigma'} G_2 = E'$. Any choice evidently depends upon a particular situation.

Corollary 4: Let (F_1, F_2) be an irreducible E-connected pair and $\Phi_{F_i} \in \mathcal{C}(F_i, \sigma)$, $i = 1, 2$. If there exists a finite-dimensional space E' equipped with a symplectic form σ' and an irreducible E'-connected pair (G_1, G_2) such that Φ_{F_i}, $i = 1, 2$, is the restriction to F_i of an absolutely integrable elementary function on $F_i \oplus^{\delta} G_i$, then $D_E(\Phi_{F_1}) \times D_E(\Phi_{F_2}) \in \mathcal{C}(E, \sigma)$.

Corollary 5: Let (F_1, F_2) be an E-connected pair and Φ_{F_i} be in $\mathcal{C}(F_i, \sigma)$, $i = 1, 2$. Suppose there exists a finite-dimensional space E' equipped with a symplectic form σ' and a pair (G_1, G_2) of σ'-orthogonal subspaces of E' such that Φ_{F_i}, $i = 1, 2$, is the restriction to F_i of an elementary function on $F_i \oplus \hat{G}_i$ satisfying the condition

$$\int_{F_i} d\eta_i \left(\int_{D \times K_i \times G_i} d\eta_D\, d\kappa_i\, d\gamma_i\, |\Phi_i(\eta_i, \eta_D, \kappa_i, \gamma_i)|^2 \right)^{\frac{1}{2}} < \infty. \tag{33'}$$

Then $D_E(\Phi_{F_1}) \times D_E(\Phi_{F_2}) \in \mathcal{C}(E, \sigma)$.

In the case of an irreducible E-connected pair (F_1, F_2), this last corollary gives the following kind of results; let

$$\Phi_{F_i}(\eta_{F_i}) = (a_{F_i})^{-1} \sum_n \lambda_n (h_n^i|\, \mathfrak{U}_{F_i}(\eta_{F_i})\, |f_n^i), \quad \eta_{F_i} \in F_i,$$

be the spectral decomposition of $\Phi_{F_i} \in \mathcal{C}(F_i, \sigma)$. Then, if

$$\int_{F_i} d\eta_{F_i} \left[\sum_n |\lambda_n|^2\, |(h_n^i|\, \mathfrak{U}_{F_i}(\eta_{F_i})\, |f_n^i)|^2 \right]^{\frac{1}{2}} < \infty,$$

the distribution $D_E(\Phi_{F_1}) \times D_E(\Phi_{F_2}) \in \mathcal{C}(E, \sigma)$.

Corollary 6: Let $(F_1, F_2, \cdots, F_n)$ be a set of regular subspaces of E such that $\sum_{i=1}^n F_i = E$ and each F_i is σ-orthogonal to F_j, $i \neq j$, except possibly for $j = i \pm 1$. Let $D_i^{\pm} = F_i \cap F_{i\pm1}$ and $K_i^{\pm} = F_i \cap (F_{i\pm1})'$. Then, if $\Phi^{|h_-{}^i)(h_+{}^i|}$, $h_{\pm}^i \in \mathcal{H}_{F_i}$, is an elementary function on F_i, a sufficient condition in order that

$$\bigtimes_{i=1}^n D_E(\Phi_i) \in \mathcal{C}(E, \sigma)$$

is that $\varphi^{|h^i)(h^i|}$ satisfies (33), with $D = D_i^{\pm}$ and $K_i = K_i^{\pm}$.

This could be proved using Corollary 5 and a recurrence process, but that would involve too many notations. We just give here a sketch of a direct proof.

Let $\Omega^{\pm}_{F_i} = \Omega_i \cdot \Omega_{D_i} \cdot \Omega_{K_i}{}^{\pm}$ be as in Lemma 7, and let $\omega^i_{\pm}$ be the associated vector in $\mathcal{K}_{F_i}$. Let Φ^-_i (resp. Φ^+_i) be the elementary function on F_i associated with $|h^i_-)(\omega^i_-|$ (resp. $|\omega^i_+)(h^i_+|$). We shall also have to consider $\Delta_i = \varphi^{|\omega_-{}^i)(\omega_+{}^i|}$. We then have, owing to $D_E(\Phi_i) = D_E(\Phi^-_i) \times D_E(\Delta_i) \times D_E(\Phi^+_i)$,

$$D_E(\Phi^+_1) \times D_E(\Phi_2) \times \cdots \times D_E(\Phi^-_n) = \bigtimes_{i=1}^{n-1} ([D_E(\Phi^+_i) \times D_E(\Phi^-_{i+1})] \times D_E(\Delta_{i+1})).$$

We first indicate how to show that

$$\bigtimes_{i=1}^{n-1} ([D_E(\Phi^+_i) \times D_E(\Phi^-_{i+1})]) \in \mathcal{C}(E, \sigma).$$

Owing to our hypothesis and Theorem 4, each term $D_E(\Phi^+_i) \times D_E(\Phi^-_{i+1})$ is the extension to E of an element in $\mathcal{C}(F_i + F_{i+1}, \sigma)$. This element can be expressed as an integral with summable trace-norm. In fact, its integrand is the product of a positive summable function by a $\mathcal{C}(F_i + F_{i+1})$-valued function which can be shown, via (34) and (35), to have the form

$$\Omega_{D_{i+1}{}^-} \cdot t_{K_{i+1}{}^-} \cdot \Phi_{i,i+1} \cdot t_{K_i{}^+},$$

where t_{K_i} is bounded in $\mathcal{C}(K_i)$ and $\Phi_{i,i+1}$ is, owing to (26') and (35), a test function on the σ-orthogonal complement in $F_i + F_{i+1}$ of $D^-_{i+1} \oplus^\sigma K^-_{i+1} \oplus^\sigma K^+_i$, with constant trace-norm. Since K^-_{i+1} and $\Omega_{D_i{}^+} = \Omega_{D_{i+1}{}^-}$ (resp. K^+_i) are σ-orthogonal to all $F_j, j < i$ (resp. $j > i + 1$), the function

$$\bigtimes_{i=1}^{n-1} (D_E(\Phi^+_i) \times D_E(\Phi^-_{i+1}))$$

can be expressed as an integral whose integrand is the product of a positive summable function by the function (on E)

$$\left(\prod_{i=1}^{n-1} \Omega_{D_{i+1}{}^-} \cdot t_{K_{i+1}{}^-}\right) \cdot \Phi \cdot \left(\prod_{i=1}^{n-1} t_{K_i{}^+}\right),$$

where Φ is in

$$\mathcal{S}\left(E \ominus^\sigma \left(\bigoplus_{i=1}^{n-1} [D^-_{i+1} \oplus^\sigma K^-_{i+1} \oplus K^+_i]\right)\right)$$

and can be shown, as in (35), to have a constant trace-norm. Hence this integrand has summable $\mathcal{C}(E)$ norm and the integral defines an element in $\mathcal{C}(E, \sigma)$. We now claim that each Δ_i is absolutely summable on F_i and that since

$$D_E(\Delta_i) = \int \Delta_i(\eta) D_E(\delta^{F_i}_\eta),$$

one can express

$$\bigtimes_{i=1}^{n-1} ([D_E(\Phi^+_i) \times D_E(\Phi^-_{i+1})] \times D_E(\Delta_{i+1}))$$

as a trace-norm summable integral of such elements; consequently, it is itself, and also

$$\bigtimes_{i=1}^{n-1} D_E(\Phi_i), \quad \text{in } \mathcal{C}(E, \sigma).$$

5. SOME CONNECTED PRODUCTS IN QUANTUM MECHANICS OF N-PARTICLE SYSTEMS

The symplectic space is here the $6N$-dimensional phase space $E^{(N)}$ of an N-particle system. The symplectic form σ on $E^{(N)}$ is defined as follows: Let η be a vector in $E^{(N)}$ describing the system when the coordinates of the position and momentum of particle (i) in a given reference frame are x^i_α and p^i_α, $\alpha = (1, 2, 3)$; if η' corresponds to another state $(x'^i_\alpha, p'^i_\alpha)$, then one defines

$$\sigma(\eta, \eta') = \sum_{i=1}^{N} \left(\sum_{\alpha=1}^{3} x^i_\alpha p'^i_\alpha - x'^i_\alpha p^i_\alpha\right).$$

We shall say that a basis $S = (\xi_n, \Pi_n), n = 1, 2, \cdots, 3N$, of $E^{(N)}$ is symplectic if it satisfies $\sigma(\Pi_n, \Pi_m) = \sigma(\xi_n, \xi_m) = 0$ and $\sigma(\Pi_n, \xi_m) = \delta_{nm}$. We define a particular symplectic basis $S^{(N)} = (\xi^i_\alpha, \Pi^i_\alpha)$ as the basis in which the above vector η is expressed as $\sum_{i=1}^{N} (\sum_{\alpha=1}^{3} x^i_\alpha \xi^i_\alpha + p^i_\alpha \Pi^i_\alpha)$. For later purposes we first describe some connected subspaces appearing in three-particle systems. Let E_i be the regular subspace of $E^{(3)}$ generated by (ξ^i_α) and (Π^i_α). Then $E^{(3)} = E_1 \oplus E_2 \oplus E_3$ (we shall henceforth omit the symbol σ on $\oplus$). In $E_1 \oplus E_2$ we introduce the new symplectic basis

$$\xi^{12}_\alpha = \xi^1_\alpha - \xi^2_\alpha, \qquad \Pi^{12}_\alpha = \frac{m_2\Pi^1_\alpha - m_1\Pi^2_\alpha}{m_1 + m_2},$$

$$\xi_{12,\alpha} = \frac{m_1\xi^1_\alpha + m_2\xi^2_\alpha}{m_1 + m_2}, \quad \Pi_{12,\alpha} = \Pi^1_\alpha + \Pi^2_\alpha,$$

m_i = mass of particle i.

Let E^{12}_{rel} (resp. E_{12}) be the regular subspace generated by the sets (ξ^{12}_α) and (Π^{12}_α) [resp. $(\xi_{12,\alpha})$ and $(\Pi_{12,\alpha})$]. We then have

$$E_1 \oplus E_2 = E_{12} \oplus E^{12}_{\text{rel}},$$

E^{12}_{rel} is the phase space for the relative motion of particles 1 and 2; E_{12} is the phase space for their center of mass motion. Decomposing in the same way $E_{12} \oplus E_3$, considering this center of mass as a particle, we get

$$E^{(3)} = E_{123} \oplus E^{12}_{\text{rel}} \oplus E^{(12,3)}.$$

We obtain other decompositions of E by permutation of (123). We define

$$E_{\text{rel}}^{\{3\}} = E_{\text{rel}}^{12} \oplus E^{(12,3)}.$$

This is the phase space for the relative motion of the three particles. In addition to the σ-orthogonal components of E_{rel}, another irreducible $E_{\text{rel}}^{\{3\}}$-connected pairs are provided by $(E_{\text{rel}}^{23}, E_{\text{rel}}^{12})$ and those obtained by permutation of (123), as can be seen from simple calculations performed on the previously defined symplectic bases. In these bases the matrix form for the operators $\mathcal{M}_1^{1'}$ and $\mathcal{M}_2^{1'}$, when $F_1 = E_{\text{rel}}^{23}$ and $F_2 = E_{\text{rel}}^{12}$, is

$$\mathcal{M}_1^{1'} = \begin{pmatrix} \nu_{123}^{-1}\eta_{12}(I) & 0 \\ 0 & \eta_{32}(I) \end{pmatrix},$$

$$\mathcal{M}_2^{1'} = \begin{pmatrix} \nu_{123}^{-1}(I) & 0 \\ 0 & (I) \end{pmatrix},$$

where $\eta_{ij} = m_i/(m_i + m_j)$, $\nu_{123} = 1 - \eta_{12}\eta_{32}$, and (I) is the 3×3 identity matrix.

We now consider general N-particle systems. Let C be some p-particle cluster contained in the system $\{N\}$; we define E^C as the regular subspace of $E^{\{N\}}$ generated by the set $(\xi_\alpha^i, \Pi_\alpha^i)$, $i \in C$, $\alpha = 1, 2, 3$. Let E_C be the regular subspace of E^C generated by the set

$$\left(\xi_{C,\alpha} = \sum_{i \in C} \frac{m_1}{m_C}\, \xi_\alpha^i\right) \quad \text{and} \quad \left(\Pi_{C,\alpha} = \sum_{i \in C} \Pi_\alpha^i\right), \qquad \alpha = 1, 2, 3,$$

where $m_C = \sum_{i \in C} m_i$; let E_{rel}^C be its σ-orthogonal complement in E^C; one then has

$$E^C = E_C \oplus E_{\text{rel}}^C. \tag{37}$$

It is easily verified that vectors of E_{rel}^C describe states of the system $\{N\}$ in which the $(N - p)$ particles not belonging to C rest at the origin and particles in C satisfy the center of mass condition $\sum_{i \in C} m_i x_{i,\alpha} = 0$, $\sum_{i \in C} p_{i,\alpha} = 0$. As to E_C, it can be identified as the phase space for a particle with mass m_C. If C and C' are disjoint clusters, we can perform, on $E_C \oplus E_{C'}$, the canonical reduction to the center of mass system described above for two-particle systems; for this, we introduce the canonical symplectic basis $(\xi_\alpha^{(C,C')}, \Pi_\alpha^{(C,C')})$ as if C and C' were single particles; one has then

$$E_C \oplus E_{C'} = E_{C \cup C'} \oplus E^{(C,C')}. \tag{38}$$

We derive then from (37) and (38) that

$$E_{\text{rel}}^{C \cup C'} = E^{(C,C')} \oplus E_{\text{rel}}^C \oplus E_{\text{rel}}^{C'}. \tag{39}$$

Iterating (39), we can decompose $E_{\text{rel}}^{C \cup C'}$ as a direct sum of σ-orthogonal two-body (particle or center of mass) relative phase spaces. The union of the canonical symplectic bases of each of these σ-orthogonal components is a symplectic basis for $E_{\text{rel}}^{C \cup C'}$; we call it again canonical although it is not unique, owing to the various possibilities of decomposing $E_{\text{rel}}^{C \cup C'}$. The subspace of some E_{rel}^C or $E^{(C,C')}$ spanned by the ξ vectors (resp. Π vectors) of a canonical basis will be called the configuration (resp. momentum) subspace of E_{rel}^C or $E^{(C,C')}$; if $\eta^C \in E_{\text{rel}}^C$, we shall denote by x^C and p^C its components on these subspaces.

We now briefly describe the usual representation of CCR's on $(E_{\text{rel}}^C, \sigma)$ or $(E^{(C,C')}, \sigma)$. Let $\mathcal{H}^C$ be the Hilbert space of square-integrable functions with respect to the Lebesgue measure on the configuration subspace of E^C. Then we define, for $h \in \mathcal{H}^C$,

$$(\mathfrak{U}^C(\eta^C)h)(a^C) = e^{-\frac{1}{2}\sigma(x^C,p^C)} e^{+i\sigma(p^C,a^C)} h(a^C - x^C). \tag{40}$$

The canonical commutation relations for $\mathfrak{U}^C$ are easily verified. In the same way one defines a representation $\mathfrak{U}^{(C,C')}$ of CCR's on $(E^{(C,C')}, \sigma)$ in the Hilbert space $\mathcal{H}^{(C,C')}$ of square-integrable functions on the configuration subspace of $E^{(C,C')}$. If we denote by (x_n^C), (p_n^C), $n = 1, \cdots, 3(p-1)$, the coordinates of x^C and p^C in some canonical symplectic basis, then $\sigma(x^C, p^C)$ takes the Cartesian form $\sum_n x_n^C \cdot p_n^C$. We prove in the Appendix the following tensor decompositions:

$$\mathcal{H}^{C \cup C'} = \mathcal{H}^C \otimes \mathcal{H}^{C'} \otimes \mathcal{H}^{(C,C')} \tag{41a}$$

and

$$\mathfrak{U}^{C \cup C'} = \mathfrak{U}^C \otimes \mathfrak{U}^{C'} \otimes \mathfrak{U}^{(C,C')} \tag{41b}$$

for any pair of disjoint clusters C and C'. Let A^C be some bounded (or at least self-adjoint) operator on $\mathcal{H}^C$; then we shall again denote by A^C the operator on $\mathcal{H}^{C \cup C'}$ obtained by ampliation of A^C to $\mathcal{H}^{C \cup C'}$ Relations (41) allow to give some explicit formulations of results stated in the preceding sections in some situations commonly encountered in quantum mechanics, which we now specify.

Lemma 8: Let $(C_1, C_2, \cdots, C_n)$ be a set of clusters whose union is $\{N\}$ and such that $(\bigcup_{i=1}^k C_i) \cap C_{k+1}$ is nonempty. Then $E_{\text{rel}}^{\{N\}}$ is generated by the set of subspaces $(E_{\text{rel}}^{C_1}, C_{\text{rel}}^{C_2}, \cdots, E_{\text{rel}}^{C_n})$.

Proof: It is sufficient to consider the case $n = 2$. We define $C = C_1 \cap C_2$ and $C_i' = C_j - C = \{N\} - C_i$, $(i,j) = (1,2)$. We derive then from (39) that

$$E_{\text{rel}}^{C_1} + E_{\text{rel}}^{C_2} = (E_{\text{rel}}^{C_1'} \oplus E_{\text{rel}}^{C} \oplus E_{\text{rel}}^{\{C_2'\}}) \oplus (E^{(C,C_1')} + E^{(C,C_2')}).$$

From the above study of three-particle systems, there results that $E^{(C,C_1')} + E^{(C,C_2')} = E^{(C,C_1')} \oplus E^{(C,C_2')}$; then two other applications of (39) give the desired result.

Theorem 5: Let $(C_1, C_2, \cdots, C_n)$ be a set of clusters whose union is $\{N\}$ and which can be rearranged in an order for which they satisfy conditions of Lemma 8. Then, if A^{C_i} is a Hilbert–Schmidt (resp. compact) operator on $\mathcal{H}^{C_i}$, the product $\prod_{i=1}^n A^{C_i}$ is a Hilbert–Schmidt (resp. compact) operator on $\mathcal{H}^{\{N\}}$.

We omit the proof which involves a simple recurrence process, Theorem 2, Corollary 2, and Lemma 8.

In order to get such an explicit formulation of Theorem 4 and its corollaries, we now look for sufficient conditions ensuring that elementary functions associated with rank-one operators in $\mathcal{H}^C$ satisfy (33) in the simplest situation of an $E^{\{N\}}$ connected pair $(E_{\text{rel}}^{C_1}, E_{\text{rel}}^{C_2})$. We first introduce some definitions: Let (n) denote a multi-index $(n_1, n_2, \cdots, n_{3(p-1)})$, where each n_i is a positive integer; we define $|(n)| = \sum_i n_i$. We consider then on $\mathcal{H}^C$ the following self-adjoint operators

$$(x^C)^{(n)} = (x_1^C)^{n_1}, \cdots, (x_{3(p-1)}^C)^{n_{3(p-1)}}$$

and

$$(-i\nabla^C)^{(n)} = (-i\partial/\partial x_1^C)^{n_1}, \cdots, (-i\partial/\partial x_{3(p-1)}^C)^{n_{3(p-1)}}$$

and the dense subspace of $\mathcal{H}^C$:

$$D_2^C = \bigcap_{\substack{|(l)|\leq 2 \\ |(m)|\leq 2}} D((x^C)^{(l)}(-i\nabla^C)^{(m)}).$$

One introduces on D_2^C the norm

$$\|f\|_2^C = \sup_{\substack{|(l)|\leq 2 \\ |(m)|\leq 2}} \|(x^C)^{(l)}(-i\nabla^C)^{(m)} f\|^C$$

(remark that with this norm the natural embedding of D_2^C into $\mathcal{H}^C$ is compact). We then have the following.

Lemma 9: Let $(E_{\text{rel}}^{C_1}, E_{\text{rel}}^{C_2})$ be an $E^{\{N\}}$-connected pair. In order that $\Phi_i = \varphi^{|f_i|(h_i|}, f_i, h_i \in \mathcal{H}^{C_i}$, $i = 1, 2$, satisfy condition (33) it is sufficient that f_i and $h_i \in \mathfrak{D}_2^{C_i}$.

Proof: Let us consider the quadratic forms on the subspaces E_{rel}^C given by

$$T(p^C) = \sum_{j\in C} \frac{|p_j|^2}{m_j} \quad \text{and} \quad Q(x^C) = \sum_{j\in C} m_j |x_j|^2,$$

where, for example, $|p_j|^2 = \sum_{\alpha=1,2,3} |p_j, \alpha|^2$. Then, if C and C' are disjoint clusters, one verifies easily that writing $\eta^{C\cup C'} = \eta^C + \eta^{C'} + \eta^{(C,C')}$; one has

$$T(p^{C\cup C'}) = T(p^C) + T(p^{C'}) + \frac{|p^{(C,C')}|^2}{m^{(C,C')}} \quad (42)$$

and

$$Q(x^{C\cup C'}) = Q(x^C) + Q(x^{C'}) + m^{(C,C')}|x^{(C,C')}|^2, \quad (43)$$

where $m^{(C,C')}$ is the reduced mass $m_C m_{C'}/(m_C + m_{C'})$. We now look at formula (33) in the above situation. It results from the proof of Lemma 8 that, by defining $C_i' = \{N\} - C_i$ and $C = C_1 \cap C_2$, (39) gives the decomposition (31) of $E_{\text{rel}}^{C_i}$ with $D = E_{\text{rel}}^C$, $K_i = E_{\text{rel}}^{C_i'}$, and $F_i = E^{(C,C_1')}$. Using Schwartz's inequality (42) and Eq. (43), one has then

$$\int d\eta^{(C,C_i')} \left(\int d\eta^C \, d\eta^{C_i'} |\Phi(\eta^{C_i})|^2 \right)^{\frac{1}{2}} \leq (I_1 I_2)^{\frac{1}{2}},$$

with

$$I_1 = \int d\eta^{(C,C_i')} \times \left(\left(1 + \frac{|p^{(C,C_i')}|^2}{m^{(C,C_i')}} \right) (1 + m^{(C,C_i')}|x^{(C,C_i')}|^2) \right)^{-2}$$

and

$$I_2 = \int d\eta^{C_i} |[1 + T(p^{C_i})][1 + Q(x^{C_i})]\Phi(\eta^{C_i})|^2.$$

Since $d\eta^{(C,C_i')} = d^3x^{(C,C_i')} \cdot d^3p^{(C,C_i')}$, the integral I_1 is finite. Let us estimate I_2. For this, we now omit the index C_i; owing to (40), one has

$$|\Phi(\eta)|^2 = \left| \int e^{i\sigma(p,a)} h(a - \tfrac{1}{2}x) f(a + \tfrac{1}{2}x) d^3a \right|^2;$$

using the Cartesian form of $\sigma(p, a) = \sum_n a_n \cdot p_n$ and the Parseval equality, we get

$$I_2 = (2\Pi)^{3(p-1)} \int d^3x d^3a \{[1 + Q(x)][1 + P(-i\nabla_a)] \times h(a - \tfrac{1}{2}x) f(p + \tfrac{1}{2}x)\}^2,$$

where ∇_a is the gradient vector with respect to a. For the last part of the proof we only need to use explicitly the fact that Q and P are quadratic forms; this allows us to decompose suitably $Q((\frac{1}{2}x - a) + (\frac{1}{2}x + a))$ and $P(-\frac{1}{2}i(\nabla_{a-\frac{1}{2}x} + \nabla_{a+\frac{1}{2}x}))$ in order that the hypothesis can be explicitly used.

Theorem 6: Let $C_1, C_2, \cdots, C_n$ be a set of clusters whose union is $\{N\}$ and such that $C_i \cap C_j$ is empty (resp. nonempty) for $j \neq i \pm 1$ (resp. $j = i \pm 1$). Let

$$A^{C_i} = \sum_p |\lambda_p| \, |f_p^i)(h_p^i|$$

be the spectral decomposition of a trace-class operator on $\mathcal{H}^{C_i}$. Then, if, for all $i = 1, 2, \cdots, n$, the sums

$$\sum_p |\lambda_p| \, (\|f_p^i\|_2^{C_i})^2 \quad \text{and} \quad \sum_p |\lambda_p| \, (\|h_p^i\|_2^{C_i})^2$$

are finite; the operator $\prod_{i=1}^{n} A^{C_i}$ is in the trace class on $\mathcal{H}^{\{N\}}$.

Proof: To prove this theorem, we use the method described in Sec. 4 for the treatment of general trace-class operators which consists in introducing elementary extensions of the functions $\varphi^{(A_i^{C_i})}$ to larger symplectic spaces in such a way that our results on connected products of elementary σ-positive-type functions can be used; these larger spaces must be chosen in such a way that the restriction to $E_{\text{rel}}^{\{N\}}$ of the connected product of extensions is precisely

$$\underset{i=1}{\overset{n}{\times}} D_{E_{\text{rel}}^{\{N\}}}(\varphi^{(A^{C_i})}).$$

Actually, we want to apply Corollary 6 to our situation. We consider then the set $\{\hat{N}\}$ of particles obtained by adjoining to the system $\{N\}$ a set $\{N'\}$ of fictitions particles which is the union of disjoint clusters $\bar{C}_i$, $i = 1, 2, \cdots, n$, where $\bar{C}_i$ contains the same number and species of particles as C_i. The symplectic form $\hat{\sigma}$ on $E_{\text{rel}}^{\{\hat{N}\}}$ is the canonical one. We consider then the following elements in $\mathcal{H}^{C_i \cup \bar{C}_i}$:

$$f^i = \sum_p |\lambda_p|^{\frac{1}{2}} f_p^i \otimes h_p^i \otimes s_i,$$
$$h^i = \sum_p |\lambda_p|^{\frac{1}{2}} h_p^i \otimes h_p^i \otimes s_i,$$

where $h_p^i \in \mathcal{H}^{\bar{C}_i} = \mathcal{H}^{C_i}$ and s_i is a Schwartz-test function in $\mathcal{H}^{(C_i, \bar{C}_i)}$. Then the restriction of $\varphi^{|f^i)(h^i|}$ to $E_{\text{rel}}^{C_i}$ is $\varphi^{(A^{C_i})}$, so that by (26) and a recurrence process the restriction of

$$\underset{i=1}{\overset{n}{\times}} D_{E_{\text{rel}}^{\{N\}}}(\varphi^{|f_i)(h_i|})$$

to $E_{\text{rel}}^{\{N\}}$ is

$$\underset{i=1}{\overset{n}{\times}} D_{E_{\text{rel}}^{\{N\}}}(\varphi^{(A^{C_i})}).$$

Furthermore, the subspaces $E_{\text{rel}}^{C_i \cup \bar{C}_i}$, $i = 1, 2, \cdots, n$, satisfy the conditions of Corollary 6. It remains to show then, in order to use the result of this corollary, that f_i and h_i are in $\mathfrak{D}_2^{C_i \cup \bar{C}_i}$ (Lemma 9). But this results from the estimates

$$\|f_i\|_2^{C_i \cup \bar{C}_i} \leq C\left(\sum_p |\lambda_p| (\|f_p^i\|_2^{C_i})^2\right)^{\frac{1}{2}} \left(\sum_p |\lambda_p| (\|h_p^i\|_2^{\bar{C}_i})^2\right)^{\frac{1}{2}},$$
$$\|h_i\|_2^{C_i \cup \bar{C}_i} \leq C\left(\sum_p |\lambda_p| (\|h_p^i\|_2^{\bar{C}_i})^2\right),$$

obtained with the help of Schwartz's inequality. Since

$$\underset{i=1}{\overset{n}{\times}} D_{E_{\text{rel}}^{\{N\}}}(\varphi^{(A^{C_i})})$$

is the restriction to $E_{\text{rel}}^{\{N\}}$ of a function in $\mathcal{C}(E_{\text{rel}}^{\{\hat{N}\}}, \hat{\sigma})$, it is itself in $\mathcal{C}(E_{\text{rel}}^{\{N\}}, \sigma)$.

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APPENDIX

We want to prove tensor decompositions (41a) and (41b) for any pair of disjoint clusters C and C'. Let us first prove (41a). If $h^C \in \mathcal{H}^C$, $h^{C'} \in \mathcal{H}^{C'}$, and $h^{(C,C')} \in \mathcal{H}^{(C,C')}$, we define their tensor product as the element of $\mathcal{H}^{C \cup C'}$ given by

$$(h^C \otimes h^{C'} \otimes h^{(C,C')})(a^{C \cup C'}) = h^C(a^C) \cdot h^{C'}(a^{C'}) \cdot h^{(C,C')}(a^{(C,C')}); \quad \text{(A1)}$$

here a^C, $a^{C'}$, and $a^{(C,C')}$ are the components of $a^{C \cup C'}$ in the configuration subspaces of E_{rel}^C, $E_{\text{rel}}^{C'}$, and $E^{(C,C')}$, respectively. The scalar product $(f|g) = \int \bar{f} \cdot g \, da^{C \cup C'}$ on $\mathcal{H}^{C \cup C'}$ defines a pre-Hilbertian structure on the space of linear combinations of these vectors such that

$$(h^C \otimes h^{C'} \otimes h^{(C,C')} \mid g^C \otimes g^{C'} \otimes g^{(C,C')}) = (h^C \mid g^C) \cdot (h^{C'} \mid g^{C'}) \cdot (h^{(C,C')} \mid g^{(C,C')}),$$

where, for example, $(f^C \mid g^C) = \int \bar{f}^C g^C \, da^{\{C\}}$. This is obvious since with our choice of canonical symplectic basis one has $da^{C \cup C'} = da^C \, da^{C'} \, da^{(C,C')}$. Hence the closure of this pre-Hilbertian space is the right tensor product $\mathcal{H}^C \otimes \mathcal{H}^{C'} \otimes \mathcal{H}^{(C,C')}$, which is consequently contained in $\mathcal{H}^{C \cup C'}$. But, owing to (43), this tensor product contains the set of translates of $\exp[-Q(a^{C \cup C'})]$, which is a total set in $\mathcal{H}^{C \cup C'}$ owing to Wiener theorem. Hence one has the equality (41a). Now, in order to prove (41b), it is sufficient to verify it on the total set of vectors $h^C \otimes h^{C'} \otimes h^{(C,C')}$, where, owing to (39) and definition (40), it is immediate.

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Polynomial Bases for Representations of Semisimple Lie Algebras

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It is shown that the polynomial bases for representations of a semisimple Lie algebra are just the various terms of typical concomitants of the Lie algebra. Consequently, the construction of polynomial bases reduces to a problem in the theory of invariants.

INTRODUCTION

In the evaluation of Wigner coefficients, fractional parentage coefficients, matrix elements of operators such as angular momentum, etc., it is useful to realize the Lie algebras that one comes across as differential operators in certain indeterminates and their representation spaces as homogeneous polynomials in these indeterminates.[1] The construction of a basis set of polynomials which is suitable to the problem at hand is often required. The aim of this article is to show that the problem is closely related to the theory of invariants[2] which was developed long ago by mathematicians.

I. ABSOLUTE, RELATIVE, AND SEMI-INVARIANTS

Following Weyl,[3] we give definitions of the absolute and relative invariants of a semisimple Lie algebra $\mathfrak{L}$ as follows: Let $\{A\}$ be the set of matrices representing $\mathfrak{L}$ in a certain irreducible representation (IR). We denote the vectors in its carrier space by $x = (x_1, \cdots, x_n)$. A homogeneous polynomial[4] $f(x_1, \cdots, x_n)$ is said to be an absolute invariant of $\mathfrak{L}$ with respect to the representation $\{A\}$ if

$$d(A)f = \sum dx_i \frac{\partial f}{\partial x_i} = 0 \quad \text{for all} \quad A \in \{A\},$$

where $dx = (dx_1, \cdots, dx_n) = Ax^T$. $f(x_1, \cdots, x_n)$ is said to be a relative invariant of $\mathfrak{L}$ if $d(A)f = k(A)f$ for all $A \in \{A\}$, where $k(A)$ is a real number.

We define semi-invariants of $\mathfrak{L}$ as follows: A homogeneous polynomial $f(x_1, \cdots, x_n)$ is said to be a semi-invariant if $d(A)f = k(A)f$ whenever A represents an element $a \in \mathfrak{K}$ and if $d(A)f = 0$ whenever A represents an $a \in \mathfrak{L}$, where $\mathfrak{L} = \mathfrak{K} + \mathfrak{L}^+ + \mathfrak{L}^-$ is the decomposition of $\mathfrak{L}$ into the Cartan subalgebra $\mathfrak{K}$, the positive root algebra $\mathfrak{L}^+$ and negative root algebra $\mathfrak{L}^-$.

These three definitions enable us to state and prove Theorems 1–4.

Theorem 1: There exist a finite set of absolute invariants (with respect to $\{A\}$) such that every absolute invariant (with respect to $\{A\}$) can be written as a polynomial in them. The finite set is called the finite integrity basis for the absolute invariants.

Proof: It is easily seen that (i) the operators $d(A) = \sum dx_i \partial/\partial x_i$ when acting on a space of polynomials in $x_1, \cdots, x_n$ span a Lie algebra $d(\mathfrak{L}, x)$ which is isomorphic to $\mathfrak{L}$ with the multiplication

$$[d(A), d(B)] = d(B)\, d(A) - d(A)\, d(B).$$

(ii) The space of polynomials $\{df\}$, where f is a homogeneous polynomial in $x_i, \cdots, x_n$ and d's are polynomials in the operators $d(A)$, $A \in \{A\}$, is finite dimensional.

By the Hilbert basis theorem[5] there exist a finite number of absolute invariants $I_1, \cdots, I_k$ such that every absolute invariant I may be written

$$I = F_1 I_1 + \cdots + F_k I_k,$$

where $F_1, \cdots, F_k$ are homogeneous but not necessarily invariants. Consider the spaces $V_i = \{dF_i\}$; the d's are polynomials in the operators $d(A)$, $A \in \{A\}$ and $i = 1, \cdots, k$. These are invariant under $d(\mathfrak{L}, x)$, and each space is completely reducible with respect to $d(\mathfrak{L}, x)$.

The space of an IR of $d(\mathfrak{L}, x)$ is determined by an extreme weight vector P, i.e., one such that $d(A)P = \lambda(A)P$ for each A corresponding to an $a \in \mathfrak{K}$ and $d(A)P = 0$ for each A corresponding to an $a \in \mathfrak{L}^+$, in other words, an extreme weight vector and a semi-invariant are identical. The numbers $\lambda(A)$ arranged in a fixed order are called the weight of P. If P is extreme and of weight zero, then it can be shown that P is an absolute invariant.

Let $v_{ij}, j = 1, 2, \cdots$, be a basis for all the extreme vectors of V_i. Let $\xi_1, \cdots, \xi_m$ be a maximal linearly independent set of vectors picked out from all the extreme vectors $v_{11}I_1, v_{12}I_1, \cdots, v_{k1}I_k, v_{k2}I_k, \cdots$. Then the spaces U_p, $p = 1, \cdots, m$, determined by $\xi_1, \cdots, \xi_m$, are linearly independent,[6] and the vectors in each U_p have one of the $I_1, \cdots, I_k$ as a factor. Consider the direct sum $U_1 + \cdots + U_m = V$. Then $F_1 I_1 \in V$ because $F_1 I_1$ belongs to the direct sum of the spaces determined by $v_{11}I_1, v_{12}I_1, \cdots$. Similarly,

$F_2I_2, \cdots, F_kI_k$ all belong to V. Hence $I \in V$. Consequently, $I = \eta_1 + \cdots + \eta_m$, where $\eta_i \in U_i$ and is an extreme vector of weight zero[6] and hence an absolute invariant. Each η is of the form $v_{ij}I_j$, where v_{ij} is extreme and I_j is an absolute invariant. Hence v_{ij} is also an absolute invariant. Hence v_{ij} is again expressible as $\sum_{i=1}^{k} L_{iq}I_q$. Repeating the argument as often as required, since the degree of I is finite, we conclude that I is expressible in terms of $I_1, \cdots, I_k$ only.

II. CONCOMITANTS

Let $\{A\}$ and $\{B\}$ be two IR's of $\mathfrak{L}$. We denote by $x = (x_1, \cdots, x_n)$ and $y = (y_1, \cdots, y_m)$, vectors in the carrier spaces of $\{A\}$ and $\{B\}$, respectively. We define a concomitant of $\mathfrak{L}$ with respect to the two representations $\{A\}$ and $\{B\}$ as follows.

For a semisimple Lie algebra $\mathfrak{L}$, there exists an automorphism θ such that $\theta h = -h$ for $h \in \mathfrak{H}$ and $\theta a_\alpha = a_{-\alpha}$ for $a_\alpha \in \mathfrak{L}^+$, where α is a positive root and $a_{-\alpha} \in \mathfrak{L}^-$. Further, θ^2 is the identity transformation.

A polynomial $f(x_1, \cdots, x_n, y_1, \cdots, y_m)$ homogeneous in x's and homogeneous in y's is said to be a concomitant of $\mathfrak{L}$ with respect to $\{A\}$ and $\{B\}$ if

$$[d_x(A) + d_y(\theta B)]f = \sum_{i=1}^{n} dx_i \frac{\partial f}{\partial x_i} + \sum_{j=1}^{m} dy_i \frac{\partial f}{\partial y_i} = 0,$$

for every $A \in \{A\}$ and $B \in \{B\}$, where A and B represent the same element, $a \in \mathfrak{L}$, in the two representations, respectively, $dx = (dx_1, \cdots, dx_n) = Ax^T$, and $dy = (dy_1, \cdots, dy_m) = \theta By^T$.

Theorem 2: The system of concomitants of $\mathfrak{L}$ (with respect to the representations $\{A\}$ and $\{B\}$) have a finite integrity basis.

Proof: Let

$$D(a) = \sum_{i=1}^{n} dx_i \frac{\partial}{\partial x} + \sum_{i=1}^{m} dy_i \frac{\partial}{\partial y_i}.$$

The operators $D(a)$, $a \in \mathfrak{L}$, span a Lie algebra $D(\mathfrak{L})$ under the multiplication $[D(a), D(b)] = D(b)D(a) - D(a)D(b)$, when they act upon the space of all polynomials in $x_1, \cdots, x_n, y_1, \cdots, y_m$. $D(\mathfrak{L})$ is isomorphic to $\mathfrak{L}$. Observing that a concomitant is then an extreme vector of $D(\mathfrak{L})$ with weight zero, we can prove the theorem exactly as Theorem 1.

Theorem 3: Let $f_1(x), \cdots, f_k(x)$ be a basis for the carrier space of an IR of $d(\mathfrak{L}, x)$ such that the matrix of $d(\theta A)$ is the negative of the transpose of the matrix of $d(A)$. Let $g_1(y), \cdots, g_k(y)$ be a similar basis for the space of an equivalent IR of $d(\mathfrak{L}, y)$. Then $f_1(x)g_1(y) + \cdots + f_k(x)g_k(y)$ is a concomitant of $\mathfrak{L}$.

Remark: It can be shown that it is possible to choose a basis with the property stated in the theorem and also such that the polynomials $f_1(x)$ and $g_1(y)$ are extreme.[5]

Proof: Let

$$d_x(A)f_i(x) = \sum_{j=1}^{k} D(A)_{ij} f_j.$$

Then

$$d_x(\theta A)f_i(x) = -\sum_{j=1}^{k} D(A)_{ji} f_j.$$

Let

$$d_y(B)g_i(y) = \sum_{j=1}^{k} D(B)_{ij} g_j;$$

then

$$d_y(\theta B)g_i(y) = -\sum_{j=1}^{k} D(B)_{ji} g_j,$$

where A and B represent the same element $a \in \mathfrak{L}$ and $D(A)_{ij}$ and $D(B)_{ij}$ are numerical coefficients. We have

$$\begin{aligned} D(a)&[f_1(x)g_1(y) + \cdots + f_k(x)g_k(y)] \\ &= \sum_{i=1}^{k} [d_x(A)f_i(x)g_i(y) + f_i(x)\, d_y(\theta B)g_i(y)] \\ &= \sum_{i=1}^{k} \left(\sum_{j=1}^{k} D(A)_{ij} f_j(x)g_i(y) - \sum_{j=1}^{k} D(B)_{ji} g_j(y)f_i(x) \right) \\ &= \sum_{p=1}^{k} \sum_{q=1}^{k} f_p(x)f_q(y)[D(A)_{pq} - D(B)_{pq}] = 0. \end{aligned}$$

As the basis, $f_1, \cdots, f_k$ and $g_1, \cdots, g_k$ are similarly transformed by $d(A)$ and $d(B)$, respectively.

Theorem 4: If $\phi(x_1, \cdots, x_n, y_1, \cdots, y_m)$ is a concomitant, then ϕ is a sum of concomitants of the form

$$f = f_1(x)g_1(y) + \cdots + f_k(x)g_k(y),$$

where f_1 and g_1 are extreme; the two sets $f_1, \cdots, f_k$ and $g_1, \cdots, g_k$ are bases for spaces irreducibly invariant under $d(\mathfrak{L}, x)$ and $d(\mathfrak{L}, y)$, respectively, such that the representations are equivalent representations of $\mathfrak{L}$.

Proof: Let

$$\phi = \sum_{p_1 \cdots p_n, q_1 \cdots q_m} x_1^{p_1} \cdots x_{n_n}^{p_n} y_1^{q_1} \cdots y_m^{q_m}.$$

$$\begin{aligned} D(a)\phi = &\sum_{p_1 \cdots p_n, q_1 \cdots q_m} d(A)x_1^{p_1} \cdots x_n^{p_n} y_1^{q_1} \cdots y_m^{q_m} \\ &+ \sum_{p_1 \cdots p_n, q_1 \cdots q_m} x_1^{p_1} \cdots x_n^{p_n}\, d(\theta B) y_1^{q_1} \cdots y_m^{q_m} = 0, \end{aligned}$$

which shows that the monomonials $x_1^{p_1} \cdots x_n^{p_n}$ span a space $\mathfrak{U}$ invariant under $d(\mathfrak{L}, x)$. Also, the monomials $y_1^{q_1} \cdots y_m^{q_m}$ span a space invariant under $d(\mathfrak{L}, y)$.

Let the number of distinct monomials $x_1^{p_1}\cdots x_n^{p_n}$ be not greater than that of the distinct monomials $y_1^{q_1}\cdots y_m^{q_m}$. Without loss of generality, we assume that the space $\mathfrak{V}$ is irreducible; otherwise, ϕ will be found to be merely a sum of two concomitants. Let $f_1\cdots f_k$ be a basis of $\mathfrak{V}$ with respect to which the matrix of $d(\theta A)$ is the negative of the transpose of the matrix of $d(A)$, and let f_1 be extreme. Expressing all $x_1^{p_1}\cdots x_n^{p_n}$ in terms of $f_1\cdots f_k$, we have

$$\phi = f_1(x)g_1 + \cdots + f_k(x)g_k(y),$$

where $g_1, \cdots, g_k$ are seen to be linearly independent and span a space V invariant under $d(\mathfrak{L}, y)$. If this space is reducible for $d(\mathfrak{L}, y)$, then ϕ would again be a sum of two concomitants, which implies that $\mathfrak{V}$ is reducible. Hence it follows that $g_1, \cdots, g_k$ span V, which is also irreducible.

Let

$$d_x(A)f_i = \sum F(A)_{ij}f_j \quad \text{and} \quad d_y(B)g_i = \sum G(B)_{ij}g_j.$$

Then

$$D(a)\phi = \sum_i d_x(A)f_i g_i + \sum_i f_i\, d_y(\theta B)g_i$$
$$= \sum_i\sum_j F(A)_{ij}f_j g_i + \sum_i f_i \sum G(\theta B)_{ij}g_j = 0.$$

The coefficient of $f_i g_j$ in the above is $F(A)_{ji} + G(\theta B)_{ij} = 0$. By our choice of the basis $f_1, \cdots, f_k$, $F(A)_{ji} = -F(\theta A)_{ij}$; hence, the above equation implies that the representations of $d(\mathfrak{L}, x)$ in $\mathfrak{V}$ and of $d(\mathfrak{L}, y)$ in V are equivalent representations of $\mathfrak{L}$.

$g_1(y)$ is also extreme because

$$d_x(A)f_1 = \sum_{j=1}^{k} F(A)_{1j}f_j = 0$$

for matrices A corresponding to each $a \in \mathfrak{L}^+$, and therefore

$$d_y(B)g_1 = \sum G(B)_{ij}g_j = \sum F(A)_{1j}g_j = 0,$$

for every B representing the same $a \in \mathfrak{L}^+$ as the matrix A.

Thus it is seen that, corresponding to any two semi-invariants of equal weights with respect to the representations $\{A\}$ and $\{B\}$, respectively, there is a concomitant of $\mathfrak{L}$ with respect to the two representations. Conversely, every concomitant is a sum of concomitants, each of which is determined by two semi-invariants with respect to $\{A\}$ and $\{B\}$ and has equal weights.

In the case of the Lie algebras A_n, B_n, C_n, and D_n, choosing $\{B\}$ as the so-called self-representation, one obtains the concomitants of the full linear, orthogonal, and symplectic groups thoroughly discussed by mathematicians long ago.

Now the semi-invariants of $\mathfrak{L}$ with respect to an IR $\{A\}$ of $\mathfrak{L}$ also have a finite subsystem in terms of which all the semi-invariants can be expressed as polynomials (that the highest weight polynomials have a finite subset in terms of which every highest weight polynomial could be expressed has been observed by Sharp and Lam[7]; we point out here the source where it was proved) because the semi-invariants are nothing but the relative invariants of the solvable Lie algebra $\mathfrak{L}^+ + \mathfrak{H}$. For the proof we refer to Weitzenböck,[8] who showed the existence of such a finite subsystem for the relative invariants of solvable groups which he called the finite integrity basis. He obtains the relative invariants of each linear operator as the simultaneous semi-invariants of a certain set of binary forms (see Ref. 5, p. 227, for the definition of the semi-invariant of a binary form).

In invariant theory a finite set of concomitants is said to be complete if every concomitant can be expressed as a polynomial in the members of the set. Theorems were established to examine whether a given set of covariants of given binary forms is complete.[2] The invariant theory shows that the number of elements in the finite integrity basis increases tremendously with the rank of the Lie algebra $\mathfrak{L}$; their determination becomes extremely tedious, and no induction argument for asserting the completeness of a given set of concomitants which holds good for any algebra $\mathfrak{L}$ is found in the theory developed so far.

It may not be out of place to remark that the highest weight polynomials determined in a series of papers[9] in this journal are merely semi-invariants of certain semisimple Lie algebras.

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Kinks and the Dirac Equation

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In a model quantum theory of interacting mesons, the motion of certain conserved particlelike structures is discussed. It is shown how collective coordinates may be introduced to describe them, leading, in lowest approximation, to a Dirac equation.

1. INTRODUCTION

It has often been suggested that the particle sources of fields might really be very localized bound states of the same fields. There are at least two important reasons for seeking theoretical models of this type; first they should reduce the number of independent fundamental variables, and second they might lead to a theory of interactions that is free from the difficulties associated with point interactions. In such a model the localized particlelike states may behave like point sources for interaction with weak external fields, but exhibit a structure in strong fields.

This paper is mainly concerned with a model theory of a self-interacting meson-like field. Considered classically, the theory has particlelike solutions; in particular there are solutions that describe static localized concentrations of field strength. The problem is to find the analogs of these in the quantized theory; the analysis suggests that these may appear as states with fermion symmetry characters, and a systematic method of solution is developed starting from an approximation in which the particlelike states are described by independent variables satisfying a Dirac equation.

Although the starting point is a relativistic theory, the discussion is presented in a form that is not manifestly covariant, following the canonical quantization procedures. At this stage a nonrelativistic description exhibits more clearly the physical ideas inherent in the model.

The problem is that of describing certain collective motions of a quantized system. That is analyzed in the usual way by introducing auxiliary redundant coordinates to describe the collective modes and imposing constraints through supplementary conditions that link them to the original variables.

2. THE ONE-DIMENSIONAL MODEL (A)

A simple one-dimensional model was considered earlier, and it will be useful to refer to it as Model A. The field variable is an angle $\alpha(x, t)$ and all physically observable quantities depend only on $\alpha \bmod (2\pi)$; the Lagrangian density is taken to be

$$-\frac{1}{8\pi}\left[\left(\frac{\partial\alpha}{\partial x}\right)^2-\left(\frac{\partial\alpha}{\partial t}\right)^2\right]-\frac{K^2}{4\pi}(1-\cos\alpha),$$

where K is a mass constant [units with $\hbar = c = 1$ will be used throughout].

The vacuum condition is taken as $\cos\alpha = 1$, and all solutions are assumed to satisfy the boundary condition that

$$\cos\alpha \to 1 \quad \text{as} \quad x \to \infty.$$

There is then a conserved current giving rise to the quantum number

$$N=\frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\frac{\partial\alpha}{\partial x}\right)dx=\frac{1}{2\pi}[\alpha(+\infty)-\alpha(-\infty)].$$

This is interpreted as a particle number. There is a localized static solution of the classical field equation for which $\alpha(-\infty) = 0$ and $\alpha(+\infty) = 2\pi$.

This field theory may be quantized in the canonical manner, with the conjugate variable

$$\beta(x,t)=\frac{1}{4\pi}\frac{\partial\alpha}{\partial t}.$$

So long as the fields are weak, $1-\cos\alpha \sim \frac{1}{2}\alpha^2$, and the theory describes "mesons" with mass K, in states with $N = 0$. A state with $N = 1$ may be created by operating upon an $N = 0$ state, e.g., the vacuum, with the (singular) operator,

$$K=\exp\left[2\pi i\int_{x_0}^{\infty}\beta\,dx\right],$$

that sends $\alpha(x) \to \alpha(x) + 2\pi\theta(x - x_0)$, a step at $x = x_0$; this is interpreted as an ideal particle singularity at x_0, but is not by itself a stationary state. It was shown, however, that the operators FK, where $F = \exp(\pm\frac{1}{2}i\alpha(x_0))$, satisfy the equations

$$\left[\pm\frac{\partial}{\partial x_0}-\frac{\partial}{\partial t}\right]FK=0,$$

so that FK may be identified with a particle creation or annihilation operator at the point x_0; furthermore,

these operators associated with different x_0 anticommute. This "particle" is a massless neutrinolike object that can be introduced as a starting point for the description of massive particles.

3. THE THREE-DIMENSIONAL MODEL (B)

A three-dimensional model was suggested that has rather similar classical properties[1]; this will be called model B and is the main subject of this paper. The field variables are four, $\phi_\rho(\mathbf{x}, t)$, $\rho = 0, 1, 2, 3$, constrained to satisfy $\sum \phi_\rho^2 = 1$ everywhere; it is convenient to describe them alternatively by a quaternion

$$U(\mathbf{x}, t) = \phi_0 + i\tau_\alpha \phi_\alpha .$$

(Indices such as α are summed from 1 to 3; τ_α denote a standard set of Pauli matrices, which will often but *not* always be associated with an "isobaric spin.")

The fields are described by the gradients $B_{\alpha\mu}$ defined by

$$\partial_\mu U = i\tau_\alpha B_{\alpha\mu} U$$

and so satisfy conditions

$$\partial_\nu B_{\alpha\mu} - \partial_\mu B_{\alpha\nu} = 2\epsilon_{\alpha\beta\gamma} B_{\alpha\mu} B_{\gamma\nu},$$

the $\epsilon_{\alpha\beta\gamma}$ being the structure constants associated with the quaternion algebra. The Lagrangian density of the model B is taken as

$$-(\epsilon/8\pi^2)[(B_{\alpha\mu}B_{\alpha\mu})^2 - (B_{\alpha\mu}B_{\alpha\nu})(B_{\beta\mu}B_{\beta\nu}) + 2K^2(B_{\alpha\mu}B_{\alpha\mu})],$$

where K is a mass constant and ϵ a dimensionless parameter, whose value should probably be $\frac{1}{2}(\hbar c)$.

The vacuum condition is taken to be $U = 1$, and there is the boundary condition

$$U(\mathbf{x}, t) \to 1 \quad \text{as} \quad \mathbf{x} \to \infty.$$

There is a conserved current that leads to the quantum number

$$N = \frac{1}{2\pi^2} \int \det(B_{\alpha i})\, d^3x.$$

There are localized solutions of the classical field equations for which $N = 1$ and which have properties that are classical analogs of particles with spin and isobaric spin $\frac{1}{2}$. Weak field solutions describe a triplet of massless mesons. Meson mass could be introduced by an additional term in the Lagrangian destroying its high symmetry, but this is not particularly relevant to the problem of the existence of particlelike structures, whose finite mass is governed classically by the constant K.

The field theory may be quantized in the canonical manner. The conjugate variables are (apart from a numerical factor) the local rotation operators (fourth components of spin currents)

$$I_\alpha(\mathbf{x}) = \frac{\epsilon}{4\pi^2}[(B_{\gamma i}B_{\gamma i} + K^2)\delta_{\alpha\beta} - (B_{\alpha i}B_{\beta i})]B_{\beta 0} = G_{\alpha\beta}B_{\beta 0}$$

(i denotes the space indices, summed from 1 to 3, 0 is the real time index), with the fundamental commutation relations

$$[I_\alpha(\mathbf{x}'), U(\mathbf{x})] = -\tfrac{1}{2}\tau_\alpha U(\mathbf{x})\delta(\mathbf{x}' - \mathbf{x}),$$

from which

$$[I_\alpha(\mathbf{x}'), B_{\beta i}(\mathbf{x})] = i\epsilon_{\alpha\beta\gamma}B_{\gamma i}(\mathbf{x})\delta(\mathbf{x}' - \mathbf{x}) + \tfrac{1}{2}i\delta_{\alpha\beta}\partial_i\delta(\mathbf{x} - \mathbf{x}').$$

In terms of these variables I and B, the physical quantities are:

Hamiltonian:

$$H(I, B) = \int I_\alpha(\mathbf{x})G^{-1}_{\alpha\beta}I_\beta(\mathbf{x})\, d^3x + \frac{\epsilon}{8\pi^2}\int \{[(B_{\alpha i}B_{\alpha i})^2 - (B_{\alpha i}B_{\alpha j})(B_{\beta i}B_{\beta j})] + 2K^2(B_{\alpha i}B_{\alpha i})\}\, d^3x,$$

where $G_{\alpha\beta}(B)$ is the inertia tensor relating I_α with $B_{\beta 0}$, defined above;

momentum:

$$P_i = 2\int I_\alpha B_{\alpha i}\, d^3x;$$

angular momentum:

$$J_i = 2\epsilon_{ijk}\int I_\alpha x_j B_{\alpha k}\, d^3x.$$

There are two internal symmetries leading to the conserved quantities

$$H_\alpha = \int I_\alpha\, d^3x$$

and

$$\tilde{H}_\alpha = \int \tilde{I}_\alpha\, d^3x;$$

here I_α rotates U "on the right":

$$[\tilde{I}_\alpha(\mathbf{x}'), U(\mathbf{x})] = U(\tfrac{1}{2}\tau_\alpha)\delta(\mathbf{x}' - \mathbf{x}).$$

The $\tilde{I}_\alpha$ are an orthogonal transformation of the I_α, defined by

$$\tau_\alpha \tilde{I}_\alpha = U^+\tau_\beta I_\beta U,$$

and commute with the I_α.

4. TOPOLOGY

A particular field distribution, such as $U(\mathbf{x})$, is a mapping from coordinate space onto the space of field values. In model A the latter is a circle; in model B it is a three-dimensional sphere S^3. In both cases

"infinity" is mapped onto a fixed point; it is then possible to regard the coordinate space as a spherical rather than Euclidean space, so that in both models the mapping is from one sphere to another of the same dimension, with a fixed point of one mapping into a fixed point of the other. The quantum number N is then just the degree of the mapping, which is the only topological characteristic of the mapping of one sphere onto another.

The topological significance of N means that the mapping space (the space of all maps with a fixed pair of corresponding points) is composed of subspaces labeled by N, so that maps in one subspace are all deformable into one another but not into those of another subspace. The classical evolution of the system may be pictured as a deformation of the map, thus showing alternatively how N must be a classical constant of the motion.

A quantum state may be regarded as a functional of $U(\mathbf{x})$, i.e., a function defined on the mapping space. As N commutes with H, a state initially defined on just one subspace will remain on that subspace.

A map with $N = 1$ will have, by Brouwer's theorem, at least one point where $U = -1$ and $\det B_{\alpha i} > 0$; this point may be identified with the "center" of the particle. More generally there may be $m > 1$ points at which $U = -1$ and $\det B > 0$; then there will also be $(m - 1)$ points at which $U = -1$ and $\det B < 0$; this situation would be identified with a configuration containing m particles and $(m - 1)$ antiparticles.

The difficulty in trying to associate these states with fermions having spinor symmetries is that the latter could not be (proper single-valued) functions defined on the mapping space. In model A indeed, the operators associated with particles involved $F = \exp(\frac{1}{2}i\alpha)$, which is a double-valued function on the circle of values $\exp(i\alpha)$.

To define such functions properly, we must go to the covering space of the mapping space, which in the case of model A means using the angle α instead of the basic field variables $\cos\alpha$, $\sin\alpha$. It does not seem possible to give such a simple explicit representation in the three-dimensional case. However, it is known that the covering space for maps from S^3 to S^3 is double sheeted; in particular, a 2π rotation of a map of degree one is nontrivial, corresponding to a path from a point on one sheet to its mate on the other. This gives the possibility of defining spinor quantities on the covering space.

A map with $N = 1$ may be deformed so that the region where U is significantly different from 1 is very small; the field distribution is then generally called a "kink," [2] e.g., a steep step of 2π in model A. Maps with $N = 2$ may be constructed by putting two kinks at different points, and so on. These could be added in either order giving the same maps, but the operations correspond to opposite points in the covering space, as it is known[2] that a path interchanging two kinks is nontrivial; it is therefore equivalent to a path corresponding with a 2π rotation, so that antisymmetry of the particle operators is naturally associated with change of sign on 2π rotation. Williams[3] showed functions of this type could be formed for the model B; these constructs, however, were not evidently associated with particle structures, and the object of this paper is to show how more realistic structures may be defined.

5. PARTICLE COORDINATES

If quantum particlelike states exist they will be characterized by quantum numbers such as momentum, spin, etc; we introduce some corresponding variables.

Evidently one such variable should be a position, denoted by $\mathbf{x}_0$ with a corresponding momentum $\mathbf{p}_0 = -i\nabla_0$. In model A this is all; there are just particles and antiparticles, steps propagating to the right and to the left, respectively; the operators FK depend only on the parameter x_0.

In model B there must be some internal spin variables. To find the appropriate choice, consider the static classical field solutions. The only ones that have been found are characterized by the central position $\mathbf{x}_0$ and by a proper orthogonal matrix $e_{\alpha i}$ that links the space and isospin directions. The classical theory, moreover, has many similarities to the semiclassical theory of the symmetrical pseudoscalar meson field[4] in which the spin operators $\sigma_i\tau_\alpha$ (of the usual meaning) become replaced by $e_{\alpha i}$. This suggests that we should introduce such a matrix as an internal coordinate. Conjugate to $e_{\alpha i}$ are the rotation operators t_α, s_i that rotate the corresponding coordinate labels and are related by the identity

$$s_i + e_{\alpha i}t_\alpha = 0,$$

so that $s_i s_i = t_\alpha t_\alpha$, and s_i, t_α have eigenstates with the same total spin values (in terms of Eulerian angles these are just the solid harmonics).

A particle operator depending on $\mathbf{x}_0$ and $e_{\alpha i}$ would then describe not just one fermion or doublet of fermions but a family of isobars; the operator would be a generating function from which the different states could be projected. This seems both reasonable and quite desirable.

6. COLLECTIVE COORDINATES

We seek to introduce the particle variables as collective coordinates, identifying them with appropriate functions of the original field variables.

In a general notation the standard procedure is this. We want to find solutions of the Schrödinger equation

$$H\psi(q) = E\psi(q),$$

where q denotes the set of independent physical variables. We introduce auxiliary variables q_a and supplementary conditions A_k, acting only in the q_a space, with

$$[A_k, A_l] = 0, \quad [H, A_k] = 0,$$

so that the system

$$H\psi(q, q_a) = E\psi(q), \quad A_k\psi(q, q_a) = 0$$

is trivially equivalent to the original one. We then make a suitable canonical transformation in the complete space; denote this by S so that

$$H' = SHS^{-1}, \quad A' = SAS^{-1}, \quad \psi' = S\psi,$$

with new dynamical equations $H'\psi' = 0$, $A'\psi' = 0$.

Suppose now $H^* = H' + \sum A'_k\lambda_k$, where the λ_k are some multipliers, arbitrary functions of the variables, and that ψ^* is an eigenstate of H^*,

$$H^*\psi^* = E\psi^*;$$

then we can form an eigenstate of H' by projecting onto the subspace allowed by the supplementary conditions

$$\psi' = \delta(A')\psi^*,$$

for, since $[H', A'] = 0$,

$$H'\psi' = \delta(A')H'\psi^* = \delta(A')H^*\psi^* = E\psi'.$$

In the original description the projected state is

$$\psi = S^\dagger\delta(A')\psi^* = \delta(A)S^\dagger\psi^*.$$

This analysis is quite general; it is useful if we can find multipliers λ_k such that H^* has the form $H + H_a + H_{\text{int}}$, where H_a is a suitable Hamiltonian describing motion of the collective coordinates and H_{int} can be treated as a perturbation. There will be different states ψ^* that project into the same state; this redundancy arises because the same original state may be described either in the original variables or with the help of the auxiliary ones; this is not generally a serious problem when the collective states are clearly physically distinguishable.

In our application we can describe particle states either by kinks in the meson fields or by the auxiliary coordinates, and there will not be any difficulty provided that in the H^* description we avoid any kinks in the meson fields, as indeed we should like to do since they cannot be generated by perturbations.

The structure of the transformations has the following typical form. Suppose we want to identify q_a with q and that p_a, p are the corresponding conjugate variables. We start with

$$H(q, p)\psi = E\psi, \quad \delta(q_a)\psi = 0.$$

The first step is to make the supplementary condition identify q_a with q; this is achieved by $S_1 = \exp(-ip_aq)$, giving

$$H(q, p + p_a) \quad \text{and} \quad \delta(q_a - q)\psi = 0.$$

The second step is to replace q by $q + q_a$; $S_2 = \exp(iq_ap)$ gives

$$H(q + q_a, p_a) \quad \text{with} \quad \delta(-q)\psi = 0.$$

The complete transformation is

$$S = S_2S_1 = \exp(iq_ap)\exp(-ip_aq).$$

7. APPLICATION TO MODEL A

The original variables are $\alpha(x)$, $\beta(x)$, with Hamiltonian

$$H = \int_{-\infty}^{\infty}\left[2\pi\beta^2 + \frac{1}{8\pi}\left(\frac{\partial\alpha}{\partial x}\right)^2 + \frac{K^2}{4\pi}(1 - \cos\alpha)\right]dx.$$

Introduce the auxiliary variables x_0, p_0 with the original supplementary condition

$$A\psi = p_0\psi = 0.$$

An appropriate transformation is

$$S = \exp\left[i\int_{x_0}^{\infty} 2\pi\beta\, dx\right]\exp[\tfrac{1}{2}i\alpha(x_0)],$$

which gives

$$H(\beta, \alpha) \to H(\beta - \tfrac{1}{2}\delta(x - x_0), \alpha + 2\pi\theta(x - x_0)) = H'$$

and

$$p_0 \to p_0 + 2\pi\beta(x_0) - \tfrac{1}{2}\left(\frac{\partial\alpha}{\partial x}\right)_{x_0} - \pi\delta(0) = p_0'.$$

Then

$$H' = H + \tfrac{1}{2}\alpha'(x_0) - 2\pi\beta(x_0) + \pi\delta(0),$$

and

$$H_+^* = H' + p_0' = H + p_0$$

exhibits a complete separation of the modes.

A similar transformation may be made with the factor $e^{\frac{1}{2}i\alpha}$ replaced by $e^{-\frac{1}{2}i\alpha}$; then

$$H_-^* = H' - p_0' = H - p_0.$$

These transformations introduce variables describing massless right- and left-going particles. The coordinate description of the particles can easily be generalized to a field description, and then, as described before,

they can be used as a basis for a self-consistent description of a massive particle.

This analysis is somewhat unsatisfactory because of the singular nature of the operators S. Alternatively the following method may be followed which provides a better analog of that appropriate in three dimensions. The sharp step described by $\theta(x - x_0)$ is replaced by some suitable smooth approximation to it, $\theta_1(x - x_0)$, which has a small finite width

$$S = \exp\left(i2\pi\int\beta(x)\theta_1(x - x_0)\right) \times \exp\left(i\tfrac{1}{2}\int\alpha(x)\theta_1'(x - x_0)\right).$$

The only difference in the analysis is that now there is a contribution from the "potential energy" term in H, so that

$$H_+^* = H' + p_0' = H + p_0 + \frac{K^2}{4\pi}\int[\cos\alpha - \cos(\alpha + 2\pi\theta_1)]\,dx.$$

If we treat the last term in perturbation, the first approximation to it is a constant

$$\frac{K^2}{4\pi}\int(1 - \cos 2\pi\theta_1)\,dx = m$$

proportional to the width of the step. However, the form $(p_0 + m)$ is not a relativistic particle Hamiltonian, and so this does not give a suitable starting point. To describe a massive particle, we need a two-component description with a Hamiltonian of the form $(\alpha p_0 + \beta m)$, where α and β are anticommuting matrices.

The two-component description can be introduced quite naturally by considering together the two transformations that lead to H_+^* and H_-^*. Introduce an additional auxiliary variable which labels these, so that

$$S(x_0, \rho) = \exp\left[i2\pi\int\beta\theta_1\right]\exp\left[\rho i\tfrac{1}{2}\int\alpha\theta_1'\right],$$

where ρ can take on the values ± 1. This gives

$$H' + p_0'\rho = H + p_0\rho + m$$

in the first approximation. This is not a suitable form for H^*; however, we are free to add to it multiples of the supplementary conditions, and there must be a condition associated with the new variable ρ; we take this to have the form

$$(\xi + 1)\psi = 0$$

in the original description, where ξ anticommutes with ρ. Then we can add to H' the term $-(\xi' + 1)m$ giving

$$H^* = H + p_0\rho - m\xi'.$$

Here

$$\xi' = S\xi S^\dagger = \exp\left(-\rho i\int(\alpha + 2\pi\theta_1)\theta_1'\,dx\right) = \xi\exp\left(-\rho i\int\alpha\theta_1'\right)$$

since $\int\theta_1\theta_1'\,dx = \frac{1}{2}$. So in lowest order $H^* = H + p_0\rho + m\xi e^{-\rho i\int\alpha\theta'}{}_1$, which has a relativistic form [ξ, ρ are the analogs of $\gamma_4\cdot\gamma_5$ in the usual Dirac equation notation].

The first approximation to an eigenstate of H^* has the form

$$\psi^* = \psi_0(\alpha)u_k e^{ikx_0},$$

where $(k\rho + m\xi)u_k = Eu_k$ and $\psi_0(\alpha)$ is the vacuum state of the meson field. In the original description the projected state is

$$\psi(\alpha) = \delta(p_0)\delta(\xi + 1)S^\dagger(x_0, \rho)\psi^* = \int[v^+S^\dagger(x_0, \rho)u_k e^{ikx_0}]\,dx_0\psi_0,$$

where v satisfies $(\xi + 1)v = 0$. This shows how $S^\dagger$ is a generating function for particle creation.

To develop a proper self-consistent theory, the analysis must be generalized to a field description of the particles, introducing an auxiliary two-component field $\psi(x_0)$. The transformation is similar but leads to additional two-particle interaction terms which in a one-particle state give a mass contribution proportional to a^{-1}, just as in the classical theory the kinetic energy terms give a similar contribution to be balanced against the K^2a contribution of the potential energy.

8. THE THREE-DIMENSIONAL PROBLEM

In a three-dimensional problem, such as posed by model B, we seek a similar type of transformation with two factors, $S = S_2S_1$, where S_2, analogous to $\exp(i\int 2\pi\beta\theta)$, introduces a kink and S_1 identifies the auxiliary momentum and spin variables with field quantities.

It is easy to construct a suitable S_2. Since the field values U form a group (here SU_2), a transformation $U \to U' = U_0U$, where U_0 is any one-kink field configuration, suffices. It is natural and convenient to choose a U_0 that has a symmetry similar to that of the classical field solutions; a specially simple choice is

$$U_0(\mathbf{x}; \mathbf{x}_0, e_i) = \frac{a + i\tau_\alpha e_{\alpha i}(\mathbf{x} - \mathbf{x}_0)_i}{-a + i\tau_\alpha e_{\alpha i}(\mathbf{x} - \mathbf{x}_0)_i},$$

depending on the auxiliary variables $\mathbf{x}_0$ and $e_{\alpha i}$; a is a length measuring the size of the kink. The transformation is described by the operator

$$S_2 = \exp\left(i\int I_\alpha(\mathbf{x})\frac{e_{\alpha i}(x - x_0)_i}{r}\,\omega(r)\,d^3x\right),$$

where $r = |\mathbf{x} - \mathbf{x}_0|$ and $\omega(r)$ is a suitable angle function.

S_1, analogous to $\exp(\frac{1}{2}i\alpha)$ of model A, should identify the auxiliary momentum vector $\mathbf{p}_0$ with a suitable field expression, and the $e_{\alpha i}$ with a matrix characterizing the field orientation. It must also introduce the spinor character. For U_0, the fields $B_{\alpha i}$ near $\mathbf{x} = \mathbf{x}_0$ are proportional to $e_{\alpha i}$, suggesting that $e_{\alpha i}$ should be identified with the "direction" of $B_{\alpha i}$ near $\mathbf{x} = \mathbf{x}_0$. In general, however, $B_{\alpha i}$ will not be proportional to an orthogonal matrix, but it can be used to define one uniquely by noting that any matrix with positive determinant can be written uniquely as the product of a real symmetric positive definite matrix with a proper orthogonal matrix, that is,

$$B_{\alpha i} = c_{\alpha\beta} f_{\beta i},$$

with $c_{\alpha\beta}$ symmetric and $f_{\beta i}$ orthogonal; $f_{\alpha i}$ is also the orthogonal matrix such that $B_{\alpha i} f_{\alpha i}$ is maximal. We can then try to identify the auxiliary variables $e_{\alpha i}$ with the local values of the $f_{\alpha i}$.

It is convenient to describe the orthogonal matrices by corresponding quaternions $\hat{E}$, $\hat{F}$, which are uniquely defined, apart from sign, by

$$\tau_\alpha e_{\alpha i} = \hat{E}\tau_i\hat{E}^\dagger, \quad \tau_\alpha f_{\alpha i} = \hat{F}\tau_i\hat{F}^\dagger;$$

(that is, we are describing O_3 by its double-valued SU_2 representation). Then $\hat{F}$ is defined, apart from sign, in terms of $B_{\alpha i}$ by the eigenvalue equation

$$\tau_\alpha B_{\alpha i}\hat{F}\tau_i = \lambda\hat{F},$$

with the maximum value of λ. Alternatively we may write the 2×2 matrix $\hat{F}$ as a four-component vector ϕ, and the corresponding equation is

$$\sigma_i\tau_\alpha B_{\alpha i}\phi = -\lambda\phi,$$

where σ and τ are two sets of Pauli matrices acting on the four-component ϕ, which is therefore seen to be a spinor in both the spaces labeled by α and i.

The quantity ϕ satisfies the reality condition $\phi^* = \sigma_2\tau_2\phi$, in the usual conventions, which is consistent with the eigenvalue equation. It is this that enables us to define a spinor quantity uniquely apart from sign in terms of the fields B. In contrast, a spinor quantity cannot be defined by a single vector; for a vector $\mathbf{a}$, the equation

$$(\boldsymbol{\tau}\cdot\mathbf{a})\chi = a\chi$$

might seem to define χ, but its phase cannot be assigned in any way independently of the coordinates.

$\hat{F}$ is a double-valued function of the field, but it is single valued on the covering space; the sign of $\hat{F}$ must be fixed arbitrarily for one particular map taken as reference point, and is then uniquely defined for a map obtained by a given path from the reference one, *provided* that we avoid points for which $\det B = 0$.

We can then write $\hat{F} = e^{i\frac{1}{2}\tau_\alpha\theta_\alpha}$, where $\boldsymbol{\theta}$ is a function of the map in the covering space. The transformation $S = \exp(it_\alpha\theta_\alpha)$, where t_α are the rotation operators for the $e_{\alpha i}$, then gives

$$S\hat{E}S^{-1} = e^{-i\frac{1}{2}\tau_\alpha\theta_\alpha}\hat{E} = \hat{F}^\dagger\hat{E}.$$

So a supplementary condition $\hat{E} = 1$ is transformed into $\hat{E} = \hat{F}$ as wanted. At the same time, as will be seen below, S identifies the momentum $\mathbf{p}_0$ with an appropriate field quantity.

9. APPLICATION TO MODEL B

We apply these ideas to the model B defined in Sec. 3. The transformation considered is $S_+ = S_2S_1$ where S_2 was defined above to introduce a kink so that $U(\mathbf{x}) \to U_0(\mathbf{x}; \mathbf{x}_0, e_{\alpha i})U(\mathbf{x})$.

S_2 induces the following consequential changes on the field variables:

$$B_{\alpha i} \to B^0_{\alpha i} + W_{\alpha\beta}B_{\beta i} = W_{\alpha\beta}(-\tilde{B}^0_{\beta i} + B_{\beta i}),$$
$$I_\alpha \to W_{\alpha\beta}I_\beta, \quad \tilde{I}_\alpha \to \tilde{I}_\alpha.$$

Here $B^0_{\alpha i}$ is the field due to the source U_0

$$B^0_{\alpha i} = b(r)e_{\alpha j}R_{ji}(\mathbf{x} - \mathbf{x}_0), \quad r = |\mathbf{x} - \mathbf{x}_0|,$$

$b(r) = 2a(a^2 + r^2)^{-1}$, and R_{ji} is the orthogonal matrix

$$R_{ji}(\mathbf{x}) = [\delta_{ji}(a^2 - r^2) + 2x_ix_j + 2a\epsilon_{jik}x_k](a^2 + r^2)^{-1},$$

with

$$\tau_jR_{ji} = \hat{R}\tau_i\hat{R}^\dagger, \quad \hat{R} = \frac{a + i\tau_\alpha x_\alpha}{(a^2 + r^2)^{\frac{1}{2}}} = [-U_0(\mathbf{x}; 0, 1)]^{\frac{1}{2}}.$$

$W_{\alpha\beta}(\mathbf{x} - \mathbf{x}_0)$ is an orthogonal matrix describing the rotation of the fields induced by S_2:

$$W_{\alpha\beta} = e_{\alpha j}(R^2)_{ji}e_{\beta i}.$$

It is convenient to introduce also $\tilde{B}^0_{\alpha i}$ so that

$$B^0_{\alpha i} = -W_{\alpha\beta}\tilde{B}^0_{\beta i}, \quad \tilde{B}^0_{\alpha i} = -W_{\beta\alpha}B^0_{\beta i} = -b(r)e_{\alpha j}R_{ij};$$

the significance of $\tilde{B}$ will be discussed further below.

We define S_1 as in the last section, using for the $B_{\alpha i}$ a suitable average of the field values near the sources. For the particular shape of U_0 used in S_2, it appears best to define an average by

$$V_{\alpha i}(B; \mathbf{x}_0) = \frac{1}{2\pi^2}\int B_{\alpha j}(\mathbf{x})R_{ij}(\mathbf{x} - \mathbf{x}_0)b^2(r)\,d^3x;$$

then, in particular, when $B = B^0$,

$$V_{\alpha i} = e_{\alpha i}.$$

So $S_1 = \exp(it_\alpha\theta_\alpha)$, where $\hat{F} = e^{i\frac{1}{2}\tau_\alpha\theta_\alpha}$ satisfies

$$\tau_\alpha V_{\alpha i}\hat{F}\tau_i = \lambda\hat{F}, \quad \text{with maximum } \lambda.$$

The transformation S_1 makes $\hat{E} \to \hat{F}^\dagger \hat{E}$, as shown above, and rotates the vector t_α; it leaves unchanged the vector s_i and the fields $B_{\alpha i}$. The field rotation operators $I_\alpha(\mathbf{x})$ transform to

$$I_\alpha(\mathbf{x}) + A_{\alpha\beta}(\mathbf{x}, B; \mathbf{x}_0)t_\alpha,$$

where

$$A_{\alpha\beta}t_\beta = \int_0^1 e^{\lambda i t\cdot\theta t_\gamma/\gamma} e^{-\lambda i t\cdot\theta}\, d\lambda [i\theta_\gamma(B, \mathbf{x}_0), I_\alpha(\mathbf{x})];$$

the commutator at the end is a function only of the B and $\mathbf{x}$, $\mathbf{x}_0$.

In particular $\int A_{\alpha\beta}(\mathbf{x}, B, \mathbf{x}_0)\, d^3x = \delta_{\alpha\beta}$. This follows from a simple argument. It is clear from the definition of $\hat{F}$ that it must behave as a spinor for rotation of the $B_{\alpha i}$ induced by the total spin operator

$$H_\alpha = \int I_\alpha(x)\, d^3x,$$

that is,

$$[H_\alpha, \hat{F}] = -\tfrac{1}{2}\tau_\alpha \hat{F} \quad \text{or} \quad \hat{F} H_\alpha F^\dagger = H_\alpha + \tfrac{1}{2}\tau_\alpha.$$

Then

$$S_1 H_\alpha S_1^\dagger = H_\alpha + t_\alpha$$

since, if we expand the left side in a series of commutators, all terms after the second involve only the mutual commutators of the t_α, which are similar to those of the $\frac{1}{2}\tau_\alpha$.

The total effect of the transformation $S_2 S_1$ on the field variables is then

$$B'_{\alpha i} = SB_{\alpha i}S^{-1} = B^0_{\alpha i} + W_{\alpha\beta}B_{\beta i} = W_{\alpha\beta}(-\tilde{B}^0_{\beta i} + B_{\beta i}),$$
$$I'_\alpha = SI_\alpha S^{-1} = W_{\alpha\beta}I_\beta + A_{\alpha\beta}(\mathbf{x}, B^0 + WB, \mathbf{x}_0)\left[t_\beta + \int (\delta_{\beta\gamma} - W_{\beta\gamma})I_\gamma\right].$$

The transformation of t_β by S_2 exhibited in the last factor is derived by noting that the total spin $t_\beta + H_\beta = t_\beta + \int I_\beta\, d^3x$ commutes with S_2.

For the auxiliary variables the transformation of $\mathbf{p}_0$ is most easily found by noting that S is translationally invariant and must therefore commute with the total linear momentum $(\mathbf{p}_0)_i + 2\int I_\alpha B_{\alpha i}\, d^3x$.

$\hat{E}$ is transformed into $\hat{F}^\dagger(B^0 + WB, \mathbf{x}_0)\hat{E}$; but $\hat{F}(B^0, \mathbf{x}_0) = \hat{E}$ so that the transformed supplementary condition $\hat{E}' = I$ is identically satisfied in its leading term (compare the end of Sec. 6).

The consequences of this transformation combined with the supplementary conditions

$$\mathbf{p}_0\psi = 0, \quad (\hat{E} - I)\psi = 0$$

are considered in the following sections.

10. MOMENTA AND SPINS

As mentioned above, $p'_{0i} + 2\int I'_\alpha B'_{\alpha i}\, d^3x = p_{0i} + 2\int I_\alpha B_{\alpha i}\, d^3x$, so that the condition $\mathbf{p}'_0 = 0$ gives

$$p_{0i} = 2\int [I'_\alpha B'_{\alpha i} - I_\alpha B_{\alpha i}]\, d^3x.$$

The term independent of the new fields is then

$$2\int A_{\alpha\beta}(\mathbf{x}, B^0, \mathbf{x}_0)B^0_{\alpha i}\, d^3x t_\beta.$$

To evaluate $A_{\alpha\beta}$, we calculate the commutator of $I_\alpha(\mathbf{x})$ with $\hat{F}(\mathbf{x}_0)$ from the eigenvalue equations, using the selected definition of the average $V_{\alpha i}$, and express the result in the form

$$[I_\alpha(\mathbf{x}), \hat{F}(\mathbf{x}_0)] = -A_{\alpha\beta}\tfrac{1}{2}\tau_\beta \hat{F}.$$

Putting $B = B^0$ in the formula, we obtain the simple result

$$A^0_{\alpha\beta} = A_{\alpha\beta}(\mathbf{x}, B^0, \mathbf{x}_0) = (1/2\pi^2)b^3(r)\delta_{\alpha\beta}, \qquad r = |\mathbf{x} - \mathbf{x}_0|.$$

So the leading term for $\mathbf{p}_{0i}$ is

$$\frac{1}{\pi^2}\int e_{\alpha j}R_{ji}b^4(r)\, d^3x t_\alpha = \frac{1}{a}e_{\alpha i}t_\alpha = -\frac{1}{a}s_i.$$

The total angular momentum of the system is, originally,

$$J_i = 2\epsilon_{ijk}\int I_\alpha x_j B_{\alpha k}\, d^3x.$$

To see how this transforms, it is convenient to use the supplementary conditions to begin instead with

$$J_i + L_i + s_i + t_i,$$

where $\mathbf{L} = \mathbf{x}_0 \times \mathbf{p}_0$ is the auxiliary orbital angular momentum. The additional terms are zero because of the conditions $\mathbf{p}_0 = 0$ and $e_{\alpha i} = \delta_{\alpha i}$. By a similar argument to that used for H_α, we see that

$$[J_i + L_i, \hat{F}] = \hat{F}\tfrac{1}{2}\tau_i$$

and so, as before, $S_1(J_i + L_i + t_i)S_1^\dagger = J_i + L_i$. Also S_1 commutes with s_i, and so does S_2 with $J_i + L_i + s_i$ since it is rotationally symmetric; thus the transformed angular momentum is

$$S(J_i + L_i + s_i + t_i)S^\dagger = J_i + L_i + s_i.$$

The internal symmetry operators are $H'_\alpha = H_\alpha + t_\alpha$, $\tilde{H}'_\alpha = H_\alpha$.

11. HAMILTONIAN

The transformed Hamiltonian is

$$H'(I, B) = H(I', B').$$

Consider the terms independent of the new fields.

These are

$$\int A^0_{\alpha\beta}t_\beta(G_0^{-1})_{\alpha\gamma}A^0_{\gamma\delta}t_\delta\,d^3x + \frac{\epsilon}{8\pi i}\int[(B^0_{\alpha i}B^0_{\alpha i})^2 - (B^0_{\alpha i}B^0_{\alpha j})(B^0_{\beta i}B^0_{\beta j}) + 2K^2(B^0_{\alpha i}B^0_{\alpha i})]\,d^3x,$$

where

$$(G_0)_{\alpha\beta} = (\epsilon/4\pi^2)[(B^0_{\gamma i}B^0_{\gamma i} + K^2)\delta_{\alpha\beta} - (B^0_{\alpha i}B^0_{\beta i})].$$

Now $B^0_{\alpha i}B^0_{\beta i} = b^2(r)\delta_{\alpha\beta}$, and so

$$G^0_{\alpha\beta} = (\epsilon/4\pi^2)(2b^2(r) + K^2)\delta_{\alpha\beta},$$

while, as above,

$$A^0_{\alpha\beta} = (1/2\pi^2)b^3(r)\delta_{\alpha\beta}.$$

So the leading terms in H' are

$$\left(\frac{1}{2\pi^2}\int\frac{b^6(r)}{b^2(r) + \frac{1}{2}K^2}\,d^3x\right)t_\beta t_\beta + \frac{\epsilon}{4\pi^2}\int(3b^4 + K^2b^2)\,d^3x.$$

For comparison with the usual field theories, it may be convenient to introduce a point particle as auxiliary (although this may not give the best scheme of approximation), i.e., to regard a as very small. Then we may neglect K in the integrals to give

$$(1/\epsilon a)t_\alpha t_\alpha + 3\epsilon/2a.$$

Suppose also that we are only concerned with spin-$\frac{1}{2}$ states; then we should want H^* to contain a term $\pm p_{0i}(2s_i)$. If we took $H^* = H' - p'_{0i}2s_i$, the leading terms in H^* would be

$$H + (1/\epsilon a)t_\alpha t_\alpha - (2/a)s_i s_i + 3\epsilon/2a.$$

If $\epsilon = \frac{1}{2}$, the first two terms cancel, leaving a mass term from the potential energy, whose divergence should be largely cancelled by the self-energy corrections.

However, the terms $(-p'_{0i}2s_i + m)$ are not a relativistic particle Hamiltonian; to achieve that, we must introduce an extra variable like ρ for model A, associated with the parity symmetry.

12. PARITY

Consider the symmetry properties of the system under inversion. The original meson field theory is obviously invariant for the transformations

$$R: U(x) \to U(-\mathbf{x}) \quad \text{and} \quad C: U(\mathbf{x}) \to U^\dagger(\mathbf{x}).$$

C is a charge conjugation operation and R appears to correspond to "CP." In connection with C it is convenient to introduce the charge conjugate fields $\tilde{B}$ defined by $\partial_\mu U^\dagger = i\tau_\alpha\tilde{B}_{\alpha\mu}U^\dagger$ so that $\tilde{B}_{\alpha i} = -g_{\alpha\beta}B_{\beta i}$, where $U\tau_\alpha U^\dagger = g_{\alpha\beta}\tau_\beta$; corresponding to them are the conjugates $\tilde{I}_\alpha = -g_{\alpha\beta}I_\beta$ (see also Sec. 3). Then C gives $B \to \tilde{B}$, $I \to \tilde{I}$, in particular the particle density $\det B \to |\tilde{B}| = -\det B$, since g is proper orthogonal, and so, in the suggested interpretation, will change particles into antiparticles.

The space inversion defined by R makes $B_{\alpha i}(\mathbf{x}) \to -B_{\alpha i}(-\mathbf{x})$ and therefore also changes the sign of $\det B$, suggesting that it should be regarded as a "CP" operation.

The combined operation RC appears to be the proper parity operation:

$$RC: U(\mathbf{x}) \to U^\dagger(-\mathbf{x}), \quad B_{\alpha i}(\mathbf{x}) \to -\tilde{B}_{\alpha i}(-\mathbf{x}), \quad I_\alpha(\mathbf{x}) \to \tilde{I}_\alpha(-\mathbf{x}).$$

Consider the effect of RC on the transformation S, supposing that R also transforms $\mathbf{x}_0$ to $-\mathbf{x}_0$. In S_2 the effect is to change I_α into $\tilde{I}_\alpha$ and to change the sign of the factor $(\mathbf{x} - \mathbf{x}_0)$; it is the operator which makes $U^\dagger(\mathbf{x}) \to U_0^\dagger(\mathbf{x}, \mathbf{x}_0, e)U^\dagger$, i.e. $U \to UU_0$. It is obviously as reasonable to introduce a kink by multiplying U on the right as on the left, and we would expect the two operations to enter symmetrically into a theory.

On S_1 the effect is to transform it to $\tilde{S}_1$, defined similarly in terms of a local field average, which becomes

$$\tilde{V}_{\alpha i} = \frac{1}{2\pi^2}\int[-\tilde{B}_{\alpha j}(\mathbf{x})]R_{ji}(\mathbf{x} - \mathbf{x}_0)b^2(r)\,d^3x.$$

The new transformation $\tilde{S}$ then gives $\tilde{B}'_{\alpha i} = \tilde{B}^0_{\alpha i} + W_{\beta\alpha}\tilde{B}_{\beta i}$, and $\tilde{V}_{\alpha i}$ evaluated for $\tilde{B} = \tilde{B}^0$ is again equal to $e_{\alpha i}$.

In the transformed Hamiltonian, the leading additional terms are the same as with S. The leading term in the momentum, however, changes sign, as it should for a parity transformation, so that with this S we should naturally consider $H^*_- = H' + p'_{0i}(2s_i)$, of which the leading terms are $H + p_{0i}(2s_i) + m$.

13. DIRAC HAMILTONIAN

We can treat these two equally good types of transformation in a symmetrical manner by introducing extra variables ρ, ξ just as for model A; these are anticommuting matrices with eigenvalues ± 1. It is natural to use a representation in which ρ is diagonal,

$$\rho = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad \xi = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}.$$

In this representation the transformations are combined as $\binom{S0}{0S}$, which we now simply write as S. We introduce the supplementary condition $(\xi - 1)\psi = 0$.

ξ transforms into

$$\xi' = S\xi S^\dagger = \begin{pmatrix} 0 & S\tilde{S}^\dagger \\ \tilde{S}S^\dagger & 0 \end{pmatrix}.$$

$\tilde{S}S^\dagger$ differs from unity because $U_0U \neq UU_0$, but the difference is small when the transformed fields can be regarded as small: This can easily be verified by detailed study of the operator.

We therefore consider $H^* = H' - p'_{0i}(2s_i\rho) + (\xi' - 1)m$ so that, for a suitable choice of m,

$$H^* = H - p_{0i}(2s_i\rho) + m\xi + \text{interaction terms}.$$

For states with spin $\frac{1}{2}$, the expression $[-p_{0i}(2s_i\rho) + m\xi]$ has exactly the structure of the Dirac Hamiltonian $(\alpha \cdot \mathbf{p} + \beta m)$.

We have thus shown that a Dirac Hamiltonian can be introduced in a quite natural way to describe the particlelike modes of the meson field.

14. COMMENTS

To investigate whether this analysis does give a starting point from which valid solutions describing particles can be constructed, the transformations must first be written with auxiliary fields for the particles rather than coordinates; then the interaction terms can be investigated by standard field theoretic methods, and it is possible that, for some suitable choice of kink U_0, perturbation theory might lead to a solution free from divergences.

The model should also contain isobaric states of higher spin; the choice made for H^* is evidently inappropriate for these as it is certainly not then relativistic.

[1] T. H. Skyrme, Proc. Roy. Soc. (London) **A260**, 127 (1961).
[2] D. Finkelstein, J. Math. Phys. **7**, 1218 (1966).
[3] J. G. Williams, J. Math. Phys. **11**, 2611 (1970).
[4] W. Pauli, *Meson Theory of Nuclear Forces* (Interscience, New York, 1946).

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Comment on a Paper of Chiang

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(Received 13 May 1971)

This is a rebuttal to a paper by Chiang [J. Math. Phys. **10**, 2098 (1969)].

It seems necessary to defend my paper[1] against presumed errors noted by Chiang,[2] who uses the gamma function in his argument. Ever since the time of Newton and through all the work of Euler, Abel, *et al.*, it has been correct to define the binomial coefficients by the formula

$$\binom{x}{n} = \frac{x(x-1)\cdots(x-n+1)}{n!} \tag{1}$$

whenever n is a nonnegative integer and x is an arbitrary complex number. From this definition it is trivial to verify the truth of the identity

$$\binom{-x}{n} = (-1)^n\binom{x+n-1}{n}, \tag{2}$$

which I gave in my paper and which result is standard in any text on combinatorial theory. Chiang believes that (2) as well as the Vandermonde addition theorem noted in my paper are incorrect because use of the gamma function gives

$$\binom{x}{n} = \frac{\Gamma(x+1)}{n!\,\Gamma(x-n+1)}, \tag{3}$$

which is at first blush indeterminate for negative integers x. However, what he ignores is that the gamma function satisfies the functional relation

$$\Gamma(x+1) = x\Gamma(x), \tag{4}$$

a standard and well-known property by which the range of meaning of the gamma function is extended. See Artin's monograph for a good treatment.[3] Repeated use of (4) gives us

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JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 8 AUGUST 1971

Useful Procedure for Computing the Lattice Green's Function—Square, Tetragonal, and bcc Lattices

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A recurrence relation, which gives the values of the lattice Green's function along the diagonal direction from a couple of the elliptic integrals of the first and second kind, is derived for the square lattice by an elementary partial integration. The values of the square lattice Green's function at an arbitrary site are then calculated in a successive way with the aid of the difference equation defining the function. Discussions are given of the application of this result to the calculation of the lattice Green's function of the tetragonal and body-centered cubic lattices.

1. INTRODUCTION

For the rectangular lattice, the lattice Green's function has been investigated with the aid of the Mellin–Barnes type integral by Katsura and Inawashiro.[1] The function along the diagonal direction was expressed in terms of the hyper-geometric function. For the special case of the square lattice, the lattice Green's function at an arbitrary lattice site can be calculated from the values along the diagonal direction. Thus they obtained the lattice Green's function at an arbitrary site for the square lattice.

With the aid of the expression obtained by Katsura and Inawashiro, the present author[2] derived a recurrence relation which gives the values along the diagonal direction from a couple of values of complete elliptic integrals of the first and the second kind for the rectangular lattice. Thus the calculation is simplified for the lattice Green's function along the diagonal direction for the rectangular lattice and for the function at an arbitrary site for the square lattice.

In the present paper, we show that an elementary consideration leads to a simpler recurrence relation which gives the function along the diagonal direction from a couple of values of complete elliptic integrals of the first and the second kind for the case of the square lattice.

In a separate paper,[2] the present author provided a procedure for calculating the lattice Green's function at an arbitrary site for the orthorhombic lattice.

We show that the present method of calculating the square lattice Green's function provides a simpler procedure for calculating the lattice Green's function at an arbitrary site for the case of the tetragonal lattice. We also obtain a procedure for calculating the function at an arbitrary site for the body-centered cubic lattice.

2. BASIC FORMULAS FOR THE SQUARE LATTICE

The lattice Green's function for the square lattice is the solution of the difference equation which involves the δ-function type inhomogeneous term:

$$2tG(t; m, n) - \gamma G(t; m+1, n) - \gamma G(t; m-1, n) - \gamma G(t; m, n+1) - \gamma G(t; m, n-1) = 2\delta_{m,0}\delta_{n,0}. \quad (2.1)$$

The required boundary value is zero at $m^2 + n^2 \to \infty$. The solution of this equation is

$$G(t; m, n) = \frac{1}{\pi^2}\int_0^\pi dy \int_0^\pi dz \frac{\cos my \cos nz}{t - \gamma \cos y - \gamma \cos z}. \quad (2.2)$$

In Fig. 1, two natural ways of introducing the coordinate axes are shown for the square lattice. Fig. 1(a) is the ordinary way and has been adopted in writing equations (2.1) and (2.2). If we adopt the way of Fig. 1(b), we write the difference equation as follows:

$$2tG'(t; m', n') - \gamma G'(t; m'+1, n'+1) - \gamma G'(t; m'-1, n'-1) - \gamma G'(t; m'+1, n'-1) - \gamma G'(t; m'-1, n'+1) = 2\delta_{m',0}\delta_{n',0}, \quad (2.3)$$

where $m' + n'$ must always be even. The boundary value is zero at $m'^2 + n'^2 \to \infty$. The solution is

$$G'(t; m', n') = \frac{1}{\pi^2}\int_0^\pi dy' \int_0^\pi dz' \frac{\cos m'y \cos n'z}{t - 2\gamma \cos y' \cos z'}. \quad (2.4)$$

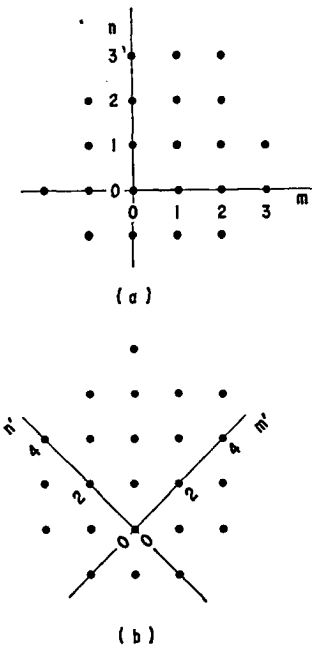

FIG. 1. Two ways of introducing the coordinate axes in the square lattice. (a) The ordinary way. (b) An alternative way.

The transformation from (2.1) and (2.2) to (2.3) and (2.4) is achieved by

$$\begin{aligned} y' &= (y+z)/2, \quad z' = (y-z)/2, \\ m' &= m+n, \qquad n' = m-n, \\ G'(t; m', n') &= G(t; (m'+n')/2, (m'-n')/2), \\ G'(t; m+n, m-n) &= G(t; m, n). \end{aligned} \tag{2.5}$$

3. SQUARE LATTICE: ALONG THE DIAGONAL DIRECTION

The square lattice Green's function along the diagonal direction is expressed as $G(t; m, m)$, which is equal to $G'(t; 2m, 0)$ by (2.5). By (2.4), it is expressed as follows:

$$G(t; m, m) = \frac{1}{\pi}\int_0^\pi dy \frac{\cos 2my}{(t^2 - 4\gamma^2\cos^2 y)^{\frac{1}{2}}}. \tag{3.1}$$

In terms of the definite integral $F_n(k^2)$ defined by

$$F_n(k^2) \equiv \int_0^\pi dy \frac{\cos ny}{(1 - k^2\cos^2 y)^{\frac{1}{2}}}, \tag{3.2}$$

$G(t; m, m)$ is expressed as follows:

$$G(t; m, m) = \frac{1}{\pi t} F_{2m}\left(\frac{4\gamma^2}{t^2}\right). \tag{3.3}$$

In order to derive a recurrence relation for $G(t; m, m)$, the following integral

$$\int_0^\pi dy \cos ny(1 - k^2\cos^2 y)^{\frac{1}{2}} \tag{3.4}$$

is expressed in two ways, in terms of $F_n(k^2)$. First, we write (3.4) as

$$\begin{aligned} \int_0^\pi dy \frac{\cos ny(1 - k^2\cos^2 y)}{(1 - k^2\cos^2 y)^{\frac{1}{2}}} &= -(k^2/4)F_{n+2}(k^2) + (1 - k^2/2)F_n(k^2) \\ &\quad - (k^2/4)F_{n-2}(k^2). \end{aligned} \tag{3.5}$$

On the other hand, by a partial integration, (3.4) is reduced to

$$\begin{aligned} -\frac{1}{n}\int_0^\pi dy \sin ny \frac{k^2\cos y \sin y}{(1 - k^2\cos^2 y)^{\frac{1}{2}}} &= -(k^2/4n)[F_{n-2}(k^2) - F_{n+2}(k^2)]. \end{aligned} \tag{3.6}$$

By equating (3.5) and (3.6), one obtains the following recurrence relation for $F_n(k^2)$:

$$\begin{aligned} F_{n+2}(k^2) &= [2n/(n+1)](2/k^2 - 1)F_n(k^2) \\ &\quad - [(n-1)/(n+1)]F_{n-2}(k^2). \end{aligned} \tag{3.7}$$

Applying formula (3.7) to (3.3), one obtains

$$\begin{aligned} &G(t; m+1, m+1) \\ &= [4m/(2m+1)](t^2/2\gamma^2 - 1)G(t; m, m) \\ &\quad - [(2m-1)/(2m+1)]G(t; m-1, m-1). \end{aligned} \tag{3.8}$$

When $m = 0$ and 1, (3.1) gives

$$G(t; 0, 0) = (2/\pi t)\mathbf{K}(2\gamma/t) \tag{3.9}$$

and

$$\begin{aligned} &G(t; 1, 1) \\ &= (2/\pi t)[(t^2/2\gamma^2 - 1)\mathbf{K}(2\gamma/t) - (t^2/2\gamma^2)\mathbf{E}(2\gamma/t)]. \end{aligned} \tag{3.10}$$

All the diagonal values $G(t; m, m)$ are now calculated by the recurrence formula (3.8) from the knowledge of the complete elliptic integrals of the first and the second kind, $\mathbf{K}(2\gamma/t)$ and $\mathbf{E}(2\gamma/t)$.

If $t > 2\gamma$, one uses (3.9), (3.10). For arbitrary complex values of t, one may use them.[3] But if $t = s - i\epsilon$ and $0 < s < 2\gamma$, it is more convenient to use their analytic continuations, which are obtained by replacing $\mathbf{K}(1/k)$ and $\mathbf{E}(1/k)$ in (3.9) and (3.10), by the right-hand sides of the following equations:

$$\mathbf{K}(1/k) = k[\mathbf{K}(k) + i\mathbf{K}(k')], \tag{3.11}$$

$$\mathbf{E}(1/k) = (1/k)[\mathbf{E}(k) - i\mathbf{E}(k') - k'^2\mathbf{K}(k) + ik^2\mathbf{K}(k')], \tag{3.12}$$

where

$$k' = (1 - k^2)^{\frac{1}{2}} \tag{3.13}$$

and

$$1/k = 2\gamma/(s - i\epsilon) = (2\gamma/s) + i\epsilon.$$

4. SQUARE LATTICE: ARBITRARY SITE

By the difference equation (2.3) or (2.1) one obtains the square lattice Green's function at an arbitrary site from the values along the diagonal direction.[2] The steps to be followed are

$$G(t; 1, 0) = [2tG(t; 0, 0) - 2]/4\gamma, \tag{4.1}$$

$$G(t; m + 1, m) = [2tG(t; m, m) - 2\gamma G(t; m, m - 1)]/2\gamma. \tag{4.2}$$

If $0 < n < m$, one has

$$\begin{aligned} G(t; m + 1, n) &= [2tG(t; m, n) - \gamma G(t; m - 1, n) \\ &\quad - \gamma G(t; m, n + 1) - \gamma G(t; m, n - 1)]/\gamma. \end{aligned} \tag{4.3}$$

The values on the axes are obtained by

$$\begin{aligned} G(t; m + 1, 0) = [2tG(t; m, 0) &- \gamma G(t; m - 1, 0) \\ &- 2\gamma G(t; m, 1)]/\gamma. \end{aligned} \tag{4.4}$$

5. TETRAGONAL LATTICE: ARBITRARY SITE

The lattice Green's function for the tetragonal lattice is given by

$$\begin{aligned} G(t; l, m, n) &= \frac{1}{\pi^3} \int_0^\pi dx \int_0^\pi dy \\ &\quad \times \int_0^\pi dz \frac{\cos lx \cos my \cos nz}{t - \gamma_1 \cos x - \gamma \cos y - \gamma \cos z}. \end{aligned} \tag{5.1}$$

Comparing with (2.2), we write this as follows:

$$G(t; l, m, n) = \frac{1}{\pi} \int_0^\pi dx \cos lx G(t - \gamma_1 \cos x; m, n). \tag{5.2}$$

If this function is calculated for the square coordinate plane, namely for $l = 0$, the values for nonzero l are calculated by the difference equation defining the function:

$$\begin{aligned} G(t; 1, m, n) &= [2tG(t; 0, m, n) - 2\delta_{m,0}\delta_{n,0} \\ &\quad - \gamma G(t; 0, m + 1, n) - \gamma G(t; 0, m - 1, n) \\ &\quad - \gamma G(t; 0, m, n + 1) - \gamma G(t; 0, m, n - 1)]/2\gamma_1. \end{aligned} \tag{5.3}$$

For $l \geq 1$, one has

$$\begin{aligned} G(t; l + 1, m, n) &= [2tG(t; l, m, n) - \gamma_1 G(t; l - 1, m, n) \\ &\quad - \gamma G(t; l, m + 1, n) - \gamma G(t; l, m - 1, n) \\ &\quad - \gamma G(t; l, m, n + 1) - \gamma G(t; l, m, n - 1)]/\gamma_1. \end{aligned} \tag{5.4}$$

6. bbc LATTICE: ARBITRARY SITE

The lattice Green's function for the bcc lattice is given by

$$G(t; l, m, n) = \frac{1}{\pi^3} \int_0^\pi dx \int_0^\pi dy \int_0^\pi dz \frac{\cos lx \cos my \cos nz}{t - \gamma \cos x \cos y \cos z}. \tag{6.1}$$

This is expressed as follows in terms of the function G' for the square lattice:

$$G(t; l, m, n) = \frac{2}{\pi} \int_0^\pi dx \frac{\cos lx}{\cos x} G'\left(\frac{t}{\gamma \cos x}; m, n\right). \tag{6.2}$$

For this case again, we can show that the values at an arbitrary site can be calculated from the values on a coordinate plane with the aid of the difference equation satisfied by the lattice Green's function.

7. CONCLUDING REMARKS

The lattice Green's function for the square lattice has been numerically computed from the complete elliptic integrals of the first and the second kind, via the formulas (3.8)–(3.13) and (4.1)–(4.4). The result obtained agrees with the one given by Katsura and Inawashiro.[1] Since the arithmetic-geometric mean procedure allows us to calculate the complete elliptic integrals to the desired accuracy with ease,[3,4] the present method is a quite convenient one.

In a recent article, Horiguchi[5] presented a calculation of the lattice Green's function $G(s - i\epsilon, l, m, n)$ of the simple cubic lattice for the sites with $l + m + n \leq 5$ and $l, m, n \geq 0$. He first calculated the function along an axis and then used the difference equation defining the function. The present method is superior to this in the respect that it allows the calculation of the lattice Green's function at an arbitrary site. There is not much difference in the respect of programming of the computations.

In the present paper, an elementary partial integration is used to give a recurrence formula. The same technique has been found useful to give recurrence relations for the values along the axes and the diagonal directions of the lattice Green's function for

the rectangular lattice. That result is applicable to the calculation of the orthorhombic lattice Green's function.[2] The same method has also been found to allow the calculation of the lattice Green's function for the fcc lattice. Those formulas and numerical computations with the aid of them will be published in the near future.

The computer NEAC 2200 in the Computer Center of Tohoku University was used to calculate the square lattice Green's function by the method presented in this paper.

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Canonical Perturbation Theory for Nonlinear Quantum Oscillators and Fields

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The method of successive canonical transformation is developed to study both the classical and quantum versions of a system of n weakly interacting nonlinear oscillators. The method reproduces the essential features of the solutions to these nonlinear differential equations. A general quartic polynomial in the oscillator coordinates is taken as the interaction Hamiltonian. After the canonical transformations to the desired order, the classical system is quantized, resulting in immediate identification of the raising and lowering operators for the perturbed eigenstates in the nonresonant case. In the resonant case (commensurable frequencies) the transformed operators lead to finite-dimensional subspaces within which eigenstates lie, and are obtained by matrix methods. In each case the Heisenberg equations for the operators are solved as fully as presently possible. A particular case of two quantum oscillators is studied in detail, both for the resonant and nonresonant cases. Finally, the method is generalized to the continuum and applied to the Lee model. The usual results for the lowest sector are obtained to second order: the physical V particle and the mass shift of the V. Instability of this particle is related to the occurrence of nonlinear resonance in the lowest-order "interaction."

1. INTRODUCTION

Perturbation expansions for the differential equation satisfied by a single classical nonlinear oscillator have been known for some time, and the characteristic features of the nonlinearity are well understood. On the other hand, relatively little has been established in the more difficult search for approximations for autonomous *systems* of interacting classical nonlinear oscillators.

Internal resonance occurs in a system of n oscillators, frequencies $\{\omega_j\}$, when these frequencies satisfy at least one linear commensurability relation

$$\sum_{j=1}^{n} i_j\omega_j \equiv \mathbf{i}\cdot\boldsymbol{\omega} = 0. \tag{1.1}$$

(Some, but not all, of the i_j can be zero.)

In general, the smaller the integers in the relation, the stronger the resonance effects, that is, the shorter the $\mathbf{i}$ vector in integer space.

Certain rather elegant results for such classical systems in the presence of resonance have been achieved recently.[1] These we shall rely on heavily later, and defer for now. As for earlier work, the literature of celestial mechanics, from Poincaré on, has wrestled with these effects, where the problem goes by the name "the problem of small divisors." Several phenomena in planetary orbits have been traced to nonlinear resonance. Stability of motion under resonant conditions has been a question studied extensively, with encouraging recent progress.[2]

As for other efforts, the presence of resonance is necessary for equipartition of energy to be established, at least in a one-dimensional model studied by Ford[3] and others.

In a particular system of two classical resonant oscillators, Brown[4] has shown that "entrainment" or synchronous oscillation is stable for a certain range of initial conditions, even though the amplitude dependence of the frequencies could destroy phase coherence, in principle. Qualitative statements of this fact can be found in mathematical literature,[5] where it is asserted that *near* equality of the frequencies is enough to produce synchronous oscillation. A system of three classical nonlinear oscillators with $\omega_1 + \omega_2 - \omega_3 = 0$ is treated by Ibragovima,[6] whose results can easily be extended to show that a certain relative angle between the oscillators is itself a periodic function of the time. This is a type of phase coherence.

In addition to the intrinsic value of understanding systems of coupled nonlinear oscillators, especially the quantum versions of such systems, the extended problem of an infinite collection of coupled nonlinear oscillators leads to interesting questions concerning quantum field theories.

The Heisenberg field equations of any nontrivial quantum field theory are nonlinear partial differential equations for the field operators as functions of space–time. In weakly coupled theories, it is traditional to use a perturbative expansion for approximating operators and matrix elements, especially if the theory is renormalizable. The equivalence of a Feynman–Dyson expansion (with or without diagrams) to iterative schemes based on the *LSZ* integral equations with adiabatic switching for definition of the singular contribution from the Green's function is now well known. All such accepted methods suffer from any limitation which may exist on a Green's function approach to an iterative solution of a nonlinear

equation. That there are such limitations in general has been argued recently in nonlinear equations ranging from the one-dimensional anharmonic oscillator (classical and quantum)[7] to the field equation for a $\lambda\phi^4$ self-coupled scalar field.[8]

This paper affords a perturbative method for either solving directly or greatly simplifying these equations while reproducing the essentially nonlinear properties (or "parts") of the solution. It is these essentially nonlinear parts which are given improperly by Green's function techniques. The technique developed here is not new, except in the extension to the quantized version of the problem and to continuum problems. It is the method of successive canonical transformation first enunciated by Birkhoff[9] for the classical problem of a mechanical system of n degrees of freedom near equilibrium, and it has since gained wide acceptance and usage. Dealing as it does with the classical equivalents of the raising and lowering operators, the method allows quantization very directly and simply.

In Sec. 2 the basic method is outlined for a very simple system: the anharmonic classical oscillator with a perturbing potential. This system is quantized and the operator-valued frequency recovered in agreement with the previous treatment of this problem.[7] Details of the transformation are deferred to Appendix A.

Systems of n coupled nonlinear oscillators are next discussed in Sec. 3 with a general quartic interaction in the oscillator coordinates. (The restriction to a quartic is inessential.) The existence of approximate, separating constants of the motion beside H is discussed in both resonant and nonresonant cases drawing on the work by Gustavson[1] mentioned above. The implications for the quantized version of the system are drawn. There exists a set of conserved "number operators" made up of the nonconserved number operators of the separate oscillators. The problem of finding the energy eigenpairs in the harder resonant case is discussed.

Next a concrete quantum two-oscillator problem is worked to first order in the coupling, both without resonance and with it, in Sec. 4. In the nonresonant case, the Heisenberg equations of motion for the position operators $x_j(t)$ are integrated directly. One again gets operator-valued frequencies. The Hamiltonian is a function of the two conserved "renormalized" (or transformed) number operators so that the eigenpairs of H are immediate. In the resonant case the canonical transformation can only simplify the problem. One identifies finite-dimensional invariant subspaces within which the eigenpairs of H are sought by ordinary matrix methods.

Finally, we apply an extended version of the method to the Lee model (a continuum problem) in Sec. 5. The low sectors of the Lee model are exactly soluble, and show only some of the effects of the nonlinearity in the equations of motion. Nonlinear resonance between different $\mathbf{k}$-modes of the field seems not to lead to important effects in the lowest sector. But the method reproduces the usual results of this sector when carried to second order in the coupling: (i) the identity of the physical V as a mixture of bare V and bare $N\theta$ states, (ii) the mass shift accurate to order g_0^2, (iii) $N\theta$ scattering. The details of the mass shift problem are left for Appendix B.

Thus, the method of successive canonical transformation seems to be a good candidate for further calculation in weakly-coupled field theories to obtain any new effects due to the intrinsic nonlinearity which the methods based on Green's functions or "switching" have either omitted or modified.

2. THE CANONICAL APPROXIMATION FOR ONE OSCILLATOR

As an example of the quantization procedure to be employed for the quantum case in Heisenberg representation, let us consider a well-studied problem. A massive particle moves in one dimension with the following Hamiltonian ($m = 1$, $\hbar = 1$):

$$H = \tfrac{1}{2}(p^2 + \omega^2 q^2) + \tfrac{1}{4}\epsilon\omega^2 q^4. \tag{2.1}$$

Hamilton's equations imply at once a second-order equation for $q(t)$:

$$\ddot{q} + \omega^2 q = -\epsilon\omega^2 q^3. \tag{2.2}$$

The solution to this equation has been widely considered as a kind of prototype for all nonlinear differential systems.[10] It is for one thing the first correction to the motion of a string pendulum, where q is the angle and $\epsilon = -\frac{1}{6}$. Many perturbation methods for successive approximation to $q(t)$ have been detailed. However, the method of successive canonical transformation gives a very direct perturbative approach to the solution and is perhaps the most meaningful in the extension to quantum mechanics. In the quantum case it enables one to deal directly with the classical equivalents of the raising and lowering operators.

Let us introduce a new complex variable $\eta(t)$ in place of the two real variables, which is a coordinate canonical to its complex conjugate $\xi(t) = \eta^*(t)$, with respect to a "Hamiltonian" $H' = -iH$:

$$\eta(t) = i(2\omega)^{-\frac{1}{2}}[p(t) - i\omega q(t)]. \tag{2.3}$$

The function η is the coordinate and ξ the conjugate momentum. Explicitly, the Hamiltonian takes the following form:

$$H' = -i\omega\xi\eta - i(\epsilon/16)(\xi + \eta)^4. \tag{2.4}$$

A sequence of canonical transformations $(\xi, \eta) \rightarrow (\bar{\xi}, \bar{\eta})$ is to be carried out, to successively higher orders in ϵ and successively higher powers of $(\bar{\xi}, \bar{\eta})$. The method is standard,[1,9] and leads to the following form for $H'(\bar{\xi}, \bar{\eta})$:

$$H' = -i\omega\left[\sum_{j=0}^{\infty} \epsilon^j d_j (\bar{\xi}\bar{\eta})^{j+1}\right], \tag{2.5}$$

where $d_0 = 1$, $d_1 = \frac{3}{8}\omega^{-1}$, $d_2 = -\frac{17}{64}\omega^{-2}$. Having succeeded in this, the solution to the rest of the problem is trivial. Hamilton's equations for $\bar{\xi}$ and $\bar{\eta}$ are

$$\dot{\bar{\xi}} = i\omega\bar{\xi}\left(\sum_{j=0}^{\infty} \epsilon^j d_j (j+1)(\bar{\xi}\bar{\eta})^j\right), \tag{2.6}$$

$$\dot{\bar{\eta}} = -i\omega\bar{\eta}\left(\sum_{j=0}^{\infty} \epsilon^j d_j (j+1)(\bar{\xi}\bar{\eta})^j\right). \tag{2.7}$$

One finds immediately a constant of the motion

$$\frac{d}{dt}(\rho^2) \equiv \frac{d}{dt}(\bar{\xi}\bar{\eta}) = 0$$
$$\Rightarrow \rho^2 \text{ is a constant in time, } \rho^2 > 0. \tag{2.8}$$

If the initial conditions on $\bar{\eta}$ are parametrized as $\bar{\eta}(0) = \rho \exp(-i\theta)$, then these equations [(2.6) and (2.7)] become the following:

$$\frac{d\bar{\xi}}{dt} = i\Omega\bar{\xi}, \tag{2.9a}$$

$$\frac{d\bar{\eta}}{dt} = -i\Omega\bar{\eta}, \tag{2.9b}$$

where

$$\Omega = \omega\left[\sum_{j=0}^{\infty} \epsilon^j d_j (j+1)(\rho^2)^j\right]. \tag{2.9c}$$

The solutions are immediate:

$$\bar{\eta}(t) = \bar{\xi}(t)^* = \rho \exp[-i(\Omega t + \theta)]. \tag{2.10}$$

Thus, one can achieve quite directly one of the major results of such nonlinear problems (and the general method is in no way restricted by the type or order of polynomial one chooses for H_1). They are known in many cases to be solved by Fourier expansions, not in the "unrenormalized" frequency ω, but in a "renormalized" frequency Ω, shifted by an amplitude-dependent amount. Failure to account for this behavior leads to the difficulty known as secularity, which the present method avoids in a natural way.

Convergence of the expansion of H in Eq. (2.5) and of Ω in Eq. (2.9c) is neither proven nor disproven here. To comment, we observe that convergence, if it occurs, must be limited to some region of initial conditions, the effective expansion parameter being $\epsilon\rho^2$, not simply ϵ. In fact, the expansion is only believable, even asymptotically, for $\epsilon\rho^2 < 1$, corresponding to H_1/H_0 small. But, in defense of possible convergence, one should note that neither expansion is a simple power series in ϵ. If they were, it would rule out convergence on grounds of the analyticity of the exact elliptic integral solution to Eq. (2.2) in ϵ. However, the constant ρ^2 is related to the initial conditions $x(0)$ and $p(0)$ by a series expansion as well. If $\eta(0) = \sigma \exp(-i\phi)$, then

$$\sigma \exp(-i\phi) = \sum_{j=0}^{\infty} \epsilon^j b_j \rho^{2j+1} f_j(\theta). \tag{2.11}$$

Thus, to obtain $\rho^2(\sigma, \phi)$, one would have to invert this series. Such a dual expansion may, in fact, converge for small σ.[1]

The details of the transformation method for this case and results to order ϵ^2 are given in Appendix A for reference. There we also outline the method for arbitrary order. At this point let us direct attention to the quantum version of this problem. As usual, the transformation $(\xi, \eta) \rightarrow (\bar{\xi}, \bar{\eta})$ induces a parallel canonical transformation $(p, q) \rightarrow (\bar{p}, \bar{q})$ and leads to a new form for H:

$$H = \sum_{j=0}^{\infty} \epsilon^j d_j \omega^{-j} [\tfrac{1}{2}(\bar{p}^2 + \omega^2\bar{q}^2)]^{j+1}. \tag{2.12}$$

It is in terms of $(\bar{p}, \bar{q})$ that quantization will now be carried out. One disposes of most of the complexity of the problem by greatly simplifying the classical Hamiltonian and only introduces the added difficulty of operators at this stage.[11] Since the Poisson bracket of q and p at any time is 1, the operator representatives of $\bar{q}$ and $\bar{p}$ (call them $\hat{q}$ and $\hat{p}$) must be chosen to satisfy the usual commutation relations

$$[\hat{q}(t), \hat{p}(t)] = i. \tag{2.13}$$

Let us introduce raising and lowering operators in the usual way:

$$\alpha(t) = i(2\omega)^{-\frac{1}{2}}[\hat{p}(t) - i\omega\hat{q}(t)], \tag{2.14a}$$

$$\alpha^\dagger(t) = -i(2\omega)^{-\frac{1}{2}}[\hat{p}(t) + i\omega\hat{q}(t)]. \tag{2.14b}$$

The commutator of α and $\alpha^\dagger$ is just 1, as usual.

Assuming there is a state of the system which is annihilated by $\alpha(t)$ for all time, call it $|0\rangle$,[12] one can construct a set of states at any time t just as in the usual harmonic oscillator.

$$|n\rangle_t = (n!)^{-\frac{1}{2}}[\alpha^\dagger(t)]^n |0\rangle. \tag{2.15}$$

Of course, these states are eigenstates of the renormalized number operator $N(t) = \alpha^\dagger(t)\alpha(t)$, with

$$N(t)\,|n\rangle_t = n\,|n\rangle_t. \tag{2.16}$$

Since $N(t)$ commutes with H at any time, it is a constant of the motion. In fact, H has a direct expression in terms of N alone. As is well known, the association between classical functions of $\bar{p}$ and $\bar{q}$ and quantum-mechanical operator representatives, $\hat{p}$ and $\hat{q}$, is not unique.[13] One must pick an ordering convention with the correct physical properties. We shall adhere to the Weyl ordering convention, where the operator to be associated with the classical monomial $\bar{p}^m\bar{q}^n$ is the coefficient of $[(m+n)!/m!\,n!] \times \lambda^m\mu^n$ in the expansion of the product $(\lambda\hat{p} + \mu\hat{q})^{m+n}$. This ordering gives an Hermitian association and positive-definite probability density. Under this convention, we obtain

$$H = (N + \tfrac{1}{2})\omega + \tfrac{3}{8}\epsilon(N^2 + N + \tfrac{1}{2})\omega. \tag{2.17}$$

One can also solve for the time dependence of the operator $\alpha(t)$ in terms of its initial (operator) value at $t = 0$, $\alpha_0 \equiv \alpha(0)$:

$$\dot{\alpha} = -i[\alpha, H] = -i\Omega\alpha, \tag{2.18a}$$

where

$$\Omega = \omega[1 + \tfrac{3}{4}\epsilon(N + 1)]. \tag{2.18b}$$

It follows upon integrating Eq. (2.18) that, by taking care to maintain the correct ordering of operators, since $[\alpha, N] \neq 0$,

$$\alpha(t) = \exp(-i\Omega t)\alpha_0. \tag{2.19}$$

The relationship of the set of basis states at $t = 0$ to those at arbitrary t, obtainable in several ways, results trivially from Eq. (2.15):

$$|n\rangle_t = \exp\left[i\left(\sum_{j=0}^{n-1}\omega_j\right)t\right]|n\rangle_0, \tag{2.20}$$

where ω_j is the eigenvalue of Ω in the state $|j\rangle_t$. It can also be verified simply that the coefficient of the factor (it) in the exponential is just $E_n^{(1)} - E_0^{(1)}$, where $H\,|n\rangle_t = E_n^{(1)}\,|n\rangle_t$. Thus, as a basis of the Hilbert state the set $\{|n\rangle_t\}$ is essentially the same set regardless of t. Henceforth, we shall use $\{|n\rangle_0\}$, denoting each state simply by $|n\rangle$. If one compares Eqs. (2.17) and (2.18) with the results of Ref. 7, remembering that $N = a^\dagger a + O(\epsilon)$, the coefficients of the N^2 terms here agrees with that of the $N^2 = (a^\dagger a)^2$ terms there, while the other coefficients differ, as they must.

To complete the discussion of one oscillator, let us consider the question of the convergence status of the approximation. Loeffel, Martin, Simon, and Wightman[14] have recently offered a proof that the Rayleigh–Schrödinger perturbation series for the ground state energy of the x^4 perturbed oscillator is asymptotic to the exact eigenvalue. They further prove that the Padè approximants constructed from the Rayleigh–Schrödinger coefficients (given to 75th order by Bender and Wu[15]) *converge* to the eigenvalue. It is expected that the proof can be extended to E_n, but they offer no rigorous statement on the status of the Rayleigh–Schrödinger approximation for the eigenfunctions. The canonical method also gives an infinite series for E_n for every ordering choice but normal ordering. The order λ^1 coefficient agrees with the RS value, while λ^2 and λ^3 differ slightly. We expect the λ^n coefficient to differ also, for $n \geq 4$. Since an asymptotic expansion is unique, we conclude that the power series generated by the canonical method is not asymptotic. Some reflection suggests why this difference exists. Knowledge of the operators $x(t)$ [and $p(t)$ and H which are implied by x] would yield a global solution. It would give *all* of the eigenvalues and eigenstates. In the Schrödinger representation one is solving for a *single* eigenpair at a time. If these expansions are no better than asymptotic, one expects power series expansions of the operator H, $x(t)$, and $p(t)$ to be less convergent. Thus, the expansions for eigenvalues generated by the expansion of the operator will not be asymptotic. But the physical approximations behind the canonical method are valid and yield expansions for low-lying eigenvalues which closely approximate the eigenvalues. This has been verified numerically for small λ (< 0.1) to third order in the case at hand. The first few orders, then, "converge" toward the true values. Such approximations are very common in physics and very useful, as long as they are qualitatively correct as well. Finally, we generate approximate eigenvectors in the sense discussed above. The references to the Schrödinger representation studies[14] defer on this question.

3. n OSCILLATORS WITH QUARTIC INTERACTION

The techniques and results to be described here are more general than the limitation to quartic interaction would suggest. Gustavson[1] uses them for a classical two-oscillator problem from celestial mechanics with cubic interaction, while his general results assume an arbitrary power series expansion of the Hamiltonian, convergent in some neighborhood of an equilibrium point. For the purposes at hand the complexity of the completely general case is unnecessary. The issues to be met are difficult enough with a single order for the nonlinear coupling term. Second, for at least one sign of the coupling constant the energy surface is well

behaved for all values of the coordinates, making generalization to the quantum case more reliable. (The cut in the coupling constant plane along the negative real axis for a one-dimensional λx^4 oscillator arises, physically, from the possibility of escape to infinity in finite time for a quantum particle in a negative x^4 potential via tunneling.) Finally, to shed light on the $\lambda\phi^4$ field problem, we select an interaction as much like it as possible. In a box the denumerably infinite set of coupled oscillator equations arising from decomposition into normal modes has a quartic interaction, which is just an infinite generalization of exactly the interaction to be considered.

At first the discussion will focus on the classical case, drawing heavily on the results, methods, and some of the notation of Gustavson. Then the problems associated with quantization will be discussed. Consider, then, a set of n interacting, nonlinear oscillators with the following Hamiltonian:

$$H = H_0 + H_1, \tag{3.1a}$$

$$H_0 = \sum_{\nu=1}^{n} \tfrac{1}{2}(p_\nu^2 + \omega_\nu^2 q_\nu^2), \tag{3.1b}$$

$$H_1 = \sum_{|\mathbf{i}|+|\mathbf{j}|=4} a_{\mathbf{ij}} q^{\mathbf{i}} p^{\mathbf{j}}. \tag{3.1c}$$

In the notation used here $\mathbf{i}$ and $\mathbf{j}$ represent an n-vector with nonnegative integer components, $|\mathbf{i}| = \sum_{\nu=1}^{n} i_\nu$, and $q^{\mathbf{i}} = \prod_{\nu=1}^{n} q_\nu^{i_\nu}$.

Next we must define precisely the notion, degree, and order of resonance present in the system. The system has resonance of *degree* r when the frequencies $\{\omega_\nu\}$ are connected by exactly r linear integer commensurability relations

$$\sum_{\nu=1}^{n} c_\nu^{(\sigma)} \omega_\nu = 0, \quad \sigma = 1, 2, \cdots, r, \tag{3.2}$$

and the $c_\nu^{(\sigma)}$ are arbitrary integers. (Examples are $\omega_1 - \omega_2 = 0$, $\omega_1 + \omega_2 - \omega_3 = 0$, etc.) The case $r = 0$ is called the nonresonant case. The *order* of each such relation is defined as the length of the $\mathbf{c}^{(\sigma)}$ vector in integer space. (Assume the $c_\nu^{(\sigma)}$ are chosen relatively prime.) We have

$$l_\sigma = \sum_{\nu=1}^{n} |c_\nu^{(\sigma)}|, \quad \sigma = 1, 2, \cdots, r.$$

Thus, for a given set of n frequencies we identify resonance of degree r with orders $\{l_1, l_2, \cdots, l_r\}$.

The results of Gustavson may be summarized as follows: The original variables may be expressed as a formal infinite series of homogeneous polynomials of increasing order in canonically transformed variables, which bring H into a "normal form" in the new variables. In our notation we will discuss this normal form shortly. It is attained by a succession of canonical transformations, just as in the case of one oscillator. In addition he shows that there are $n - r$ independent formal integrals or constants of the motion. If $r \neq 0$, the $n - r$ integrals are independent of H (itself an integral, of course). If $r = 0$, then there are n independent integrals and H is a function of them.

Again let us introduce the complex variables η_ν, n in number,

$$\eta_\nu(t) = i(2\omega_\nu)^{-\frac{1}{2}}[p_\nu(t) - i\omega_\nu q_\nu(t)],$$
$$\xi_\nu(t) = [\eta_\nu(t)]^*. \tag{3.3}$$

After re-expressing H in terms of these variables, we obtain

$$H_0 = \sum_{\nu=1}^{n} \omega_\nu(\xi_\nu \eta_\nu), \tag{3.4a}$$

$$H_1 = \epsilon \sum_{|\mathbf{i}|+|\mathbf{j}|=4} b_{\mathbf{ij}} \xi^{\mathbf{i}} \eta^{\mathbf{j}}. \tag{3.4b}$$

Here the multi-index notation is implicit as above. The parameter ϵ is assumed small and $|b_{\mathbf{ij}}| \lesssim 1$. The goal is to find a new set of variables $\{\bar{\eta}_\nu\}(\Rightarrow \{\bar{\xi}_\nu\})$ in terms of which H takes on greatly simplified normal form and the integrals mentioned above become simple functions of the $\{\bar{\eta}_\nu\}$. The transformation is to be exhibited as a formal power series:

$$\eta_\nu = \bar{\eta}_\nu + \sum_{\mu=1}^{\infty} \epsilon^\mu f_\nu^{(2\mu+1)}(\bar{\eta}_\nu, \bar{\xi}_\nu),$$
$$\xi_\nu = \bar{\xi}_\nu + \sum_{\mu=1}^{\infty} \epsilon^\mu [f_\nu^{(2\mu+1)}(\bar{\eta}_\nu, \bar{\xi}_\nu)]^*. \tag{3.5}$$

The functions $f_\nu^{(2\mu+1)}$ are homogeneous polynomials of order $2\mu + 1$ in the indicated variables:

$$f_\nu^{(2\mu+1)} = \sum_{|\mathbf{i}|+|\mathbf{j}|=2\mu+1} \gamma_{\mathbf{ij}}^{(\nu,2\mu+1)} \bar{\xi}^{\mathbf{i}} \bar{\eta}^{\mathbf{j}}. \tag{3.6}$$

The choice of the generating functions for the sequence of transformations is given by Gustavson in slightly different variables. Here let us carry out only the lowest order to indicate concretely how the procedure works:

$$K_4(\eta_\nu, \bar{\xi}_\nu) = \epsilon \sum_{|\mathbf{i}|+|\mathbf{j}|=4} k_{\mathbf{ij}} \bar{\xi}^{\mathbf{i}} \eta^{\mathbf{j}}, \tag{3.7a}$$

$$\bar{K}_4(\bar{\eta}_\nu, \bar{\xi}_\nu) = \epsilon \sum_{|\mathbf{i}|+|\mathbf{j}|=4} k_{\mathbf{ij}} \bar{\xi}^{\mathbf{i}} \bar{\eta}^{\mathbf{j}}. \tag{3.7b}$$

The transformation generated is, as before,

$$\eta_\nu = \bar{\eta}_\nu - \frac{\partial K_4(\eta, \bar{\xi})}{\partial \bar{\xi}_\nu}, \tag{3.8a}$$

$$\xi_\nu = \bar{\xi}_\nu + \frac{\partial K_4(\eta, \bar{\xi})}{\partial \eta_\nu}. \tag{3.8b}$$

But, we can use $\tilde{K}_4$ to order ϵ as well, introducing differences only in higher order:

$$\eta_\nu = \bar{\eta}_\nu - \frac{\partial \tilde{K}_4(\bar{\eta}, \bar{\xi})}{\partial \bar{\xi}_\nu} + O(\epsilon^2), \tag{3.9a}$$

$$\xi_\nu = \bar{\xi}_\nu + \frac{\partial \tilde{K}_4(\bar{\eta}, \bar{\xi})}{\partial \bar{\eta}_\nu} + O(\epsilon^2). \tag{3.9b}$$

If $H^{(\mu)}$ represents the order μ terms in H in terms of transformed variables, then our results due to this substitution for $H^{(0)}$ and $H^{(1)}$ are

$$H^{(0)} = \sum_{\nu=1}^{n} \omega_\nu(\bar{\xi}_\nu \bar{\eta}_\nu), \tag{3.10a}$$

$$H^{(1)} = \sum_{\nu=1}^{n} \omega_\nu\left(\bar{\eta}_\nu \frac{\partial \tilde{K}_4}{\partial \bar{\eta}_\nu} - \bar{\xi}_\nu \frac{\partial \tilde{K}_4}{\partial \bar{\xi}_\nu}\right) + \epsilon \sum_{|\mathbf{i}|+|\mathbf{j}|=4} b_{\mathbf{ij}} \bar{\xi}^{\mathbf{i}} \bar{\eta}^{\mathbf{j}}. \tag{3.10b}$$

The first term in $H^{(1)}$ can be calculated from Eq. (3.7b):

$$\sum_{\nu=1}^{n} \omega_\nu\left(\bar{\eta}_\nu \frac{\partial \tilde{K}_4}{\partial \bar{\eta}_\nu} - \bar{\xi}_\nu \frac{\partial \tilde{K}_4}{\partial \bar{\xi}_\nu}\right) = \epsilon \sum_{|\mathbf{i}|+|\mathbf{j}|=4} k_{\mathbf{ij}}\left(\sum_{\nu=1}^{n}(j_\nu - i_\nu)\omega_\nu\right) \bar{\xi}^{\mathbf{i}} \bar{\eta}^{\mathbf{j}}. \tag{3.11}$$

For a given pair of vectors $\{\mathbf{i}, \mathbf{j}\}$ let $(\mathbf{i} - \mathbf{j}, \boldsymbol{\omega})$ represent the n-vector scalar product $\sum_{\nu=1}^{n}(i_\nu - j_\nu)\omega_\nu$. Then the expression for $H^{(1)}$ can be written as follows:

$$H^{(1)} = \epsilon \sum_{|\mathbf{i}|+|\mathbf{j}|=4} \{b_{\mathbf{ij}} - k_{\mathbf{ij}}(\mathbf{i} - \mathbf{j}, \boldsymbol{\omega})\} \bar{\xi}^{\mathbf{i}} \bar{\eta}^{\mathbf{j}}. \tag{3.12}$$

All such terms become zero by appropriate choice of $k_{\mathbf{ij}}$ except those which satisfy $(\mathbf{i} - \mathbf{j}, \boldsymbol{\omega}) = 0$:

$$k_{\mathbf{ij}} = (\mathbf{i} - \mathbf{j}, \boldsymbol{\omega})^{-1} b_{\mathbf{ij}}. \tag{3.13}$$

The case $\mathbf{i} = \mathbf{j}$ automatically fails to satify Eq. (3.13). To the present order of approximation this represents at most n^2 terms. The first feature of "normal form," then, is that it contains all terms of the type $\bar{\xi}^{\mathbf{i}} \bar{\eta}^{\mathbf{i}}$ which were there originally with $|\mathbf{i}| = 2$. Similar terms will be induced in higher order by the transformation and this statement will extend, although $|\mathbf{i}|$ will be greater. Let us call these terms the nonresonant irreducible Hamiltonian, since their presence does not require any resonance condition of the type in Eq. (3.2).

Second, Eq. (3.13) can fail to be valid if one of the resonance conditions has order 4 or less. In this case we shall call the terms which cannot be removed by transformation the resonant part of the irreducible Hamiltonian. As the process is carried to arbitrary order, all of the resonance conditions will eventually come into play.

One important caution is necessary here concerning a pitfall which the formal considerations tend to conceal. If for some $\mathbf{i}$ and $\mathbf{j}$, $b_{\mathbf{ij}} \sim 1$ and $(\mathbf{i} - \mathbf{j}, \boldsymbol{\omega}) \approx 0$, but not exactly, then the coefficient $k_{\mathbf{ij}}$ in Eq. (3.13) will be very large. As a perturbative approach, then, this iteration scheme will become suspect at this order of approximation. This is, the author believes, a very deep but unresolved point, which probably means that the approximate integrals of the motion remain constant only on a certain time scale. For *arbitrary* $\{\omega_\nu\}$, even if $r = 0$, there is an integer vector $\mathbf{i}$ such that $(\mathbf{i}, \boldsymbol{\omega})$ is arbitrarily close to zero. Such vectors may have to be very "long" in integer space, in fact usually are if $r = 0$. A study of two oscillators by the author, with $\omega_1 - \omega_2 \approx 0$, shows that all of the characteristic features of resonance, such as synchronous oscillation, persist in low order at least. One might then be led to suspect that for arbitrarily high order the actual motion of the system approaches the case $n = r$ for long times, and the only remaining constant of the motion is H itself.

Having chosen $k_{\mathbf{ij}}$ as mentioned above and, with Gustavson, taken as zero all $k_{\mathbf{ij}}$ such that $(\mathbf{i} - \mathbf{j}, \boldsymbol{\omega}) = 0$, we arrive at a unique choice for $\tilde{K}_4$. The function K_4 then follows by simple substitution, $\bar{\eta}_\nu \to \eta_\nu$. The Hamiltonian is now in normal form or, in present terminology, is irreducible, to order ϵ. But, as outlined explicitly in Appendix A, Eq. (A7)ff., for one oscillator, the transformation to order ϵ has generated ϵ^2 terms which are degree six monomials and also ϵ^3 terms of degree eight. The same procedure, then, is followed to achieve an irreducible H to order ϵ^2 by choice of K_6, and so on to arbitrary order.[16]

At any order in the iteration the formal constants of the motion—constant to the order in question, subject to the caution above concerning small divisors—are found as follows: Let $\mathbf{A}$ be the $r \times n$ matrix whose first row is $\mathbf{c}^{(1)}$, second row $\mathbf{c}^{(2)}$, etc. Let $\boldsymbol{\mu}^{(\tau)}$ be $n - r$ independent solutions of the equation

$$\mathbf{A}\boldsymbol{\mu}^{(\tau)} = 0. \tag{3.14}$$

Then, if $I^{(\tau)}$ denotes the τth constant, $1 \leq \tau \leq n - r$,

$$I^{(\tau)} = \sum_{\nu=1}^{n} \mu_\nu^{(\tau)}(\bar{\xi}_\nu \bar{\eta}_\nu) \tag{3.15a}$$

$$= \tfrac{1}{2} \sum_{\nu=1}^{n} \omega_\nu^{-1} \mu_\nu^{(\tau)}(\bar{p}_\nu^2 + \omega_\nu^2 \bar{q}_\nu^2). \tag{3.15b}$$

Of course, the $I^{(\tau)}$ are not unique, as independent linear combinations of them are also constants of the motion.

With respect to the new (approximate) canonical variables $\{\bar{p}_\nu, \bar{q}_\nu\}$, the constancy of the $\{I^{(\tau)}\}$ means that their Poisson bracket with H must vanish to the order of concern. Quantization will then proceed

exactly as for one oscillator subject to the same ordering ambiguities. But, whatever the ordering, these $n-r$ integrals give us at once $n-r$ good quantum numbers with which to label our states.

Let $\alpha_\nu(t)$ and $\alpha_\nu^\dagger(t)$ be the raising and lowering operators for the νth oscillator. The operators $N_\nu(t) \equiv \alpha_\nu^\dagger(t)\alpha_\nu(t)$ are not constants of the motion unless $r=0$. In the case $r=0$ we may choose $I^{(\nu)} = \frac{1}{2}(p_\nu^2 + \omega_\nu^2 q_\nu^2)$, $1 \le \nu \le n$. After quantization, this implies the constancy in time of the number operators N_ν:

$$\frac{dN_\nu(t)}{dt} = -i[N_\nu(t), H] = 0 \quad \text{for all } t. \tag{3.16}$$

In the presence of resonance, however, a set of $n-r$ "number operators" do commute with H, although at least some of the $N_\nu(t)$ will not separately. These are not unique, and either convenience or physical considerations should be served by their choice. We have

$$\mathcal{N}^{(\tau)}(t) \equiv \sum_{\nu=1}^{n} \mu_\nu^{(\tau)} N_\nu(t), \quad 1 \le \tau \le n-\nu, \tag{3.17}$$

$$\Rightarrow \frac{d\mathcal{N}_\nu^{(\tau)}(t)}{dt} = -i[\mathcal{N}^{(\tau)}, H] = 0. \tag{3.18}$$

The oscillator states obtained from the vacuum using $\alpha_\nu^\dagger(0)$ will be taken as the basis of the Hilbert space:

$$|m_1, m_2, \cdots, m_n\rangle = \left[\prod_{\nu=1}^{n} m_\nu!\right]^{-\frac{1}{2}} [\alpha_1^\dagger(0)]^{m_1} \cdots [\alpha_n^\dagger(0)]^{m_n} |0\rangle, \tag{3.19}$$

where $\alpha_\nu(0)|0\rangle = 0$, $1 \le \nu \le n$. In the case $r=0$, the previous remarks make it clear that these are already eigenstates of H, and the eigenvalue problem is completely solved to this order. This follows from the fact that the nonresonant irreducible classical Hamiltonian contains only $\bar\xi^{\mathbf{i}}\bar\eta^{\mathbf{i}}$ terms, which when quantized give a polynomial in the N_ν, regardless of ordering chosen. Further, the equations of motion for $\alpha_\nu(t)$ can be solved exactly:

$$\dot\alpha_\nu(t) = -i[\alpha_\nu(t), H] = -i\alpha_\nu(t)\Omega_\nu(N_1, N_2, \cdots, N_n) \tag{3.20a}$$

$$\Rightarrow \alpha_\nu(t) = \alpha_\nu(0)\exp[-i\Omega_\nu(N_1, N_2, \cdots, N_n)t]. \tag{3.20b}$$

Again one obtains an operator-valued Hermitian frequency, dependent now in general on the occupation number of every oscillator.

In the resonant case ($r \neq 0$) the states defined in Eq. (3.19) are not eigenstates of H. But the $\mathcal{N}^{(\tau)}$ define finite-dimensional subspaces within which H can be diagonalized by standard matrix methods. Thus, the eigenvalue problem can be solved, albeit not so directly as in the nonresonant case. But the equations of motion for the $\alpha_\nu(t)$ become highly intractable. A forthcoming paper by the author on a particular case of $n=2$, where the corresponding classical equations are solved to order ϵ, shows the complexity of these equations even without the added issue raised by noncommutativity of the variables.

To give content to these rather general and formal considerations, a case with $n=2$ and $\omega_1 - \omega_2 = 0$ is taken up in the next section.

4. TWO QUASILINEAR OSCILLATORS: $H_1 = \frac{1}{4}\epsilon\omega_1\omega_2 q_1^2 q_2^2$

Consider a system of two oscillators near equilibrium ($q_1 = q_2 = 0$) governed by the following Hamiltonian:

$$H_0 = \tfrac{1}{2}(p_1^2 + \omega_1^2 q_1^2) + \tfrac{1}{2}(p_2^2 + \omega_2^2 q_2^2), \tag{4.1a}$$

$$H_1 = \tfrac{1}{4}\epsilon\omega_1\omega_2 q_1^2 q_2^2. \tag{4.1b}$$

If $\omega_1 = \omega_2 = (\mathbf{k}^2 + m^2)^{\frac{1}{2}}$, then this system corresponds to the coupling of only two modes in the $\lambda\phi^4$ field Hamiltonian decomposed into normal modes, the mode of wave number $\mathbf{k}$ and that of $-\mathbf{k}$.

If $\omega_1 - \omega_2 \neq 0$, then the system is nonresonant, whereas if $\omega_1 - \omega_2 = 0$ or $\omega_1 - \omega_2 \approx 0$ to order ϵ, the system is resonant of degree 1, order 2. Let us consider first the nonresonant case and introduce the new variables η_1 and η_2 from Eq. (3.3):

$$H_0 = \omega_1\xi_1\eta_1 + \omega_2\xi_2\eta_2, \tag{4.2a}$$

$$H_1 = (\epsilon/16)(\xi_1 + \eta_1)^2(\xi_2 + \eta_2)^2. \tag{4.2b}$$

In terms of the transformed variables $\{\bar\eta_1, \bar\eta_2, \bar\xi_1, \bar\xi_2\}$, the irreducible Hamiltonian will contain only one term corresponding to $\mathbf{i} = (1,1)$:

$$H_0 = \omega_1\bar\xi_1\bar\eta_1 + \omega_2\bar\xi_2\bar\eta_2, \tag{4.3a}$$

$$H_1 = (\epsilon/4)(\bar\xi_1\bar\eta_1)(\bar\xi_2\bar\eta_2) + O(\epsilon^2). \tag{4.3b}$$

The choice of K_4 which must be made is

$$\begin{aligned}\tilde K_4 = (\epsilon/32)[&(\omega_1+\omega_2)^{-1}\bar\xi_1^2\bar\xi_2^2 + (2/\omega_1)\bar\xi_1^2\bar\xi_2\bar\eta_2 \\ &+ (\omega_1-\omega_2)^{-1}\bar\xi_1^2\bar\eta_2^2 - (\omega_1-\omega_2)^{-1}\bar\xi_2^2\bar\eta_1^2 \\ &+ (2/\omega_2)\bar\xi_1\bar\xi_2^2\bar\eta_1 - (2/\omega_2)\bar\xi_1\bar\eta_1\bar\eta_2^2 \\ &- (2/\omega_1)\bar\xi_2\bar\eta_1^2\bar\eta_2 - (\omega_1+\omega_2)^{-1}\bar\eta_1^2\bar\eta_2^2].\end{aligned} \tag{4.4}$$

Of course K_4 has the same form as $\tilde K_4$ with $\bar\eta_j$, replaced by η_j. The transformation generated by K_4 from the pairs (ξ_j, η_j) to $(\bar\xi_j, \bar\eta_j)$ may be found from Eq. (3.8)

to order ϵ:

$$\eta_1 = \xi_1^* = \bar{\eta}_1 - (\epsilon/8)[(\omega_1 + \omega_2)^{-1}\bar{\xi}_1\bar{\xi}_2^2 + (2/\omega_1)\bar{\xi}_1\bar{\xi}_2\eta_2 + (\omega_1 - \omega_2)^{-1}\bar{\xi}_1\eta_2^2 + \omega_2^{-1}\bar{\xi}_2^2\eta_1 - \omega_2^{-1}\eta_1\eta_2^2], \tag{4.5a}$$

$$\eta_2 = \xi_2^* = \bar{\eta}_2 - (\epsilon/8)[(\omega_1 + \omega_2)^{-1}\bar{\xi}_1^2\bar{\xi}_2 + \omega_1^{-1}\bar{\xi}_1^2\eta_2 - (\omega_1 - \omega_2)^{-1}\bar{\xi}_2\eta_1^2 + (2/\omega_2)\bar{\xi}_1\bar{\xi}_2\eta_1 - \omega_1^{-1}\eta_1^2\eta_2]. \tag{4.5b}$$

To the same order of accuracy, we can replace η_1 and η_2 in the order-ϵ terms on the right-hand side of Eqs. (4.5) by $\bar{\eta}_1$ and $\bar{\eta}_2$, thus giving the new variables in terms of the old by inversion of a set of implicit cubic equations. Numerically, an iteration procedure would be the indicated method of solution. One can see that order-ϵ^2 terms as functions of the once-transformed variables are induced in H, coming both from H_0 and H_1, as well as terms of order ϵ^3, ϵ^4, and ϵ^5. All of the order-ϵ^2 terms are obtained by simple substitution of Eqs. (4.5) (in terms of $\bar{\xi}_j$, $\bar{\eta}_j$ on rhs) into Eqs. (4.2), except for those introduced by a further transformation to order ϵ^2 generated by K_6. However, until K_6 is chosen to give irreducible form for H to order ϵ^2, one cannot complete the enumeration of the order ϵ^3 induced terms. The formal procedure, of course, is as outlined in Appendix A, and extends to arbitrary order. Suffice it here simply to enumerate the types of terms in the irreducible Hamiltonian to order ϵ^2:

$$\mathbf{i} = (3, 0): \quad (\bar{\xi}_1\bar{\eta}_1)^3; \tag{4.6a}$$

$$\mathbf{i} = (2, 1): \quad (\bar{\xi}_1\bar{\eta}_1)^2(\bar{\xi}_2\bar{\eta}_2); \tag{4.6b}$$

$$\mathbf{i} = (1, 2): \quad (\bar{\xi}_1\bar{\eta}_1)(\bar{\xi}_2\bar{\eta}_2)^2; \tag{4.6c}$$

$$\mathbf{i} = (0, 3): \quad (\bar{\xi}_2\bar{\eta}_2)^3. \tag{4.6d}$$

In terms of a transformed pair of position–momentum variables, the Hamiltonian now has simple form to order ϵ:

$$H_0 = \tfrac{1}{2}\sum_{j=1}^{2}(\bar{p}_j^2 + \omega_j^2\bar{q}_j^2), \tag{4.7a}$$

$$H_1 = [\epsilon/(16\omega_1\omega_2)](\bar{p}_1^2 + \omega_1^2\bar{q}_1^2)(\bar{p}_2^2 + \omega_2^2\bar{q}_2^2). \tag{4.7b}$$

One next introduces the operator representatives of $\bar{p}_j$ and $\bar{q}_j$, defines raising and lowering operators, and generates a space of states from the ground state in the usual way. In terms of the number operators $N_j = \alpha_j^\dagger\alpha_j$, the quantum version of H with symmetric ordering is

$$H = (N_1 + \tfrac{1}{2})\omega_1 + (N_2 + \tfrac{1}{2})\omega_2 + (\epsilon/4)(N_1 + \tfrac{1}{2})(N_2 + \tfrac{1}{2}). \tag{4.8}$$

It is evident here that N_1 and N_2 commute with H, and thus have no time dependence. The time dependence of the operator α_j is obtained in the usual way:

$$\dot{\alpha}_j = -i[\alpha_j, H] = -i\Omega_j\alpha_j, \quad j = 1, 2, \tag{4.9a}$$

where

$$\Omega_1 = \omega_1 + (\epsilon/4)(N_2 + \tfrac{1}{2}) \tag{4.9b}$$

and

$$\Omega_2 = \omega_2 + (\epsilon/4)(N_1 + \tfrac{1}{2}). \tag{4.9c}$$

These equations are integrated easily to give the same type of operator-valued frequencies as we found in the case of one oscillator. The first-order spectrum is trivial from Eq. (4.8) since the states $|n_1, n_2\rangle$ generated by $\alpha_j^\dagger(0)$ are seen to be energy eigenstates:

$$E^{(1)}_{n_1,n_2} = (n_1 + \tfrac{1}{2})\omega_1 + (n_2 + \tfrac{1}{2})\omega_2 + (\epsilon/4)(n_1 + \tfrac{1}{2})(n_2 + \tfrac{1}{2}). \tag{4.10}$$

This very direct and complete treatment of the problem to first order is possible only in the nonresonant case. The steps outlined above apply to arbitrary order, although one encounters large numbers of distinct monomial terms in higher orders.

In the resonant or near-resonant cases the situation is rather different. If $\omega_1 - \omega_2$ is zero or near zero, then two of the terms in $\tilde{K}_4$, Eq. (4.4), are either undefined or have coefficients which are large and not of order ϵ, those with factors of $(\omega_1 - \omega_2)^{-1}$. Let us perform a reduced canonical transformation in either case, generated by $\tilde{K}_4$ with omission of these terms. The irreducible Hamiltonian has the following form in this case:

$$H_0 = (\omega - \Delta)(\bar{\xi}_1\bar{\eta}_1) + (\omega + \Delta)(\bar{\xi}_2\bar{\eta}_2), \tag{4.11a}$$

$$H_1 = (\epsilon/16)[\bar{\xi}_1^2\bar{\eta}_2^2 + 4(\bar{\xi}_1\bar{\eta}_1)(\bar{\xi}_2\bar{\eta}_2) + \bar{\xi}_2^2\bar{\eta}_1^2], \tag{4.11b}$$

where $\omega = \frac{1}{2}(\omega_1 + \omega_2)$ and $0 < \Delta = \frac{1}{2}(\omega_2 - \omega_1)$. In terms of the transformed momentum and position operators, the interaction Hamiltonian is as follows:

$$H_1 = [\epsilon/32(\omega^2 - \Delta^2)] \times \{2[\bar{p}_1^2 + (\omega - \Delta)^2\bar{q}_1^2][\bar{p}_2^2 + (\omega + \Delta)^2\bar{q}_2^2] + [\bar{p}_1^2 - (\omega - \Delta)^2\bar{q}_1^2][\bar{p}_2^2 - (\omega + \Delta)^2\bar{q}_2^2]\} + (\epsilon/8)\bar{q}_1\bar{p}_1\bar{q}_2\bar{p}_2. \tag{4.12}$$

Again let us introduce the transformed raising and lowering operators, and calculate the quantum H, using symmetric ordering. (Of course, in this case $\{\alpha_j, \alpha_j^\dagger\}$ have different meaning than in the nonresonant case, because the transformation is different.) We have

$$H = (N_1 + N_2 + 1)\omega + (N_2 - N_1)\Delta + (\epsilon/4)(N_1 + \tfrac{1}{2})(N_2 + \tfrac{1}{2}) + (\epsilon/16)(\alpha_1^{\dagger 2}\alpha_2^2 + \alpha_2^{\dagger 2}\alpha_1^2). \tag{4.13}$$

The additional terms here, not found in Eq. (4.8), radically alter the nature of the solution. As mentioned earlier, neither N_1 nor N_2 commute with H. Thus, neither is a constant of the motion. But $N = N_1 + N_2$ does commute with H and is time-independent. The operators (H, N) are, then, a possible choice of quantum representatives of the two independent constants of the motion which exist in the $n = 2$ case with one commensurability relation, as asserted in Gustavson's theorem. Further, the $\{\alpha_j(t)\}$ do not obey an easily integrable equation such as Eq. (4.8). No direct integration of the equations satisfied by α_1 and α_2 has been found as yet.

Let us define a basis of the Hilbert space at time t using $\alpha_1^\dagger$ and $\alpha_2^\dagger$, where the ground state satisfies $\alpha_1 |0\rangle = \alpha_2 |0\rangle = 0$ (any t) and it is an eigenstate of H:

$$|n_1, n_2\rangle_t = (n_1!\, n_2!)^{-\frac{1}{2}}[\alpha_1^\dagger(t)]^{n_1}[\alpha_2^\dagger(t)]^{n_2} |0\rangle. \quad (4.14)$$

At $t = 0$, this set of states is denoted simply by $\{|n_1, n_2\rangle\}$ and will be the actual reference basis for finding the eigenpairs. Within the subspaces spanned by $\{|n_1, n_2\rangle_t\}$ with $n_1 + n_2 = n$, the Hamiltonian can be diagonalized and the eigenpairs found. The constancy in time of N assures that the states $\{|n_1, n_2\rangle_t\}$, with the fixed value of $n = n_1 + n_2$, span the same $(n + 1)$-dimensional subspace of the Hilbert space for all t. Let $\mathbf{H}$ be the $(n + 1) \times (n + 1)$ matrix to order ϵ of the Hamiltonian in this subspace, where $n_1 = n$, $n_2 = 0$ corresponds to index 1 and $n_1 = 0$, $n_2 = n$ to index $n + 1$. The energy eigenvalues can be found as usual in the degenerate case of perturbation theory. They are the $(n + 1)$ roots of the secular equation.

$$\text{Det}\,\{\mathbf{H} - E\mathbf{I}\} = 0. \quad (4.15)$$

Let $E_{n,\sigma}$ be these eigenvalues, the lowest being $\sigma = 0$, the highest being $\sigma = n + 1$. Further, let $|n, \sigma)$ be the corresponding eigenstates. Then, the eigenpairs are given in Table I. One sees that the $n = 0$ and $n = 1$ subspaces are still eigenstates with the same eigenvalues as in the nonresonant case, since the new terms in H have zero matrix elements in these subspaces. For $n = 2$, the characteristic effects of the near-frequency and equal-frequency cases begin to occur.

If one assumes $\epsilon/\delta \ll 1$ for $n = 2$, which should give results in agreement with case (1), the three eigenvalues and the states to order ϵ become the following [cf. Eq. (4.10)]:

$$E_{2,0} = \tfrac{1}{2}(\omega_1 + 5\omega_2) + \tfrac{5}{16}\epsilon, \quad |2, 0) = -|0, 2\rangle, \quad (4.16a)$$

$$E_{2,1} = \tfrac{1}{2}(5\omega_1 + \omega_2) + \tfrac{5}{16}\epsilon, \quad |2, 1) = |2, 0\rangle, \quad (4.16b)$$

$$E_{2,2} = \tfrac{1}{2}(3\omega_1 + 3\omega_2) + \tfrac{9}{16}\epsilon, \quad |2, 2) = |1, 1\rangle. \quad (4.16c)$$

The other limit which interests us, because it corresponds to two modes of a ϕ^3 quantum field with equal and opposite momenta, is $\omega_1 = \omega_2 = \omega$. In this limit

TABLE I. Eigenstates and eigenvalues of H in the $n = 0, 1, 2$ subspaces for two unequal-frequency quantum nonlinear oscillators, $Hint = \frac{1}{4}\epsilon\omega_1\omega_2 q_1^2 q_2^2$. The form of H in terms of the transformed operators is given in Eq. (4.13) and the states $|n_1, n_2\rangle$ are created by $\alpha_1^\dagger(0)$ and $\alpha_2^\dagger(0)$.

$n = 0$	$E_{0,0} = \frac{1}{2}(\omega_1 + \omega_2) + \frac{1}{16}\epsilon$
	$\|0, 0) = \|0, 0\rangle$
$n = 1$ $(\omega_1 < \omega_2)$	$E_{1,0} = \frac{1}{2}(3\omega_1 + \omega_2) + \frac{3}{16}\epsilon$
	$E_{1,1} = \frac{1}{2}(\omega_1 + \omega_2) + \frac{3}{16}\epsilon$
	$\|1, 0) = \|1, 0\rangle$
	$\|1, 1) = \|0, 1\rangle$
	Let $\omega = \frac{1}{2}(\omega_1 + \omega_2), \delta = \omega_1 - \omega_2, \gamma = [1 + \epsilon^2/(64\delta^2)]^{\frac{1}{2}}$ and $\eta = 8\delta(\gamma + 1)$
$n = 2$	$E_{2,0} = 3\omega + \frac{5}{16}\epsilon - \delta\gamma$
	$E_{2,1} = 3\omega + \frac{5}{16}\epsilon + \delta\gamma$
	$E_{2,2} = 3\omega + \frac{9}{16}\epsilon$
	$\|2, 0) = (\epsilon^2 + \eta^2)^{-\frac{1}{2}}(\epsilon\|2, 0\rangle - \eta\|0, 2\rangle)$
	$\|2, 1) = (\epsilon^2 + \eta^2)^{-\frac{1}{2}}(\eta\|2, 0\rangle + \epsilon\|0, 2\rangle)$
	$\|2, 2) = \|1, 1\rangle$

from Table I with $\delta\gamma = \epsilon/8$ and $\eta = \epsilon$, one obtains

$$E_{2,0} = 3\omega + \tfrac{3}{16}\epsilon, \quad |2,0) = 2^{-\frac{1}{2}}(|2,0\rangle - |0,2\rangle), \tag{4.17a}$$

$$E_{2,1} = 3\omega + \tfrac{7}{16}\epsilon, \quad |2,1) = 2^{-\frac{1}{2}}(|2,0\rangle + |0,2\rangle), \tag{4.17b}$$

$$E_{2,2} = 3\omega + \tfrac{9}{16}\epsilon, \quad |2,2) = |1,1\rangle. \tag{4.17c}$$

In this limit, the ordering of the eigenvalues accords with the earlier convention. For $\epsilon < 0$, a less reliable region for the approximation due to the physical possibility of tunneling, both $E_{2,2}$ and $E_{2,3}$ are less than twice $E_{1,1} = E_{1,2}$. Now the states $|1,2)$ and $|1,3)$ would correspond to single-particle states, while the states $|2,1)$, $|2,2)$, and $|2,3)$ would correspond to two-particle states. It is not possible here to define asymptotic states, since the perturbation does not damp in $|t|$. But since two of these two-particle states have energy lower than twice the one-particle energy, we might suggest an analogy here with binding in the field problem. On heuristic grounds it is expected that correct treatment of the nonlinearity in the field problem will lead to appearance of binding and/or resonance.[8] The equal-frequency eigenpairs for $n = 3$ are also given here:

$$\begin{aligned}
E_{3,0} &= E_{3,1} = 4\omega + (\epsilon/16)(11 - 2\sqrt{7}),\\
|3,0) &= -(\sqrt{7}+2)/\sqrt{3}\,|3,0\rangle + b\,|1,2\rangle,\\
|3,1) &= b\,|2,1\rangle - (\sqrt{7}+2)/\sqrt{3}\,|0,3\rangle,\\
E_{3,2} &= E_{3,3} = 4\omega + (\epsilon/16)(11 + 2\sqrt{7}),\\
|3,2) &= (\sqrt{7}-2)/\sqrt{3}\,|3,0\rangle + a\,|1,2\rangle,\\
|3,3) &= a\,|2,1\rangle + (\sqrt{7}-2)/\sqrt{3}\,|0,3\rangle,
\end{aligned}$$

where

$$a = [4(7 - \sqrt{7})/3]^{-\frac{1}{2}}, \quad b = [4(7 + \sqrt{7})/3]^{-\frac{1}{2}}.$$

The absence of regularity in the spectrum and states shows up for $n = 3$, whereas one might be mislead in the $n = 2$ case by the symmetry or antisymmetry of the eigenstates to expect such regularity in the higher subspaces.

5. OBSERVATIONS ON THE LEE MODEL[17]

The purpose of the following discussion is not to present new results for the Lee model, although a solution of the operator differential equations would probably have this significance. Rather the aim is to show how the canonical method presented above generalizes to the continuum quantum problem and how it gives quite naturally a reasonable choice of the dressed or renormalized asymptotic particles in agreement with the usual "physical V particle." Further, we shall see that the possibility of an unstable V particle coincides with the kind of frequency commensurability relation we have come to associate with the onset of nonlinear resonance.

The Lee model Hamiltonian is defined as follows:

$$H = H_0 + H_1, \tag{5.1a}$$

where

$$H_0 = \int d\mathbf{p}[m_{V0}a_V^\dagger(\mathbf{p})a_V(\mathbf{p}) + m_{N0}a_N^\dagger(\mathbf{p})a_N(\mathbf{p}) + \omega(\mathbf{p})a_\theta^\dagger(\mathbf{p})a_\theta(\mathbf{p})], \quad \omega(\mathbf{p}) = \omega_{\mathbf{p}} = (\mathbf{p}^2 + \mu^2)^{\frac{1}{2}} \tag{5.1b}$$

and

$$H_1 = g_0(2\pi)^{-\frac{3}{2}}\int d\mathbf{k}(2\omega_{\mathbf{k}})^{-\frac{1}{2}}\int d\mathbf{p}[a_V^\dagger(\mathbf{p})a_N(\mathbf{p}-\mathbf{k})a_\theta(\mathbf{k}) + a_V(\mathbf{p})a_N^\dagger(\mathbf{p}-\mathbf{k})a_\theta^\dagger(\mathbf{k})]f(\omega_{\mathbf{k}}). \tag{5.1c}$$

One usually looks for the physical states as eigenstates of the full Hamiltonian

$$|V,\mathbf{p}\rangle_d = Z^{-\frac{1}{2}}\left(|V,\mathbf{p}\rangle_0 + \int d\mathbf{k}\Phi(\mathbf{p},\mathbf{k})\,|N,\mathbf{p}-\mathbf{k};\theta,\mathbf{k}\rangle_0\right). \tag{5.2}$$

A standard calculation yields the function

$$\Phi(\mathbf{p},\mathbf{k}) = -g_0(2\pi)^{-\frac{3}{2}}\frac{(2\omega_{\mathbf{k}})^{-\frac{1}{2}}f(\omega_{\mathbf{k}})}{m_V - m_{N0} - \omega_{\mathbf{k}}}. \tag{5.3}$$

Here m_V is the "physical" mass of the V, and $m_V - m_{V0}$ and $Z^{-\frac{1}{2}}$ are found in terms of integrals of Φ in the standard fashion. A point that is seldom discussed is that, while $|V,\mathbf{p}\rangle_d$ is an eigenstate with time dependence $\exp(-im_V t)$, the "bare" states, $|\ \rangle_0$, are not. In fact, the whole asymptotic field problem is hidden in this formulation. One defines the operators $a(\mathbf{p})$, $a^\dagger(\mathbf{p})$ as satisfying canonical commutation relations at a time t hence creating and annihilating the "bare" particles. But, the commutator of $\alpha_V^\dagger(\mathbf{p})$ with H (at $t = 0$, say) is an operator not involving a_V or $a_V^\dagger$, rather than a c-number times $a_V^\dagger(\mathbf{p})$ as it would be for a free field. The restriction $[a(\mathbf{p},t), a^\dagger(\mathbf{p}',t)] = \delta(\mathbf{p}-\mathbf{p}')$ is assumed. Thus, without solving the Heisenberg equation for these operators, one cannot relate the bare quanta at time t to those at time 0, although the physical V remains the same superposition of $|V\rangle_0|_t$ and bare $|N,\theta\rangle_0|_t$ at time t as it is at $t = 0$. This fact and the interpretive difficulties it raises should be borne in mind when the statement that the Lee model, though a truncated field theory, is "exactly soluble" in the lowest sector is made. These issues are discussed to some extent by Ezawa.[18]

What we now show is that a kind of interaction representation exists, in which the physical V has the usual expansion in $|V\rangle_{0,t}$ and $|N,\theta\rangle_{0,t}$ and, further,

identify the physical one-particle $|N\rangle_d$ and $|\theta\rangle_d$ states as corresponding to the bare states. These results fail to hold when the V particle is unstable, as far as bare masses are concerned. Equations of motion for renormalized operators are discussed, but not solved.

Let us consider a classical Hamiltonian in terms of conventional variables, whose quantized version gives the Lee model.

The following momentum and position operators for wave number $\mathbf{k}$ are defined, and $H_{0,V}$ is taken as the part of H_0 involving only the V particle:

$$Q_v(\mathbf{k}) = (2m_{v0})^{-\frac{1}{2}}[a_V(\mathbf{p}) + a_V^\dagger(\mathbf{p})], \tag{5.4a}$$

$$P_v(\mathbf{k}) = -i(2m_{v0})^{-\frac{1}{2}}[a_V(\mathbf{p}) - a_V^\dagger(\mathbf{p})]. \tag{5.4b}$$

Then

$$H_{0,V} = \tfrac{1}{2}\int d\mathbf{k}[P_V(\mathbf{k})P_V(\mathbf{k}) + m_{V0}^2 Q_V(\mathbf{k})Q_V(\mathbf{k})]. \tag{5.5}$$

Similar expressions can be worked out for $H_{0,N}$, $H_{0,\theta}$, and H_1. Let p_V and q_V be the classical coordinates, where quantum representatives are P_V and Q_V. Further, let us introduce the classical equivalents of $a^\dagger$ and a as before, canonical with respect to $-iH$:

$$H_0 = \int d\mathbf{p}[m_{V0}\xi_V(\mathbf{p})\eta_V(\mathbf{p}) + m_{N0}\xi_N(\mathbf{p})\eta_N(\mathbf{p}) + \omega_{\mathbf{p}}\xi_\theta(\mathbf{p})\eta_\theta(\mathbf{p})], \tag{5.6a}$$

$$H_1 = g_0(2\pi)^{\frac{3}{2}}\int d\mathbf{p}\int d\mathbf{k}[(2\omega_{\mathbf{k}})^{-\frac{1}{2}}f(\omega_{\mathbf{k}})] \times [\xi_V(\mathbf{p})\eta_N(\mathbf{p}-\mathbf{k})\eta_\theta(\mathbf{k}) + \text{c.c.}]. \tag{5.6b}$$

Hamilton's equations now read in terms of functional derivatives:

$$\dot{\eta}_V(\mathbf{k}) = -i\frac{\delta H}{\delta \xi_V(\mathbf{k})}, \tag{5.7a}$$

$$\Rightarrow \dot{\xi}_V(\mathbf{k}) = i\frac{\delta H}{\delta \eta_V(\mathbf{k})}. \tag{5.7b}$$

To remove the third-order terms from H_1 in so far as possible, one chooses a generating function

$$K(\eta_V, \bar{\xi}_V; \eta_N, \bar{\xi}_N; \eta_\theta, \bar{\xi}_\theta)$$

as an order-3 integrated polynomial in η's and $\bar{\xi}$'s with the usual meaning for $\tilde{K}$[19]:

$$\tilde{K}_3 = g_0\int d\mathbf{q}\int d\mathbf{q}'[F(\mathbf{q},\mathbf{q}')\bar{\xi}_V(\mathbf{q})\bar{\eta}_N(-\mathbf{q}'-\mathbf{q})\bar{\eta}_\theta(\mathbf{q}') + F^*(\mathbf{q},\mathbf{q}')\bar{\eta}_V(\mathbf{q})\bar{\xi}_N(-\mathbf{q}'-\mathbf{q})\bar{\xi}_\theta(\mathbf{q}')]. \tag{5.8}$$

The transformed variables are as follows:

$$\eta_V(\mathbf{k}) = \bar{\eta}_V(\mathbf{k}) + ig_0\left(\frac{\delta\tilde{K}_3}{\delta\bar{\xi}_V(\mathbf{k})}\right),$$

$$\Rightarrow \xi_V(\mathbf{k}) = \bar{\xi}_V(\mathbf{k}) - ig_0\left(\frac{\delta\tilde{K}_3}{\delta\bar{\eta}_V(\mathbf{k})}\right). \tag{5.9}$$

The transformed V part of H_0 is, then,

$$H_{0,V} = m_{V0}\int d\mathbf{p}\bar{\xi}_V(\mathbf{p})\bar{\eta}_V(\mathbf{p}) + m_{V0}g_0\int d\mathbf{p}\left[\bar{\eta}_V(\mathbf{p})\frac{\delta\tilde{K}_3}{\delta\bar{\eta}_V(\mathbf{p})} - \bar{\xi}_V(\mathbf{p})\frac{\delta\tilde{K}_3}{\delta\bar{\xi}_V(\mathbf{p})}\right]. \tag{5.10}$$

When this is done for all three particles, the free Hamiltonian $\tilde{H}_0$ has the same form as Eq. (5.6a), but in terms of the transformed variables. The new interaction in light of Eqs. (5.6b), (5.8), and (5.10) is

$$\tilde{H}_1 = g_0\int d\mathbf{q}\int d\mathbf{q}'\{[(2\pi)^{-\frac{3}{2}}(2\omega_{\mathbf{q}'})^{-\frac{1}{2}}f(\omega_{\mathbf{q}'}) - (m_{V0} - m_{N0} - \omega_{\mathbf{q}'})F(\mathbf{q},\mathbf{q}')] \times \bar{\xi}_V(\mathbf{q})\bar{\eta}_N(-\mathbf{q}'-\mathbf{q})\bar{\eta}_\theta(\mathbf{q}') + \text{c.c.}\}. \tag{5.11}$$

A suitable choice of F then removes this part of the interaction completely. What remains are terms proportional to g_0^2 and higher and involving order-4 integrated polynomials in the operators and higher. A choice of a $\tilde{K}_4$ ($\Rightarrow K_4$) will then allow some of that part to be removed. In other words, most of the interaction can be pushed to higher and higher order.

The choice of F is, clearly,

$$F(\mathbf{q},\mathbf{q}') = (2\pi)^{-\frac{3}{2}}f(\omega_{\mathbf{q}'})/[(2\omega_{\mathbf{q}'})^{\frac{1}{2}}(m_{V0} - m_{N0} - \omega_{\mathbf{q}'})]. \tag{5.12}$$

Now, in the case of a stable V particle, there is *no* mass renormalization to order $(g_0, 3)$; $m_V = m_{V0}$, where the quantized version of $\bar{\xi}_V$ will create the physical V particles. In this case, to order g_0 we have the following stability condition

$$m_{V0} < m_{N0} + \mu. \tag{5.13}$$

If the V is unstable, then the function F in Eq. (5.12) has a singularity. Some region around this singularity *must* be omitted and some third-order term left in H_1 to avoid violating the perturbative approach. The condition $m_{V0} - m_{N0} - \omega_{\mathbf{K}} = 0$ for some $\mathbf{k}$ is the kind of linear commensurability relationship we have come to associate with nonlinear resonance and the presence of approximate, separating constants of the motion beside H itself. This establishes a connection between instability of a particle and presence of nonlinear resonance in the Heisenberg equations, when we quantize $H_0 + H_1$ as follows.[20] (In the fourth-order term the presence of resonance is unavoidable. There it is associated with scattering and the forces between particles.) To quantize, one writes H in terms of $(\bar{q}_v, \bar{p}_v; \bar{q}_N, \bar{p}_N; \bar{q}_\theta, \bar{p}_\theta)$ and associates the usual kind of operators, $\bar{P}_v(\mathbf{k})$ and $\bar{Q}_v(\mathbf{k})$ for example, and the

associated raising and lowering operators $\alpha_v^\dagger(\mathbf{k})$ and $\alpha_v(\mathbf{k})$. Aside from the crucial question of order of operators, when one takes the operator representative for mixed pq terms mentioned previously, the net effect is simply to replace $\bar{\xi}_v$ in H by $\alpha_v^\dagger$ and $\bar{\eta}_v$ by α_v, etc.

If $H^{(n)}$ denotes the Hamiltonian transformed to order n [inaccurate, then, in order (g_0^{n-2}, n)] and $H^{(n)} = \sum_{j=2}^{n} \tilde{H}_j$, we have the following results in the stable case:

$$\tilde{H}_2 = m_{V0}\int d\mathbf{p}\alpha_V^\dagger(\mathbf{p})\alpha_V(\mathbf{p}) + m_{N0}\int d\mathbf{p}\alpha_N^\dagger(\mathbf{p})\alpha_N(\mathbf{p}) + \int d\mathbf{p}\omega_{\mathbf{p}}\alpha_\theta^\dagger(\mathbf{p})\alpha_\theta(\mathbf{p}), \tag{5.14}$$

$$\tilde{H}_3 = 0, \tag{5.15}$$

$$\tilde{H}_4 = (g_0^2/4)\int d\mathbf{k}_1 \cdots \int d\mathbf{k}_4 \delta(\mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_2 - \mathbf{k}_4) \times G(\mathbf{k}_1, \cdots, \mathbf{k}_4)[\alpha_V(\mathbf{k}_2)\alpha_V^\dagger(\mathbf{k}_1) - \alpha_V^\dagger(\mathbf{k}_1)\alpha_V(\mathbf{k}_2)] \times [\alpha_N^\dagger(\mathbf{k}_3)\alpha_N(\mathbf{k}_4) - \alpha_N(\mathbf{k}_4)\alpha_N^\dagger(\mathbf{k}_3)] + (\text{similar } V - \theta \text{ and } N - \theta \text{ terms}). \tag{5.16}$$

The functions G_1, G_2, and G_3 are given in Appendix B, and all further correction terms are of order $(g_0^3, 5)$ or higher. Symmetric or Weyl ordering has been used here in a generalized version for bosons and antisymmetric for fermions. One sees that H_4, the lowest-order interaction, has as eigenstates $|0\rangle$, $|V, \mathbf{p}\rangle$, $|\theta, \mathbf{p}\rangle$, and $|N, \mathbf{p}\rangle$. In each case it has different eigenvalues. These eigenvalues correspond to the shift of the zero point of E, ΔM_V, ΔM_θ, and ΔM_N, respectively.

The expressions have the same basic form as the usual equation for $m_V - m_{V0}$. We do have shifts to renormalized masses, then, in order $(g_0^2, 4)$. Of course, we obtain $\Delta M_\theta = \Delta M_N = 0$.

A further observation is that the $N\theta$ terms in H_4 will account for $N\theta$ scattering. Also, the transformation Eq. (5.9) with $\tilde{K}_3$ from Eq. (5.8) and F from Eq. (5.12), gives lowest-order relationships between $(\alpha_V^\dagger, \alpha_N^\dagger, \alpha_\theta^\dagger)$ and $(a_V^\dagger, \alpha_N^\dagger, \alpha_\theta^\dagger)$. The one of greatest interest concerns $\alpha_V^\dagger(p)$,

$$\alpha_V^\dagger(\mathbf{p}) \cong a_V^\dagger(\mathbf{p}) + g_0(2\pi)^{-\frac{3}{2}}\int d\mathbf{q}(2\omega_{\mathbf{q}})^{-\frac{1}{2}} \frac{f(\omega_{\mathbf{q}})}{m_{V0} - m_{N0} - \omega_{\mathbf{q}}} \times a_N^\dagger(\mathbf{p} - \mathbf{q})a_\theta^\dagger(\mathbf{q}). \tag{5.17}$$

Thus, the usual result in Eqs. (5.2) and (5.3) is reproduced if we remember that $Z = 1 + O(g_0^2)$. As a final note, when $f(\omega_{\mathbf{q}}) = 1$, all $\mathbf{q}$, we find that ${}_a\langle V \mid V\rangle_a$ is ∞. $\delta(\mathbf{p} - \mathbf{p}')$ if ${}_0\langle V \mid V\rangle_0$ and ${}_0\langle N, \theta \mid N, \theta\rangle_0$ are the usual δ functions, because the following integral fails to converge:

$$\int dk(\omega_{\mathbf{k}})^{-1}(m_{V0} - m_{N0} - \omega_{\mathbf{k}})^{-2} = \infty. \tag{5.18}$$

Thus the transformation carries one out of the original Hilbert space without a cutoff. However, the physical result for ΔM_V also becomes infinite in this limit.

If we choose normal ordering rather than symmetric ordering, then the four energy (mass) shifts are zero. Issues related to ordering choice are briefly discussed also in Appendix B.

It is clear that much development is needed for these techniques to give valuable new insight into better approximate solutions to the field problem than any perturbation method basically equivalent to a Green's function approach, which will not give a fully accurate solution to the nonlinear field equations. That much development of the canonical method is warranted has been suggested in this paper, as we have shown in simple cases that the technique does reproduce the characteristic behavior of solutions to this type of nonlinear equation. In particular the behavior of oscillator systems in the presence of nonlinear resonance must be understood. A solution to the equations of motion under resonant conditions for two classical oscillators will be presented in a later paper by the author. It is hoped that the points made above will help to stimulate the needed development.

APPENDIX A: THE TRANSFORMATION FOR ONE OSCILLATOR

In this appendix the details of the canonical transformation for a single anharmonic oscillator will be presented. Let us begin with the example of Sec. 2 in the complex variables $\{\xi, \eta\}$, let $H' = -iH$, then

$$H' = -i\omega\xi\eta - i(\epsilon/16)(\xi + \eta)^4. \tag{A1}$$

A canonical transformation is generated by means of a generating function $K(\eta, \bar{\xi})$,[21] to new variables $(\bar{\xi}, \bar{\eta})$:

$$\eta = \bar{\eta} - \frac{\partial K}{\partial \bar{\xi}}, \tag{A2a}$$

$$\xi = \bar{\xi} + \frac{\partial K}{\partial \eta}. \tag{A2b}$$

If one chooses K to be a polynomial of degree n, the terms involving K above are of degree $n - 1$. Thus, to begin with a function K which is of order ϵ and a polynomial of degree four will give fourth-order terms in the Hamiltonian to cancel some of the $\epsilon(\xi + \eta)^4$ terms. Let $K_4(\eta, \bar{\xi})$ be such a polynomial and $\tilde{K}_4(\bar{\eta}, \bar{\xi})$ the same polynomial with the simple

replacement $\eta \to \bar{\eta}$. To order ϵ, the use of K_4 in Eq. (A2) will not affect the transformation. Correct to order ϵ, then, the Hamiltonian becomes

$$H = -i\omega\bar{\xi}\bar{\eta} - i\left[\omega\left(\bar{\eta}\frac{\partial\tilde{K}_4}{\partial\bar{\eta}} - \bar{\xi}\frac{\partial\tilde{K}_4}{\partial\bar{\xi}}\right) + \frac{\epsilon}{16}(\bar{\xi}+\bar{\eta})^4\right] + O(\epsilon^2). \tag{A3}$$

Each term in $\tilde{K}_4$ is to be of the form $\beta\bar{\xi}^m\bar{\eta}^n$ with $m+n=4$. These terms are eigenfunctions of the operator $(\bar{\eta}\partial/\partial\bar{\eta} - \bar{\xi}\partial/\partial\bar{\xi})$ with eigenvalue $m-n$. Thus, the coefficients β can be chosen to cancel every term in $\epsilon(\bar{\xi}+\bar{\eta})^4$ except $\epsilon(\bar{\xi}\bar{\eta})^2$. Gustavson selects a zero coefficient for all such "diagonal" terms in the transformation at each stage (terms in the null space of the operator). But, to maintain a conjugate relationship between $\bar{\xi}$ and $\bar{\eta}$, one must use this freedom and add the diagonal terms to K in order ϵ^2 and higher with the correct coefficient so that $\bar{\xi} = \bar{\eta}^*$. The selection of K_4 is evident at this point:

$$\tilde{K}_4(\bar{\eta},\bar{\xi}) = (\epsilon/64\omega)(\bar{\xi}^4 + 8\bar{\xi}^3\bar{\eta} - 8\bar{\xi}\bar{\eta}^3 - \bar{\eta}^4) \tag{A4a}$$

$$\Rightarrow K_4(\eta,\bar{\xi}) = (\epsilon/64\omega)(\bar{\xi}^4 + 8\bar{\xi}^3\eta - 8\bar{\xi}\eta^3 - \eta^4). \tag{A4b}$$

The canonical transformation to order ϵ now follows from Eqs. (A4) and (A2):

$$\eta = \bar{\eta} + \epsilon(16\omega)^{-1}(2\bar{\eta}^3 - 6\bar{\xi}^2\bar{\eta} - \bar{\xi}^3), \tag{A5a}$$

$$\xi = \bar{\xi} + \epsilon(16\omega)^{-1}(2\bar{\xi}^3 - 6\bar{\xi}^2\bar{\eta} - \bar{\eta}^3). \tag{A5b}$$

Finally, with this transformation the Hamiltonian takes on "normal form" to order ϵ:

$$H' = -i\omega(\bar{\xi}\bar{\eta}) - i(3\epsilon/8)(\bar{\xi}\bar{\eta})^2 + O(\epsilon^2). \tag{A6}$$

We call this form the irreducible Hamiltonian.

To proceed to second order, let us first here outline the procedure for arbitrary order. In order ϵ^j we introduce a generating function $K_{2j+2}(\eta,\bar{\xi})$, where K_{2j+2} is a polynomial of order $2j+2$ in the variables $\{\eta,\bar{\xi}\}$ times a factor ϵ^j. Suppose the transformation has been calculated to order ϵ^{j-1} by selection of K_4 through K_{2j}, giving the functions $\tilde{K}_4$ through $\tilde{K}_{2j}$ by the substitution $\bar{\eta} \to \eta$. (One also obtains K_{2j+2} by this substitution once $\tilde{K}_{2j+2}$ has been chosen, of course.) Letting η_k and ξ_k be the kth approximation to η and ξ as polynomials in $\bar{\xi}$ and $\bar{\eta}$, one obtains the transformation to order ϵ^j as follows:

$$\eta = \bar{\eta} - \frac{\partial K_4}{\partial\bar{\xi}}\bigg|_{\eta=\eta_{j-1}} - \frac{\partial K_6}{\partial\bar{\xi}}\bigg|_{\eta=\eta_{j-2}} - \cdots - \frac{\partial K_{2j}}{\partial\bar{\xi}}\bigg|_{\eta=\eta_1} - \frac{\partial\tilde{K}_{2j+2}}{\partial\bar{\xi}}, \tag{A7a}$$

$$\xi = \bar{\xi} + \frac{\partial K_4}{\partial\eta}\bigg|_{\eta=\eta_{j-1}} + \frac{\partial K_6}{\partial\eta}\bigg|_{\eta=\eta_{j-2}} + \cdots + \frac{\partial K_{2j}}{\partial\eta}\bigg|_{\eta=\eta_1} + \frac{\partial\tilde{K}_{2j+2}}{\partial\bar{\eta}}. \tag{A7b}$$

When these two expressions are substituted into H' as given in Eq. (A1), all of the terms of order ϵ^j in H' are generated as explicit polynomials of order $2j+2$ in $\bar{\xi}$ and $\bar{\eta}$ as well as the term

$$i\omega\left(\bar{\eta}\frac{\partial}{\partial\bar{\eta}} - \bar{\xi}\frac{\partial}{\partial\bar{\xi}}\right)\tilde{K}_{2j+2}.$$

All of these explicit terms in order ϵ^j may be cancelled by properly selected terms in $\tilde{K}_{2j+2}$ except $(\bar{\xi}\bar{\eta})^{j+1}$, whose coefficient in $\tilde{K}_{2j+2}$ is fixed to insure that $\bar{\xi}$ and $\bar{\eta}$ are conjugate to order ϵ^j.

To achieve an order ϵ^2 transformation, then, we introduce $\tilde{K}_6(\bar{\xi},\bar{\eta})$. The transformation to this order reads as follows:

$$\eta = \bar{\eta} - \epsilon(64\omega)^{-1}(4\bar{\xi}^3 + 24\bar{\xi}^2\eta - 8\eta^3)\big|_{\eta=\eta_1} - \frac{\partial\tilde{K}_6}{\partial\bar{\xi}}, \tag{A8a}$$

$$\xi = \bar{\xi} + \epsilon(64\omega)^{-1}(8\bar{\xi}^3 - 24\bar{\xi}\eta^2 - 4\eta^3)\big|_{\eta=\eta_1} + \frac{\partial\tilde{K}_6}{\partial\bar{\eta}}, \tag{A8b}$$

where

$$\eta_1 = \bar{\eta} + \epsilon(16\omega)^{-1}(2\bar{\eta}^3 - 6\bar{\xi}^2\bar{\eta} - \bar{\xi}^3). \tag{A8c}$$

The Hamiltonian H' to order ϵ^2, then, is the following:

$$iH' = \omega(\bar{\xi}\bar{\eta}) + (3\epsilon/8)(\bar{\xi}\bar{\eta})^2 + \epsilon^2\left[\epsilon^{-2}\omega\left(\bar{\eta}\frac{\partial\tilde{K}_6}{\partial\bar{\eta}} - \bar{\xi}\frac{\partial\tilde{K}_6}{\partial\bar{\xi}}\right) + (64\omega)^{-1}(2\bar{\xi}^6 + 3\bar{\xi}^5\bar{\eta} - 18\bar{\xi}^4\bar{\eta}^2 - 17\bar{\xi}^3\bar{\eta}^3 - 15\bar{\xi}^2\bar{\eta}^4 - 9\bar{\xi}\bar{\eta}^5 - \bar{\eta}^6)\right] + O(\epsilon^3). \tag{A9}$$

The function $\tilde{K}_6$ is now chosen just as was $\tilde{K}_4$, since terms of the form $\beta\bar{\xi}^m\bar{\eta}^n$, where $m+n=6$, are eigenfunctions of the operator $(\bar{\eta}\partial/\partial\bar{\eta} - \bar{\xi}\partial/\partial\bar{\xi})$ with eigenvalue $m-n$. The entire ϵ^2 part of H' may thus

be cancelled except $(\bar{\xi}\bar{\eta})^3$ with the following choice:

$$\tilde{K}_6 = \epsilon^2(1536\omega^2)^{-1}(8\bar{\xi}^6 + 8\bar{\xi}^5\bar{\eta} - 216\bar{\xi}^4\bar{\eta}^2 - 123\bar{\xi}^3\bar{\eta}^3 + 180\bar{\xi}^2\bar{\eta}^4 + 54\bar{\xi}\bar{\eta}^5 + 4\bar{\eta}^6), \quad \text{(A10a)}$$

$$K_6(\eta, \bar{\xi}) = \tilde{K}_6(\bar{\eta}, \bar{\xi})|_{\bar{\eta}=\eta}. \quad \text{(A10b)}$$

And, of course, we then have the entire transformation to order ϵ^2:

$$\eta = \bar{\eta} + \epsilon(16\omega)^{-1}(2\bar{\eta}^3 - 6\bar{\xi}^2\bar{\eta} - \bar{\xi}^3) + \epsilon^2(1536\omega^2)^{-1} \times (36\bar{\xi}^5 + 216\bar{\xi}^4\bar{\eta} - 36\bar{\xi}^3\bar{\eta}^2 + 81\bar{\xi}^2\bar{\eta} - 360\bar{\xi}\bar{\eta}^4 + 18\bar{\eta}^5) + O(\epsilon^3). \quad \text{(A11)}$$

The diagonal term in $\tilde{K}_6$ was fixed so that $\bar{\xi}^* = \bar{\eta}$, whence the equation for ξ is implied by Eq. (A11) by conjugation. Thus, the Hamiltonian has the following irreducible form to second order:

$$iH' = \omega(\bar{\xi}\bar{\eta}) + (3\epsilon/8)(\bar{\xi}\bar{\eta})^2 - (17\epsilon^2)(64\omega)^{-1}(\bar{\xi}\bar{\eta})^3 + O(\epsilon^3). \quad \text{(A12)}$$

It would be desirable, clearly, in applications to use a digital computer to perform the polynomial algebra and to find the value of the conserved quantity $(\bar{\xi}\bar{\eta}) = \rho^2$ in terms of the particular initial conditions selected.

APPENDIX B

In this appendix we present the Lee model results to second order (for completeness) in the stable V-particle case. Generalizing the higher-order procedure outlined in Appendix A to the continuum, we obtain a $\tilde{K}_4$ which generates the transformation of the classical Lee model coordinates to order g_0^2:

$$\tilde{K}_4 = g_0^2\int d\mathbf{k}\int d\mathbf{k}'\int d\mathbf{k}''\Delta(\mathbf{k}')\frac{G(\mathbf{k}'^2) - G(\mathbf{k}''^2)}{\omega_{\mathbf{k}''} - \omega_{\mathbf{k}'}} \times v(\omega_{\mathbf{k}''} - \omega_{\mathbf{k}'}) \times [\bar{\xi}_N(\mathbf{k} - \mathbf{k}')\bar{\eta}_N(\mathbf{k} - \mathbf{k}'')\bar{\xi}_\theta(\mathbf{k}')\bar{\eta}_\theta(\mathbf{k}'') - \bar{\xi}_V(\mathbf{k})\bar{\eta}_V(\mathbf{k} - \mathbf{k}'' + \mathbf{k}')\bar{\xi}_\theta(\mathbf{k}')\bar{\eta}_\theta(\mathbf{k})], \quad \text{(B1)}$$

where

$$\Delta(\mathbf{k}) = m_{V0} - m_{N0} - \omega_{\mathbf{k}},$$
$$G(\mathbf{k}^2) = (2\pi)^{-\frac{3}{2}}(2\omega_{\mathbf{k}})^{-\frac{1}{2}}\Delta_{\mathbf{k}}^{-1}f(\omega_k^2),$$

and

$$v(x) = \begin{cases} 1, & |x| > \delta \\ 0, & |x| < \delta, \quad \text{for some} \quad \delta > 0. \end{cases}$$

The region $|\mathbf{k}'| \approx |\mathbf{k}''|$ corresponds to near commensurability of field oscillator frequencies, and the large coefficients in $\tilde{K}_4$ due to $(\omega_{\mathbf{k}''} - \omega_{\mathbf{k}'})^{-1}$ are excluded by the step function $v(x)$. One element of arbitrariness here, then, is the choice of δ. Obviously, certain other types of function for $v(x)$ would also be acceptable.

The irreducible form for the Lee model Hamiltonian to order g_0^2 is then easy to obtain:

$$H_0 = \int d\mathbf{p}[m_{V0}\bar{\xi}_V(\mathbf{p})\bar{\eta}_V(\mathbf{p}) + m_{N0}\bar{\xi}_N(\mathbf{p})\bar{\eta}_N(\mathbf{p}) + \omega_{\mathbf{p}}\bar{\xi}_\theta(\mathbf{p})\bar{\eta}_\theta(\mathbf{p})], \quad \text{(B2a)}$$

$$H_1 = g_0^2\int d\mathbf{k}\int d\mathbf{k}'\int d\mathbf{k}'' \times \{\Delta_{\mathbf{k}'}G(\mathbf{k}'^2)G(\mathbf{k}''^2)\phi(\omega_{\mathbf{k}'} - \omega_{\mathbf{k}''}) \times [\bar{\xi}_N(\mathbf{k} - \mathbf{k}')\bar{\eta}_N(\mathbf{k} - \mathbf{k}'') - \bar{\xi}_V(\mathbf{k} - \mathbf{k}')\bar{\eta}_v(\mathbf{k} - \mathbf{k}'')]\bar{\xi}_\theta(\mathbf{k}')\bar{\eta}_\theta(\mathbf{k}'') - \Delta_{\mathbf{k}'}[G(\mathbf{k}'^2)]^2\bar{\xi}_V(\mathbf{k})\bar{\eta}_V(\mathbf{k}'')\bar{\xi}_N(\mathbf{k}'' - \mathbf{k}')\bar{\eta}_N(\mathbf{k} - \mathbf{k}')\} \quad \text{(B2b)}$$

where

$$\phi(x) = 1 - v(x).$$

One now reintroduces $\bar{p}(\mathbf{k})$ and $\bar{q}(\mathbf{k})$ functions by the usual relationship $(\bar{\xi}(\mathbf{k}), \bar{\eta}(\mathbf{k})) \leftrightarrow (\bar{p}(\mathbf{k}), \bar{q}(\mathbf{k}))$ for each field, obtains H in terms of the $\bar{p}$'s and $\bar{q}$'s, and then introduces operator representatives. These details need not be repeated here; but the effect of the quantization is to replace $\bar{\xi}(\mathbf{k})$ by $\alpha^\dagger(\mathbf{k})$ and $\bar{\eta}(\mathbf{k})$ by $\alpha(\mathbf{k})$, subject to the correct choice of the ordering of the operators.

For fermions we cannot use symmetric ordering, as $\frac{1}{2}[a^\dagger(\mathbf{p})a(\mathbf{p}') + a(\mathbf{p}')a^\dagger(\mathbf{p})] = \frac{1}{2}\delta(\mathbf{p} - \mathbf{p}')$ and is not a Q number. It turns out that antisymmetric ordering gives the correct result for Δm_V and we shall rely on it here:

$$\bar{\xi}_V(\mathbf{p})\bar{\eta}_V(\mathbf{p}') \to \tfrac{1}{2}[\alpha_V^\dagger(\mathbf{p})\alpha_V(\mathbf{p}') - \alpha_V(\mathbf{p}')\alpha_V^\dagger(\mathbf{p})] = \alpha_V^\dagger(\mathbf{p})\alpha_V(\mathbf{p}') - \delta^3(\mathbf{p} - \mathbf{p}'). \quad \text{(B3)}$$

The Hamiltonian operator then has the following expression:

$$H_0 = \int d\mathbf{p}[m_{V0}\alpha_V^\dagger(\mathbf{p})\alpha_V(\mathbf{p}) + m_{N0}\alpha_N^\dagger(\mathbf{p})\alpha_N(\mathbf{p}) + \omega_{\mathbf{p}}\alpha_\theta^\dagger(\mathbf{p})\alpha_\theta(\mathbf{p})] - \tfrac{1}{2}\delta(\mathbf{o})\int d\mathbf{p}(m_{V0} + m_{N0} - \omega_{\mathbf{p}}), \quad \text{(B4a)}$$

$$H_1 = -g_0^2\int d\mathbf{k}\int d\mathbf{k}'\int d\mathbf{k}''\Delta(\mathbf{k}')G(\mathbf{k}'^2)\{G(\mathbf{k}''^2) \times \phi(\omega_{\mathbf{k}'} - \omega_{\mathbf{k}''})[\alpha_N^\dagger(\mathbf{k} - \mathbf{k}')\alpha_N(\mathbf{k} - \mathbf{k}'') - \alpha_V^\dagger(\mathbf{k} - \mathbf{k}')\alpha_V(\mathbf{k} - \mathbf{k}'')]\alpha_\theta^\dagger(\mathbf{k}')\alpha_\theta(\mathbf{k}'') - G(\mathbf{k}'^2)\alpha_V^\dagger(\mathbf{k})\alpha_V(\mathbf{k}'')\alpha_N^\dagger(\mathbf{k}'' - \mathbf{k}')\alpha_N(\mathbf{k} - \mathbf{k}')\} - g_0^2\int d\mathbf{k}\int d\mathbf{k}'\Delta(\mathbf{k}')[G(\mathbf{k}'^2)]\alpha_V^\dagger(\mathbf{k})\alpha_V(\mathbf{k}) - (g_0^2/4)\left(\int d\mathbf{k}\int d\mathbf{k}'\Delta(\mathbf{k}')[G(\mathbf{k}'^2)]^2\right)\delta(\mathbf{o}). \quad \text{(B4b)}$$

Now both H_0 and H_1 have the vacuum as eigenstate with divergent eigenvalues. These are the infinite zero-point contributions and are removed by "mass renormalization." The renormalized Hamiltonian to second order, then, follows:

$$H_0 = \int d\mathbf{p}[m_{V0}\mathcal{N}_V(\mathbf{p}) + m_{N0}\mathcal{N}_N(\mathbf{p}) + \omega_p\mathcal{N}_\theta(\mathbf{p})], \tag{B5a}$$

$$\begin{aligned} H_1 = &-g_0^2\int d\mathbf{k}\int d\mathbf{k}'\int d\mathbf{k}'' \\ &\times \Delta_{\mathbf{k}'}G(\mathbf{k}'^2)\{\phi(\omega_{\mathbf{k}'} - \omega_{\mathbf{k}''})G(\mathbf{k}''^2) \\ &\times [\alpha_N^\dagger(\mathbf{k}-\mathbf{k}')\alpha_N(\mathbf{k}-\mathbf{k}'') \\ &- \alpha_V^\dagger(\mathbf{k}-\mathbf{k}')\alpha_V(\mathbf{k}-\mathbf{k}'')]\alpha_\theta^\dagger(\mathbf{k}')\alpha_\theta(\mathbf{k}'') \\ &- G(\mathbf{k}'^2)\alpha_V^\dagger(\mathbf{k})\alpha_V(\mathbf{k}')\alpha_N^\dagger(\mathbf{k}''-\mathbf{k}')\alpha_N(\mathbf{k}-\mathbf{k}')\} \\ &- g_0^2\Gamma\int d\mathbf{k}\mathcal{N}_V(\mathbf{k}), \end{aligned} \tag{B5b}$$

where

$$\Gamma = \int dk'(2\pi)^{-3}(2\omega_{\mathbf{k}'})^{-1}(m_{V0} - m_{N0} - \omega_{\mathbf{k}'})^{-1}\,|f(\mathbf{k}'^2)|^2$$

and

$$\mathcal{N}_V(\mathbf{p}) = \alpha_V^\dagger(\mathbf{p})\alpha_V(\mathbf{p}).$$

The first term in H with the single integral has the one-particle states as eigenvectors; the eigenvalues are the mass (energy) shifts of these states to second order:

$$(H_0 + H_1)\alpha_V^\dagger(\mathbf{q})\,|0\rangle = (m_{V0} - g_0^2\Gamma)\alpha_V^\dagger(\mathbf{q})\,|0\rangle, \tag{B6a}$$

$$(H_0 + H_1)\alpha_N^\dagger(\mathbf{q})\,|0\rangle = m_{N0}\alpha_N^\dagger(\mathbf{q})\,|0\rangle, \tag{B6b}$$

$$(H_0 + H_1)\alpha_\theta^\dagger(\mathbf{q})\,|0\rangle = \omega_q\alpha_\theta^\dagger(\mathbf{q})\,|0\rangle \tag{B6c}$$

$$\Rightarrow \Delta m_V = -g_0^2\Gamma,$$

$$\Delta m_N = \Delta E_\theta = 0$$

to order g_0^2. These results accord entirely with the usual expressions to this order. One has $\Delta m_N \equiv 0$ and $\Delta E_\theta \equiv 0$, but the expression for Δm_V is as follows:

$$\begin{aligned} &m_V - m_{V0} \\ &= -g_0^2(2\pi)^{-3}\int d\mathbf{k}(2\omega_{\mathbf{k}})^{-1}(m_V - m_{N0} - \omega_{\mathbf{k}})^{-1}\,|f(\mathbf{k}^2)|^2. \end{aligned} \tag{B7}$$

If we expand m_V in the denominator in powers of g_0 and the denominator itself about $m_V - m_{N0} - \omega_{\mathbf{k}} = m_{V0} - m_{N0} - \omega_{\mathbf{k}}$, then we regain the result in Eq. (B6a).

An investigation of higher sectors to this order, and higher orders as well, should prove quite interesting. We have yet to demonstrate effects due to nonlinearity at odds with a Green's function expansion. At least we have reproduced several typical results in the exactly soluble sectors of the Lee model.

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Tensor and Spinor Spherical Harmonics and the Spin-s Harmonics ${}_sY_{lm}(\theta, \phi)$*

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A set of Cartesian tensor spherical harmonics is constructed from the spin weighted harmonics of Newman and Penrose, ${}_sY_{lm}(\theta, \phi)$. It is shown that these tensor harmonics are eigenfunctions of total angular momentum, z component of total angular momentum, total spin and radial component of spin. In particular, $-s$ may be thought of as a helicity for outgoing radiation. Tensor operators are introduced which lower and raise this helicity. They are shown to correspond to the operators $\eth$ and $\bar{\eth}$ introduced by Newman and Penrose. Because the ${}_sY_{lm}(\theta, \phi)$ can be defined for half-integer values of l, m, and s, a set of spinor spherical harmonics is also constructed which has properties paralleling those of the tensor harmonics.

1. INTRODUCTION

In a paper on the Bondi–Metzner–Sachs group, Newman and Penrose[1] introduced a set of spin-s spherical harmonics ${}_sY_{lm}(\theta, \phi)$ and the operator $\eth$. In a subsequent paper, Goldberg, MacFarlane, Newman, Rohrlich, and Sudarshan[2] pointed out the relationship between these functions and representation matrices of the rotation group R_3. They also showed that $\eth$ plays the role of an angular momentum raising operator, as did Newman and Penrose.

In the present paper we introduce a set of symmetric, traceless, Cartesian tensor spherical harmonics which are constructed from the ${}_sY_{lm}(\theta, \phi)$. By using the angular momentum operators for tensor representations of R_3, we show that these tensor harmonics are eigenfunctions of the square of the total angular momentum with eigenvalue $l(l+1)$, of the z component of the total angular momentum with eigenvalue m, and of the radial component of the spin with eigenvalue $-s$. They are also eigenfunctions of the square of the spin operator with eigenvalue depending on their tensor rank. If these tensor harmonics are used in expansions of outgoing tensor spherical waves, $-s$ can be interpreted as a helicity.

The operator $\eth$ can be related to a particular spherical component of the total angular momentum operator. When used along with a spherical component of the spin operator, it gives us a helicity lowering operator. We have then a correspondence between the ${}_sY_{lm}(\theta, \phi)$ and helicity states with helicity $-s$ and between $\eth$ and a helicity lowering operator.

As Newman and Penrose and Goldberg *et al.* pointed out, the definition of the ${}_sY_{lm}(\theta, \phi)$ can be extended to include half-integer values of l, m, and s. This extended definition is used to construct a set of spinor spherical harmonics which have properties similar to those of the tensor harmonics. In particular, $-s$ and $\eth$ will have the same interpretation as above.

In Sec. 2 we briefly review the properties of the ${}_sY_{lm}(\theta, \phi)$. In Sec. 3 we introduce the tensor harmonics. The spinor harmonics are discussed in Sec. 4. In the Appendix we list tensor harmonics of rank $n = 1, 2$, and 3.

2. A REVIEW OF THE PROPERTIES OF ${}_sY_{lm}(\theta, \phi)$

As we stated in the introduction, we will construct our tensor and spinor harmonics from the spin harmonics ${}_sY_{lm}(\theta, \phi)$. These spin harmonics for integer values of l, m, and s can be obtained from the ordinary spherical harmonics $Y_{lm}(\theta, \phi)$ by repeated applications of $\eth$. The operator $\eth$ is defined specifically in terms of the function on which it operates, that is, its specific form depends on the so-called spin weight of the function.

Newman and Penrose[1] define spin weight by considering rotations, around the radial direction, of unit vectors tangent to a sphere. Suppose $\mathbf{a}$ and $\mathbf{b}$ are such unit vectors which are perpendicular to each other. If we define the complex unit vector $\mathbf{m} \equiv (1/\sqrt{2})(\mathbf{a} + i\mathbf{b})$, then the rotation we want is given by

$$\mathbf{m}' = e^{i\psi}\mathbf{m}, \tag{2.1}$$

where ψ is the angle of rotation. We say that any function η defined on the sphere has spin weight s if under transformation (2.1) η transforms according to

$$\eta' = e^{si\psi}\eta. \tag{2.2}$$

As examples, the quantities $\mathbf{m} \cdot \mathbf{A}$ and $\mathbf{m}^* \cdot \mathbf{A}$, where $\mathbf{A}$ is some fixed vector, have respectively spin weights $+1$ and -1.

We can now define the operator $\eth$. For our purposes it will be convenient to define this operator in terms of the usual orbital angular momentum operator $\mathbf{L} \equiv -i\mathbf{r} \times \nabla$. Using the function η, with spin weight

s, we have

$$\begin{aligned}\eth\eta &\equiv -(\sin\theta)^s\{(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})\cdot\mathbf{L}\}(\sin\theta)^{-s}\eta \\ &= -(\sin\theta)^s\left\{\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi}\right\}(\sin\theta)^{-s}\eta \\ &= -\left\{\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi} - s\cot\theta\right\}\eta, \qquad (2.3)\end{aligned}$$

with $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\phi}}$ the polar and azimuthal unit vectors. A companion operator $\bar{\eth}$ is defined in a similar way by

$$\begin{aligned}\bar{\eth}\eta &\equiv (\sin\theta)^{-s}\{(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}})\cdot\mathbf{L}\}(\sin\theta)^{s}\eta \\ &= (\sin\theta)^{-s}\left\{-\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi}\right\}(\sin\theta)^{s}\eta \\ &= \left\{-\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi} - s\cot\theta\right\}\eta. \qquad (2.4)\end{aligned}$$

If we now let $\mathbf{a} = \hat{\boldsymbol{\theta}}$ and $\mathbf{b} = \hat{\boldsymbol{\phi}}$ so that $\mathbf{m} = (1/\sqrt{2})(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})$, we see that we may take $\eth$ to have spin weight $+1$, if we hold the coordinates fixed during transformation (2.1). Similarly $\bar{\eth}$ has spin weight -1 and the functions $\eth\eta$ and $\bar{\eth}\eta$ have respectively spin weights $s+1$ and $s-1$.

For our definition of ${}_sY_{lm}$ for integer values of l, m, and s, we use the following set of equations:

$$\begin{aligned}&{}_0Y_{lm}(\theta,\phi) \equiv Y_{lm}(\theta,\phi), \\ &\eth[{}_sY_{lm}] = [(l-s)(l+s+1)]^{\frac{1}{2}}\,{}_{s+1}Y_{lm}, \qquad (2.5)\\ &\bar{\eth}[{}_sY_{lm}] = -[(l+s)(l-s+1)]^{\frac{1}{2}}\,{}_{s-1}Y_{lm}.\end{aligned}$$

We note that, with the spin weight of Y_{lm} understood to be zero, the spin weight of ${}_sY_{lm}$ will be s. Furthermore, $\eth$ annihilates ${}_lY_{lm}$ and $\bar{\eth}$ annihilates ${}_{-l}Y_{lm}$. We therefore do not define ${}_sY_{lm}$ for $|s| > l$. It is clear that $\eth$ operating on Y_{lm} s times will give ${}_sY_{lm}$ and $\bar{\eth}$ on Y_{lm} s times will give ${}_{-s}Y_{lm}$.

The ${}_sY_{lm}$ defined by (2.5) form a complete orthonormal set for any function of θ and ϕ with spin weight s. That is,

$$\int_{4\pi} {}_sY^*_{l'm'}\,{}_sY_{lm}\,d\Omega = \delta_{ll'}\delta_{mm'}, \qquad (2.6)$$

and

$$\sum_{\substack{l,m\\ l\geq|s|}} {}_sY^*_{lm}(\theta',\phi')\,{}_sY_{lm}(\theta,\phi) = \delta(\phi-\phi')\delta(\cos\theta-\cos\theta'). \qquad (2.7)$$

Goldberg *et al.*[2] showed that ${}_sY_{lm}$ is proportional to $D^l_{-sm}(\phi,\theta,0)$, which is a representation matrix for the rotation group R_3, i.e.,

$$\begin{aligned}{}_sY_{lm}(\theta,\phi) &= [(2l+1)/4\pi]^{\frac{1}{2}}D^l_{-sm}(\phi,\theta,0) \\ &= \left[\frac{(l+m)!\,(l-m)!}{(l-s)!\,(l+s)!}\frac{(2l+1)}{4\pi}\right]^{\frac{1}{2}}(\sin\tfrac{1}{2}\theta)^{2l} \\ &\quad\times\sum_p\binom{l-s}{p}\binom{l+s}{p-m+s}(-)^{l-s-p} \\ &\quad\times e^{im\phi}(\cos\tfrac{1}{2}\theta)^{2p-m+s} \\ &= [(2l+1)/4\pi]^{\frac{1}{2}}\,d^l_{-sm}(\theta)e^{im\phi}, \qquad (2.8)\end{aligned}$$

where $\binom{p}{q}$ is the usual binomial coefficient and p is summed over the integers. The functions $D^l_{m'm}(\alpha\beta\gamma)$ and $d^l_{m'm}(\beta)$ are discussed in some detail in Ref. 2.[3]

This relationship between ${}_sY_{lm}$ and D^l_{-sm} gives us some additional properties of the spin harmonics which we will need. If we introduce the usual orbital angular momentum raising and lowering operators

$$\begin{aligned}L_\pm &= L_x \pm iL_y \\ &= \pm e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right), \qquad (2.9)\end{aligned}$$

along with the commutation relations

$$\begin{aligned}[L_z, L_\pm] &= \pm L_\pm, \\ [L_+, L_-] &= 2L_z,\end{aligned} \qquad (2.10)$$

with

$$L_z = -i\frac{\partial}{\partial\phi},$$

then we find that the operators

$$\begin{aligned}\Lambda_z &\equiv L_z, \\ \Lambda_\pm &= \Lambda_x \pm i\Lambda_y \\ &\equiv L_\pm - s\csc\theta e^{\pm i\phi}\end{aligned} \qquad (2.11)$$

satisfy the commutation relations

$$\begin{aligned}[\Lambda_z, \Lambda_\pm] &= \pm\Lambda, \\ [\Lambda_+, \Lambda_-] &= 2\Lambda_z,\end{aligned} \qquad (2.12)$$

i.e., $\boldsymbol{\Lambda}$ obeys the commutation relations of an angular momentum operator. Using these operators, we find

$$\begin{aligned}\Lambda^2\,{}_sY_{lm} &= l(l+1)\,{}_sY_{lm}, \\ \Lambda_z\,{}_sY_{lm} &= m\,{}_sY_{lm}, \\ \Lambda_\pm\,{}_sY_{lm} &= [(l\mp m)(l\pm m+1)]^{\frac{1}{2}}\,{}_sY_{lm\pm1}.\end{aligned} \qquad (2.13)$$

Thus the ${}_sY_{lm}$ are eigenfunctions of Λ^2, and Λ_z and $\Lambda_\pm$ raise and lower m.

Finally we note that we can allow l, m, and s to take on half-integer values, and all of the above results still hold as long as we now take Eqs. (2.8) to give us our basic definition of ${}_sY_{lm}$. Of course, we cannot generate the half-integer harmonics from Y_{lm}, but

given one, say ${}_{\frac{1}{2}}Y_{lm}$, we could generate the others for this l and m, by using relations (2.5). However, Eqs. (2.8) give ${}_sY_{lm}$ explicitly, and so we have no need for this generating procedure.

3. TENSOR SPHERICAL HARMONICS

The fact that spin weight is defined in terms of rotations around the radial direction indicates that it corresponds to an eigenvalue associated with the radial component of an angular momentum. That it is a "magnetic" quantum number associated with l is indicated by relations (2.5) for $\eth\,{}_sY_{lm}$ and $\bar{\eth}\,{}_sY_{lm}$. Goldberg *et al.*[2] have, in fact, shown this more explicitly by using the connection between ${}_sY_{lm}$ and the D^l_{-sm} functions. We will see the same thing here when we construct tensor harmonics. We will also see that s corresponds to a helicity.

We first define a set of Cartesian vector harmonics and, by examining their properties, we will see how we can generalize to tensor harmonics of any higher rank. The vector harmonics $T_i(s, l, m; \hat{\mathbf{r}})$ are defined by

$$\begin{aligned} T_i(+1, l, m; \hat{\mathbf{r}}) &\equiv m_i[{}_{-1}Y_{lm}(\theta, \phi)], \\ T_i(0, l, m; \hat{\mathbf{r}}) &\equiv \hat{r}_i[{}_0Y_{lm}(\theta, \phi)], \\ T_i(-1, l, m; \hat{\mathbf{r}}) &\equiv -m_i^*[{}_{+1}Y_{lm}(\theta, \phi)], \end{aligned} \tag{3.1}$$

with $\hat{\mathbf{r}}$ the unit vector in the radial direction and $\mathbf{m} = (1/\sqrt{2})(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})$ as before. The three unit vectors $\hat{\mathbf{r}}$, $\mathbf{m}$, and $\mathbf{m}^*$ clearly satisfy the relations

$$\begin{aligned} \hat{\mathbf{r}} \cdot \mathbf{m} = \hat{\mathbf{r}} \cdot \mathbf{m}^* = \mathbf{m} \cdot \mathbf{m} = \mathbf{m}^* \cdot \mathbf{m}^* = 0, \\ \hat{\mathbf{r}} \cdot \hat{\mathbf{r}} = \mathbf{m} \cdot \mathbf{m}^* = 1. \end{aligned} \tag{3.2}$$

If we combine relations (3.2) with the orthonormality conditions for ${}_sY_{lm}$ given in Eq. (2.6), we find

$$\int_{4\pi} T_i^*(s', l', m')T^i(s, l, m)\, d\Omega = \delta_{ss'}\delta_{ll'}\delta_{mm'}, \tag{3.3}$$

where we have introduced the abbreviated notation $T_i(s, l, m) = T_i(s, l, m; \hat{\mathbf{r}})$. If we use the completeness relation (2.7) along with the fact that $r_ir_i + m_im_j^* + m_i^*m_j = \delta_{ij}$, we see that

$$\begin{aligned} \sum_{\substack{s,l,m \\ |s|\le l}} T_i(s, l, m; \hat{\mathbf{r}}')T_j(s, l, m; \hat{\mathbf{r}}) \\ = \delta_{ij}\delta(\phi - \phi')\delta(\cos\theta - \cos\theta'). \end{aligned} \tag{3.4}$$

These vector harmonics, therefore, form a complete set for vector functions of θ and ϕ. In fact, the $T_i(s, l, m)$ are the usual vector harmonics used in electrodynamics,[4] although in a somewhat disguised form.[5]

The total angular momentum operator for these harmonics, which is the generator of rotations for vector functions, is given by[6]

$$\begin{aligned} (J_k)_{ij} &= \delta_{ij}L_k + (S_k)_{ij}, \\ (S_k)_{ij} &= -i\epsilon_{ijk}, \end{aligned} \tag{3.5}$$

with $\mathbf{L} = -i\mathbf{r} \times \nabla$ the usual orbital angular momentum operator introduced earlier. The spin operator given in (3.5) is that for Cartesian 3-vectors. (The more familiar representation for spin-1 systems is given by using the complex coordinates z and $x \pm iy$ instead of x, y, and z.)

Using (3.5) along with the specific forms for $L_\pm$ and L_z given in (2.9) and (2.10), we can derive the following operator relations:

$$\begin{aligned} (J_\pm)_i^j\hat{r}_j &= \hat{r}_iL_\pm, \\ (J_z)_i^j\hat{r}_j &= \hat{r}_iL_z, \\ (J_\pm)_i^jm_j &= m_i(L_\pm + \csc\theta e^{\pm i\phi}), \\ (J_z)_i^jm_j &= m_iL_z, \\ (J_\pm)_i^jm_j^* &= m_i^*(L_\pm - \csc\theta e^{\pm i\phi}), \\ (J_z)_i^jm_j^* &= m_i^*L_z, \end{aligned} \tag{3.6}$$

with $J_\pm \equiv J_x + iJ_y$ as usual. In addition we have

$$\begin{aligned} (\hat{\mathbf{r}} \cdot \mathbf{S})_i^j\hat{r}_j &= 0, \\ (\hat{\mathbf{r}} \cdot \mathbf{S})_i^jm_j &= m_i, \\ (\hat{\mathbf{r}} \cdot \mathbf{S})_i^jm_j^* &= -m_i^*. \end{aligned} \tag{3.7}$$

Finally we note that $(S^2)_{ij} = (S_k)_i^p(S^k)_{pj} = 2\delta_{ij}$.

The operator relations (3.6) allow us to establish a correspondence between $(\mathbf{J})_{ij}$ and the operator $\boldsymbol{\Lambda}$ introduced in Sec. 2. From inspection of the definition of $\boldsymbol{\Lambda}$ given in (2.11), we see that

$$\begin{aligned} (\mathbf{J})_i^jT_j(+1, l, m) &= m_i[\boldsymbol{\Lambda}_{-1}Y_{lm}], \\ (\mathbf{J})_i^jT_j(0, l, m) &= \hat{r}_i[\boldsymbol{\Lambda}_0Y_{lm}], \\ (\mathbf{J})_i^jT_j(-1, l, m) &= -m_i^*[\boldsymbol{\Lambda}_{+1}Y_{lm}]. \end{aligned} \tag{3.8}$$

Because the ${}_sY_{lm}$ are eigenfunctions of Λ^2 and Λ_z, the $T_i(s, l, m)$ are eigenfunctions of $(J^2)_{ij}$ and $(J_z)_{ij}$.

Putting together the results in (3.7) and (3.8) along with (2.13), we have

$$\begin{aligned} (J^2)_i^jT_j(s, l, m) &= l(l + 1)T_i(s, l, m), \\ (J_z)_i^jT_j(s, l, m) &= mT_i(s, l, m), \\ (J_\pm)_i^jT_j(s, l, m) &= [(l \mp m)(l \pm m + 1)]^{\frac{1}{2}} \\ &\quad \times T_i(s, l, m \pm 1), \\ (S^2)_i^jT_j(s, l, m) &= 2T_i(s, l, m), \\ (\hat{\mathbf{r}} \cdot \mathbf{S})_i^jT_j(s, l, m) &= sT_i(s, l, m). \end{aligned} \tag{3.9}$$

Since $(\hat{\mathbf{r}} \cdot \mathbf{J})_{ij} = (\hat{\mathbf{r}} \cdot \mathbf{S})_{ij}$, the last equation holds for $\mathbf{J}$ as well. [The implication of the results in (3.9) is that $(\hat{\mathbf{r}} \cdot \mathbf{S})_{ij}$ commutes with $(\mathbf{J})_{ij}$ and, of course, with $(S^2)_{ij}$. This can be easily verified.]

We are therefore able to relate l to a total angular

momentum, m to its z projection, and s to the radial component of spin. If we think in terms of outgoing radiation, s can be thought of as a helicity. We note that this helicity is the negative of the spin weight of the ${}_sY_{lm}$ used to construct a vector harmonic. This is easy to understand from the definition of spin weight. A spin weight $+1$ quantity, e.g., $\mathbf{m}\cdot\mathbf{A}$, is obtained by contracting $\mathbf{m}$ into a vector, but this projects out the function multiplying $\mathbf{m}^*$ in the vector, and $\mathbf{m}^*$ has helicity -1.

Missing from Eqs. (3.9) are a raising and a lowering operator for s. Any such operators must be related to $\eth$ and $\bar{\eth}$. In order to construct the operator we need, we note first the operator relations

$$\begin{aligned}
[(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}})\cdot\mathbf{J}]^j_i \hat{r}_j &= \hat{r}_i\left\{\pm\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi}\right\},\\
[(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}})\cdot\mathbf{J}]^j_i m_j &= m_i\left\{\pm\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi} + \cot\theta\right\},\\
[(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}})\cdot\mathbf{J}]^j_i m^*_j &= m^*_i\left\{\pm\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi} - \cot\theta\right\}.
\end{aligned} \tag{3.10}$$

In addition we have

$$\begin{aligned}
[(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]^j_i m_j &= [(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]^j_i m^*_j = 0,\\
[(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]^j_i m_j &= -2^{\frac{1}{2}}\hat{r}_i,\\
[(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]^j_i m^*_j &= +2^{\frac{1}{2}}\hat{r}_i,\\
[(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]^j_i \hat{r}_j &= -2^{\frac{1}{2}}m_i,\\
[(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]^j_i \hat{r}_j &= +2^{\frac{1}{2}}m^*_i.
\end{aligned} \tag{3.11}$$

Comparing the right-hand sides in (3.10) with the definitions of $\eth$ and $\bar{\eth}$ given in (2.3) and (2.4) suggests that we define the operators

$$\begin{aligned}
\theta_{ij} &\equiv [(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]^k_i[(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})\cdot\mathbf{J}]_{kj},\\
\bar{\theta}_{ij} &\equiv [(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]^k_i[(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}})\cdot\mathbf{J}]_{kj}.
\end{aligned} \tag{3.12}$$

These operators are related to $\eth$ and $\bar{\eth}$ in the following way:

$$\begin{aligned}
(m_i\theta^{ij}\hat{r}_j)\,{}_0Y_{lm} &= -2^{\frac{1}{2}}\eth\,{}_0Y_{lm},\\
(\hat{r}_i\theta^{ij}m_j)\,{}_{-1}Y_{lm} &= +2^{\frac{1}{2}}\eth\,{}_{-1}Y_{lm},\\
(m^*_i\bar{\theta}^{ij}\hat{r}_j)\,{}_0Y_{lm} &= -2^{\frac{1}{2}}\bar{\eth}\,{}_0Y_{lm},\\
(\hat{r}_i\bar{\theta}^{ij}m^*_j)\,{}_{+1}Y_{lm} &= +2^{\frac{1}{2}}\bar{\eth}\,{}_{+1}Y_{lm},
\end{aligned} \tag{3.13}$$

as one can easily verify using (3.10), (3.11) and (2.3), (2.4).

Combining the results of (3.13) with the raising and lowering properties of $\eth$ and $\bar{\eth}$ given in (2.5), we find from our definitions of the $T_i(s, l, m)$ that

$$\begin{aligned}
\theta^j_i T_j(s, l, m) &= [2(l+s)(l-s+1)]^{\frac{1}{2}}T_i(s-1, l, m),\\
\bar{\theta}^j_i T_j(s, l, m) &= [2(l-s)(l+s+1)]^{\frac{1}{2}}T_i(s+1, l, m).
\end{aligned} \tag{3.14}$$

Thus θ_{ij}, which corresponds to $\eth$, lowers the helicity by one and $\bar{\theta}_{ij}$, which corresponds to $\bar{\eth}$, raises the helicity by one. [The results of (3.14) when compared with Eqs. (3.9) imply that both θ_{ij} and $\bar{\theta}_{ij}$ commute with $(\mathbf{J})_{ij}$ and $(S^2)_{ij}$.]

We have treated the vector harmonics here in some detail for two reasons. One is that they illustrate general properties we will find for higher rank tensor harmonics. The other is that operator relations (3.6) and (3.10) are actually of a very general nature. If one uses the specific form of $(\mathbf{J})_{ij}$ in terms of $\mathbf{L}$ which is given in (3.5), relations (3.6) and (3.10) tell how to commute $\mathbf{L}$ and $(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}})\cdot\mathbf{L}$ through several factors of $\hat{r}_i$, m_i, and m^*_i. The effects of $(\hat{\mathbf{r}}\cdot\mathbf{S})_{ij}$ and $[(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}]_{ij}$ on $\hat{r}_i$, m_i, and m^*_i given in (3.7) and (3.11) are also general in that, as we will see below, $-i\epsilon_{ijk}$ is involved in the spin operator for higher-rank tensors. These facts will allow us to write down the higher-rank harmonics and their properties with little difficulty.

For nth-rank tensor functions, the total angular momentum operator is

$$\begin{aligned}
(J_k)_{i_1\cdots i_n j_1\cdots j_n} &= \delta_{i_1 j_1}\cdots\delta_{i_n j_n}L_k + (S_k)_{i_1\cdots i_n j_1\cdots j_n},\\
(S_k)_{i_1\cdots i_n j_1\cdots j_n} &= -i\sum_{t=1}^{n}\delta_{i_1 j_1}\cdots\delta_{i_{t-1}j_{t-1}}\epsilon_{i_t j_t k}\delta_{i_{t+1}j_{t+1}}\delta_{i_n j_n},
\end{aligned} \tag{3.15}$$

which is the generalization of (3.5). In order to make our notation more compact, we will adopt the convention for indices that

$$i(n) \equiv i_1 i_2\cdots i_n,$$

which we will use wherever possible.

Suppose that $\tau_{i(n)}(p, q)$ is an nth-rank tensor made up of p factors of m_i, q of $-m^*_i$, $p+q \le n$, with the rest of the indices assigned to factors of $\hat{r}_i$. Clearly there are, in general, many ways of doing this, since the ith index could have any of the three unit vectors assigned to it, while maintaining the same values of p and q. For the moment we will not worry about these possible variations.

Consider then the tensor harmonic

$$\tau_{i(n)}(p, q)[{}_{-(p-q)}Y_{lm}].$$

From the definition of $(J_k)_{i(n)j(n)}$ given in (3.15) and repeated use of operator relations (3.6), we can show that

$$(\mathbf{J})^{j(n)}_{i(n)}\tau_{j(n)}(p, q)[{}_{-(p-q)}Y_{lm}] = \tau_{i(n)}(p, q)[\boldsymbol{\Lambda}\,{}_{-(p-q)}Y_{lm}]. \tag{3.16}$$

Using the definition of $(S_k)_{i(n)j(n)}$ and (3.7), we also find

$$(\hat{\mathbf{r}}\cdot\mathbf{S})^{j(n)}_{i(n)}\tau_{j(n)}(p, q) = (p-q)\tau_{i(n)}(p, q). \tag{3.17}$$

From these two results, we see that these tensor harmonics are eigenfunctions of J^2, J_z, and $\hat{\mathbf{r}} \cdot \mathbf{S}$ and that $J_\pm$ are the raising and lowering operators for m. They are not, in general, eigenfunctions of S^2.

For two reasons, one physical and the other mathematical, we will restrict ourselves to symmetric, traceless[7] tensor harmonics. Frequently the tensor fields we use in physics are symmetric and traceless. Such fields correspond to eigenfunctions of S^2.[8] Mathematically we know that any nth-rank tensor can be decomposed uniquely into a term which is symmetric and traceless and is an eigenfunction of $(S^2)_{i(n)j(n)}$ with eigenvalue $n(n+1)$ and terms which can be related to successively lower rank symmetric, traceless tensors.[3] This decomposition can be understood if we think of an nth-rank tensor as a direct product of n spin-1 states. For such a direct product we find total spins ranging from 0 up to n, with only one possible way to obtain spin n.

What we need is a set of $\tau_{i(n)}$ which are symmetric and traceless and eigenfunctions of $(\hat{\mathbf{r}} \cdot \mathbf{S})_{i(n)j(n)}$. One such $\tau_{i(n)}$ is easy to construct. Consider[9]

$$\begin{aligned}\tau_{i(n)}(n) &\equiv \tau_{i(n)}(p = n, q = 0)\\ &= m_{i_1} m_{i_2} \cdots m_{i_n},\end{aligned} \tag{3.18}$$

which clearly satisfies

$$\begin{aligned}(\hat{\mathbf{r}} \cdot \mathbf{S})^{j(n)}_{i(n)} \tau_{j(n)}(n) &= n\tau_{i(n)}(n),\\ \tau^*_{i(n)}(n)\tau^{i(n)}(n) &= 1.\end{aligned} \tag{3.19}$$

Since this tensor is symmetric and traceless, it must also satisfy

$$(S^2)^{j(n)}_{i(n)} \tau_{j(n)}(n) = n(n+1)\tau_{i(n)}(n). \tag{3.20}$$

This result can be verified directly from the definition of $(S)_{i(n)j(n)}$. Another symmetric, traceless $\tau_{i(n)}$ which is normalized to unity and has eigenvalue, for $\hat{\mathbf{r}} \cdot \mathbf{S}$, equal to $-n$ is

$$\begin{aligned}\tau_{i(n)}(-n) &\equiv \tau_{i(n)}(p = 0, q = n)\\ &= (-)^n m^*_i m^*_{i_2} \cdots m^*_{i_n}.\end{aligned} \tag{3.21}$$

It also satisfies (3.20).

We can obtain all the other $\tau_{i(n)}$ we need from either one of these, since $[(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}}) \cdot \mathbf{S}]_{i(n)j(n)}$ are the spin raising and lowering operators which go with $(\hat{\mathbf{r}} \cdot \mathbf{S})_{i(n)j(n)}$. We note from the definition of $(\mathbf{S})_{i(n)j(n)}$, that when it operates on a symmetric, traceless tensor, it leaves a symmetric, traceless tensor. We obtain $\tau_{i(n)}(s)$ by stepping down $\tau_{i(n)}(n)$ $n - s$ times. Let us assume that $\tau_{i(n)}(s)$ is normalized to unity and that we use a phase convention consistent with (3.21) and the vector case. We have then

$$\begin{aligned}&[(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}}) \cdot \mathbf{S}]^{j(n)}_{i(n)} \tau_{j(n)}(s)\\ &\quad = -[(n \mp s)(n \pm s + 1)]^{\frac{1}{2}} \tau_{i(n)}(s \pm 1).\end{aligned} \tag{3.22}$$

If we either step down from $\tau_{i(n)}(n)$ or up from $\tau_{i(n)}(-n)$ to obtain $\tau_{i(n)}(s)$, we find

$$\begin{aligned}\tau_{i(n)}(s) &= (-)^{n-s}\left[\frac{(n+s)!}{(2n)!\,(n-s)!}\right]^{\frac{1}{2}}\\ &\quad \times \{[(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}}) \cdot \mathbf{S}]^{n-s}\}^{j(n)}_{i(n)} \tau_{j(n)}(n)\\ &= (-)^{n+s}\left[\frac{(n-s)!}{(2n)!\,(n+s)!}\right]^{\frac{1}{2}}\\ &\quad \times \{[(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}}) \cdot \mathbf{S}]^{n+s}\}^{j(n)}_{i(n)} \tau_{j(n)}(-n).\end{aligned} \tag{3.23}$$

Noting that $\tau^*_{i(n)}(n) = (-)^n \tau_{i(n)}(-n)$ and $(S_k)^*_{i(n)j(n)} = -(S_k)_{i(n)j(n)}$, we have

$$\tau^*_{i(n)}(s) = (-)^s \tau_{i(n)}(-s), \tag{3.24}$$

which means we only need to step down $\tau_{i(n)}(n)$ to $s = 0$ [or step up $\tau_{i(n)}(-n)$ to $s = 0$] to obtain all the $\tau_{i(n)}(s)$.

It is clear that $\tau_{i(n)}(s)$ is made up of terms which contain $\tau_{i(n)}(p, q)$, all with $p - q = s$. This means that results (3.16) and (3.17) will still hold if we replace $\tau_{i(n)}(p, q)$ with $\tau_{i(n)}(s)$ and $p - q$ with s. We define then the nth-rank, symmetric, traceless tensor harmonics as

$$T_{i(n)}(s, l, m; \hat{\mathbf{r}}) \equiv \tau_{i(n)}(s)[{}_sY_{lm}(\theta, \phi)], \tag{3.25}$$

which are eigenfunctions of J^2, J_z, S^2, and $\hat{\mathbf{r}} \cdot \mathbf{S}$, with $J_\pm$ the raising and lowering operators for m. Recalling that $Y^*_{lm} = (-)^m Y_{l,-m}$ and using the definition of ${}_sY_{lm}$ given in Sec. 2 along with the result in (3.24), we find

$$T^*_{i(n)}(s, l, m) = (-)^m T_{i(n)}(-s, l, -m). \tag{3.26}$$

These harmonics form a complete set of nth-rank, symmetric, traceless tensors. We have

$$\int_{4\pi} T^*_{i(n)}(s', l', m') T^{i(n)}(s, l, m)\, d\Omega = \delta_{ss'}\delta_{ll'}\delta_{mm'} \tag{3.27}$$

and

$$\begin{aligned}&\sum_{\substack{s,l,m\\ |s|\le l}} T^*_{i(n)}(s, l, m; \hat{\mathbf{r}}') T_{j(n)}(s, l, m; \hat{\mathbf{r}})\\ &\quad = P_{i(n)j(n)}\delta(\phi - \phi')\delta(\cos\theta - \cos\theta'),\end{aligned} \tag{3.28}$$

with

$$P_{i(n)j(n)} = \sum_{s=-n}^{n} \tau^*_{i(n)}(s)\tau_{j(n)}(s), \tag{3.29}$$

where $P_{i(n)j(n)}$ is a projection operator which projects out the symmetric, traceless part of any nth-rank tensor. The results in (3.27) and (3.28) are easily

obtained from the properties of the $\tau_{i(n)}(s)$ and the ${}_sY_{lm}$.

In complete analogy with the vector case, we define operators $\theta_{i(n)j(n)}$ and $\bar{\theta}_{i(n)j(n)}$ which will lower and raise s. We have

$$\theta_{i(n)j(n)} \equiv [(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}}) \cdot \mathbf{S}]^{k(n)}_{i(n)}[(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}}) \cdot \mathbf{J}]_{k(n)j(n)},$$
$$\bar{\theta}_{i(n)j(n)} \equiv [(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}}) \cdot \mathbf{S}]^{k(n)}_{i(n)}[(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}}) \cdot \mathbf{J}]_{k(n)j(n)}. \tag{3.30}$$

Using operator relations (3.10) repeatedly, we can show that

$$[(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}}) \cdot \mathbf{J}]^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = -\tau_{i(n)}(s)[\eth\, {}_sY_{lm}].$$
$$[(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}}) \cdot \mathbf{J}]^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = \tau_{i(n)}(s)[\bar{\eth}\, {}_sY_{lm}]. \tag{3.31}$$

{Actually, (3.31) is most easily proved for $\tau_{i(n)}(p, q) \times [{}_{-(p-q)}Y_{lm}]$, but, as we have seen, $T_{i(n)}(s, l, m)$ is just a linear combination of these with $p - q = s$.}

Combining the results of (3.31) and the effects of $(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}}) \cdot \mathbf{S}$ on $\tau_{i(n)}(s)$ given in (3.22), we see that $\theta_{i(n)j(n)}$ and $\eth$, $\bar{\theta}_{i(n)j(n)}$ and $\bar{\eth}$ are related in that

$$[\tau^*_{i(n)}(s-1)\theta^{i(n)j(n)}\tau_{j(n)}(s)]\, {}_sY_{lm} = [(n+s)(n-s+1)]^{\frac{1}{2}}\eth\, {}_sY_{lm},$$
$$[\tau^*_{i(n)}(s+1)\bar{\theta}^{i(n)j(n)}\tau_{j(n)}(s)]\, {}_sY_{lm} = -[(n-s)(n+s+1)]^{\frac{1}{2}}\bar{\eth}\, {}_sY_{lm}. \tag{3.32}$$

Collecting together all our results, we have

$$(J^2)^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = l(l+1)T_{i(n)}(s, l, m),$$
$$(J_z)^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = mT_{i(n)}(s, l, m),$$
$$(J_\pm)^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = [(l \mp m)(l \pm m + 1)]^{\frac{1}{2}} \times T_{i(n)}(s, l, m \pm 1),$$
$$(S^2)^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = n(n+1)T_{i(n)}(s, l, m),$$
$$(\hat{\mathbf{r}} \cdot \mathbf{S})^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = sT_{i(n)}(s, l, m), \tag{3.33}$$
$$\theta^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = [(n+s)(n-s+1)(l+s)(l-s+1)]^{\frac{1}{2}} \times T_{i(n)}(s-1, l, m),$$
$$\bar{\theta}^{j(n)}_{i(n)}T_{j(n)}(s, l, m) = [(n-s)(n+s+1)(l-s)(l+s+1)]^{\frac{1}{2}} \times T_{i(n)}(s+1, l, m).$$

Once again we note that $\hat{\mathbf{r}} \cdot \mathbf{S} = \hat{\mathbf{r}} \cdot \mathbf{J}$ so that s is a radial eigenvalue of $\mathbf{J}$ as well. It is interesting that this dual role for s also shows up in θ and $\bar{\theta}$.

In the Appendix we tabulate these tensor harmonics for $n = 1$, 2, and 3.

4. SPINOR SPHERICAL HARMONICS

Because the ${}_sY_{lm}$ are defined for half-integer values of s, l, and m, we can use the techniques of Sec. 3 to construct spinor spherical harmonics from them. To do this, we need a set of spinors which will play the same role as $\hat{\mathbf{r}}$, $\mathbf{m}$, and $\mathbf{m}^*$ do in the construction of $\tau_{i(n)}(s)$.

The spinors

$$u(\theta, \phi) \equiv \begin{pmatrix} \cos(\theta/2)e^{-i/2\phi} \\ \sin(\theta/2)e^{i/2\phi} \end{pmatrix},$$
$$v(\theta, \phi) \equiv \begin{pmatrix} \sin(\theta/2)e^{-i/2\phi} \\ -\cos(\theta/2)e^{i/2\phi} \end{pmatrix}, \tag{4.1}$$

are the ones we will use. They are normalized and orthogonal so that $u^+u = v^+v = 1$ and $u^+v = 0$. They also satisfy

$$\hat{\mathbf{r}} \cdot \boldsymbol{\sigma}u = u,$$
$$\hat{\mathbf{r}} \cdot \boldsymbol{\sigma}v = -v,$$
$$(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}}) \cdot \boldsymbol{\sigma}u = (\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}}) \cdot \boldsymbol{\sigma}v = 0, \tag{4.2}$$
$$(\hat{\boldsymbol{\theta}} - i\hat{\boldsymbol{\phi}}) \cdot \boldsymbol{\sigma}u = -2v,$$
$$(\hat{\boldsymbol{\theta}} + i\hat{\boldsymbol{\phi}}) \cdot \boldsymbol{\sigma}v = -2u,$$

where $\boldsymbol{\sigma} = \sigma_1\mathbf{i} + \sigma_2\mathbf{j} + \sigma_3\mathbf{k}$ with σ_1, σ_2, and σ_3 the usual Pauli spin matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

If we define the total angular momentum operator

$$\mathbf{J} = \mathbf{L} + \mathbf{S},$$
$$\mathbf{S} = \tfrac{1}{2}\boldsymbol{\sigma}, \tag{4.3}$$

then we can obtain the operator relations

$$J_\pm u = u(L_\pm + \tfrac{1}{2}\csc\theta e^{\pm i\phi}),$$
$$J_z u = uL_z,$$
$$J_\pm v = v(L_\pm - \tfrac{1}{2}\csc\theta e^{\pm i\phi}),$$
$$J_z v = vL_z, \tag{4.4}$$
$$[(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}}) \cdot \mathbf{J}]u = u\left(\pm\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi} + \tfrac{1}{2}\cot\theta\right),$$
$$[(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}}) \cdot \mathbf{J}]v = v\left(\pm\frac{\partial}{\partial\theta} + i\csc\theta\frac{\partial}{\partial\phi} - \tfrac{1}{2}\cot\theta\right),$$

which are the spin-$\frac{1}{2}$ analogs of (3.6) and (3.10).

Via all these properties, it is easy to see that $u[{}_{-\frac{1}{2}}Y_{lm}]$ and $v[{}_{+\frac{1}{2}}Y_{lm}]$ are the spinor harmonics we want for spin-$\frac{1}{2}$ systems.

For higher-spin systems we take direct products of u's and v's. For a system which involves $2n$ factors in

this direct product, with n either an integer or half-integer, the total angular momentum operator will be

$$(J_k)_{\alpha_1\cdots\alpha_{2n}\beta_1\cdots\beta_{2n}} = \delta_{\alpha_1\beta_1}\cdots\delta_{\alpha_{2n}\beta_{2n}}L_k + (S_k)_{\alpha_1\cdots\alpha_{2n}\beta_1\cdots\beta_{2n}},$$
$$(S_k)_{\alpha_1\cdots\alpha_{2n}\beta_1\cdots\beta_{2n}} = \tfrac{1}{2}\sum_{t=1}^{2n}\delta_{\alpha_1\beta_1}\cdots\delta_{\alpha_{t-1}\beta_{t-1}}(\sigma_k)_{\alpha_t\beta_t}\delta_{\alpha_{t+1}\beta_{t+1}}\cdots\delta_{\alpha_{2n}\beta_{2n}}, \tag{4.5}$$

where we use Greek letters for spinor indices. We will again use the convention that $\alpha(2n)$ stands for the $2n$ indices α_1–α_{2n}.

Following the procedure of the last section, we will construct spinor quantities $\tau_{\alpha(2n)}(s)$ and from them the spinor harmonics. We start with the normalized quantities

$$\tau_{\alpha(2n)}(n) \equiv u_{\alpha_1}u_{\alpha_2}\cdots u_{\alpha_{2n}}, \tag{4.6}$$

or

$$\tau_{\alpha(2n)}(-n) \equiv v_{\alpha_1}v_{\alpha_2}\cdots v_{\alpha_{2n}}, \tag{4.7}$$

which are eigenstates of $(\hat{\mathbf{r}}\cdot\mathbf{S})_{\alpha(2n)\beta(2n)}$ with eigenvalues n and $-n$, respectively.

Because of our choice of phases for u and v, the stepping operators $(\hat{\boldsymbol{\theta}} \pm i\hat{\boldsymbol{\phi}})\cdot\mathbf{S}$ will have exactly the same effect on $\tau_{\alpha(2n)}(s)$ here as it does on $\tau_{i(n)}(s)$ in (3.22). In fact all we need do is replace the indices $i(n)$ by $\alpha(2n)$, etc., and Eqs. (3.23) will give us $\tau_{\alpha(2n)}(s)$ in terms of $\tau_{\alpha(2n)}(n)$ and $\tau_{\alpha(2n)}(-n)$. Once we have constructed the $\tau_{\alpha(2n)}(s)$, everything else parallels our construction of the tensor harmonics exactly.

If we define the spinor harmonics

$$\Sigma_{\alpha(2n)}(s, l, m; \hat{\mathbf{r}}) \equiv \tau_{\alpha(2n)}(s)[{}_{-s}Y_{lm}(\theta, \phi)], \tag{4.8}$$

then all the relations in Sec. 3 for $T_{i(n)}(s, l, m)$ from (3.27) on will hold for $\Sigma_{\alpha(2n)}(s, l, m)$ if we replace Cartesian indices $i(n)$ with spinor indices $\alpha(2n)$, etc. This includes the definitions of θ and $\bar{\theta}$. The difference here is that n may take on half-integer as well as integer values.

Actually, the spinor harmonics for integer values of n are completely equivalent to the tensor harmonics. We see this most easily by noting that

$$\begin{aligned} \hat{r}_1 &= u_1v_1 - u_2v_2, \\ \hat{r}_2 &= i(u_1v_1 + u_2v_2), \\ \hat{r}_3 &= -(u_1v_2 + u_2v_1), \\ m_1 &= (1/\sqrt{2})(u_1^2 - u_2^2), \\ m_2 &= (i/\sqrt{2})(u_1^2 + u_2^2), \\ m_3 &= (\sqrt{2})u_1u_2, \end{aligned} \tag{4.9}$$

with similar expressions for $\mathbf{m}^*$. Thus, only the spinor harmonics for half-integer values of n give us anything new.

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APPENDIX

We list here the tensor harmonics for rank $n = 1, 2$, and 3. Since these harmonics have the form

$$T_{i(n)}(s, l, m) = \tau_{i(n)}(s)[{}_{-s}Y_{lm}],$$

we list the $\tau_{i(n)}(s)$ and ${}_sY_{lm}$ separately. Also, because $\tau_{i(n)}(-s) = (-)^s\tau^*_{i(n)}(+s)$, we list $\tau_{i(n)}(s)$ for $s \geq 0$ only:

$n = 1$:

$$\tau_i(+1) = m_i, \quad \tau_i(0) = \hat{r}_i; \tag{A1}$$

$n = 2$:

$$\begin{aligned} \tau_{ij}(+2) &= m_im_j, \\ \tau_{ij}(+1) &= (1/\sqrt{2})(\hat{r}_im_j + m_i\hat{r}_j), \\ \tau_{ij}(0) &= (1/\sqrt{6})(2\hat{r}_i\hat{r}_j - m_i^*m_j - m_im_j^*); \end{aligned} \tag{A2}$$

$n = 3$:

$$\begin{aligned} \tau_{ijk}(+3) &= m_im_jm_k, \\ \tau_{ijk}(+2) &= (1/\sqrt{3})(\hat{r}_im_jm_k + m_i\hat{r}_jm_k + m_im_j\hat{r}_k), \\ \tau_{ijk}(+1) &= (1/\sqrt{15})(2\hat{r}_i\hat{r}_jm_k + 2\hat{r}_im_j\hat{r}_k + 2m_i\hat{r}_j\hat{r}_k \\ &\quad - m_i^*m_jm_k - m_im_j^*m_k - m_im_jm_k^*), \\ \tau_{ijk}(0) &= (1/\sqrt{10})(2\hat{r}_i\hat{r}_j\hat{r}_k - \hat{r}_im_j^*m_k - \hat{r}_im_jm_k^* \\ &\quad - m_i^*\hat{r}_jm_k - m_i\hat{r}_jm_k^* - m_i^*m_j\hat{r}_k \\ &\quad - m_im_j^*\hat{r}_k). \end{aligned} \tag{A3}$$

For the ${}_sY_{lm}$ we have

$$\begin{aligned} {}_0Y_{lm} &\equiv Y_{lm}, \\ {}_{\pm1}Y_{lm} &= \frac{1}{[l(l+1)]^{\frac{1}{2}}}\left(\mp\frac{\partial}{\partial\theta} - i\csc\theta\frac{\partial}{\partial\phi}\right)Y_{lm}, \\ {}_{\pm2}Y_{lm} &= \frac{1}{[(l-1)l(l+1)(l+2)]^{\frac{1}{2}}} \\ &\quad\times\left(\mp\frac{\partial}{\partial\theta} - i\csc\theta\frac{\partial}{\partial\phi} \pm \cot\theta\right) \\ &\quad\times\left(\mp\frac{\partial}{\partial\theta} - i\csc\theta\frac{\partial}{\partial\phi}\right)Y_{lm}, \\ {}_{\pm3}Y_{lm} &= \frac{1}{[(l-2)(l-1)l(l+1)(l+2)(l+3)]^{\frac{1}{2}}} \\ &\quad\times\left(\mp\frac{\partial}{\partial\theta} - i\csc\theta\frac{\partial}{\partial\phi} \pm 2\cot\theta\right) \\ &\quad\times\left(\mp\frac{\partial}{\partial\theta} - i\csc\theta\frac{\partial}{\partial\phi} \pm \cot\theta\right) \\ &\quad\times\left(\mp\frac{\partial}{\partial\theta} - i\csc\theta\frac{\partial}{\partial\phi}\right)Y_{lm}. \end{aligned} \tag{A4}$$

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[3] For discussions of both representations of the rotation group and tensor representations, see M. Hamermesh, *Group Theory* (Addison-Wesley, Reading, Mass., 1962), Chaps. 9 and 10.

[4] Vector spherical harmonics in electrodynamics are discussed by J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962), Chap. 16.

[5] For a discussion of several different sets of vector harmonics and their relationships see R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), Chap. 2.

[6] The tensor ϵ_{ijk} is the usual antisymmetric tensor density for three dimensions.

[7] By traceless for an nth-rank tensor, we mean traceless on any pair of indices.

[8] This follows from the fact that symmetric, traceless tensors form bases for irreducible representations of the rotation group. See Ref. 3.

[9] What we are doing here, of course, is constructing direct products of spin-1 states.

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Quantum Potentials on Lattices

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The existence and analyticity of thermodynamic states of ν-dimensional lattices is proved for non-number-conserving potentials at all values of fugacity for sufficiently high temperatures.

The existence and analyticity of the correlation functions of a lattice gas in the thermodynamic limit have been proved for sufficiently high temperatures at all values of fugacity only for a class of potentials which are number conserving.[1–3] In this paper we demonstrate how integral equation techniques can be used to prove the existence of infinite-volume correlation functions for a large class of non-number-conserving potentials.[4]

We associate with each bounded subset Λ of the ν-dimensional lattice $\mathbf{Z}^\nu$ the Hilbert space tensor product $\mathcal{H}_\Lambda = \otimes_{x\in\Lambda} \mathcal{H}_x$, where $\mathcal{H}_x$ is a two-dimensional vector space, and define creation and annihilation operators a_x^+ and a_x on $\mathcal{H}_x$ to satisfy Fermi–Dirac statistics at the site x and commutation between different lattice sites. Then there is a one-to-one map between the subsets of Λ and the basis vectors of $\mathcal{H}_\Lambda$, and we may label the basis vectors as

$$|Y\rangle = a^+(Y)\,|\varnothing\rangle \quad \text{for} \quad Y \subset \Lambda$$

and

$$a^+(Y) \equiv \prod_{y\in Y} a^+(y).$$

We let $\mathcal{A}$ be the quasilocal C^*-algebra generated by the local algebras $\mathcal{B}(\mathcal{H}_\Lambda)$ of all bounded operators on $\mathcal{H}_\Lambda$.

We shall assume that the system is specified by Hamiltonians $H(\Lambda)$ which are given by potential functions $\varphi(X)$, $X \subset \Lambda$, satisfying the following requirements: $\varphi(X) \in \mathcal{B}(\mathcal{H}_X)$ is Hermitian, translation invariant, $\varphi(x) = -\mu a_x^+ a_x$, and φ is bounded in λ-norm $\| \ \|_\lambda$:

$$\|\varphi\|_\lambda = \sum_{\substack{X\subset \mathbf{Z}^\nu \\ 0\in X}} \|\varphi(X)\|\, \lambda^{N(X)} < \infty$$

for all $\lambda > 0$. Here the local Hamiltonians $H(\Lambda)$ are

$$H(\Lambda) = \sum_{\substack{X\subset X \\ X\neq\varnothing}} \varphi(Y).$$

Then the finite-volume correlation functions are defined by

$$\rho_\Lambda(X, Y) = Z_\Lambda^{-1}\, \mathrm{Tr}_{\mathcal{H}_\Lambda}\, [e^{-\beta H(\Lambda)} a^+(X) a(Y)],$$

where $Z_\Lambda = \mathrm{Tr}_{\mathcal{H}_\Lambda}(e^{-\beta H(\Lambda)})$ is the partition function. For further details, see Ref. 5.

In Ref. 1 it was proved that the correlation functions ρ_Λ, considered as elements of the Banach space L_ν^∞ of bounded functions on the set of finite subsets of $\mathbf{Z}^\nu$, are the solution of the Banach space equations

$$\rho_\Lambda = K_\Lambda \rho_\Lambda + \chi_\Lambda \alpha,$$

where $\chi_\Lambda \alpha \in L_\nu^\infty$ and K_Λ is a bounded operator on L_ν^∞. More precisely, $\chi_\Lambda(X)$ is the characteristic function of the subset Λ, $\delta(A = B) = 1$ if $A = B$, zero otherwise,

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[5] For a discussion of several different sets of vector harmonics and their relationships see R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), Chap. 2.

[6] The tensor ϵ_{ijk} is the usual antisymmetric tensor density for three dimensions.

[7] By traceless for an nth-rank tensor, we mean traceless on any pair of indices.

[8] This follows from the fact that symmetric, traceless tensors form bases for irreducible representations of the rotation group. See Ref. 3.

[9] What we are doing here, of course, is constructing direct products of spin-1 states.

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Quantum Potentials on Lattices

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The existence and analyticity of thermodynamic states of ν-dimensional lattices is proved for non-number-conserving potentials at all values of fugacity for sufficiently high temperatures.

The existence and analyticity of the correlation functions of a lattice gas in the thermodynamic limit have been proved for sufficiently high temperatures at all values of fugacity only for a class of potentials which are number conserving.[1–3] In this paper we demonstrate how integral equation techniques can be used to prove the existence of infinite-volume correlation functions for a large class of non-number-conserving potentials.[4]

We associate with each bounded subset Λ of the ν-dimensional lattice $\mathbf{Z}^\nu$ the Hilbert space tensor product $\mathcal{H}_\Lambda = \otimes_{x\in\Lambda} \mathcal{H}_x$, where $\mathcal{H}_x$ is a two-dimensional vector space, and define creation and annihilation operators a_x^+ and a_x on $\mathcal{H}_x$ to satisfy Fermi–Dirac statistics at the site x and commutation between different lattice sites. Then there is a one-to-one map between the subsets of Λ and the basis vectors of $\mathcal{H}_\Lambda$, and we may label the basis vectors as

$$|Y\rangle = a^+(Y)\,|\varnothing\rangle \quad \text{for} \quad Y \subset \Lambda$$

and

$$a^+(Y) \equiv \prod_{y\in Y} a^+(y).$$

We let $\mathcal{A}$ be the quasilocal C^*-algebra generated by the local algebras $\mathcal{B}(\mathcal{H}_\Lambda)$ of all bounded operators on $\mathcal{H}_\Lambda$.

We shall assume that the system is specified by Hamiltonians $H(\Lambda)$ which are given by potential functions $\varphi(X)$, $X \subset \Lambda$, satisfying the following requirements: $\varphi(X) \in \mathcal{B}(\mathcal{H}_X)$ is Hermitian, translation invariant, $\varphi(x) = -\mu a_x^+ a_x$, and φ is bounded in λ-norm $\| \ \|_\lambda$:

$$\|\varphi\|_\lambda = \sum_{\substack{X\subset \mathbf{Z}^\nu \\ 0\in X}} \|\varphi(X)\|\, \lambda^{N(X)} < \infty$$

for all $\lambda > 0$. Here the local Hamiltonians $H(\Lambda)$ are

$$H(\Lambda) = \sum_{\substack{X\subset X \\ X\neq\varnothing}} \varphi(Y).$$

Then the finite-volume correlation functions are defined by

$$\rho_\Lambda(X, Y) = Z_\Lambda^{-1}\, \mathrm{Tr}_{\mathcal{H}_\Lambda}\, [e^{-\beta H(\Lambda)} a^+(X) a(Y)],$$

where $Z_\Lambda = \mathrm{Tr}_{\mathcal{H}_\Lambda}(e^{-\beta H(\Lambda)})$ is the partition function. For further details, see Ref. 5.

In Ref. 1 it was proved that the correlation functions ρ_Λ, considered as elements of the Banach space L_ν^∞ of bounded functions on the set of finite subsets of $\mathbf{Z}^\nu$, are the solution of the Banach space equations

$$\rho_\Lambda = K_\Lambda \rho_\Lambda + \chi_\Lambda \alpha,$$

where $\chi_\Lambda \alpha \in L_\nu^\infty$ and K_Λ is a bounded operator on L_ν^∞. More precisely, $\chi_\Lambda(X)$ is the characteristic function of the subset Λ, $\delta(A = B) = 1$ if $A = B$, zero otherwise,

$\alpha(X, Y) = \delta(X \cup Y = \varnothing)$, and the kernel K_Λ is

$$K_\Lambda(X, Y; P, (Y - y) \cup R) = \begin{cases} \sum_{\substack{V \subset R \cap P \\ R \cap (y \cup X) \subset V}} (-1)^{N(V)} \langle P - V | e^{\beta H(\Lambda)} a_y e^{-\beta H(\Lambda)} \\ \qquad \times |X \cup (R - V)\rangle \\ \qquad \text{if} \quad Y \neq \varnothing, \quad (X \cup y) \cap R \subset P \\ \sum_{\substack{V \subset R \cap [P - (X - x)] \\ x \cap P \subset V}} (-1)^{N(V)} \langle P - (X - x) - V | \\ \qquad \times e^{-\beta H(\Lambda)} a_x^+ e^{\beta H(\Lambda)} |R - V\rangle \\ \qquad \text{if} \quad Y = \varnothing, \quad (X - x) \subset P, \quad (x \cap P) \subset R \\ \text{zero otherwise} \end{cases}$$

for y, x distinguished elements of Y, X, respectively, and $z = e^{-\beta\mu}$, the fugacity.

To study the thermodynamic limit, we wish to estimate the norm

$$\|K_\Lambda\| = \sup_{X, Y} \sum_{P, R \subset \mathbf{Z}^\nu} |K_\Lambda(X, Y; P, R)|.$$

Theorem 1:

$$\|K_\Lambda\| \leq \alpha z \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{2\beta}{\alpha}\right)^n \sum_{k_1=2}^{N(\Lambda)} \cdots \sum_{k_n=2}^{N(\Lambda)} \|\varphi\|_{\alpha\hat{z}, k_1} \cdots \|\varphi\|_{\alpha\hat{z}, k_n} \times \prod_{j=1}^{n-1} \left(\sum_{i=1}^{j} (k_i - 1) + 1\right),$$

where $\alpha = 2\sqrt{2} + 1$, $\hat{z} = \max\{z, z^{-1}\}$, and

$$\|\varphi\|_{\lambda, j} = \sum_{\substack{Y \subset \mathbf{Z}^\nu \\ N(Y) = j}} \|\varphi(Y)\| \lambda^j.$$

Proof: Use the Dyson expansion and locality to obtain

$$e^{\beta H(\Lambda)} a_y e^{-\beta H(\Lambda)} = \sum_{n \geq 0} \sum_{y_2 \in S_1} \cdots \sum_{y_n \in S_{n-1}} \sum_{\substack{Y_1 \subset \Lambda \\ Y_1 \cap y = \varnothing}} \cdots \sum_{\substack{Y_n \subset \Lambda \\ Y_n \cap y_n = \varnothing}} \times \int_{1 > t_1 > \cdots > t_n > 0} dt_1 \cdots dt_n \times \beta^n [e^{\beta\mu t_1 N} \varphi(Y_n \cup y_n) e^{-\beta\mu t_1 N}, \cdots, [e^{\beta\mu t_n N} \varphi(Y_1 \cup y) e^{-\beta\mu t_n N}, e^{-\beta\mu} a_y], \cdots]$$

for N the number operator in $\mathcal{H}_\Lambda$ and $S_i = Y_i \cup Y_{i-1} \cup \cdots \cup Y_1 \cup y$. In evaluating

$$\sum_{R, P \subset \Lambda} |K_\Lambda(X, Y; P, Y' \cup R)|,$$

we may interchange the order of summation and sum last over n and the arguments $Y_1, y_2, Y_2, \cdots, y_n, Y_n$ of the potentials. The cancellations proceed analogously to those in Ref. 1. The result for $Y \neq \varnothing$ is

$$\sum_{R, P \subset \Lambda} |K_\Lambda(X, Y; P, Y' \cup R)| \leq \sum_{n=1}^{\infty} \sum_{y_2 \in S_1} \cdots \sum_{y_n \in S_{n-1}} \sum_{\substack{Y_1 \subset \Lambda \\ Y_1 \cap y = \varnothing}} \cdots \sum_{\substack{Y_n \subset \Lambda \\ Y_n \cap y_n = \varnothing}} \sum_{\substack{P, R \subset S_n \\ R \cap X' = \varnothing \\ (X \cup y) \cap R \subset P}} \times \sum_{W \subset R \cap P - (X \cup y) \cap (R \cap P)} \frac{z\beta^n}{n!} (\hat{z})^{\sum_{i=1}^{n} N(Y_i \cup y_i)} \times |\langle P - (R \cap P) + W | [\varphi(Y_n \cup y_n), \cdots, [\varphi(Y_1 \cup y), a_y] \cdots]| (X \cap S_n) \cup (R - R \cap P + W)\rangle|,$$

and the Schwarz inequality is used to complete the proof.

The infinite-volume correlation functions $\rho(X, Y)$ are defined to be the solution of the integral equations

$$\rho = K\rho + \alpha,$$

where K is defined pointwise by $K(X, Y; P, R) = \lim K_\Lambda(X, Y; P, R)$ as $\Lambda \to \infty$. The proof of Theorem 1 shows $K_\Lambda \to K$ in the sense of strong operator convergence of the adjoints in the predual of L_ν^∞. This and the uniform bound for $\|K_\Lambda\|$ proves $\rho(X, Y)$ is unique, analytic in its parameters, and the pointwise limit of the finite volume correlation functions for fugacities and temperatures for which the kernels are strict contractions. We have the following.

Theorem 2: The infinite-volume correlation functions are unique and analytic in the region of the (β, z) plane defined by

$$\alpha z \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{2\beta}{\alpha}\right)^n \sum_{k_1=2}^{\infty} \cdots \sum_{k_n=2}^{\infty} \|\varphi\|_{\alpha\hat{z}, k_1} \cdots \|\varphi\|_{\alpha\hat{z}, k_n} \times \prod_{j=1}^{n-1} \left(\sum_{i=1}^{j} (k_i - 1) + 1\right) < 1$$

and including a neighborhood of the (positive) z axis. If $\Lambda \to \infty$ in the sense of van Hove, then

$$\rho(X, Y) = \lim_{\Lambda \to \infty} \rho_\Lambda(X, Y).$$

By extending these arguments to the dual potential,

$$(\mathfrak{L}\varphi)(X) = (-1)^{N(X)} \sum_{\substack{Y \subset \mathbf{Z}^\nu \\ Y \supset X}} \mathrm{Tr}_{\mathcal{H}_{Y - X}} \varphi(Y)$$

in the case $\|\mathfrak{L}\varphi\|_\lambda < \infty$, it can be seen that the correlation functions extend analytically to the region defined by replacing φ by $\mathfrak{L}\varphi$ and z by z^{-1} in Theorem 2.

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Linear Canonical Transformations and Their Unitary Representations*

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We show that the group of linear canonical transformations in a $2N$-dimensional phase space is the real symplectic group $Sp(2N)$, and discuss its unitary representation in quantum mechanics when the N coordinates are diagonal. We show that this $Sp(2N)$ group is the well-known dynamical group of the N-dimensional harmonic oscillator. Finally, we study the case of n particles in a q-dimensional oscillator potential, for which $N = nq$, and discuss the chain of groups $Sp(2nq) \supset Sp(2n) \times O(q)$. An application to the calculation of matrix elements is given in a following paper.

1. INTRODUCTION

It is well known that some of the powerful techniques for solving mechanics problems are based on the symmetry group of canonical transformations, i.e., the transformations in phase space that leave the Hamiltonian and the Poisson brackets of coordinates and momenta invariant. In some cases these transformations concern the coordinates alone, i.e., are point transformations, as is the case when there is invariance under translations, rotations, or permutations of the particles. Symmetry groups of point transformations have been discussed extensively in the literature[1–3] both in their applications to classical and quantum mechanics. Groups of canonical transformations have been less extensively applied particularly in quantum mechanics, in which we require their unitary representation in an appropriate Hilbert space.[4] We shall discuss in this note the group of linear canonical transformations in a $2N$-dimensional phase space and their unitary representation when the N coordinates are diagonal. The linear canonical transformations constitute the dynamical group of the N-dimensional harmonic oscillator.[5] Their unitary representation plays a fundamental role in the understanding of the properties of harmonic oscillator states[5] and their use in many-body calculations.[6]

2. THE SYMPLECTIC GROUP OF LINEAR CANONICAL TRANSFORMATIONS

A canonical transformation is a transformation in phase space which leaves invariant the Poisson brackets

$$\{x_i, p_j\} = \delta_{ij}, \quad \{x_i, x_j\} = \{p_i, p_j\} = 0, \qquad i,j = 1, \cdots N. \tag{2.1}$$

To understand the nature of the group that these transformations form, we introduce the notation z_α, $\alpha = 1, 2, \cdots, 2N$, for a vector in phase space defined by

$$z_i \equiv x_i, \quad z_{i+N} \equiv p_i, \quad i = 1, \cdots N. \tag{2.2}$$

The Poisson bracket of two observables f, g is then

$$\{f, g\} = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x_i} \right) = \sum_{\alpha,\beta=1}^{2N} \frac{\partial f}{\partial z_\alpha} K_{\alpha\beta} \frac{\partial g}{\partial z_\beta}, \tag{2.3}$$

where the matrix

$$\mathsf{K} = \|K_{\alpha\beta}\| = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{2.4}$$

has all its submatrices of dimension $N \times N$.

If we now pass from the vector $\{z_\alpha\}$ in phase space to a new one $\{\bar{z}_\alpha\}$ whose components are functions of the previous one, the transformation will be canonical if

$$\sum_{\gamma,\delta} \frac{\partial \bar{z}_\alpha}{\partial z_\gamma} K_{\gamma\delta} \frac{\partial \bar{z}_\beta}{\partial z_\delta} = K_{\alpha\beta}. \tag{2.5}$$

If, in particular, the transformation between the new and the old vectors in phase space is linear, i.e.,

$$\bar{z}_\alpha = \sum_\beta S_{\alpha\beta} z_\beta, \tag{2.6}$$

the transformation will be canonical if

$$\mathsf{S}\mathsf{K}\tilde{\mathsf{S}} = \mathsf{K}, \tag{2.7}$$

where $\mathsf{S} = \|S_{\alpha\beta}\|$ and the tilde stands for transposed. The matrix S will be assumed real so that $\bar{x}_i$ and $\bar{p}_i$ remain Hermitian when x_i and p_i are represented by Hermitian operators.

The matrix K is the one usually associated with the symplectic group.[3,7] Thus the matrices S satisfying (2.7) are elements of a $2N$-dimensional real symplectic group. We shall write these matrices in the form

$$\mathsf{S} = \begin{pmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{C} & \mathsf{D} \end{pmatrix}, \tag{2.8}$$

where the real submatrices are all of dimension $N \times N$ with components

$$\mathsf{A} = \|a_{ij}\|, \quad \mathsf{B} = \|b_{ij}\|, \quad \mathsf{C} = \|c_{ij}\|, \quad \mathsf{D} = \|d_{ij}\|. \tag{2.9}$$

The restriction (2.7) leads then to the equations

$$\mathsf{B}\tilde{\mathsf{A}} = \mathsf{A}\tilde{\mathsf{B}}, \tag{2.10a}$$

$$\mathsf{C}\tilde{\mathsf{D}} = \mathsf{D}\tilde{\mathsf{C}}, \tag{2.10b}$$

$$\mathsf{D}\tilde{\mathsf{A}} - \mathsf{C}\tilde{\mathsf{B}} = \mathsf{I}. \tag{2.10c}$$

We first consider the case when the matrix B is nonsingular. We can then use (2.10c) to determine C by

$$\mathsf{C} = (\mathsf{D}\tilde{\mathsf{A}} - \mathsf{I})\tilde{\mathsf{B}}^{-1}. \tag{2.11a}$$

From this equation and (2.10a) and (2.10b) we see that the restrictions on the remaining submatrices A, B, and D are given by

$$\mathsf{B}\tilde{\mathsf{A}} = \mathsf{A}\tilde{\mathsf{B}}, \tag{2.11b}$$

$$\tilde{\mathsf{B}}\mathsf{D} = \tilde{\mathsf{D}}\mathsf{B}. \tag{2.11c}$$

Equations (2.11) are then the ones that determine the general matrices S of the real symplectic group when

$$\det \mathsf{B} \neq 0. \tag{2.12}$$

When B is singular, we proceed to show that it is always possible to find a nonsingular diagonal matrix B′ such that

$$\begin{pmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{C} & \mathsf{D} \end{pmatrix} = \begin{pmatrix} \mathsf{I} & \mathsf{B}' \\ 0 & \mathsf{I} \end{pmatrix} \begin{pmatrix} \mathsf{A} - \mathsf{B}'\mathsf{C} & \mathsf{B} - \mathsf{B}'\mathsf{D} \\ \mathsf{C} & \mathsf{D} \end{pmatrix} \tag{2.13}$$

and

$$\det (\mathsf{B} - \mathsf{B}'\mathsf{D}) \neq 0. \tag{2.14}$$

To prove (2.14), let us denote the components of B′ by

$$\mathsf{B}' = \|b_i'\delta_{ij}\|, \quad b_i' \neq 0. \tag{2.15}$$

If, for all choices of the b_i', the matrix

$$\mathsf{B} - \mathsf{B}'\mathsf{D} \tag{2.16}$$

is singular, then it is possible to find a set of real γ_k, not all zero, such that

$$\gamma_k(b_{ik} - b_i'd_{ik}) = 0, \tag{2.17}$$

where in what follows all repeated Latin indices are summed from 1 to N. As this relation must be valid for any nonzero value of b_i', we can conclude that it implies the existence of a set γ_k, not all zero, for which

$$\gamma_k b_{ik} = \gamma_k d_{ik} = 0. \tag{2.18}$$

But this indicates that a linear combination of columns in the right-hand side of (2.8) gives zero, which implies that in this case S is singular. We have though from (2.7) that

$$(\det \mathsf{S})^2 = 1, \tag{2.19}$$

and thus we are led to a contradiction. We conclude, therefore, that it is possible to find a diagonal nonsingular matrix B′ for which (2.14) holds when B itself is singular.

In the particular case when S is a point transformation, i.e.,

$$\mathsf{S} = \begin{pmatrix} \mathsf{A} & 0 \\ 0 & \tilde{\mathsf{A}}^{-1} \end{pmatrix} = \begin{pmatrix} \mathsf{I} & \mathsf{I} \\ 0 & \mathsf{I} \end{pmatrix} \begin{pmatrix} \mathsf{A} & -\tilde{\mathsf{A}}^{-1} \\ 0 & \tilde{\mathsf{A}}^{-1} \end{pmatrix}, \tag{2.20}$$

we can express it in the form (2.13)–(2.14) with B = I.

As the matrix

$$\begin{pmatrix} \mathsf{I} & \mathsf{B}' \\ 0 & \mathsf{I} \end{pmatrix} \tag{2.21}$$

satisfies the conditions (2.11), we have decomposed the matrix S of (2.8) when B is singular, into the product of two matrices belonging to the symplectic group for both of which the submatrix in the upper right corner is nonsingular. We later show that we can obtain in an elementary fashion the unitary representation of the matrix S when B is nonsingular. Thus the development (2.13) allows us to obtain the unitary representation of the matrix S when B is singular, as a product of two unitary representations of matrices for which the submatrix in the upper right corner is nonsingular.

3. THE UNITARY REPRESENTATION OF LINEAR CANONICAL TRANSFORMATIONS

We wish to find in the quantum mechanical picture the unitary representation of the linear canonical transformations discussed in the previous section. We denote the states in which the coordinates x_i are diagonal by the bras and kets $\langle \mathbf{x}' |$ and $|\mathbf{x}''\rangle$, where whenever something is characterized by the eigenvalues of *all* the coordinates x_i, $i = 1, \cdots, N$, we suppress the index i. The matrix elements of the operators x_i and p_i with respect to this basis are then[4]

$$\langle \mathbf{x}' | x_i | \mathbf{x}'' \rangle = x_i'\delta(\mathbf{x}' - \mathbf{x}''), \tag{3.1a}$$

$$\langle \mathbf{x}' | p_i | \mathbf{x}'' \rangle = -\frac{1}{i}\frac{\partial}{\partial x_i''}\delta(\mathbf{x}' - \mathbf{x}''), \tag{3.1b}$$

where $\hbar$ is taken as 1 and

$$\delta(\mathbf{x}' - \mathbf{x}'') = \prod_{i=1}^{N} \delta(x_i' - x_i''). \tag{3.1c}$$

If we now pass to another set of coordinates and momenta,

$$\bar{x}_i = a_{ij}x_j + b_{ij}p_j, \tag{3.2a}$$

$$\bar{p}_i = c_{ij}x_j + d_{ij}p_j, \tag{3.2b}$$

which are canonical, i.e., for which the matrices A, B, C, and D satisfy the relations (2.10), then it is clear[4] that the matrix elements of $\bar{x}_i$ and $\bar{p}_i$ between

the bras and kets $(\bar{\mathbf{x}}'|$ and $|\bar{\mathbf{x}}'')$ will have the same form as (3.1). We use a round bracket notation for states in which $\bar{x}_i$ is diagonal to distinguish them from the states in which x_i is diagonal, in case we take the same numerical value for the eigenvalues of $\bar{x}_i$ and x_i.

Clearly we could make the development

$$|\bar{\mathbf{x}}') = \int |\mathbf{x}')\, d\mathbf{x}'\, \langle \mathbf{x}' \,|\, \bar{\mathbf{x}}'), \tag{3.3}$$

where $d\mathbf{x}' = dx_1' \cdots dx_N'$ and we have an N-dimensional integration. The transformation bracket in (3.3) satisfies the equations[4]

$$\left(a_{ij}x_j' - ib_{ij}\frac{\partial}{\partial x_j'}\right)\langle \mathbf{x}' \,|\, \bar{\mathbf{x}}') = \bar{x}_i' \langle \mathbf{x}' \,|\, \bar{\mathbf{x}}'), \qquad i = 1, \cdots, N. \tag{3.4}$$

It is important to notice that Eqs. (3.4) do not completely determine the transformation bracket $\langle \mathbf{x}' \,|\, \bar{\mathbf{x}}')$. In particular, if we multiply $\langle \mathbf{x}' \,|\, \bar{\mathbf{x}}')$ by an arbitrary function of $\bar{\mathbf{x}}'$, it continues to satisfy Eqs. (3.4). We could, though, fully determine the transformation bracket $\langle \mathbf{x}' \,|\, \bar{\mathbf{x}}')$ up to a constant phase by the further requirements that the matrix elements of $\bar{x}_i$ and $\bar{p}_i$ with respect to the states $(\mathbf{x}'|$ and $|\bar{\mathbf{x}}'')$ have the form (3.1), i.e., that the transformation be canonical, which implies[4]

$$(\bar{\mathbf{x}}'|\, \bar{x}_i\, |\bar{\mathbf{x}}'') = \int (\bar{\mathbf{x}}' \,|\, \mathbf{x}')\left(a_{ij}x_j' - ib_{ij}\frac{\partial}{\partial x_j'}\right)\langle \mathbf{x}' \,|\, \bar{\mathbf{x}}'')\, d\mathbf{x}' = \bar{x}_i' \delta(\bar{\mathbf{x}}' - \bar{\mathbf{x}}''), \tag{3.5a}$$

$$(\bar{\mathbf{x}}'|\, \bar{p}_i\, |\bar{\mathbf{x}}'') = \int (\bar{\mathbf{x}}' \,|\, \mathbf{x}')\left(c_{ij}x_j' - id_{ij}\frac{\partial}{\partial x_j'}\right)\langle \mathbf{x}' \,|\, \bar{\mathbf{x}}'')\, d\mathbf{x}' = -\frac{1}{i}\frac{\partial}{\partial \bar{x}_i''}\delta(\bar{\mathbf{x}}' - \bar{\mathbf{x}}''), \tag{3.5b}$$

where[4]

$$(\bar{\mathbf{x}}' \,|\, \mathbf{x}') = \langle \mathbf{x}' \,|\, \bar{\mathbf{x}}')^*. \tag{3.5c}$$

Once we have these transformation brackets, we can easily identify them with the unitary representation of the canonical transformation (3.2). For this purpose, we note, for example, that the matrix elements of $\bar{x}_i$ with respect to the basis in which the x_i are diagonal can be written as

$$\langle \mathbf{x}'|\, \bar{x}_i\, |\mathbf{x}''\rangle = \int \langle \mathbf{x}' \,|\, \bar{\mathbf{x}}')\, d\bar{\mathbf{x}}' (\bar{\mathbf{x}}'|\, \bar{x}_i\, |\bar{\mathbf{x}}'')\, d\bar{\mathbf{x}}'' (\bar{\mathbf{x}}'' \,|\, \mathbf{x}'') = \int \langle \mathbf{x}' \,|\, \bar{\mathbf{x}}')\, d\bar{\mathbf{x}}' \bar{x}_i' \delta(\bar{\mathbf{x}}' - \bar{\mathbf{x}}'')\, d\bar{\mathbf{x}}'' (\bar{\mathbf{x}}'' \,|\, \mathbf{x}''). \tag{3.6}$$

Now $\bar{x}_i'$, $\bar{x}_i''$ are not operators but just variables over which we carry out integrations, and thus, using (3.1a), we can write

$$\bar{x}_i' \delta(\bar{\mathbf{x}}' - \bar{\mathbf{x}}'') = \langle \bar{\mathbf{x}}'|\, x_i\, |\bar{\mathbf{x}}''\rangle, \tag{3.7}$$

where we stress the angular, rather than round, brackets of the matrix elements. To express then (3.6) as a matrix multiplication, we define the matrix elements of a unitary matrix U in a basis in which the x_i are diagonal[4] as

$$\langle \mathbf{x}'|\, U\, |\mathbf{x}''\rangle \equiv \langle \mathbf{x}' \,|\, \mathbf{x}''), \quad \text{which implies} \quad \langle \mathbf{x}'|\, U^{-1}\, |\mathbf{x}''\rangle = (\mathbf{x}' \,|\, \mathbf{x}''\rangle, \tag{3.8}$$

thus getting

$$\langle \mathbf{x}'|\, \bar{x}_i\, |\mathbf{x}''\rangle = \int \langle \mathbf{x}'|\, U\, |\bar{\mathbf{x}}')\, d\bar{\mathbf{x}}'\, \langle \bar{\mathbf{x}}'|\, x_i\, |\bar{\mathbf{x}}'')\, d\bar{\mathbf{x}}''\, \langle \bar{\mathbf{x}}''|\, U^{-1}\, |\mathbf{x}''\rangle. \tag{3.9}$$

In operator language we have then[4]

$$\bar{x}_i = Ux_iU^{-1}, \tag{3.10}$$

and it is clear that an entirely similar analysis gives us

$$\bar{p}_i = Up_iU^{-1}. \tag{3.11}$$

If we carry out in succession two canonical transformations that give rise to the unitary representations U and V, the new coordinates and momenta in the quantum mechanical picture are affected by the transformation VU. Thus we have the quantum mechanical equivalent[4] of the classical canonical transformations and therefore also a unitary representation of the general symplectic group of which they form a part.

We now proceed to determine $\langle \mathbf{x}'|\, U\, |\mathbf{x}''\rangle$ explicitly when, in the canonical transformation (2.6), the matrix S is given by (2.8), where the submatrix B is nonsingular. We shall use the notation

$$\langle \mathbf{x}' \,|\, \mathbf{x}'') = \langle \mathbf{x}'|\, U\, |\mathbf{x}''\rangle \equiv \phi(\mathbf{x}', \mathbf{x}''), \tag{3.12}$$

and proceed to show that ϕ must have the form

$$\phi(\mathbf{x}', \mathbf{x}'') = \alpha \exp\left[i(\lambda_{ij}x_i'x_j' + \mu_{ij}x_i'x_j'' + \nu_{ij}x_i''x_j'')\right], \tag{3.13}$$

where α is a constant, the $N \times N$ matrices

$$\mathfrak{L} = \|\lambda_{ij}\|, \quad \mathfrak{M} = \|\mu_{ij}\|, \quad \mathfrak{N} = \|\nu_{ij}\| \tag{3.14}$$

are real, and $\mathfrak{L}$ and $\mathfrak{N}$ are symmetric. These parameters can be determined as follows: First, as $\langle \mathbf{x}' \,|\, \bar{\mathbf{x}}')$ satisfies Eqs. (3.4), we obtain that

$$\left(a_{ij}x_j' - ib_{ij}\frac{\partial}{\partial x_j'}\right)\phi(\mathbf{x}', \mathbf{x}'') = x_i''\phi(\mathbf{x}', \mathbf{x}''), \tag{3.15}$$

which implies that

$$\left[a_{ij}x_j' + b_{ij}(2\lambda_{jk}x_k' + \mu_{jk}x_k'')\right]\phi(\mathbf{x}', \mathbf{x}'') = x_i''\phi(\mathbf{x}', \mathbf{x}''), \tag{3.16a}$$

which in matrix notation takes the form

$$\mathsf{A}\mathbf{x}' + 2\mathsf{B}\mathfrak{L}\mathbf{x}' + \mathsf{B}\mathcal{M}\mathbf{x}'' = \mathbf{x}''. \tag{3.16b}$$

As $\mathbf{x}'$ and $\mathbf{x}''$ are arbitrary independent vector and B is nonsingular, this implies that

$$\mathfrak{L} = -\tfrac{1}{2}\mathsf{B}^{-1}\mathsf{A}, \quad \mathcal{M} = \mathsf{B}^{-1}. \tag{3.17}$$

The matrix $\mathfrak{L}$ is symmetric, as it should be, as a consequence of (2.11b). Passing now to Eq. (3.5a), we see from (3.16a), using the notation (3.12), that it implies

$$\int \phi^*(\mathbf{x}', \bar{\mathbf{x}}')\phi(\mathbf{x}', \bar{\mathbf{x}}'')\, d\mathbf{x}' = \delta(\bar{\mathbf{x}}' - \bar{\mathbf{x}}''). \tag{3.18}$$

Thus we must have the restriction

$$\begin{aligned} &|\alpha|^2 \exp\left[i\nu_{ij}(-\bar{x}_i'\bar{x}_j' + \bar{x}_i''\bar{x}_j'')\right] \\ &\qquad \times \int \exp\left\{-ix_i'[\mu_{ij}(\bar{x}_j' - \bar{x}_j'')]\right\} d\mathbf{x}' \\ &= |\alpha|^2 \exp\left\{i\nu_{ij}(-\bar{x}_i'\bar{x}_j' + \bar{x}_i''\bar{x}_j'')\right\}(2\pi)^N \\ &\qquad \times \prod_{i=1}^{N} \delta[\mu_{ij}(\bar{x}_j'' - \bar{x}_j')] \\ &= |\alpha|^2 (2\pi)^N |\det \mathsf{B}|\, \delta(\bar{\mathbf{x}}'' - \bar{\mathbf{x}}'). \end{aligned} \tag{3.19}$$

In (3.19) we made use of the fact that if

$$y_i'' = \mu_{ij}\bar{x}_j'' \tag{3.20a}$$

or

$$\bar{x}_i'' = b_{ij}y_j'', \tag{3.20b}$$

and similarly for $\bar{x}_i'$, then

$$\prod_{i=1}^{N} \delta(y_i'' - y_i') = |J| \prod_{i=1}^{N} \delta(\bar{x}_i'' - \bar{x}_i'), \tag{3.21}$$

where J is the Jacobian of the transformation (3.20b), i.e.,

$$J = \left|\frac{\partial \bar{x}_i''}{\partial y_j''}\right| = \det \mathsf{B}. \tag{3.22}$$

Thus the restriction that $\bar{x}_i$ must have its canonical form (3.5a) leads, up to a phase, to the value

$$\alpha = [(2\pi)^N |\det \mathsf{B}|]^{-\frac{1}{2}}. \tag{3.23}$$

The next step is to make use of Eq. (3.5b), which leads to

$$\begin{aligned} &\int \phi^*(\mathbf{x}', \bar{\mathbf{x}}')\left[\left(c_{ij}x_j' - id_{ij}\frac{\partial}{\partial x_j'}\right)\phi(\mathbf{x}', \bar{\mathbf{x}}'')\right] d\mathbf{x}' \\ &= \int \phi^*(\mathbf{x}', \bar{\mathbf{x}}')[c_{ij}x_j' + d_{ij}(2\lambda_{jk}x_k' + \mu_{jk}\bar{x}_k'')]\phi(\mathbf{x}', \bar{\mathbf{x}}'')\, d\mathbf{x}' \\ &= -\frac{1}{i}\frac{\partial}{\partial \bar{x}_i''}\delta(\bar{\mathbf{x}}' - \bar{\mathbf{x}}''). \end{aligned} \tag{3.24a}$$

But, making use of (3.18), we see that

$$\begin{aligned} &-\frac{1}{i}\frac{\partial}{\partial \bar{x}_i''}\delta(\bar{\mathbf{x}}' - \bar{\mathbf{x}}'') \\ &= \int \phi^*(\mathbf{x}', \bar{\mathbf{x}}')[-\mu_{ji}x_j' - 2\nu_{ji}\bar{x}_j'']\phi(\mathbf{x}', \bar{\mathbf{x}}'')\, d\mathbf{x}'. \end{aligned} \tag{3.24b}$$

From Eqs. (3.24) we obtain the following relation in matrix notation,

$$(\mathsf{C} + 2\mathsf{D}\mathfrak{L})\mathbf{x}' + \mathsf{D}\mathcal{M}\bar{\mathbf{x}}'' = -\tilde{\mathcal{M}}\mathbf{x}' - 2\tilde{\mathcal{N}}\bar{\mathbf{x}}'', \tag{3.25}$$

and, as $\mathbf{x}'$ and $\bar{\mathbf{x}}''$ are arbitrary independent vectors, we obtain

$$\mathsf{C} = -2\mathsf{D}\mathfrak{L} - \tilde{\mathcal{M}} = \mathsf{D}\mathsf{B}^{-1}\mathsf{A} - \tilde{\mathsf{B}}^{-1} = (\tilde{\mathsf{D}}\mathsf{A} - I)\tilde{\mathsf{B}}^{-1}, \tag{3.26a}$$

$$\mathcal{N} = -\tfrac{1}{2}\tilde{\mathcal{M}}\tilde{\mathsf{D}} = -\tfrac{1}{2}\tilde{\mathsf{B}}^{-1}\tilde{\mathsf{D}} = -\tfrac{1}{2}\mathsf{D}\mathsf{B}^{-1}. \tag{3.26b}$$

Equation (3.26a) is automatically satisfied in view of the relation (2.11a), while (3.26b) gives us the explicit form of the matrix $\mathcal{N}$, which from (2.11c) is symmetric as it should be. Thus, finally, up to a constant phase factor, we can write (in matrix and vector notation) the unitary representation of the linear canonical transformation (2.6) as

$$\begin{aligned} &\langle \mathbf{x}'|\, U\, |\mathbf{x}''\rangle \\ &\quad = [(2\pi)^N |\det \mathsf{B}|]^{-\frac{1}{2}} \\ &\qquad \times \exp\left[-\tfrac{1}{2}i(\tilde{\mathbf{x}}'\mathsf{B}^{-1}\mathsf{A}\mathbf{x}' - 2\tilde{\mathbf{x}}'\mathsf{B}^{-1}\mathbf{x}'' + \tilde{\mathbf{x}}''\mathsf{D}\mathsf{B}^{-1}\mathbf{x}'')\right], \end{aligned} \tag{3.27}$$

where $\tilde{\mathbf{x}}'$ and $\tilde{\mathbf{x}}''$ are the transposed vectors $\mathbf{x}'$ and $\mathbf{x}''$. We recall though that this holds only in the case when B is nonsingular, and thus B^{-1} exists.

When B is singular, we can consider the development (2.13). To obtain the unitary representation in this case, we need to calculate the product of two unitary representations of the form (3.27). We proceed first to discuss the unitary representation of the product of two arbitrary canonical transformations

$$\begin{aligned} \begin{pmatrix} \mathsf{A}_2 & \mathsf{B}_2 \\ \mathsf{C}_2 & \mathsf{D}_2 \end{pmatrix}\begin{pmatrix} \mathsf{A}_1 & \mathsf{B}_1 \\ \mathsf{C}_1 & \mathsf{D}_1 \end{pmatrix} &= \begin{pmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{C} & \mathsf{D} \end{pmatrix} \\ &= \begin{pmatrix} \mathsf{A}_2\mathsf{A}_1 + \mathsf{B}_2\mathsf{C}_1 & \mathsf{A}_2\mathsf{B}_1 + \mathsf{B}_2\mathsf{D}_1 \\ \mathsf{C}_2\mathsf{A}_1 + \mathsf{D}_2\mathsf{C}_1 & \mathsf{C}_2\mathsf{B}_1 + \mathsf{D}_2\mathsf{D}_1 \end{pmatrix}, \end{aligned} \tag{3.28}$$

where we assume B_1 and B_2 nonsingular. We shall denote the unitary representations of the matrices in (3.28) by U_2, U_1, and U, respectively. The unitary

representation of the product of canonical transformations is then

$$\begin{aligned}&\langle \mathbf{x}'|\, U_1U_2\,|\mathbf{x}''\rangle\\&=\int\langle \mathbf{x}'|\, U_1\,|\mathbf{x}'''\rangle\, d\mathbf{x}'''\langle \mathbf{x}'''|\, U_2\,|\mathbf{x}''\rangle\\&=(2\pi)^{-N}(|\det \mathsf{B}_1|\cdot|\det \mathsf{B}_2|)^{-\frac{1}{2}}\\&\quad\times\exp\left[-\tfrac{1}{2}i(\tilde{\mathbf{x}}'\mathsf{B}_1^{-1}\mathsf{A}_1\mathbf{x}'+\tilde{\mathbf{x}}''\mathsf{D}_2\mathsf{B}_2^{-1}\mathbf{x}'')\right]\\&\quad\times\int d\mathbf{x}'''\exp\{-\tfrac{1}{2}i[\tilde{\mathbf{x}}'''(\mathsf{D}_1\mathsf{B}_1^{-1}+\mathsf{B}_2^{-1}\mathsf{A}_2)\mathbf{x}'''\\&\quad-2\tilde{\mathbf{x}}'''(\tilde{\mathsf{B}}_1^{-1}\mathbf{x}'+\mathsf{B}_2^{-1}\mathbf{x}'')]\}.\end{aligned}\tag{3.29}$$

From (2.11b) and (2.11c) we see that the real matrix $\mathsf{D}_1\mathsf{B}_1^{-1}+\mathsf{B}_2^{-1}\mathsf{A}_2$ is symmetric, and thus there exists an orthogonal transformation

$$\mathbf{x}'''=\mathcal{O}\mathbf{y}\tag{3.30}$$

that diagonalizes this matrix, i.e.,

$$\tilde{\mathcal{O}}(\mathsf{D}_1\mathsf{B}_1^{-1}+\mathsf{B}_2^{-1}\mathsf{A}_2)\mathcal{O}=\Delta=\|\delta_i\delta_{ij}\|.\tag{3.31}$$

We note furthermore that

$$\mathsf{D}_1\mathsf{B}_1^{-1}+\mathsf{B}_2^{-1}\mathsf{A}_2=\mathsf{B}_2^{-1}\mathsf{B}\mathsf{B}_1^{-1},\tag{3.32}$$

and thus the number of zeros among the real eigenvalues δ_i will be equal to the dimension minus the rank of the matrix B which we shall denote by p. We can always select the matrix $\mathcal{O}$ in such a way that the first p eigenvalues $\delta_1,\cdots,\delta_p$ are the ones that vanish. If we then denote by z the vector

$$\mathbf{z}\equiv\tilde{\mathcal{O}}(\tilde{\mathsf{B}}_1^{-1}\mathbf{x}'+\mathsf{B}_2^{-1}\mathbf{x}''),\tag{3.33}$$

the integral in (3.29) takes the form

$$\begin{aligned}&\int\cdots\int dy_1\cdots dy_N\exp\left(-\frac{i}{2}\sum_{i=p+1}^{N}\delta_i y_i^2\right)\exp\left(i\sum_{i=1}^{N}y_iz_i\right)\\&\quad=(2\pi)^N\prod_{i=1}^{p}\delta(z_i)\prod_{j=p+1}^{N}|\delta_j|^{-1}\\&\qquad\times\exp(-\tfrac{1}{4}i\pi\operatorname{sgn}\delta_j)\exp\left(\frac{i}{2}\frac{z_j^2}{\delta_j}\right),\end{aligned}\tag{3.34}$$

where we used the notation

$$\delta_i=(\operatorname{sgn}\delta_i)\,|\delta_i|.\tag{3.35}$$

Introducing then (3.34) into (3.29), we obtain explicitly the unitary representation of the product of two canonical transformations. In particular, if we want the unitary representation of a canonical transformation where B is singular, we just have to consider the product (2.13), i.e.,

$$\begin{aligned}&\mathsf{A}_2=\mathsf{D}_2=\mathsf{I},\quad \mathsf{B}_2=\mathsf{B}',\quad \mathsf{C}_2=0,\quad \mathsf{A}_1=\mathsf{A}-\mathsf{B}'\mathsf{C},\\&\mathsf{B}_1=\mathsf{B}-\mathsf{B}'\mathsf{D},\quad \mathsf{C}_1=\mathsf{C},\quad \mathsf{D}_1=\mathsf{D}.\end{aligned}\tag{3.36}$$

We note from (3.34) that the unitary representation will contain a product of as many δ functions as the nullity (i.e., dimension minus rank) of the matrix B. In particular, if we are dealing with a point transformation in which from (2.20) we have

$$\mathsf{B}'=\mathsf{I},\quad \mathsf{D}=\tilde{\mathsf{A}}^{-1},\quad \mathsf{B}=\mathsf{C}=0,\tag{3.37}$$

then we obtain

$$\langle \mathbf{x}'|\, U_1U_2\,|\mathbf{x}''\rangle=|\det \mathsf{A}|^{\frac{1}{2}}\,\delta(\mathsf{A}\mathbf{x}'-\mathbf{x}'').\tag{3.38}$$

This last result is to be expected, as for a unimodular A (i.e., $\det \mathsf{A}=1$) we see that the unitary representation transforms an arbitrary wavefunction $\psi(\mathbf{x}')$ into

$$\int\psi(\mathbf{x}')\,d\mathbf{x}'\,\langle \mathbf{x}'|\, U\,|\mathbf{x}''\rangle=\psi(\mathsf{A}^{-1}\mathbf{x}'').\tag{3.39}$$

We now return to the product of two canonical transformations (3.28) but assume that B is nonsingular. We note then that the integral (3.34) takes the form

$$\begin{aligned}&(2\pi)^N\left(\prod_{i=1}^{N}|\delta_i|^{-1}\right)\\&\quad\times\exp\left(-\tfrac{1}{4}i\pi\sum_i\operatorname{sgn}\delta_i\right)\exp\left(\tfrac{1}{2}i\sum_i(z_i^2/\delta_i)\right).\end{aligned}\tag{3.40}$$

But from (3.33) we obtain

$$\begin{aligned}&\sum_{i=1}^{N}\frac{z_i^2}{\delta_i}\\&\quad=\sum_{i=1}^{N}[(\tilde{\mathbf{x}}'\mathsf{B}_1^{-1}+\tilde{\mathbf{x}}''\tilde{\mathsf{B}}_2^{-1})\mathcal{O}]_i\frac{1}{\delta_i}[\tilde{\mathcal{O}}(\tilde{\mathsf{B}}_1^{-1}\mathbf{x}'+\mathsf{B}_2^{-1}\mathbf{x}'')]_i\\&\quad=(\tilde{\mathbf{x}}'\mathsf{B}_1^{-1}+\tilde{\mathbf{x}}''\tilde{\mathsf{B}}_2^{-1})\mathcal{O}\Delta^{-1}\tilde{\mathcal{O}}(\tilde{\mathsf{B}}_1^{-1}\mathbf{x}'+\mathsf{B}_2^{-1}\mathbf{x}'')\\&\quad=(\tilde{\mathbf{x}}'\mathsf{B}_1^{-1}+\tilde{\mathbf{x}}''\tilde{\mathsf{B}}_2^{-1})\mathsf{B}_1\mathsf{B}^{-1}\mathsf{B}_2(\tilde{\mathsf{B}}_1^{-1}\mathbf{x}'+\mathsf{B}_2^{-1}\mathbf{x}''),\end{aligned}\tag{3.41}$$

so that the unitary representation of the product of two canonical transformations for which B_1 and B_2 are nonsingular becomes in this case

$$\begin{aligned}&\langle \mathbf{x}'|\, U_1U_2\,|\mathbf{x}''\rangle\\&\quad=\exp\left(-\tfrac{1}{4}i\pi\sum_i\operatorname{sgn}\delta_i\right)\\&\qquad\times[(2\pi)^N|\det \mathsf{B}_1|\cdot|\det \mathsf{B}_2|\cdot|\det\Delta|]^{-\frac{1}{2}}\\&\qquad\times\exp\{-\tfrac{1}{2}i[\tilde{\mathbf{x}}'\mathsf{B}_1^{-1}\mathsf{A}_1\mathbf{x}'+\tilde{\mathbf{x}}''\mathsf{D}_2\mathsf{B}_2^{-1}\mathbf{x}''\\&\qquad-(\tilde{\mathbf{x}}'\mathsf{B}_1^{-1}+\tilde{\mathbf{x}}''\tilde{\mathsf{B}}_2^{-1})\mathsf{B}_1\mathsf{B}^{-1}\mathsf{B}_2(\tilde{\mathsf{B}}_1^{-1}\mathbf{x}'+\mathsf{B}_2^{-1}\mathbf{x}'')]\}.\end{aligned}\tag{3.42}$$

Making use of some of the relations between the submatrices A, B, C, and D discussed in Sec. 2, as well as of the definition (3.28), we finally obtain

$$\langle \mathbf{x}'|\, U_1U_2\,|\mathbf{x}''\rangle=\exp\left(-\tfrac{1}{4}i\pi\sum_i\operatorname{sgn}\delta_i\right)\langle \mathbf{x}'|\, U\,|\mathbf{x}''\rangle.\tag{3.43}$$

The matrix elements of U_1, U_2, and U, in a representation in which the coordinates are diagonal, are given by (3.27) when we substitute in it the corresponding canonical transformation.

As there is no way of making the phase factor disappear in (3.43) by multiplying the unitary representation (3.27) by an appropriate constant phase factor, this representation then constitutes a ray representation[8] of the $2N$-dimensional symplectic group. We have even explicitly obtained in (3.43) the phase of this ray representation in the case when the submatrices B of all the symplectic matrices (2.8) are nonsingular.

4. LINEAR CANONICAL TRANSFORMATIONS AND THE DYNAMICAL GROUP OF THE OSCILLATOR

The set of real $2N$-dimensional matrices (2.8) that satisfy the conditions (2.10) constitute the symplectic group $Sp(2N)$. A subgroup of $Sp(2N)$ is formed by the matrices (2.8) that are also orthogonal, which besides (2.10) satisfy

$$\begin{pmatrix} \tilde{\mathsf{A}} & \tilde{\mathsf{C}} \\ \tilde{\mathsf{B}} & \tilde{\mathsf{D}} \end{pmatrix}\begin{pmatrix} \mathsf{A} & \mathsf{B} \\ \mathsf{C} & \mathsf{D} \end{pmatrix} = \begin{pmatrix} \tilde{\mathsf{A}}\mathsf{A} + \tilde{\mathsf{C}}\mathsf{C} & \tilde{\mathsf{A}}\mathsf{B} + \tilde{\mathsf{C}}\mathsf{D} \\ \tilde{\mathsf{B}}\mathsf{A} + \tilde{\mathsf{D}}\mathsf{C} & \tilde{\mathsf{B}}\mathsf{B} + \tilde{\mathsf{D}}\mathsf{D} \end{pmatrix} = \begin{pmatrix} \mathsf{I} & 0 \\ 0 & \mathsf{I} \end{pmatrix}. \tag{4.1}$$

The relations (2.10) and (4.1) can also be expressed in terms of the complex matrices

$$\mathfrak{U} \equiv \mathsf{A} + i\mathsf{B}, \quad \mathfrak{U}^* \equiv \mathsf{A} - i\mathsf{B}, \quad \mathfrak{V} \equiv \mathsf{D} - i\mathsf{C}, \quad \mathfrak{V}^* \equiv \mathsf{D} + i\mathsf{C}, \tag{4.2}$$

and we showed in another publication[9] that they are satisfied if

$$\mathfrak{V} = \mathfrak{U} \text{ and } \mathfrak{U} \text{ unitary, i.e., } \mathfrak{U}^*\mathfrak{U} = \mathsf{I}. \tag{4.3}$$

Thus the subgroup of orthogonal linear canonical transformations is actually a representation of the N-dimensional unitary group $\mathfrak{U}(N)$ whose elements are

$$\begin{pmatrix} \frac{1}{2}(\mathfrak{U} + \mathfrak{U}^*) & -\frac{1}{2}i(\mathfrak{U} - \mathfrak{U}^*) \\ \frac{1}{2}i(\mathfrak{U} - \mathfrak{U}^*) & \frac{1}{2}(\mathfrak{U} + \mathfrak{U}^*) \end{pmatrix}. \tag{4.4}$$

We can construct the elements of the Lie algebra of $Sp(2N)$ and its subgroup $\mathfrak{U}(N)$ in terms of bilinear expressions in coordinates and momenta.[5] It is more convenient to do this in terms of the creation and annihilation operators defined as usual by

$$\eta_i \equiv 2^{-\frac{1}{2}}(x_i - ip_i), \quad \xi_i \equiv 2^{-\frac{1}{2}}(x_i + ip_i), \quad i = 1, \cdots, N, \tag{4.5}$$

whose commutation relations are

$$[\eta_i, \eta_j] = [\xi_i, \xi_j] = 0, \quad [\xi_i, \eta_j] = \delta_{ij}. \tag{4.6}$$

We consider the $N(2N + 1)$ bilinear operators

$$H_i = \tfrac{1}{2}(\eta_i\xi_i + \xi_i\eta_i) \equiv \mathcal{C}_{ii} + \tfrac{1}{2}, \quad i = 1, \cdots, N, \tag{4.7a}$$

$$\eta_i\xi_j \equiv \mathcal{C}_{ij}, \quad i \neq j, \quad i,j = 1, \cdots, N, \tag{4.7b}$$

$$\eta_i\eta_j, \quad i \leq j = 1, \cdots, N, \tag{4.7c}$$

$$\xi_i\xi_j, \quad i \leq j = 1, \cdots, N. \tag{4.7d}$$

From (4.6), these operators close under commutation, and, if we obtain their root vectors with respect to the set of commuting operators H_i, we find that they are the generators[5] of the group $Sp(2N)$. The set of operators $\mathcal{C}_{ij}$, $i,j = 1, \cdots, N$, of (4.7a) and (4.7b) also close under commutation, and their root vectors indicate that they are the generators of the $\mathfrak{U}(N)$ group. A subset of this last set given by

$$\mathcal{C}_{ij} - \mathcal{C}_{ji} = i(x_ip_j - x_jp_i) = x_i\frac{\partial}{\partial x_j} - x_j\frac{\partial}{\partial x_i} \tag{4.8}$$

clearly[10] gives the generators of the $\mathcal{O}(N)$ subgroup of $\mathfrak{U}(N)$.

We note that the H_i of (4.7a) are just

$$H_i = \tfrac{1}{2}(\eta_i\xi_i + \xi_i\eta_i) = \tfrac{1}{2}(p_i^2 + x_i^2), \tag{4.9}$$

and the Hamiltonian of the N-dimensional harmonic oscillator is given by

$$H = \sum_{i=1}^{N} H_i = \tfrac{1}{2}\sum_{i=1}^{N}(p_i^2 + x_i^2). \tag{4.10}$$

Thus the group $Sp(2N)$, whose generators are the operators (4.7), is the dynamical group of the N-dimensional oscillator. The group $\mathfrak{U}(N)$, whose generators are the $\mathcal{C}_{ij}$ of (4.7a) and (4.7b), is the symmetry group of the harmonic oscillator, as can be seen directly because

$$[\mathcal{C}_{ij}, H] = 0 \tag{4.11}$$

and also from the fact that the orthogonal group of canonical transformations clearly leaves H invariant.

In applications[6] we usually deal with several particles, say n, in an oscillator potential of definite number of dimensions q so that $N = nq$. Denoting by $\mu = 1, \cdots, q$ the component and by $s = 1, \cdots, n$, the particle indices, we can now express the coordinates and momenta as well as the creation and annihilation operators in the following notation:

$$\mathbf{x}_s = \{x_{\mu s}\}, \quad \mathbf{p}_s = \{p_{\mu s}\}, \quad \boldsymbol{\eta}_s = \{\eta_{\mu s}\}, \quad \boldsymbol{\xi}_s = \{\xi_{\mu s}\}. \tag{4.12}$$

Clearly we can in (4.7) substitute i by μs and contract with respect to the component index μ, thus getting

the operators

$$\mathcal{K}_s = \tfrac{1}{2}(\eta_s \cdot \xi_s + \xi_s \cdot \eta_s), \quad s = 1, \cdots, n, \tag{4.13a}$$

$$\eta_s \cdot \xi_t, \quad s \neq t, \quad s, t = 1, \cdots, n, \tag{4.13b}$$

$$\eta_s \cdot \eta_t, \quad s \leq t = 1, \cdots, n, \tag{4.13c}$$

$$\xi_s \cdot \xi_t, \quad s \leq t = 1, \cdots, n. \tag{4.13d}$$

From (4.6) these operators close under commutation and have the same type of root vectors with respect to the set of commuting operators $\mathcal{K}_s$ as we had previously for the operators (4.7) with respect to H_i. Thus the operators (4.13) are the generators of a group $Sp(2n)$ which is a subgroup of $Sp(2N) = Sp(2nq)$.

We can also contract the operators (4.7) with respect to index s, obtaining, for example,

$$\mathcal{C}_{\mu\nu} \equiv \sum_{s=1}^{n} \eta_{\mu s}\xi_{\nu s}, \tag{4.14}$$

which by a similar reasoning as above will be the generators of a group $\mathfrak{U}(q)$. The antisymmetrized part of these generators, i.e.,

$$\Lambda_{\mu\nu} \equiv \mathcal{C}_{\mu\nu} - \mathcal{C}_{\nu\mu} \quad \mu, \nu = 1, \cdots, q, \tag{4.15}$$

constitute as before the generators of an orthogonal group $\mathcal{O}(q)$. It is clear that the $\Lambda_{\mu\nu}$ and the generators of $Sp(2n)$ commute, as the latter are by construction invariant under rotations in the q-dimensional space. Thus, for the problem of n particles in a q-dimensional harmonic oscillator potential, we have the following chain of groups:

$$Sp(2nq) \supset Sp(2n) \times \mathcal{O}(q). \tag{4.16}$$

It is interesting to see in which way the subgroups $\mathcal{O}(q)$ and $Sp(2n)$ act on the coordinates $x_{\mu s}$ and momenta $p_{\mu s}$. Clearly for $\mathcal{O}(q)$ we have the orthogonal transformation $\|\mathcal{O}_{\mu\nu}\|$,

$$\bar{x}_{\mu s} = \sum_{\nu} \mathcal{O}_{\mu\nu} x_{\nu s}, \quad \bar{p}_{\mu s} = \sum_{\nu} \mathcal{O}_{\mu\nu} p_{\nu s}, \tag{4.17}$$

while for $Sp(2n)$ we obtain

$$\bar{x}_{\mu s} = \sum_{t=1}^{n} a_{st} x_{\mu t} + \sum_{t=1}^{n} b_{st} p_{\mu t},$$

$$\bar{p}_{\mu s} = \sum_{t=1}^{n} c_{st} x_{\mu t} + \sum_{t=1}^{n} d_{st} p_{\mu t}, \tag{4.18}$$

with the $2n$-dimensional matrix of the type (2.8) satisfying again the restrictions (2.10).

The set of all states of an N-dimensional harmonic oscillator belong to one of two irreducible representations of the group $Sp(2N)$. This can be seen as follows: First all states can be expressed as homogeneous polynomials of degree $r = 0, 1, \cdots$ in the creation operators η_i acting on the ground state $|0\rangle$. Using the generators $\eta_i \xi_j$, $i > j$, repeatedly, we can transform these states into

$$(r!)^{-\frac{1}{2}} \eta_N^r |0\rangle. \tag{4.19}$$

Applying then the generator ξ_N^2, we finally convert them either in

$$|0\rangle \; r \text{ even or } \eta_N |0\rangle \; r \text{ odd}. \tag{4.20}$$

The two IR's are then characterized by the eigenvalues of the N weight generators (4.7a) corresponding to the minimum weight states (4.20), i.e.,

$$[\tfrac{1}{2} \cdots \tfrac{1}{2}] = [(\tfrac{1}{2})^N] \quad \text{or} \quad [\tfrac{1}{2}\tfrac{1}{2} \cdots \tfrac{3}{2}] = [(\tfrac{1}{2})^{N-1}\tfrac{3}{2}]. \tag{4.21}$$

This result continues to hold when we have n particles in a q-dimensional oscillator in which case $N = nq$.

Now the chain of groups (4.16), which characterizes states defined by boson creation operators acting on the ground state, looks very similar to the corresponding problem for fermions[11] of spin $\frac{1}{2}$ in a given shell of angular momentum l. We briefly review the fermion case to establish the parallelism in detail. Assume that we have n different types of fermions (e.g., $n = 2$ if we have both protons and neutrons) in a shell of orbital angular momentum l. We can then define the indices

$$\mu \equiv m\sigma, \quad m = l, \cdots, -l, \quad \sigma = \tfrac{1}{2}, -\tfrac{1}{2}, \quad s = 1, \cdots, n, \tag{4.22}$$

in which μ can take $4l + 2$ values. The fermion creation and annihilation operators can then be denoted respectively by

$$b_{\mu s}^{+}, \quad b^{\mu s}. \tag{4.23}$$

The bilinear operators

$$b_{\mu s}^{+} b^{\mu' s'}, \tag{4.24a}$$

$$b_{\mu s}^{+} b_{\mu' s'}^{+}, \tag{4.24b}$$

$$b^{\mu s} b^{\mu' s'} \tag{4.24c}$$

then constitute the generators of an $\mathcal{O}[2n(4l + 2)]$ group.[11] If we contract with respect to the μ index [keeping in mind a phase factor $(-1)^{l+m+\frac{1}{2}+\sigma}$ for (4.24b) and (4.24c)], we get the generators of an $Sp_u(2n)$ group.[12] The u index here means we are dealing with the compact symplectic group (a subgroup of a unitary rather than of a linear group) since all representations we have for a fermion system are finite dimensional due to the fact that the Pauli principle limits the total number of states[13] to 2^{4l+2}.

Had we, on the other hand, contracted the operators (4.24a) with respect to the s index, we would have obtained the generators of a $(4l+2)$-dimensional unitary group $\mathfrak{U}(4l+2)$, whose compact symplectic subgroup $Sp_u(4l+2)$ has the generators

$$\sum_s [b^+_{m\sigma s} b^{m'\sigma' s} + (-1)^{m+m'+\sigma+\sigma'} b^+_{-m'-\sigma' s} b^{-m-\sigma s}]. \quad (4.25)$$

The generators of $Sp_u(2n)$ and $Sp_u(4l+2)$ clearly commute with each other since the former by construction are invariant under the transformations of the latter. Thus in the fermion case we have the chain of groups

$$\mathcal{O}(2nq) \supset Sp_u(2n) \times Sp_u(q), \quad q = 4l+2. \quad (4.26)$$

If we have just one type of particles, i.e., $n = 1$, the group $Sp_u(2)$ is identical to $SU(2)$ and the group $O(3)$, which is homeomorphic to it, is the usual quasispin group. For two types of particles, e.g., protons and neutrons, $Sp_u(4)$, which is isomorphic to $\mathcal{O}(5)$, is the generalized quasispin discussed by Hecht[14] and others.

In the fermion case all states belong to one of two IR's of $\mathcal{O}^+(2nq)$,

$$[\tfrac{1}{2} \cdots \tfrac{1}{2}\tfrac{1}{2}] \quad \text{or} \quad [\tfrac{1}{2} \cdots \tfrac{1}{2} -\tfrac{1}{2}], \quad (4.27)$$

which parallels the result (4.21) for bosons. The IR's of the subgroups $Sp_u(2n)$ and $Sp_u(q)$ for a given IR (4.27) of $\mathcal{O}^+(2nq)$ are complementary in the sense that they are in one-to-one correspondence as defined in Ref. 13. In particular this correspondence for $n = 1$ gives the relation between quasispin and seniority. In the boson chain (4.16) the IR's of $\mathcal{O}(q)$ are characterized by the partitions

$$[\lambda_1 \lambda_2 \cdots \lambda_{\frac{1}{2}q}] \quad \text{or} \quad [\lambda_1 \lambda_2 \cdots \lambda_{\frac{1}{2}(q-1)}], \quad (4.28)$$

depending on whether q is even or odd. As was shown by Chacón,[15] these partitions also characterize completely the IR's of $Sp(2n)$. Thus the groups $Sp(2n)$ and $\mathcal{O}(q)$ are complementary in the same sense as $Sp_u(2n)$ and $Sp_u(q)$ were complementary in the fermion problem. We note though that in the boson problem $Sp(2n)$ is a noncompact group and so its IR's are infinite dimensional, as we have an infinite number of harmonic oscillator states corresponding to a definite IR of $\mathcal{O}(q)$.

The group $Sp(2n)$ plays then, with respect to the boson operators associated with particles in an harmonic oscillator potential, a role similar to the one the generalized quasispin has with respect to Fermi operators. In the following paper we use this quasispin for bosons[16] in the evaluation of one-particle matrix elements with harmonic oscillator states, in a way that parallels the use of the fermion quasispin by Lawson and MacFarlane[17] for a similar problem. Later we plan to extend this viewpoint to more than one particle.

When dealing with the problem of n particles in a q-dimensional oscillator potential, we are also interested in the unitary representation of the group $Sp(2n)$ of canonical transformations (4.18). Clearly, in the case when $\mathsf{B} = \|b_{st}\|$ is nonsingular, we can immediately generalize the reasoning of Sec. 3, and obtain that the unitary representation in the basis in which the coordinates $\mathbf{x}_s$ are diagonal is, in the vector notation (4.12), given by

$$\langle \mathbf{x}' | U | \mathbf{x}'' \rangle = [(2\pi)^n |\det \mathsf{B}|]^{-\frac{1}{2}} \exp\left(-\tfrac{1}{2} i \sum_{s,t} [\tilde{\mathbf{x}}'_s (\mathsf{B}^{-1}\mathsf{A})_{st} \mathbf{x}'_t - 2\tilde{\mathbf{x}}'_s (\mathsf{B}^{-1})_{st} \mathbf{x}''_t + \tilde{\mathbf{x}}''_s (\mathsf{D}\mathsf{B}^{-1})_{st} \mathbf{x}''_t]\right). \quad (4.29)$$

A particular case is that of a single particle ($n = 1$) in a three-dimensional ($q = 3$) harmonic oscillator. Designating by $\mathbf{r} = (x_1 x_2 x_3)$ the position vector, we have that the unitary representation of $Sp(2)$ in a scheme where the coordinates are diagonal is

$$\langle \mathbf{r}' | U | \mathbf{r}'' \rangle = (2\pi |b|)^{-\frac{3}{2}} \exp[-(i/2b)(ar'^2 - 2\mathbf{r}' \cdot \mathbf{r}'' + dr''^2)]. \quad (4.30)$$

If we want the matrix U in a scheme in which the Hamiltonian H, angular momentum L^2, and projection L_z are diagonal, we can obtain it from (4.30) with the help of the relation

$$\langle n'l'm' | U | n''l''m'' \rangle = \iint \langle n'l'm' | \mathbf{r}' \rangle \, d\mathbf{r}' \langle \mathbf{r}' | U | \mathbf{r}'' \rangle \, d\mathbf{r}'' \langle \mathbf{r}'' | n''l''m'' \rangle, \quad (4.31)$$

where $\langle \mathbf{r} | nlm \rangle$ is the three-dimensional harmonic oscillator wavefunction and $\langle nlm | \mathbf{r} \rangle$ its conjugate. Using the relations[18,19] for Laguerre polynomials,

$$\int_0^\infty x^{\nu+1} e^{-\beta x^2} L_n(\alpha x^2) J_\nu(xy)\, dx = 2^{-\nu-1} \beta^{-\nu-n-1} (\beta - \alpha)^n y^\nu e^{-y^2/4\beta} L_n^\nu\left(\frac{\alpha y^2}{4\beta(\alpha - \beta)}\right), \quad (4.32)$$

$$L_n^{l+\frac{1}{2}}(\mu x^2) = \sum_{m=0}^{n} \frac{[\Gamma(n+l+\frac{3}{2})]^2}{m!\,[\Gamma(n-m+l+\frac{3}{2})]^2} \times \mu^{n-m}(1-\mu)^m L_{n-m}^{l+\frac{1}{2}}(x^2), \quad (4.33)$$

we obtain straightforwardly that the unitary representation (4.31), which is clearly diagonal in l, m and

independent of m, has the explicit form

$$\langle n'lm|\, U\, |n''lm\rangle = i^l[n'!\, n''!\, \Gamma(n'+l+\tfrac{3}{2})\Gamma(n''+l+\tfrac{3}{2})]^{\frac{1}{2}} \times (b+ia)^{-n'-l-\frac{3}{2}}(-b+ia)^{n'}\gamma^{-l-\frac{3}{2}} \times \sum_p \{[p!\,(n'-p)!\,(n''-p)!\,\Gamma(p+l+\tfrac{3}{2})]^{-1} \times [\gamma^2(a^2+b^2)]^{-p}[1-\gamma^{-1}(a^2+b^2)^{-1}]^{n'-p} \times (1-\gamma^{-1})^{n''-p}\}, \quad (4.34)$$

where γ is given by

$$\gamma = \{b(1+a^2+b^2) - i[a-d(a^2+b^2)]\}[2b(a^2+b^2)]^{-1}. \quad (4.35)$$

If we consider an element of $Sp(2)$ that belongs also to the orthogonal subgroup $\mathcal{O}(2)$ of this group, i.e.,

$$a = d = \cos\varphi, \quad b = -c = \sin\varphi, \quad (4.36)$$

we have $a^2+b^2=1$ and $\gamma=1$, and thus the unitary representation (4.34) simplifies drastically, taking the form

$$\langle n'lm|\, U\, |n''lm\rangle = \delta_{n'n''} i^{-\frac{3}{2}} e^{i(2n'+l+\frac{3}{2})\varphi}. \quad (4.37)$$

This result we, of course, expect as the state $|nlm\rangle$ can be written as an homogeneous[9] polynomial of degree $2n+l$ in the creation operators $\boldsymbol{\eta}$ acting on the ground state. The linear canonical transformation (4.36) implies then

$$\bar{\boldsymbol{\eta}} = e^{i\varphi}\boldsymbol{\eta}, \quad (4.38)$$

and thus the state $|nlm\rangle$ transforms, up to a constant phase, in the way indicated by the unitary representation (4.37).

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Canonical Transformations and Matrix Elements*

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We use the ideas on linear canonical transformations developed previously to calculate the matrix elements of the multipole operators between single-particle states in a three-dimensional oscillator potential. We characterize first the oscillator states in the chain of groups $Sp(6) \supset Sp(2) \times \mathcal{O}(3)$, $Sp(2) \supset \mathcal{O}_S(2)$, and $\mathcal{O}(3) \supset \mathcal{O}_L(2)$, and then expand the multipole operators in terms of irreducible tensors with respect to the $Sp(2) \times \mathcal{O}(3)$ group. Their matrix elements are obtained by applying the Wigner–Eckart theorem with respect to both the $Sp(2)$ and $\mathcal{O}(3)$ groups. In this way an explicit expression for the radial integral of r^k, $k > 0$, is obtained.

1. INTRODUCTION

While canonical transformations play a fundamental role in the solution of problems of classical and quantum mechanics, their application, in the latter case, to the evaluation of matrix elements has not been fully explored. In the preceding paper[1] we discussed the linear canonical transformations and showed that the symplectic group which they form is the dynamical group of the harmonic oscillator. We wish in this paper to make use of this group and its subgroups in the evaluation of the matrix elements of the multipole operators

$$\mathcal{Y}_{kt}(\mathbf{r}) \equiv r^k Y_{kt}(\theta, \varphi) \quad (1.1)$$

independent of m, has the explicit form

$$\langle n'lm|\, U\, |n''lm\rangle = i^l[n'!\, n''!\, \Gamma(n'+l+\tfrac{3}{2})\Gamma(n''+l+\tfrac{3}{2})]^{\frac{1}{2}} \times (b+ia)^{-n'-l-\frac{3}{2}}(-b+ia)^{n'}\gamma^{-l-\frac{3}{2}} \times \sum_p \{[p!\,(n'-p)!\,(n''-p)!\,\Gamma(p+l+\tfrac{3}{2})]^{-1} \times [\gamma^2(a^2+b^2)]^{-p}[1-\gamma^{-1}(a^2+b^2)^{-1}]^{n'-p} \times (1-\gamma^{-1})^{n''-p}\}, \quad (4.34)$$

where γ is given by

$$\gamma = \{b(1+a^2+b^2) - i[a-d(a^2+b^2)]\}[2b(a^2+b^2)]^{-1}. \quad (4.35)$$

If we consider an element of $Sp(2)$ that belongs also to the orthogonal subgroup $\mathcal{O}(2)$ of this group, i.e.,

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we have $a^2+b^2=1$ and $\gamma=1$, and thus the unitary representation (4.34) simplifies drastically, taking the form

$$\langle n'lm|\, U\, |n''lm\rangle = \delta_{n'n''} i^{-\frac{3}{2}} e^{i(2n'+l+\frac{3}{2})\varphi}. \quad (4.37)$$

This result we, of course, expect as the state $|nlm\rangle$ can be written as an homogeneous[9] polynomial of degree $2n+l$ in the creation operators $\boldsymbol{\eta}$ acting on the ground state. The linear canonical transformation (4.36) implies then

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We use the ideas on linear canonical transformations developed previously to calculate the matrix elements of the multipole operators between single-particle states in a three-dimensional oscillator potential. We characterize first the oscillator states in the chain of groups $Sp(6) \supset Sp(2) \times \mathcal{O}(3)$, $Sp(2) \supset \mathcal{O}_S(2)$, and $\mathcal{O}(3) \supset \mathcal{O}_L(2)$, and then expand the multipole operators in terms of irreducible tensors with respect to the $Sp(2) \times \mathcal{O}(3)$ group. Their matrix elements are obtained by applying the Wigner–Eckart theorem with respect to both the $Sp(2)$ and $\mathcal{O}(3)$ groups. In this way an explicit expression for the radial integral of r^k, $k > 0$, is obtained.

1. INTRODUCTION

While canonical transformations play a fundamental role in the solution of problems of classical and quantum mechanics, their application, in the latter case, to the evaluation of matrix elements has not been fully explored. In the preceding paper[1] we discussed the linear canonical transformations and showed that the symplectic group which they form is the dynamical group of the harmonic oscillator. We wish in this paper to make use of this group and its subgroups in the evaluation of the matrix elements of the multipole operators

$$\mathcal{Y}_{kt}(\mathbf{r}) \equiv r^k Y_{kt}(\theta, \varphi) \quad (1.1)$$

with respect to single-particle states in a three-dimensional harmonic oscillator potential. While these matrix elements can be evaluated either directly using elementary properties of special functions or with the help of more sophisticated properties associated with the group theory[2,3] behind these functions, so far as we know they have not been evaluated with the help of the canonical transformations associated with the harmonic oscillator. Thus we think the discussion can be not only instructive for the particular problem we propose to deal with here, but may also be useful in a general approach to the evaluation of matrix elements for problems in which an explicit group of canonical transformations is available.

2. THE SINGLE-PARTICLE STATES IN A THREE-DIMENSIONAL OSCILLATOR POTENTIAL

As indicated in the preceding article,[1] whose notation we shall employ, we have for a single particle in a three-dimensional oscillator potential the chain of groups

$$Sp(6) \supset Sp(2) \times \mathcal{O}(3). \tag{2.1}$$

All states of even number of quanta belong to the irreducible representation (IR) $[\frac{111}{222}]$ of the six-dimensional symplectic group $Sp(6)$, while those of odd number of quanta belong to the IR $[\frac{113}{222}]$ of the same group. The group $\mathcal{O}(3)$ is the usual rotation group in three dimensions whose generators are the components of the angular momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = -i\boldsymbol{\eta} \times \boldsymbol{\xi}, \tag{2.2}$$

where $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ are the creation and annihilation vectors defined by

$$\boldsymbol{\eta} = 2^{-\frac{1}{2}}(\mathbf{r} - i\mathbf{p}), \tag{2.3a}$$

$$\boldsymbol{\xi} = 2^{-\frac{1}{2}}(\mathbf{r} + i\mathbf{p}). \tag{2.3b}$$

The generators of the symplectic group $Sp(2)$ are formed by the bilinear expressions in the components of $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ that are invariant under rotations and thus can be expressed as

$$T_+ \equiv -\tfrac{1}{2}\boldsymbol{\eta} \cdot \boldsymbol{\eta}, \tag{2.4a}$$

$$T_0 \equiv \tfrac{1}{4}(\boldsymbol{\eta} \cdot \boldsymbol{\xi} + \boldsymbol{\xi} \cdot \boldsymbol{\eta}) = \tfrac{1}{2}(\boldsymbol{\eta} \cdot \boldsymbol{\xi} + \tfrac{3}{2}), \tag{2.4b}$$

$$T_- \equiv -\tfrac{1}{2}\boldsymbol{\xi} \cdot \boldsymbol{\xi}. \tag{2.4c}$$

The commutation rules of these operators are

$$[T_0, T_\pm] = \pm T_\pm, \tag{2.5a}$$

$$[T_+, T_-] = -2T_0, \tag{2.5b}$$

which differ in the sign of the last term from the usual ones of the rotation group. Thus we are dealing with the Lie algebra of the real symplectic group $Sp(2)$ or those locally isomorphic to it[4] such as $S\mathfrak{U}(1, 1)$ or $\mathcal{O}(2, 1)$.

The single-particle harmonic oscillator states can be expressed as[5]

$$|nlm\rangle = P_{nlm}(\boldsymbol{\eta})\,|0\rangle, \tag{2.6}$$

where $|0\rangle$ is the ground state of the oscillator and P_{nlm} is a homogeneous polynomial of degree $2n + l$ in the creation operator

$$P_{nlm}(\boldsymbol{\eta}) = A_{nl}(\boldsymbol{\eta} \cdot \boldsymbol{\eta})^n \mathcal{Y}_{lm}(\boldsymbol{\eta}), \tag{2.7a}$$

$$A_{nl} = (-1)^n \left(\frac{4\pi}{(2n + 2l + 1)!!\,(2n)!!}\right)^{\frac{1}{2}}. \tag{2.7b}$$

This state can be characterized by definite IR's of the chain of groups

$$Sp(2) \supset \mathcal{O}_S(2), \quad \mathcal{O}(3) \supset \mathcal{O}_L(2), \tag{2.8}$$

where we distinguish by indices S and L the two-dimensional orthogonal subgroups associated respectively with $Sp(2)$ (which was discussed in Ref. 1) and with $\mathcal{O}(3)$.

Clearly the state (2.7) is characterized by the IR's l of $\mathcal{O}(3)$ and m of $\mathcal{O}_L(2)$. For $Sp(2)$ we note first that when $n = 0$, the state is of lowest weight in $Sp(2)$ as

$$T_-\,|0lm\rangle = -\tfrac{1}{2}A_{nl}(\boldsymbol{\xi} \cdot \boldsymbol{\xi})\mathcal{Y}_{lm}(\boldsymbol{\eta})\,|0\rangle = 0, \tag{2.9}$$

because $\boldsymbol{\xi}$ can be interpreted as the differential operator $\partial/\partial\boldsymbol{\eta}$ when applied to polynomials in $\boldsymbol{\eta}$, due to the commutation relations between $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$.[5] Applying T_0 to $|0lm\rangle$, we obtain the eigenvalues

$$\lambda \equiv \tfrac{1}{2}(l + \tfrac{3}{2}), \tag{2.10}$$

which we may consider as the label that characterizes the IR of $Sp(2)$. The IR of $\mathcal{O}(3)$ specifies the IR of $Sp(2)$, and thus the groups are complementary in the sense discussed in the preceding article.[1,6] If we apply T_+ to the state, we do not change the IR of $Sp(2)$, and thus we see that all states $|nlm\rangle$ of fixed l, m belong to the same IR (2.10) of $Sp(2)$. They belong though to different IR's of the subgroup $\mathcal{O}_S(2)$, whose generator is T_0, as the eigenvalue of this operator is now

$$\mu = \tfrac{1}{2}(2n + l + \tfrac{3}{2}). \tag{2.11}$$

Thus the single-particle state $|nlm\rangle$ can also be written as

$$|nlm\rangle \equiv |\lambda\mu;\, lm\rangle, \tag{2.12}$$

where it is now characterized by the IR's of the chain of groups (2.8), with λ and μ given by (2.10) and (2.11), respectively.

We proceed now to show that the solid spherical harmonic (1.1) can also be expressed in terms of linear combinations of irreducible tensors in $Sp(2)$.

Thus the evaluation of the matrix elements of this solid spherical harmonic can be carried out with the help of the Wigner–Eckart theorem for both the rotation $\mathcal{O}(3)$ and symplectic $Sp(2)$ groups.

3. TENSORIAL CHARACTER OF THE MULTIPOLE OPERATORS WITH RESPECT TO THE $Sp(2) \times \mathcal{O}(3)$ GROUP

The multipole operator (1.1) is clearly an irreducible tensor of rank k and projection t with respect to the $\mathcal{O}(3)$ group. We wish now to investigate its properties with respect to the $Sp(2)$ group. As the latter group is locally isomorphic to $S\mathfrak{U}(1, 1)$, an irreducible tensor $\mathcal{C}^{\kappa}_{\tau}$, $\tau = -\kappa, -\kappa+1, \cdots, \kappa$, with respect to this group has the properties[7]

$$[T_{\pm}, \mathcal{C}^{\kappa}_{\tau}] = \pm[(\kappa \mp \tau)(\kappa \pm \tau + 1)]^{\frac{1}{2}} \mathcal{C}^{\kappa}_{\tau\pm1}, \quad (3.1a)$$

$$[T_0, \mathcal{C}^{\kappa}_{\tau}] = \tau \mathcal{C}^{\kappa}_{\tau}. \quad (3.1b)$$

The operators $\mathcal{C}^{\kappa}_{\zeta}$ form a basis for a finite-dimensional, and therefore nonunitary, IR of $S\mathfrak{U}(1, 1)$. In the following, we are going to consider double tensors $\mathcal{C}^{\kappa k}_{\tau t}$, i.e., tensors with respect to the $Sp(2) \times \mathcal{O}(3)$ group.

In order to investigate the tensorial character of the multipole operator (1.1) with respect to the $Sp(2)$ group, we first note that the operators η_t and ξ_t, for a given t ($t = 1, 0$, or -1), are the projections $+\frac{1}{2}$ and $-\frac{1}{2}$, respectively, of a tensor of rank $\frac{1}{2}$ with respect to $Sp(2)$, as

$$[T_+, \eta_t] = 0, \qquad [T_+, \xi_t] = \eta_t, \quad (3.2a)$$

$$[T_0, \eta_t] = \tfrac{1}{2}\eta_t, \qquad [T_0, \xi_t] = -\tfrac{1}{2}\xi_t, \quad (3.2b)$$

$$[T_-, \eta_t] = -\xi_t, \qquad [T_-, \xi_t] = 0. \quad (3.2c)$$

Higher-rank irreducible tensor operators can be constructed from the creation and annihilation operators by using $S\mathfrak{U}(1, 1)$ Wigner coefficients. On the other hand, it is well known[4,7] that the Wigner coefficients which couple two finite-dimensional, nonunitary IR's of the $S\mathfrak{U}(1, 1)$ group can be taken to be identical to the corresponding Wigner coefficients of the $S\mathfrak{U}(2)$ group. Therefore, the construction of higher-rank irreducible tensors only requires $S\mathfrak{U}(2)$ Wigner coefficients. In this way we can form a tensor of rank $k/2$ whose highest component is given by

$$\mathcal{C}^{\frac{1}{2}kk}_{\frac{1}{2}kt} \equiv \mathcal{Y}_{kt}(\boldsymbol{\eta}). \quad (3.3)$$

If we apply now the transformation

$$\begin{pmatrix} \mathbf{r} \\ i\mathbf{p} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{\eta} \\ \boldsymbol{\xi} \end{pmatrix} \quad (3.4)$$

to the operators $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ in the generators (2.4) of $Sp(2)$, we get new generators

$$\bar{T}_+ = -\tfrac{1}{2}\mathbf{r} \cdot \mathbf{r}, \quad (3.5a)$$

$$\bar{T}_0 = \tfrac{1}{4}i(\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}), \quad (3.5b)$$

$$\bar{T}_- = \tfrac{1}{2}\mathbf{p} \cdot \mathbf{p}, \quad (3.5c)$$

with respect to which the operators r_t and ip_t, for a given t, are the projections $+\frac{1}{2}$ and $-\frac{1}{2}$, respectively, of a tensor of rank $\frac{1}{2}$. As before, we can build from it higher-rank irreducible tensors by just using $S\mathfrak{U}(2)$ Wigner coefficients. In particular, the transformation of (3.3) leads to the multipole operator (1.1), which can be rewritten as

$$\bar{\mathcal{C}}^{\frac{1}{2}kk}_{\frac{1}{2}kt} = \mathcal{Y}_{kt}(\mathbf{r}). \quad (3.6)$$

As the construction of the tensor operators only involves the algebra of $S\mathfrak{U}(2)$ and the matrix of the transformation (3.4) is unitary, the transformed tensor is given in terms of the original one by means of a Wigner $\mathfrak{D}$ function[8]

$$\bar{\mathcal{C}}^{\frac{1}{2}kk}_{\tau t} = \sum_{\tau'} \mathcal{C}^{\frac{1}{2}kk}_{\tau' t} \mathfrak{D}^{\frac{1}{2}k}_{\tau'\tau}(0, -\tfrac{1}{2}\pi, 0). \quad (3.7)$$

Introducing in (3.7) the explicit expression of the $\mathfrak{D}$ function, we finally get the expansion of the multipole operators in terms of double tensors,

$$\mathcal{Y}_{kt}(\mathbf{r}) = \sum_{\tau=-k/2}^{k/2} \left(\frac{k!}{(k+2\tau)!!\,(k-2\tau)!!} \right)^{\frac{1}{2}} \mathcal{C}^{\frac{1}{2}kk}_{\tau t}. \quad (3.8)$$

We proceed now to use this expansion to calculate the matrix elements of (1.1) between oscillator single-particle states.

4. MATRIX ELEMENTS OF THE MULTIPOLE OPERATORS BETWEEN OSCILLATOR SINGLE-PARTICLE STATES

Using (2.12) and (3.8), we can write the matrix elements of a solid spherical harmonic between oscillator single-particle states as

$$\langle n'l'm' | \mathcal{Y}_{kt}(\mathbf{r}) | nlm \rangle = \sum_{\tau=-k/2}^{k/2} \left[\left(\frac{k!}{(k+2\tau)!!\,(k-2\tau)!!} \right)^{\frac{1}{2}} \times \langle \lambda'\mu'; l'm' | \mathcal{C}^{\frac{1}{2}kk}_{\tau t} | \lambda\mu; lm \rangle \right]. \quad (4.1)$$

The Wigner–Eckart theorem applied to both the $S\mathfrak{U}(1, 1)$ and $S\mathfrak{U}(2)$ groups enables to factorize the matrix element of the tensor operator $\mathcal{C}^{\frac{1}{2}kk}_{\tau t}$ into a product of Wigner coefficients of $S\mathfrak{U}(1, 1)$ and $S\mathfrak{U}(2)$ and the reduced matrix element of the operator

with respect to both groups,

$$\langle n'l'm'|\,\mathcal{Y}_{kt}(\mathbf{r})\,|nlm\rangle = \sum_{\tau=-k/2}^{k/2}\left[\left(\frac{k!}{(k+2\tau)!!\,(k-2\tau)!!}\right)^{\frac{1}{2}} \times \langle\lambda\,\tfrac{1}{2}k\,\mu\,\tau\,|\,\lambda'\mu'\rangle_{\mathrm{nc}}\langle l\,k\,m\,t\,|\,l'm'\rangle\right]\langle\lambda';l'\|\,\mathcal{C}^{\frac{1}{2}kk}\,\|\lambda;l\rangle. \tag{4.2}$$

We designate by $\langle\,|\,\rangle_{\mathrm{nc}}$ the Wigner coefficient of the noncompact $S\mathfrak{U}(1,1)$ group in order to distinguish it from the $S\mathfrak{U}(2)$ Wigner coefficient $\langle\,|\,\rangle$. This type of $S\mathfrak{U}(1,1)$ Wigner coefficient is the one which arises when a unitary and a nonunitary representation are coupled to get a unitary representation. Explicit expressions of it have been given by Ui.[7]

The selection rule on the $S\mathfrak{U}(2)$ Wigner coefficient[8] gives rise to the well-known selection rule on the angular part of the matrix element (4.1),

$$|l-l'|\le k\le l+l'. \tag{4.3}$$

On the other hand, the selection rule on the $S\mathfrak{U}(1,1)$ Wigner coefficient[7]

$$\mu+\tau=\mu', \tag{4.4}$$

taking into account the values of μ and μ' given by (2.11) and the fact that τ goes from $-k/2$ to $k/2$, leads us to the selection rule on the radial part of (4.1),

$$2n+l-(2n'+l')=-k,\,-k+2,\cdots,k. \tag{4.5}$$

As the angular part of (4.1) is well known, we are only interested in the explicit expression of the radial integral. To obtain it, the relation (4.2) can be rewritten by expressing the reduced matrix element, in terms of the matrix element corresponding to $n=n'=0$ or $\mu=\lambda$, $\mu'=\lambda'$, as

$$\begin{aligned}\langle n'l'm'|\,\mathcal{Y}_{kt}(\mathbf{r})\,|nlm\rangle &= \left[\left(\frac{k!}{(k+2\mu'-2\mu)!!\,(k-2\mu'+2\mu)!!}\right)^{\frac{1}{2}} \times\langle\lambda,\tfrac{1}{2}k,\mu,\mu'-\mu\,|\,\lambda'\mu'\rangle_{\mathrm{nc}}\right] \\ &\times\left[\left(\frac{k!}{(k+2\lambda'-2\lambda)!!\,(k-2\lambda'+2\lambda)!!}\right)^{\frac{1}{2}} \times\langle\lambda,\tfrac{1}{2}k,\lambda,\lambda'-\lambda\,|\,\lambda'\lambda'\rangle_{\mathrm{nc}}\right]^{-1} \\ &\times\langle 0l'm'|\,\mathcal{Y}_{kt}(\mathbf{r})\,|0lm\rangle,\end{aligned} \tag{4.6}$$

from which it follows that

$$\begin{aligned}\int_0^\infty R_{n'l'}(r)r^{k+2}R_{nl}(r)\,dr &= \left(\frac{(k+2\lambda'-2\lambda)!!\,(k-2\lambda'+2\lambda)!!}{(k+2\mu'-2\mu)!!\,(k-2\mu'+2\mu)!!}\right)^{\frac{1}{2}} \\ &\times\frac{\langle\lambda,\tfrac{1}{2}k,\mu,\mu'-\mu\,|\,\lambda'\mu'\rangle_{\mathrm{nc}}}{\langle\lambda,\tfrac{1}{2}k,\lambda,\lambda'-\lambda\,|\,\lambda'\lambda'\rangle_{\mathrm{nc}}} \\ &\times\int_0^\infty R_{0l'}(r)r^{k+2}R_{0l}(r)\,dr.\end{aligned} \tag{4.7}$$

The radial integral of the right-hand side is easily shown to be equal to

$$\int_0^\infty R_{0l'}(r)r^{k+2}R_{0l}(r)\,dr = (k+l+l'+1)!!\,[2^k(2l+1)!!\,(2l'+1)!!]^{-\frac{1}{2}}. \tag{4.8}$$

Introducing in (4.7) the explicit expression for the $S\mathfrak{U}(1,1)$ Wigner coefficients,[7] we finally get

$$\begin{aligned}\int_0^\infty R_{n'l'}(r)r^{k+2}R_{nl}(r)\,dr &= (-1)^{n+n'}\frac{(k+l+l'+1)!!\,[\frac{1}{2}(k+l-l')]!}{[\frac{1}{2}(k+l'-l)+n'-n]!} \\ &\times\left(\frac{2^{n'-n-k}n!\,n'!\,(2n'+2l'+1)!!}{(2n+2l+1)!!}\right)^{\frac{1}{2}}\sum_{p=\max(0,n-n')}^{\min(n,\frac{1}{2}(k+l-l')+n-n')} \\ &\times\left(\frac{2^p[\frac{1}{2}(k+l'-l)+n'-n+p]!}{p!\,[\frac{1}{2}(k+l-l')+n-n'-p]!\,(n-p)!\,(n'-n+p)!\,(2n'-2n+2l'+2p+1)!!}\right).\end{aligned} \tag{4.9}$$

This formula coincides with that given by Armstrong[2] using group theory related to special functions.

The approach followed in this article for the evaluation of the single-particle matrix elements for harmonic oscillator states can clearly be generalized to problems involving more particles, as well as to states associated with other type of potentials. It requires the knowledge of the chain of groups involved in the characterization of the states and of the Wigner coefficients of these groups.

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The Sound Wave Boundary Value Problem in Kinetic Theory. I

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A detailed investigation of the generation of sound waves from an oscillating piston is considered within the framework of kinetic theory. Two kinetic models appropriate to the problem are developed. Both of these are exactly solved by the Wiener–Hopf method. Under a certain special limit, gas dynamics is shown to hold. A variety of other special limits are also considered.

1. INTRODUCTION

An early investigation of the sound propagation problem by means of kinetic theory is to be found in the pioneering report of Wang Chang and Uhlenbeck.[1] In brief their method is based upon the expansion of the distribution function in terms of moments. Using this method, they showed that a series expansion for sound speed and attenuation rate in the frequency ω could be obtained. The leading terms of these yield the same results as the Euler, Navier-Stokes, and Burnett equations, etc. A numerical investigation based on this method and using an extremely large number of moments is to be found in the work of Pekeris and his co-workers.[2,3] However, these results proved to be very poor in the transition and high frequency limit when compared with the experiments of Greenspan[4] and Meyer and Sessler.[5] A discussion of these results is to be found in Sirovich and Thurber.[6] In that paper a method for investigating sound waves by means of fairly elaborate kinetic models is given. The results of their investigation showed extremely close agreement with the above-mentioned experiments.

In all of the above theoretical investigations, only the problem of sound propagation was considered. By this we mean that only the dispersion relation for a plane wave was analyzed. The boundary value problem corresponding to the experiments of Refs. 4 and 5 was not considered. This lead to a controversy (see Refs. 7 and 8) concerning the applicability of the plane wave description in the neighborhood of the oscillating wall. It was felt that in this region a free flow analysis would be more appropriate. The free flow analysis and certain experiments in their support are given in Refs. 9 and 10. However, even these new experiments provided data which fell more closely on the sound dispersion curves than on the free flow curves. It was shown in Ref. 7 that the free flow analysis is of very questionable value at high frequencies even within one mean free path of the wall.

The real issue can only be resolved by the solution of the exact boundary value problem. A certain amount of penetration into this problem has been made by Ostrowsky and Kleitman,[11] Weitzner,[12] Mason,[13,14] and Buckner and Ferziger.[15] Due to various analytical difficulties a number of restrictive assumptions had to be made in each of these investigations. To a certain extent the result of these studies was to raise more questions rather than to settle the above controversy. Notable among these new questions was the result in Ref. 11, that the falloff of a disturbance from an oscillating wall at large distances is $O[\exp(-x^{\frac{3}{2}})]$. This is in clear violation of the widely held view that gas dynamics is the valid theory at large distances, since this theory predicts a simple exponential falloff which is clearly recessive when compared with the result of Ref. 11. We mention in passing that this same peculiar falloff was also found in a study of shock wave structure by Lyubarskii.[16] The explanation for this behavior is due to the BGKW model (Bhatnagar, Gross, and Krook[17] and Welander[18]) or variations of it which were used in the above theoretical investigations, for, in this model, the collision frequency is a constant and fast molecules have unbounded free paths. This point is made in a recent paper.[19] It is also shown there that other fall-offs occur when the collision frequency is nonconstant. If we denote the collision frequency by $\nu(\xi)$ and if

$$\alpha = \lim_{\xi \to \infty} \ln \nu / (\ln \xi),$$

then in general one has a falloff $O[\exp(-x^{2/(3-\alpha)})]$. This has been demonstrated in a particular boundary value problem using a model equation (Sirovich and York[20]) and also for the full linearized Boltzmann equation (Richardson and Sirovich[21]).

The resolution of the boundary value problem can be made in terms of contributions due to the point spectrum (essentially sound propagation) and continuous spectrum (in which the collision frequency and boundary conditions play a major role). A major aim of our investigation is to better understand the interplay of these two effects. Specifically, we wish to know if and where the point and continuous spectra individually dominate. We also wish to take up the

detailed effect of collision frequency. This last part will be taken up in the second part of this study, and in the present paper we will assume a constant collision frequency.

We are critical of the previous treatments in their choice of models and in their boundary conditions. For these reasons we will (in Sec. 2) formulate the problem and treat the boundary conditions with more than usual care. It is shown that previous studies, at least implicitly, assume that the flow under investigation is distant from the piston. We develop the problem under the sole assumption that the Mach number based on piston speed is small, and a simple transformation renders the analysis valid up to the wall.

In Sec. 3 we introduce two kinetic models for the sound problem. Both are developed with the goal of faithfully describing both the plane wave and continuous spectrum contributions to the solution. These models are exactly solved by essentially the Wiener–Hopf technique in Sec. 4.

Although our solutions are explicit, they do not yield to ready analysis. For low frequencies our solution implicitly settles the above-mentioned controversy in showing that the discrete spectrum dominates over the continuous spectrum in the neighborhood of the piston. A specific solution for all frequencies must await machine calculation. In the limit of low frequency oscillations a number of results can be obtained. For one thing, in this limit the neighborhood of the piston is dominated by the discrete spectrum, ie., the plane wave solution. The role of hydrodynamics also emerges. We show that in the limit of $\nu \to \infty$ with $x\omega/(RT)^{\frac{1}{2}}$ held fixed, hydrodynamical theory (the plane wave) dominates. Also of interest is the extent of the region in which the plane wave solution dominates the continuous spectra portion of the solution. The asymptotic extent of this is $x \ll \omega^{-6}$. Beyond this region the description is essentially nonhydrodynamic. A more detailed picture of this "crossover" phenomena is given in Sec. 5.

2. STATEMENT OF THE SOUND PROPAGATION PROBLEM

We begin our discussion with the Boltzmann equation

$$\left(\frac{\partial}{\partial t'} + \xi_1' \frac{\partial}{\partial \tilde{x}'}\right) F = JF, \tag{2.1}$$

where $F = F(\tilde{x}, \boldsymbol{\xi}', t')$ is the molecular distribution function, $\tilde{x}'$ is distance measured from the mean position of a sinusoidally oscillating piston, $\boldsymbol{\xi}'$ is the molecular velocity, and t' is the time. JF is the nonlinear Boltzmann collision operator or any particular model of it.

Equation (2.1) can be nondimensionalized with respect to a constant ν, representative of molecular collision frequency, a mean molecular speed $(RT_0)^{\frac{1}{2}}$, where T_0 is the mean gas temperature, and ρ_0, the mean density. The dimensionless variables are then defined by

$$\nu\tilde{x}'/(RT_0)^{\frac{1}{2}} = \tilde{x}, \quad \boldsymbol{\xi}'/(RT_0)^{\frac{1}{2}} = \boldsymbol{\xi}, \quad \nu t' = t. \tag{2.2}$$

Since boundary conditions are applied at the piston position $\tilde{x}' = x_p'(t)$, rather than the mean position $\tilde{x}' = 0$, we make a (noninertial) transformation which takes the piston position $x_p'(t)$ into the origin of a coordinate x';

$$\tilde{x}' - x_p'(t) = x', \quad \frac{d}{dt} x_p'(t) = u_p'(t),$$

where $u_p'(t)$ is the piston velocity. $\tilde{x}_p'$, u_p' are nondimensionalized by (2.2) and we write

$$x'\nu/(RT_0)^{\frac{1}{2}} = x, \quad u_p'(t)/(RT_0)^{\frac{1}{2}} = \epsilon u_p(t),$$
$$\nu x_p'(t)/(RT_0)^{\frac{1}{2}} = x_p(t),$$

where ϵ is chosen so as to make $u_p = O(1)$ and hence is in effect the piston Mach number. Finally by writing

$$F(\tilde{x}', \boldsymbol{\xi}', t') = f(x, \boldsymbol{\xi}, t),$$

(2.1) becomes

$$\left[\frac{\partial}{\partial t} + (\xi_1 + \epsilon u_p)\frac{\partial}{\partial x}\right] f = \frac{1}{\nu} Jf. \tag{2.3}$$

We impose the following boundary conditions on (2.3):

$$\int_{-\infty}^{\infty} (\xi_1 - \epsilon u_p) f(x = 0, \boldsymbol{\xi}, t)\, d\boldsymbol{\xi} = 0, \tag{2.4a}$$

$$f(x = 0, \boldsymbol{\xi}, t) = \rho_0 (2\pi RT_0)^{-\frac{3}{2}} \rho_p (T_p)^{-\frac{3}{2}} \times \exp\left[(\boldsymbol{\xi} - \epsilon u_p)^2 (2T_p)^{-1}\right]; \quad \xi_1 > \epsilon u_p(t). \tag{2.4b}$$

Equations (2.4) have been nondimensionalized according to (2.2) and

$$\rho_p = \rho_p'/\rho_0, \quad T_p = T_p'/T_0.$$

The first condition, (2.4a), states that there is no mass flow through the piston surface. For this to be true, it must be assumed that the "waiting time" of molecules on the surface is small compared to the period of oscillations of the piston. It should be mentioned that for very high frequency oscillations this might not be the case. (In the case of specular reflection at the piston there is no waiting time and the condition is exact.) The second equation, (2.4b), specifies that the

molecules leave the piston diffusely, i.e., for $\xi_1 > \epsilon u_p$ the distribution function is Maxwellian centered at the piston speed and with a density and temperature ρ_p, T_p which must be determined. (Other "outgoing" distribution functions can be prescribed. We choose this since it seems to be the most realistic condition.) One of the unknown parameters is ultimately fixed by (2.4a). In general, to determine the other one, another boundary condition must be applied. (For example, the temperature of the piston can be given, or a heat flow condition supplied at the piston.) However, we will subsequently show that, for the model operators that we will consider, (2.4b) must satisfy a symmetry condition of the equation which effectively relates ρ_p and T_p, so that (2.4a) suffices for a complete determination. It will be seen that the method of solution holds in principle for any given outgoing distribution function. The distribution function for molecules striking the wall is of course determined with the full solution.

Equation (2.3) together with (2.4) forms a completely general framework for the sound propagation problem in a rarefied gas. The linearization is carried out by assuming that the Mach number ϵ is very much less than 1. We emphasize that this will be the sole "smallness" assumption which we make. This is in contrast to previous treatments which, at least implicitly, assume that the piston position x_p is small. This added generality is a direct consequence of the coordinate transformation.

Linearization follows from the following perturbation expansion:

$$f = f^0[1 + \epsilon\hat{g} + O(\epsilon^2)]$$

with f^0 the absolute Maxwellian,

$$f^0 = \frac{\rho_0}{(2\pi RT_0)^{\frac{3}{2}}} \exp\left[-\frac{\xi^2}{2}\right] = \frac{\rho_0}{(RT)^{\frac{3}{2}}}\Omega.$$

To $O(1)$, (2.3) is identically satisfied, and, to $O(\epsilon)$, we obtain

$$\left(\frac{\partial}{\partial t} + \xi_1\frac{\partial}{\partial x}\right)\hat{g} = \frac{1}{\nu}\frac{\partial}{\partial\epsilon}(Jf)\Big|_{\epsilon=0} = L\hat{g}. \tag{2.5}$$

Defining the inner product

$$(f, g) = \int_{-\infty}^{\infty} \Omega f^* g \, d\boldsymbol{\xi}, \tag{2.6}$$

where f^* is the complex conjugate of f, we have, for the hydrodynamical moments,

$$\rho' = \int_{-\infty}^{\infty} f\, d\boldsymbol{\xi}' = \rho_0 + \epsilon\rho_0\hat{\rho} + O(\epsilon^2),$$

$$\rho' u' = \int_{-\infty}^{\infty} \xi_1' f\, d\boldsymbol{\xi}' = \epsilon\rho_0(RT_0)^{\frac{1}{2}}\hat{u} + O(\epsilon^2),$$

$$\rho' RT' = \int_{-\infty}^{\infty} \{[(\xi_1' - u')^2 + \xi_2^2 + \xi_3^2]/3\} f\, d\boldsymbol{\xi}'$$
$$= \rho_0 RT_0 + \epsilon\rho_0 RT_0(\hat{\rho} + \hat{T}) + O(\epsilon^2),$$

with the perturbed hydrodynamical quantities given by

$$\hat{\rho} = (1, \hat{g}), \quad \hat{u} = (\xi_1, \hat{g}), \quad \hat{T} = (\tfrac{1}{3}\xi^2 - 1, \hat{g}). \tag{2.7}$$

The boundary conditions (2.4) become

$$(\xi_1, \hat{g}(x = 0)) = u_p(t) \tag{2.8a}$$

$$\hat{g}(x = 0; \boldsymbol{\xi}, t) = \hat{\alpha}_1(t) + \hat{\alpha}_2(t)(\tfrac{1}{2}\xi^2 - \tfrac{3}{2}) + \xi_1 u_p, \tag{2.8b}$$

where the unknown functions $\hat{\alpha}_1(t)$, $\hat{\alpha}_2(t)$ arise from

$$\rho_p = 1 + \epsilon\hat{\alpha}_1(t) + O(\epsilon^2),$$
$$T_p = 1 + \epsilon\hat{\alpha}_2(t) + O(\epsilon^2).$$

3. DISCUSSION OF KINETIC MODELS

The system (2.5), (2.6) is completed by specifying a particular collision operator L. We base our discussion on the well-known model operator of Bhatnagar, Gross, Krook,[17] and Welander,[18]

$$Jf = \hat{\nu}(f_0 - f). \tag{3.1}$$

Here f_0 is the local Maxwellian, $\hat{\nu} = \nu\rho'/\rho_0$, and ν is constant. Linearizing according to (2.5) becomes

$$L\hat{g} = -\hat{g} + \hat{\rho} + \xi_1\hat{u} + (\tfrac{1}{2}\xi^2 - \tfrac{3}{2})\hat{T}, \tag{3.2}$$

where we have used the definitions (2.7). We focus on the problem of an oscillating piston by taking $u_P = \exp(i\omega t)$. Collecting (2.5), (2.8), (3.2) and defining $\hat{g} = g(x, \xi)e^{i\omega t}$, $\hat{\rho} = \rho e^{i\omega t}$, $\hat{u} = ue^{i\omega t}$, $\hat{T} = Te^{i\omega t}$, $\hat{\alpha}_{1,2} = \alpha_{1,2}(\omega)e^{i\omega t}$, we have the boundary value problem defined by

$$\left(1 + i\omega + \xi_1\frac{\partial}{\partial x}\right)g = \rho + \xi_1 u + (\tfrac{1}{2}\xi^2 - \tfrac{3}{2})T, \tag{3.3}$$

$$[1, g(x = 0)] = 1, \tag{3.4a}$$

$$g(x = 0, \boldsymbol{\xi}) = \alpha_1(\omega) + \alpha_2(\omega)(\tfrac{1}{2}\xi^2 - \tfrac{3}{2}) + \xi_1, \quad \xi_1 > 0. \tag{3.4b}$$

The restriction to $\partial/\partial t = i\omega$ is, of course, the case of steady state oscillations—which corresponds to asymptotically long times. As indicated, the parameters α_1, α_2, are functions of ω, and their determination is part of the problem. From (3.4a) we note that ϵ is the normalized velocity amplitude of the piston.

Equation (3.3) is seen to be an integro-differential equation for g. The mass conservation equation [taking

the inner product (2.7) with respect to 1] is

$$i\omega\rho + \frac{\partial u}{\partial x} = 0. \tag{3.5}$$

This implies that (3.3) has really only two independent moments of g on the right-hand side. As a result it may be reduced to two coupled integral equations. Unfortunately, no procedures for exact solution are known for this type of problem. Thus for the sound problem, if one seeks exact solutions (as we do here), it is necessary to approximate (3.3) in such a way that there is only a single moment of g present. (For low-speed shear problems this is exactly the case, which accounts for the amount of success which is met with in such problems.) Several such approximations have been introduced in connection with the sound propagation problem. (Buckner and Ferziger[15] present an interesting alternative. They make no assumption on the number of moments but instead replace the boundary with a known oscillating source.) In Refs. 11, 13, and 14 the "isothermal" model ($T = 0$) is considered:

$$\left(1 + i\omega + \xi_1 \frac{\partial}{\partial x}\right) g = \rho + \xi_1 u. \tag{3.6}$$

It is of interest to note that (3.6) does not provide exact solutions to (3.3) with $T = 0$. To prove this, let us integrate (3.6) with respect to the first two moments to obtain

$$\begin{aligned} i\omega\rho + \frac{\partial u}{\partial x} &= 0, \\ i\omega u + \frac{\partial \rho}{\partial x} &= 0. \end{aligned} \tag{3.7}$$

To obtain the second, we have written

$$\frac{\partial}{\partial x}(\xi_1^2 - 1 + 1, g) = 3\frac{\partial T}{\partial x} + \frac{\partial \rho}{\partial x} = \frac{\partial \rho}{\partial x},$$

using (3.2), the fact that $g = g(x, \xi_1)$ only, and the isothermal assumption. Therefore, (3.7) and hence (3.6) permit plane wave solutions

$$e^{i\omega t - ikx}, \quad k = \omega,$$

and k is real. To see that this is impossible, we seek a plane wave solution of (3.6) directly. This then takes the form

$$(1 + i\omega - ik\xi_1)g = \rho + \xi_1 u, \tag{3.8}$$

where ρ and u are now constants. Taking the inner product with respect to g^*, we obtain

$$(1 + i\omega)\,\|g\|^2 - ik(g, \xi_1 g) = |\rho|^2 + |u|^2, \tag{3.9}$$

and $\|g\|^2 = (g, g)$. The real part of (3.9) is

$$\|g\|^2 = |\rho|^2 + |u|^2,$$

which implies that

$$g = \rho + \xi_1 u. \tag{3.10}$$

Substituting (3.10) into (3.8) demonstrates that $k = \omega$ is impossible, hence a contradiction, and hence (3.7) does not admit a solution with $T = 0$.

Another type of model is due to Weitzner.[12] There g is assumed to depend only on ξ_1 so that one has the equation

$$\left(1 + i\omega + \xi_1 \frac{\partial}{\partial x}\right) g = \rho + \xi_1 u + \tfrac{1}{2}(\xi_1^2 - 1)(\xi_1^2 - 1, g). \tag{3.11}$$

This too cannot produce a solution to (3.3). For, comparison of (3.11) with (3.3) shows that, in order for a solution of (3.11) to satisfy (3.3), the distribution can only be a function of ξ_1 in velocity space. However, imposing this on (3.3), we see that this is impossible unless $T = 0$. But this has been shown above to be incompatible with (3.3).

A related and somewhat more severe difficulty associated with (3.6) and (3.11) is that they lead to incorrect "sound speeds"; (3.6) produces sound waves travelling at $(\frac{3}{5})^{\frac{1}{2}}$ of the correct adiabatic speed and (3.11) $3/\sqrt{5}$ of the adiabatic speed. We now introduce two models which to some degree eliminate this shortcoming.

Adiabatic Model

First consider the "adiabatic" model defined by

$$\left(1 + i\omega + \xi_1 \frac{\partial}{\partial x}\right) g = \frac{\xi^2}{3}\rho + \xi_1 u. \tag{3.12}$$

This equation can be obtained by assuming that $\partial Q/\partial x = 0$ in the energy equation of (3.3), namely in

$$i\omega T + \frac{2}{3}\frac{\partial u}{\partial x} + \frac{2}{3}\frac{\partial Q}{\partial x} = 0.$$

Then this and (3.5) give $\rho = \frac{3}{2}T$, hence (3.12) from (3.3). Note that (3.12) conserves mass and momentum but not energy just as (3.6). Because of the adiabatic assumption, the dispersion relation of (3.12) gives the adiabatic sound speed, $(\frac{5}{3})^{\frac{1}{2}}$ to lowest order in the frequency ω (Appendix A). However, again an exact solution of (3.12) does not yield an exact solution of the BGKW model.

Positive Wave Model

We now introduce a second model of (3.3). Our objective will be to construct a model which faithfully portrays the plane wave solutions of (3.3), but involves only a single moment of g. For convenience we write

$$\chi = [1, \xi_1, \xi^2/\sqrt{6} - (\tfrac{3}{2})^{\frac{1}{2}}],$$

and note that $(\chi_i, \chi_j) = \delta_{ij}$. Then (3.3) can be rewritten as

$$\left(1 + i\omega + \xi_1 \frac{\partial}{\partial x}\right) g = \boldsymbol{\chi} \cdot (\boldsymbol{\chi}, g). \tag{3.13}$$

Now we seek a plane wave solution of this, i.e., we assume

$$g = G(\boldsymbol{\xi}) e^{sx}, \tag{3.14}$$

to obtain

$$(1 + i\omega + s\xi_1)G = \boldsymbol{\chi} \cdot (\boldsymbol{\chi}, G) = \boldsymbol{\chi} \cdot \mathbf{a}. \tag{3.15}$$

In order that

$$G = \boldsymbol{\chi} \cdot \mathbf{a}/(1 + i\omega + s\xi_1) \tag{3.16}$$

be a solution of (3.15), it is necessary that

$$\det [\mathbf{1} - (\boldsymbol{\chi}, \boldsymbol{\chi}/(1 + i\omega + s\xi_1))] = 0. \tag{3.17}$$

Among the possible roots s which satisfy (3.17), we choose the one $s = s_0(\omega)$ which lies in the third quadrant. Then, by taking $\omega > 0$, this gives a wave propagating to the right (and decaying in the direction of propagation). Next let $\mathbf{a} = \mathbf{a}(s_0; \omega)$ denote the eigenvector corresponding to s_0,

$$[\mathbf{1} - (\boldsymbol{\chi}, \boldsymbol{\chi}/(1 + i\omega + s_0\xi_1))] \cdot \mathbf{a} = 0, \tag{3.18}$$

and for convenience we take $\mathbf{a}^* \cdot \mathbf{a} = 1$; as before the asterisk signifies the complex conjugate.

Now consider the equation

$$\left(1 + i\omega + \xi_1 \frac{\partial}{\partial x}\right) g = \boldsymbol{\chi} \cdot \mathbf{a} v(x), \tag{3.19}$$

with

$$v(x) = (\mathbf{a} \cdot \boldsymbol{\chi}, g) \tag{3.20}$$

and $\mathbf{a}$ as defined above. A plane wave solution, (3.14), of (3.19) gives

$$G = \frac{\boldsymbol{\chi} \cdot \mathbf{a}}{1 + i\omega + s\xi_1} (\mathbf{a} \cdot \boldsymbol{\chi}, G). \tag{3.21}$$

The inner product of both sides with respect to $\boldsymbol{\chi} \cdot \mathbf{a}$ gives

$$(\mathbf{a} \cdot \boldsymbol{\chi}, G) = (\mathbf{a} \cdot \boldsymbol{\chi}\ G)\mathbf{a}^* \cdot \left(\boldsymbol{\chi}, \frac{\boldsymbol{\chi}}{1 + i\omega + s\xi_1}\right) \cdot \mathbf{a},$$

hence the dispersion relation

$$\mathbf{a}^* \cdot \left(\boldsymbol{\chi}, \frac{\boldsymbol{\chi}}{1 + i\omega + s\xi_1}\right) \cdot \mathbf{a} = 1. \tag{3.22}$$

Multiplying (3.18) on the left by $\mathbf{a}^*$ shows that $s = s_0(\omega)$ satisfies (3.22). In Appendix A it is shown that s_0 is the only solution of (3.22). By observing that $(\mathbf{a} \cdot \boldsymbol{\chi}, G)$ in (3.21) is merely a constant, it follows that (3.21) and (3.16) are identical up to a constant multiplier. Therefore, the model (3.19) has the same plane wave solution as the BGKW model (3.13).

The positive wave model (3.19) does not *a priori* satisfy the conservation equations. On the other hand, the plane wave solution does. This follows trivially from the fact that any solution of the BGKW equation satisfies the conservation equations. Hence, in any region in which the plane wave dominates, (3.19) does lead to the conservation laws. Now, although the positive wave model does not yield an exact solution of the BGKW model, it will have this property asymptotically. We will later show in what follows that the plane wave is dominant in one important region.

In the limit $\omega \to 0$, s_0 and $\mathbf{a}(s_0)$ take especially simple forms. This calculation follows from (3.17), (3.18) and yields

$$s_0 = -(\tfrac{3}{5})^{\frac{1}{2}} i\omega + O(\omega^2)$$
$$\mathbf{a}^\circ = (\tfrac{3}{10})^{\frac{1}{2}}, (\tfrac{1}{2})^{\frac{1}{2}}, (\tfrac{1}{5})^{\frac{1}{2}} + O(\omega).$$

(These are the same as would be obtained from the gasdynamic Euler equations.) Under this limit

$$\boldsymbol{\chi} \cdot \mathbf{a}^\circ = (1/\sqrt{2})(\xi_1 + \xi^2/\sqrt{15}) + O(\omega),$$

and the asymptotic positive wave model has the form

$$\left(1 + i\omega + \xi_1 \frac{\partial}{\partial x}\right) g = \frac{1}{\sqrt{2}} \left(\xi_1 + \frac{\xi^2}{\sqrt{15}}\right) w(x), \tag{3.23}$$

$$w(x) = (1/\sqrt{2})(\xi_1 + \xi^2/\sqrt{15}, g). \tag{3.24}$$

The positive wave model (3.19), (3.20) and its asymptotic form (3.23), (3.24) both yield to solution by the methods of the following section. However, since the exact calculation of $s_0(\omega)$ and $\mathbf{a}^\circ$ is difficult, all explicit calculations will refer to (3.23), (3.24).

Boundary Conditions

As stated after (2.4), the particular model operator that we choose, (3.12), (3.19), or (3.23), places a restriction on the form of (2.4b) or, in the linearized form, on (3.4b). To show this, consider (3.12) and (3.23) in the limit $\xi_1 \to 0$ for $x > 0$. As will be clear from the representation of the solution, $\partial g/\partial x$ exists for $x > 0$. Then, in the limit,

$$(1 + i\omega)g(x, \xi_1 = 0) = \begin{cases} [(\xi_2^2 + \xi_3^2)/3]\rho(x), & \text{adiabatic model,} \\ [(\xi_2^2 + \xi_3^2)/\sqrt{30}]w(x), & \text{positive wave model.} \end{cases}$$

The prescribed boundary value must also have this symmetry; hence

$$\alpha_1(\omega) = \tfrac{3}{2}\alpha_2(\omega)$$

and (3.4b) becomes

$$g_0 = g(x = 0, \boldsymbol{\xi}) = \alpha_2(\omega)\tfrac{1}{2}\xi^2 + \xi_1, \quad \xi_1 > 0. \tag{3.25}$$

Thus (3.12) or (3.23) together with (3.4a) and (3.25) form the complete boundary value problem. [A more

complicated form than (3.25) results for the model (3.19).]

4. SOLUTION OF THE BOUNDARY VALUE PROBLEM

A variety of equivalent methods are available for solving the given model equations. An approach of some generality is the normal modes method used by Cercignani.[22] Another approach is that of Weitzner,[12] who uses transforms. In this paper we use an approach which relies on the reduction of the problem to a pure integral equation of the Wiener–Hopf type.

The equations to be solved are (3.12) [for which ρ can be eliminated by (3.5)] or (3.23) with boundary conditions (3.4a) and (3.25). These can be typically represented by the equation

$$\left(1 + i\omega + \xi_1 \frac{\partial}{\partial x}\right) g = f_1(\xi) v(x) + f_2(\xi) \frac{\partial v}{\partial x}. \quad (4.1)$$

v is taken as a generic moment, depending on the model, and we write

$$v(x) = (f_3(\xi), g). \quad (4.2)$$

Thus f_1, f_2, and f_3 are known for each model. Our method of solution allows any number of derivatives of v to appear on the right-hand side of (4.1), but for simplicity we consider only one here. Integrating (4.1) gives the equation

$$\begin{aligned} g(x, \xi) = {} & H(\xi_1) g_0(\xi) \exp\left[-\frac{(1 + i\omega)}{\xi_1} x\right] \\ & + H(\xi_1) \int_0^x \frac{1}{\xi_1}\left[f_1(\xi) v(s) + f_2(\xi) \frac{\partial v}{\partial s}\right] \\ & \times \exp\left[-\frac{(1 + i\omega)}{\xi_1}(x - s)\right] ds \\ & - H(-\xi_1) \int_x^\infty \frac{1}{\xi_1}\left[f_1(\xi) v(s) + f_2(\xi) \frac{\partial v}{\partial s}\right] \\ & \times \exp\left[-\frac{(1 + i\omega)}{\xi_1}(x - s)\right] ds. \quad (4.3) \end{aligned}$$

H is the Heaviside function, g_0 is the given boundary value (3.25). Parts integrating terms in $\partial v/\partial s$ gives

$$\begin{aligned} g(x, \xi) = {} & H(\xi_1)\{g_0(\xi) - [f_2(\xi)/\xi_1] v(0)\} \\ & \times \exp\{-[(1 + i\omega)/\xi_1]x\} + [f_2(\xi)/\xi_1] v(x) \\ & + H(\xi_1) \int_0^x (1/\xi_1) \\ & \times \{f_1(\xi) - (1 + i\omega)[f_2(\xi)/\xi_1]\} v(s) \\ & \times \exp\{-[(1 + i\omega)/\xi_1](x - s)\} ds \\ & - H(-\xi_1) \int_x^\infty (1/\xi_1) \\ & \times \{f_1(\xi) - (1 + i\omega)[f_2(\xi)/\xi_1]\} v(s) \\ & \times \exp\{-[(1 + i\omega)/\xi_1](x - s)\} ds. \quad (4.4) \end{aligned}$$

Taking the inner product (4.2) of (4.4), one obtains the integral equation

$$v(x) = \int_0^\infty K(x - s) v(s)\, ds + f(x), \quad (4.5)$$

where (in the cases under study f_z is real)

$$\begin{aligned} K(x) = {} & (1/\gamma) \int_{-\infty}^\infty \Omega(\xi)[f_3(\xi)/\xi_1] \\ & \times \{f_1(\xi) - (1 + i\omega)[f_2(\xi)/\xi_1]\} \\ & \times \exp\{-[(1 + i\omega)/\xi_1]x\} \\ & \times [H(\xi_1)H(x) - H(-\xi_1)H(-x)]\, d\xi, \quad (4.6) \end{aligned}$$

$$\begin{aligned} f(x) = {} & (1/\gamma) \int_{-\infty}^\infty \Omega(\xi) f_3(\xi) H(\xi_1) \\ & \times \{g_0(\xi) - [f_2(\xi)/\xi_1] v(0)\} \\ & \times \exp\{-[(1 + i\omega)/\xi_1]x\}\, d\xi, \quad (4.7) \end{aligned}$$

$$\gamma = 1 - (f_3(\xi), [f_2(\xi)/\xi_1]). \quad (4.8)$$

In (4.5) redefine the functions as follows:

$$\begin{aligned} v(x) = v(x), \quad & x > 0, \quad f(x) = f(x), \quad x > 0, \\ = 0, \quad & x < 0, \quad = 0, \quad x < 0, \end{aligned}$$

and let

$$q(x) = \begin{cases} 0, & x > 0, \\ -\int_0^\infty K(x - s) v(s) ds, & x < 0. \end{cases}$$

Then (4.5) is extended to the integral equation

$$v(x) = \int_{-\infty}^\infty K(x - s) v(s)\, ds + f(x) + q(x). \quad (4.9)$$

The Fourier transform of (4.9) is taken using

$$g(k) = \int_{-\infty}^\infty e^{ikx} g(x)\, dx,$$

and the same functional notation is used for the transformed and untransformed function. (The argument signifies the variable under consideration.) This yields the Wiener–Hopf equation

$$v(k)[1 - K(k)] = f(k) + q(k), \quad (4.10)$$

where the transforms of (4.6) and (4.7) are

$$\begin{aligned} K(k) = {} & \frac{1}{\gamma} \int_{-\infty}^\infty \frac{\Omega(\xi) f_3(\xi)}{1 + i\omega - ik\xi_1} \\ & \times \left(f_1(\xi) - (1 + i\omega)\frac{f_2(\xi)}{\xi_1}\right) d\xi, \quad (4.11) \end{aligned}$$

$$\begin{aligned} f(k) = {} & \frac{1}{\gamma} \int_{-\infty}^\infty \frac{\Omega(\xi) f_3(\xi) H(\xi_1) \xi_1}{1 + i\omega - ik\xi_1} \\ & \times \left(g_0(\xi) - \frac{f_2(\xi)}{\xi_1} v(0)\right) d\xi. \quad (4.12) \end{aligned}$$

In (4.10), by construction, $v(k)$ is analytic for Im $k >$ 0 and $q(k)$ is analytic for Im $k < 0$. From (4.11) it is seen that $1 - K(k)$ defines two different analytic functions for Im $(1 + i\omega/ik) \gtrless 0$, i.e., across the line $L = \{k \mid 1 + i\omega - ik\xi_1 = 0, -\infty < \xi_1 < \infty\}$. Each, of course, may be continued into the other half-plane. From (4.12), $f(k)$ defines an analytic function having a cut on the half-line $L_- = \{k \mid 1 + i\omega - ik\xi_1 = 0, \xi_1 > 0\}$ in the fourth quadrant. (L_+ will denote $L - L_-$ in the second quadrant.) Considering k real, we see that both f and K are continuous at $k = 0$ and analytic elsewhere. In addition $1 - K(k) = 1 + O(1/k)$, $f(k) = O(1/k)$ for $k \to \infty$. From Appendix A we know that $1 - K$ has no zeros on the real line for $\omega \neq 0$.

In order to solve (4.10) by the Wiener–Hopf method, it is necessary to construct a splitting into upper and lower analytic functions. This is accomplished in a standard way,[23] by introducing the functions

$$Q(k) = (1/2\pi i)\int_{-\infty}^{\infty} \log [1 - K(t)]\, dt/(t - k), \quad (4.13)$$

$$P(k) = (1/2\pi i)\int_{-\infty}^{\infty} f(t) \exp [Q^-(t)]\, dt/(t - k). \quad (4.14)$$

From the above mentioned properties of f and K, (4.13) and (4.14) exist. Again P and Q define two analytic functions for Im $k \gtrless 0$. Unless otherwise stated, the particular function being considered is determined by the value of the argument, i.e., assume no analytic continuation unless specifically stated. (Analytic continuation will be denoted by the superscript $\pm$.) In particular from the Plemelj formula,[23] as Im $k \to 0$ from above and below ($\pm$ respectively),

$$Q^+(k) - Q^-(k) = \log [1 - K(k)]. \quad (4.15)$$

Next consider the function

$$\begin{aligned} A(k) &= v(k) \exp [Q(k)] - P(k), \quad \text{Im } k > 0, \\ &= q(k) \exp [Q(k)] - P(k), \quad \text{Im } k < 0. \end{aligned} \quad (4.16)$$

A is analytic by construction in the domain of definition, and, as Im $k \to 0^{\pm}$, by (4.15),

$$\begin{aligned} A^+(k) - A^-(k) &= \exp [Q^-(k)]\{v^+(k) \\ &\quad \times \exp [Q^+(k) - Q^-(k)] \\ &\quad - [P^+(k) - P^-(k)] \\ &\quad \times \exp [-Q^-(k)] - q^-(k)\} \\ &= \exp [Q^-(k)]\{v(k)[1 - K(k)] \\ &\quad - f(k) - q(k)\} \\ &= 0, \end{aligned}$$

since the term in square brackets is zero from (4.10). Thus A is analytic for Im $k \gtrless 0$ and continuous for Im $k = 0$. Hence it is analytic everywhere. In the limit of k large, Q, P are both $O(1/k)$ so that (4.16) gives for Im $k > 0$

$$v(k) = P(k) \exp [-Q(k)]. \quad (4.17)$$

Taking the inverse Fourier transform, we have

$$v(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx} P(k) \exp [-Q(k)]\, dk, \quad (4.18)$$

where the path of integration is parallel to and just above the real line.

At this point the problem is essentially solved since (4.18) can be put in (4.4) to give g for all (x, ξ). However, it is natural to push the contour of (4.18) as far as possible into the lower half-plane since the solution for $x > 0$ is desired. In doing this, we also split the solution into contributions from the point and continuous spectra. First we continue P and Q into the lower half-plane by means of (4.15) and find

$$\begin{aligned} v(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx} &\frac{\exp [-Q(k)]}{1 - K(k)} \\ &\times \{P(k) + f(k) \exp [Q(k)]\}\, dk, \end{aligned} \quad (4.19)$$

where now the contour is just below the real axis, passing through the origin, and P and Q are now defined for Im $k < 0$.

We note again that the line $L((1 + i\omega)/it, -\infty < t < \infty)$ is a cut for $K(k)$ and L_- a cut for $f(k)$. Also, for the models under study, $1 - K$ has a single root, k_0, in the lower half-plane (see Appendix A). Therefore, k_0 is a pole for $(1 - K)^{-1}$ and a branch point for ln $(1 - K)$. The branch cut is taken between k_0 and ∞ as indicated in Fig. 1. (One may easily show that the origin is an essential singularity of K.)

Considering P, (4.14), and making use of the contours indicated in Fig. 1, we find (in the following we will take Im $k < 0$, although the final results do not depend on this)

$$\begin{aligned} P(k) = &-f(k) \exp Q(k) \\ &+ \frac{1}{2\pi i}\int_{L_-} \{f(t)\} \exp Q(t) \frac{dt}{t - k}, \end{aligned} \quad (4.20)$$

where

$$\{f\} = f(t)_r - f(t)_l.$$

Here $f(t)_r$ and $f(t)_l$ signify that t approaches L from the right and left, as viewed in Fig. 1.

Using the same contours for Q, (4.13), we obtain

$$\begin{aligned} Q(k) = &-\ln (1 - K(k)) \\ &+ \frac{1}{2\pi i}\int_{L_-} \{\ln [1 - K(t)]\} \frac{dt}{t - k} \\ &+ \ln (k_0 - k). \end{aligned} \quad (4.21)$$

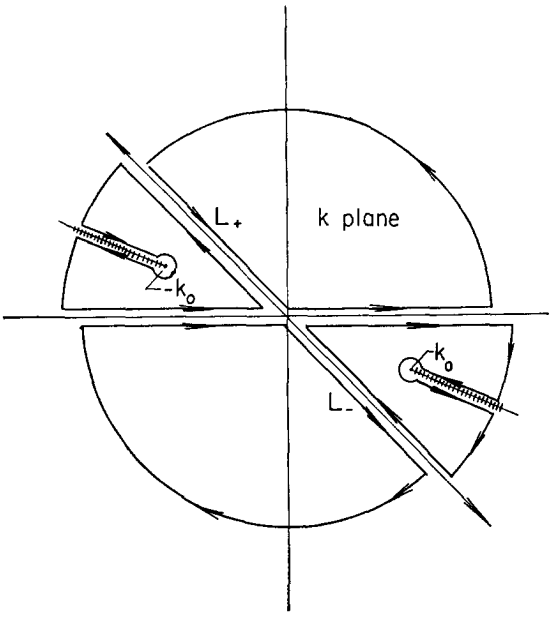

FIG. 1. Complex k plane.

Then, defining

$$X(k) = \exp\left(\frac{1}{2\pi i}\int_{L_-}\{\ln(1-K)\}\frac{dt}{t-k}\right), \quad (4.22)$$

we have from (4.21)

$$\exp(-Q)/(1-K) = [X(k)(k_0-k)]^{-1}. \quad (4.23)$$

On defining

$$N(k) = -\frac{1}{2\pi i}\int_{L_-}\{f(t)\}\exp(Q(t))\frac{dt}{t-k}, \quad (4.24)$$

(4.19) becomes

$$v(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikx}\frac{N(k)}{(k-k_0)X(k)}\,dk. \quad (4.25)$$

N and X are analytic except on L_- and the pole is explicit. Therefore, the continuation of the contour down into the lower half-plane yields

$$v(x) = -i[N(k_0)/X(k_0)]e^{-ik_0x} + (2\pi)^{-1} \times \int_{L_-}[e^{-ikx}/(k-k_0)]\{N(k)/X(k)\}\,dk, \quad (4.26)$$

where the boldface curly brackets again indicate the jump of the enclosed function across L_-.

We defer discussion of the solution to the next section and now specialize the above results to the adiabatic and positive wave models.

Adiabatic Model

For this model

$$f_1(\xi) = f_3(\xi) = \xi_1, \quad f_2(\xi) = -(1/3i\omega)\xi^2,$$

so that, from (4.8),

$$\gamma = (1 + i\omega)/i\omega.$$

Therefore, from (4.11) and (4.12) we have

$$K(k) = \frac{i\omega}{1+i\omega}\int_{-\infty}^{\infty}\frac{\Omega(t)t^2\,dt}{1+i\omega-ikt} + \frac{1}{3}\int_{-\infty}^{\infty}\frac{\Omega(t)(t^2+2)}{1+i\omega-ikt}\,dt, \quad (4.27)$$

$$f(k) = \int_0^{\infty}\frac{\Omega(t)t}{1+i\omega-ikt}\left(\frac{i\omega}{1+i\omega}tg_0(t) + \frac{(t^2+2)}{3(1+i\omega)}\right)dt. \quad (4.28)$$

Here we have integrated out the ξ_2 and ξ_3 variables and in (4.28)

$$g_0(\xi_1) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Omega(\xi_2)\Omega(\xi_3)g_0(\xi)\,d\xi_2\,d\xi_3 = \xi_1 + \alpha_2(\omega)(1 + \tfrac{1}{2}\xi_1^2).$$

In these, $\Omega(x) = (2\pi)^{-\frac{1}{2}}\exp(-x^2/2)$ is the one-dimensional Gaussian. It is clear from (4.27) that

$$K(-k) = K(k). \quad (4.29)$$

In particular, if t lies on the cut L of the function K,

$$K(t)_r = K(-t)_l.$$

From this and an obvious change of variable, we obtain

$$X(-k) = \exp\left(-\frac{1}{2\pi i}\int_{L_+}\{\ln(1-K(t))\}\frac{dt}{t-k}\right). \quad (4.30)$$

L_+ is the path indicated in Fig. 1 extending from the origin to ∞.

From (4.29) it is clear that $-k_0$ is a root of the dispersion relation $1 - K = 0$ if k_0 is a root. Therefore, as indicated in Fig. 1, $-k_0$ is a branch point of $\ln[1 - K(t)]$. On making use of the contours indicated in the upper half-plane of Fig. 1, we obtain in analogy with (4.22),

$$\exp[Q(k)] = -[X(-k)(k+k_0)]^{-1}, \quad (4.31)$$

and combining (4.22) and (4.31) gives

$$X(k)X(-k) = [1 - K(k)]/(k^2 - k_0^2). \quad (4.32)$$

Inserting (4.31) into (4.24) gives

$$N(k) = \frac{1}{2\pi i}\int_{L_-}\frac{\{f(t)\}\,dt}{X(-t)(t+k_0)(t-k)}. \quad (4.33)$$

Positive Wave Model

We have

$$f_1(\xi) = f_3(\xi) = 2^{-\frac{1}{2}}(\xi_1 + \xi^2/\sqrt{15}), \quad f_2 = 0,$$

and, from (4.8), $\gamma = 1$. From (4.11) and (4.12),

$$K(k) = \tfrac{1}{2}\int_{-\infty}^{\infty} \Omega(\xi)\left(\xi_1 + \frac{\xi^2}{\sqrt{15}}\right)^2 \frac{d\xi}{1 + i\omega - ik\xi_1}, \tag{4.34}$$

$$f(k) = \frac{1}{\sqrt{2}}\int_{-\infty}^{\infty} \Omega(\xi)H(\xi_1)\left(\xi_1 + \frac{\xi^2}{\sqrt{15}}\right) \times \xi_1 g_0(\xi)\frac{d\xi}{1 + i\omega - ik\xi_1}. \tag{4.35}$$

In analogy with (4.30) and (4.31),

$$\exp Q(k) = 1/Y(k),$$
$$Y(k) = \exp\left(\frac{-1}{2\pi i}\int_{L_+} \log\frac{1 - K(t)_r}{1 - K(t)_i}\frac{dt}{t - k}\right) \tag{4.36}$$

since there is now no root to $1 - K = 0$ in the upper half-plane (see Appendix B). From (4.23)

$$X(k)Y(k) = (1 - K)/(k_0 - k). \tag{4.37}$$

Finally, substitution into (4.24) gives

$$N(k) = \frac{-1}{2\pi i}\int_{L_-} \frac{\{f(t)\}}{Y(t)}\frac{dt}{t - k}. \tag{4.38}$$

Alternate Representation

The above results can be put in a somewhat simpler form with the transformation

$$z = (1 + i\omega)/ik.$$

This transformation takes L into the real axis [and L_- into $(0, \infty)$]. Under this transformation we also have $\{f\} \to -\langle f\rangle$, where

$$\langle f(t)\rangle = f(t)^+ - f(t)^-.$$

Here, as usual, f^+ and f^- signify the limits of $f(z)$ as z approaches the real axis from above and below, respectively. Functions of z will in general be denoted by tildes, e.g.,

$$\tilde{K}(z) = K((1 + i\omega)/iz)$$

Adiabatic model: From (4.29)

$$\tilde{K}(z) = -\frac{i\omega z}{(1 + i\omega)^2}\int_{-\infty}^{\infty} \Omega(t)t^2\frac{dt}{t - z} - \frac{z}{3(1 + i\omega)}\int_{-\infty}^{\infty}\frac{\Omega(t)(t^2 + 2)}{t - z}dt. \tag{4.39}$$

Also from (4.28),

$$\tilde{f}(z) = \int_0^{\infty} \Omega(t)t(i\omega t g_0(t) + \tfrac{1}{3}(t^2 + 2))\frac{dt}{t - z} = \frac{(1 + i\omega)^2}{z} f\left(\frac{1 + i\omega}{iz}\right). \tag{4.40}$$

Next we define

$$\tilde{X}(z) = -\frac{(1 + i\omega)^2}{\omega z_0 z} X\left(\frac{1 + i\omega}{iz}\right). \tag{4.41}$$

Then, using contours of the type shown on Fig. 1, one can show

$$\tilde{X}(z) = \frac{1}{z}\exp\left(\frac{1}{2\pi i}\int_0^{\infty}\frac{\langle \ln[1 - \tilde{K}(\tau)]\rangle}{\tau - z}d\tau\right) \tag{4.42}$$

and also

$$\tilde{X}(-z) = -\frac{1}{z}\exp\left(\frac{1}{2\pi i}\int_{-\infty}^{0}\frac{\langle \ln[1 - \tilde{K}(\tau)]\rangle}{\tau - z}d\tau\right). \tag{4.43}$$

Then from (4.32)

$$\tilde{X}(z)\tilde{X}(-z) = -\frac{1 - \tilde{K}(z)}{z^2 - z_0^2}\left(\frac{1 + i\omega}{i\omega}\right)^2. \tag{4.44}$$

We see from (4.42) and (4.43) that $\tilde{X}(z)$ and $\tilde{X}(-z)$ have cuts, respectively, on the positive and negative real axis. Therefore, from (4.48) and the Plemelj formulas, we may write

$$\tilde{X}(z) = -\frac{1}{2\pi i}\left(\frac{1 + i\omega}{i\omega}\right)^2\int_0^{\infty}\frac{\langle 1 - \tilde{K}(t)\rangle}{\tilde{X}(-t)(t^2 - z_0^2)}\frac{dt}{t - z}. \tag{4.45}$$

From (4.33) and (4.40) we find

$$\tilde{N}(z) = \frac{1}{2\pi i}\int_0^{\infty}\frac{\langle \tilde{f}(t)\rangle\, dt}{\tilde{X}(-t)(t_0 + z_0)(t - z)} = -\frac{i\omega(1 + i\omega)}{z}N\left(\frac{1 + i\omega}{iz}\right). \tag{4.46}$$

The various jump quantities are now easily obtained:

$$\langle \tilde{f}(t)\rangle = 2\pi i\Omega(t)t(i\omega t g_0(t) + \tfrac{1}{3}(t^2 + 2)), \tag{4.47}$$

$$\langle 1 - \tilde{K}(t)\rangle = 2\pi i\Omega(t)t\left(\frac{i\omega t^2}{(1 + i\omega)^2} + \frac{t^2 + 2}{3(1 + i\omega)}\right). \tag{4.48}$$

Returning to (4.26), we first recognize that $v(x) = u(x)$, the macroscopic velocity, for the adiabatic model, and, then inserting (4.41) and (4.46), we find

$$u(x) = \frac{1 + i\omega}{(i\omega)^2 z_0}\frac{\tilde{N}(z_0)}{\tilde{X}(z_0)}\exp\left(-\frac{(1 + i\omega)x}{z_0}\right) - \frac{1}{2\pi i}\int_0^{\infty}\frac{\exp[-(1 + i\omega)x/z]}{z - z_0}\frac{1 + i\omega}{(i\omega)^2 z} \times \left\langle\frac{\tilde{N}(z)}{\tilde{X}(z)}\right\rangle dz, \tag{4.49}$$

where

$$\left\langle\frac{\tilde{N}}{\tilde{X}}\right\rangle = \frac{1}{\tilde{X}^+\tilde{X}^-}(\tilde{N}^+(\tilde{X}^- - \tilde{X}^+) + \tilde{X}^+(\tilde{N}^+ - \tilde{N}^-)). \tag{4.50}$$

Then from (4.46) and (4.47)

$$\tilde{N}^+ - \tilde{N}^- = \frac{\Omega(z)z}{\tilde{X}(-z)(z+z_0)}[i\omega z g_0(z) + \tfrac{1}{3}(z^2+2)], \tag{4.51}$$

and from (4.45) and (4.48)

$$\tilde{X}^- - \tilde{X}^+ = \frac{\Omega(z)z}{\tilde{Y}(-z)(z^2-z_0^2)}\left(\frac{z^2}{i\omega} + \frac{1+i\omega}{(i\omega)^2}\frac{z^2+2}{3}\right). \tag{4.52}$$

Positive wave model: In analogy with the above treatment, we write

$$\tilde{N}(z) = \frac{1}{2\pi i}\int_0^\infty \frac{\langle \tilde{f}(t)\rangle}{Y(t)}\frac{dt}{t-z} \tag{4.53}$$

$$\tilde{X}(z) = \frac{1}{z}\exp\frac{1}{2\pi i}\int_0^\infty \log\frac{1-\tilde{K}(t)^+}{1-\tilde{K}(t)^-}\frac{dt}{t-z} \tag{4.54}$$

$$\tilde{Y}(z) = \exp\frac{1}{2\pi i}\int_{-\infty}^0 \log\frac{1-\tilde{K}(t)^+}{1-\tilde{K}(t)^-}\frac{dt}{t-z}, \tag{4.55}$$

with

$$\tilde{f}(z) = 2^{\frac{1}{2}}\int_0^\infty \frac{\Omega(t)t}{t-z} \times\left[\tfrac{1}{30}(t^4 + 2(15)^{\frac{1}{2}}t^3 + 19t^2 + 4(15)^{\frac{1}{2}}t + 8) + \frac{1}{2(15)^{\frac{1}{2}}}\left(\frac{\alpha_2(\omega)}{2} - \frac{1}{(15)^{\frac{1}{2}}}\right) \times (t^4 + (15)^{\frac{1}{2}}t^3 + 4t^2 + 2(15)^{\frac{1}{2}}t + 8)\right]dt, \tag{4.56}$$

$$1 - \tilde{K}(z) = 1 + \frac{z}{30(1+i\omega)}\int_{-\infty}^\infty \frac{\Omega(t)}{t-z}(t^4 + 2(15)^{\frac{1}{2}}t^3 + 19t^2 + 4(15)^{\frac{1}{2}}t + 8)\,dt. \tag{4.57}$$

The jumps are now

$$\langle \tilde{f}(z)\rangle = 2\pi i 2^{\frac{1}{2}}\Omega(z)z \times\left[\tfrac{1}{30}(z^4 + 2(15)^{\frac{1}{2}}z^3 + 19z^2 + 4(15)^{\frac{1}{2}}z + 8) + \frac{1}{2(15)^{\frac{1}{2}}}\left(\frac{\alpha_2(\omega)}{2} - \frac{1}{(15)^{\frac{1}{2}}}\right) \times (z^4 + (15)^{\frac{1}{2}}z^3 + 4z^2 + 2(15)^{\frac{1}{2}}z + 8)\right], \tag{4.58}$$

$$\langle 1 - \tilde{K}(z)\rangle = 2\pi i\frac{\Omega(z)z}{30(1+i\omega)}(z^4 + 2(15)^{\frac{1}{2}}z^3 + 19z^2 + 4(15)^{\frac{1}{2}}z + 8). \tag{4.59}$$

The identity analogous to (4.44) is

$$\tilde{X}(z)\tilde{Y}(z) = -\frac{1-\tilde{K}(z)}{z-z_0}\frac{1+i\omega}{i\omega}, \tag{4.60}$$

and then

$$\tilde{X}(z) = -\frac{1}{2\pi i}\frac{1+i\omega}{i\omega}\int_0^\infty \frac{\langle 1-\tilde{K}(t)\rangle}{Y(t)(t-z_0)}\frac{dt}{t-z}. \tag{4.61}$$

Finally, inverting the transform (4.53), we have

$$w(x) = +\frac{1+i\omega}{i\omega z_0}\frac{\tilde{N}(z_0)}{\tilde{X}(z_0)}\exp\left(-\frac{(1+i\omega)x}{z_0}\right) - \frac{1}{2\pi i}\int_0^\infty \frac{\exp[-(1+i\omega)x/z]}{z-z_0}\frac{1+i\omega}{i\omega z} \times\left\langle\frac{\tilde{N}(z)}{\tilde{X}(z)}\right\rangle dz, \tag{4.62}$$

with $\langle N/X\rangle$ calculated as in (4.50) with

$$\tilde{N}^+ - \tilde{N}^- = \langle \tilde{f}(z)\rangle/\tilde{Y}(z)$$

and

$$\tilde{X}^- - \tilde{X}^+ = \frac{1+i\omega}{i\omega}\frac{\langle 1-\tilde{K}(z)\rangle}{\tilde{Y}(z)(z-z_0)}. \tag{4.63}$$

To study a hydrodynamic moment of g, it is, of course, necessary to put (4.62) back into (4.3) and take the appropriate moment. Our solution in the z variable for both models has the same form as is found in Refs. 12 and 22, while in the k variable it is similar to that of Ref. 11.

5. ANALYSIS OF THE SOLUTION

Determination of $g(x = 0, \xi_1 < 0)$

Adiabatic model: As a first step in the study of the solution (4.49) we calculate the boundary value of the distribution for incoming molecules by evaluating (4.4) at $x = 0$ for $\xi_1 < 0$ with the appropriate f_1, f_2, and f_3. This gives

$$g(x=0,\xi_1<0) = -\int_0^\infty\left[1 + \frac{1+i\omega}{3i\omega}\frac{\xi^2}{\xi_1^2}\right]u(s)\exp\left[\frac{(1+i\omega)s}{\xi_1}\right]ds - \frac{1}{3i\omega}\frac{\xi^2}{\xi_1}. \tag{5.1}$$

We demonstrate that (5.1) is bounded in the limit $\xi_1 \to 0$. By Watson's Lemma we have

$$\int_0^\infty u(s)\exp\left(\frac{(1+i\omega)s}{\xi_1}\right)ds = -\frac{\xi_1}{1+i\omega}u(0) + \frac{\xi_1^2}{(1+i\omega)^2}u'(0) + O(\xi_1^2), \tag{5.2}$$

where we use $u(x) = u(0) + u'(0)x + O(x)$ which is demonstrated in Appendix B. Note that, unlike shear problems, $u'(0)$ exists—however, this is already signaled by the continuity equation (3.5). Using (5.2)

in (5.1), we find, since $u(0) = 1$, that

$$\lim_{\xi_1 \to 0^-} g(x = 0, \xi) = -\frac{(\xi_2^2 + \xi_3^2)}{3i\omega(1 + i\omega)} u'(0). \quad (5.3)$$

Positive wave model: Here we find that from (4.3)

$$g(x = 0, \xi_1 < 0) = -\frac{1}{\sqrt{2}} \int_0^\infty \left[1 + \frac{\xi^2}{\sqrt{15}\xi_1}\right] w(s) \times \exp\left[\frac{(1 + i\omega)s}{\xi_1}\right] ds \quad (5.4)$$

and in the limit for ξ_1 small, by Watson's lemma,

$$\lim_{\xi_1 \to 0^-} g(x = 0, \xi) = \frac{(\xi_2^2 + \xi_3^2)}{\sqrt{30}\,(1 + i\omega)} w(0). \quad (5.5)$$

Comparing (5.3) and (5.5) with (3.25), we see that the distribution will not be continuous at $\xi_1 = 0$ unless

$$\begin{aligned} \alpha_2(\omega) &= \tfrac{2}{3}[u'(0)/i\omega(1 + i\omega)], && \text{adiabatic,} \\ &= (2/\sqrt{30})[w(0)/(1 + i\omega)], && \text{positive wave.} \end{aligned} \quad (5.6)$$

However, α_2 is fixed by (3.4a), and (5.6) is not satisfied. Hence the distribution function is discontinuous at the wall.

Low Frequency Oscillations

Adiabatic model: We will consider the behavior of the solution (4.49) as $\omega \to 0$. The expansion of z_0 in this case is given by (A.2). Now the point spectrum contribution to (4.49) is

$$u_p(x) = \frac{1 + i\omega}{(i\omega)^2 z_0} \frac{\tilde{N}(z_0)}{\tilde{X}(z_0)} e^{-(1+i\omega)x/z_0}. \quad (5.7)$$

$\tilde{N}(z_0)$ is given by (4.40, 4.44), and using (A.2) we find to first order

$$\tilde{N}(z_0) = -\frac{1}{z_0^2} \int_0^\infty \frac{\Omega(t)t}{\tilde{X}(-t, \omega = 0)} \frac{(t^2 + 2)}{3} dt + O(\omega^3) \quad (5.8)$$

[where $1/z^2 = -(3/5)\omega^2 + O(\omega^3)$]. The dependence of $\tilde{X}$ on ω is indicated and from (4.41, 4.43) we observe that it is well behaved at $\omega = 0$. Similarly $\tilde{X}$ is expanded using (4.45), (4.49), and we find

$$\tilde{X}(z_0) = -\frac{1}{z_0^3(i\omega)^2} \int_0^\infty \frac{\Omega(t)t}{X(-t, \omega = 0)} \times \frac{(t^2 + 2)}{3} dt + O(\omega^2). \quad (5.9)$$

Then (5.8), (5.9) give in (5.7)

$$u_p(x) = [1 + O(\omega)]e^{-(1+i\omega)x/z_0}. \quad (5.10)$$

The continuous spectrum contribution to (4.49) is given by

$$u_c(x) = -\frac{1}{2\pi i} \int_0^\infty \frac{e^{-(1+i\omega)x/z_0}}{z - z_0} \frac{1 + i\omega}{(i\omega)^2 z} \left\langle \frac{\tilde{N}(z)}{\tilde{X}(z)} \right\rangle dz. \quad (5.11)$$

From (4.40), (4.44) we find that to first order

$$\tilde{X}(z) = \frac{1}{z_0} \int_0^\infty \frac{\Omega(t)t}{\tilde{X}(-t, 0)} \frac{(t^2 + 2)}{3} \frac{dt}{t - z} + O(\omega^2), \quad (5.12)$$

and

$$\tilde{X}(z) = \frac{1}{z_0^2(i\omega)^2} \int_0^\infty \frac{\Omega(t)t}{\tilde{X}(-t, 0)} \frac{(t^2 + 2)}{3} \frac{dt}{t - z} + O(\omega). \quad (5.13)$$

Therefore

$$\frac{1}{z - z_0} \frac{1 + i\omega}{(i\omega)^2 z} \frac{\tilde{N}(z)}{\tilde{X}(z)} = -\frac{1}{z} + O(\omega). \quad (5.14)$$

If we now take the jump of (5.14), it is seen to be of $O(\omega)$ since the $O(1)$ term is analytic across the real axis [while the $O(\omega)$ term is not]. Hence in the limit, for a fixed x,

$$u_c(x) = O(\omega). \quad (5.15)$$

Thus (5.10), (5.15) and the expansion of z_0 give

$$u(x, t) = [1 + O(\omega)] \exp\{i\omega[t - (\tfrac{3}{5})^{\frac{1}{2}}x] - \tfrac{2}{5}(\tfrac{3}{5})^{\frac{1}{2}}\omega^2 x + O(\omega^3 x)\} + O(\omega). \quad (5.16)$$

Hence, for any fixed value of x and as $\omega \to 0$, the flow is governed not only by the plane wave (the point spectrum) but actually by hydrodynamics, since the amplitude of the plane wave is unity, i.e., $u(0) = 1$ in the normalization.

Positive wave model: For this model, since we are interested in the velocity moment u, it is necessary to substitute the solution for w, (4.63), into (4.3) and solve for u. Hence u will have a representation such as (4.63) in terms of the point and continuous spectra, and we again write

$$u = u_p(x) + u_c(x).$$

After some calculation, the contribution from the point spectrum is found to be

$$u_p(x) = -\frac{\tilde{N}(z_0)}{i\omega \tilde{X}(z_0)} \int_{-\infty}^\infty \frac{\Omega(\xi_1)}{\sqrt{2}} \times \left(\xi_1 + \frac{\xi_1^2 + 2}{\sqrt{15}}\right) \frac{\xi_1 \, d\xi_1}{\xi_1 - z_0} e^{-(1+i\omega)x/z_0}, \quad (5.17)$$

and that of the continuous spectrum is

$$u_c(x) = \int_0^\infty \Omega(\xi_1)\xi_1[\xi_1 + \tfrac{1}{2}\alpha_2(\omega)(\xi_1^2+2)] \times \exp\left(-\frac{(1+i\omega)x}{\xi_1}\right) d\xi_1 + \frac{1}{i\omega}\int_0^\infty \frac{\Omega(\xi_1)}{\sqrt{2}}\left(\xi_1 + \frac{\xi_1^2+2}{\sqrt{15}}\right)\xi_1 e^{-(1+i\omega)x/\xi_1} \times \left(-\frac{1}{2\pi i}\int_0^\infty \frac{1}{(z-z_0)(\xi_1-z)}\left\langle\frac{\tilde N(z)}{\tilde X(z)}\right\rangle dz + \frac{\tilde N(z_0)}{\tilde X(z_0)}\frac{1}{(\xi_1-z_0)}\right) d\xi_1 + \frac{1}{2\pi i}\int_{-\infty}^\infty \frac{\Omega(\xi_1)}{\sqrt{2}}\left(\xi_1 + \frac{\xi_1^2+2}{\sqrt{15}}\right)\frac{\xi_1}{i\omega} \times \int_0^\infty \frac{e^{-(1+i\omega)x/z}}{(z-z_0)(\xi_1-z)}\left\langle\frac{\tilde N(z)}{\tilde X(z)}\right\rangle dz. \quad (5.18)$$

First consider the pole contribution for ω small. The ξ_1 integral behaves asymptotically as $-1/\sqrt{2}\, z_0 + O(\omega^2)$. The expansions of $\tilde N(z_0)$ and $\tilde X(z_0)$ follow from (4.53), (4.56) and (4.59), (4.61) respectively. We find

$$\tilde N(z_0) = -\frac{2^{\frac{1}{2}}}{z_0}\int_0^\infty \frac{\Omega(t)t}{\tilde Y(t)} \times \left[\tfrac{1}{30}(t^4 + 2(15)^{\frac{1}{2}}t^3 + 19t^2 + 4(15)^{\frac{1}{2}}t + 8) + \frac{1}{2(15)^{\frac{1}{2}}}\left(\frac{\alpha_2(0)}{2} - \frac{1}{15^{\frac{1}{2}}}\right)(t^4 + (15)^{\frac{1}{2}}t^3 + 4t^2 + 2(15)^{\frac{1}{2}}t + 8)\right]\frac{dt}{t-z} + O(\omega^2), \quad (5.19)$$

and

$$\tilde X(z_0) = -\frac{1}{i\omega z_0^2}\int_0^\infty \frac{\Omega(t)t}{\tilde Y(t)}\tfrac{1}{30}(t^4 + 2(15)^{\frac{1}{2}}t^3 + 19t^2 + 4(15)^{\frac{1}{2}}t + 8)\frac{dt}{t-z} + O(\omega^2). \quad (5.20)$$

Unlike the adiabatic model (5.17), $\alpha_2(0)$ occurs to first order in $\tilde N(z_0)$ [(5.19)]. Therefore, we must determine it to fix u_p and u_c. The condition for its determination is (3.4a), and so in the limit we have

$$1 = \lim_{\omega\to 0}[u_p(x=0) + u_c(x=0)].$$

As is easily seen by (5.17), (5.18), this is a linear equation in $\alpha_2(0)$. However, it is unnecessary to solve for it, since we observe that if

$$\alpha_2(0) = 2/\sqrt{15},$$

by (5.19), (5.20)

$$\tilde N(z_0)/\tilde X(z_0) = 2^{\frac{1}{2}}i\omega z_0 + O(\omega),$$

so that (5.17) to first order at $x = 0$ is

$$u_p(x=0) = 1 + O(\omega). \quad (5.21)$$

Also we see that

$$[\tilde N(z)/\tilde X(z)] = O(\omega).$$

The remaining calculation is analogous to that of (5.12)–(5.14) and need not be repeated. All contributions to u_c are seen to be $O(\omega)$. Therefore, altogether, we have for this model

$$u(x,t) = [1 + O(\omega)]\exp\{i\omega(t - (\tfrac{3}{5})^{\frac{1}{2}}x) - \tfrac{1}{5}(\tfrac{3}{5})^{\frac{1}{2}}\omega^2 x + O(\omega^3 x)\} + O(\omega). \quad (5.22)$$

Again for any fixed x and as $\omega \to 0$, not only does the plane wave dominate, but also hydrodynamics, since the amplitude is unity.

Limit of x Large

Adiabatic model: For x large, the contribution from the point spectrum is clear and is $O(e^{-k_0\omega x})$ where $\operatorname{Re} k_0(\omega) > 0$ for $\omega \neq 0$, i.e., the decay is exponential. Now consider the continuous spectrum. From (5.11) and (4.50)–(4.52) this is

$$u_c(x) = -\frac{1+i\omega}{(i\omega)^2(2\pi)^{\frac{1}{2}}} \times \int_0^\infty \frac{\exp[-(1+i\omega)x/z - z^2/2]}{\tilde X^+(z)\tilde X^-(z)\tilde X(-z)} \times \frac{z^2+2}{3(z^2-z_0^2)}h(z)\,dz, \quad (5.23)$$

where

$$h(z) = \tilde X^+(z)[1 + i\omega 3zg_0(z)/(z^2+2)] + \{\tilde N^+(z)/[(i\omega)^2(z-z_0)]\}[1 + i\omega 2(2z^2+1)/(z^2+2)]. \quad (5.24)$$

The integral is of the form

$$I(x) = \int_0^\infty e^{-(1+i\omega)x/z - z^2/2}q(z)\,dz.$$

Set $z = (1+i\omega)^{\frac{1}{3}}x^{\frac{1}{3}}w$ and take the principal branch of the cube root. The path can be taken as the real axis again and

$$I(x) = \int_0^\infty \exp\left[-(1+i\omega)^{\frac{2}{3}}x^{\frac{2}{3}}\left(\frac{1}{w} + \frac{w^2}{2}\right)\right] \times q[z(w)]\frac{dz}{dw}\,dw.$$

The exponential has a maximum at $w = 1$, and by Laplace's formula, for x large, $I(x) \sim (2\pi/3)^{\frac{1}{2}} \times \exp[-\frac{3}{2}z_m^2]q(z_m)$, where

$$z_m = (1+i\omega)^{\frac{1}{3}}x^{\frac{1}{3}}. \quad (5.25)$$

Therefore, (5.23) becomes

$$u_c(x) \sim -\frac{1+i\omega}{(i\omega)^2\sqrt{3}} \times \exp\left[-\tfrac{3}{2}z_m^2\right] \frac{h(z_m)}{\tilde{X}^+(z_m)\tilde{X}^-(z_m)\tilde{X}(-z_m)} \times \frac{z_m^2+2}{3(z_m^2-z_0^2)}.$$

If we keep all first-order terms for z_m large (x large), we find

$$u_c(x) \sim \frac{1+i\omega}{(i\omega)^2 3\sqrt{3}} e^{-\frac{3}{2}z_m^2} \frac{z_m^5}{z_m^2-z_0^2}\left(\frac{1}{z_m}[1+\tfrac{3}{2}i\omega z_m\alpha_2(\omega)] - \frac{\tilde{N}^+(\infty)}{z_m(i\omega)^2(z_m-z_0)}(1+4i\omega)\right), \quad (5.26)$$

with

$$\tilde{N}^+(\infty) = \int_0^\infty \frac{\Omega(t)t}{\tilde{X}(-t)} \frac{[i\omega t g_0(t) + \frac{1}{3}(t^2+2)]\,dt}{(t+z_0)}. \quad (5.27)$$

Thus in the limit of large x the continuous spectrum, being $O(\exp[-\frac{3}{2}x^{\frac{4}{3}}])$ by (5.25), (5.26), dominates the point spectrum. This result was first obtained in Ref. 11 and in another context in Ref. 16. If one takes x large as the hydrodynamic limit, then this result contradicts hydrodynamic theory which predicts that the point spectrum is dominant. Shortly we give a proper definition of what is the hydrodynamic limit, and this resolves the contradiction.

For the positive wave model, the same type of argument may be given and a result similar to (5.26) can be obtained. In view of the similarity a separate analysis does not seem warranted.

Hydrodynamic limit: We now define the hydrodynamic limit to be

$$\frac{x'\omega'}{(RT_0)^{\frac{1}{2}}} \text{ fixed}, \quad \nu \to \infty. \quad (5.28)$$

Here x' is physical distance from the walls, $(RT_0)^{\frac{1}{2}}/\omega'$ is the wavelength of the sound disturbance, and ν is the collision frequency. In dimensionless variables, the normalization (2.2), we have that (5.28) is equivalent to

$$x\omega \text{ fixed}, \quad \omega \to 0. \quad (5.29)$$

The consequences of this limit given below should serve as sufficient motivation for making this definition.

Let us consider the exponential behavior of the point and continuous spectra under this limit. The continuous spectrum for both models has the factor

$$\exp[-\tfrac{3}{2}x^{\frac{4}{3}}] = \exp[-\tfrac{3}{2}(\omega x)^{\frac{4}{3}}(1/\omega)^{\frac{4}{3}}] \sim \exp[-\tfrac{3}{2}(1/\omega)^{\frac{4}{3}}]. \quad (5.30)$$

The point spectrum, on the other hand, is, by taking the real part to first order,

$$\exp[-\tfrac{3}{5}(\tfrac{2}{5})^{\frac{1}{3}}\omega^2 x] = \exp[-\tfrac{2}{5}(\tfrac{3}{5})^{\frac{1}{3}}(\omega x)\omega] = O(1). \quad (5.31)$$

Clearly the point spectrum dominates and the hydrodynamic solution (5.16) or (5.22) results. It is of interest to consider the sequence of limits

$$\omega^n x \text{ fixed}, \quad \omega \to 0, \quad (5.32)$$

for $n = 1, 2, 3, \cdots$. By (5.30), (5.31) it is apparent that the point spectrum will still dominate for $n - 2 < 2n/3$, i.e., $n < 6$. Hence hydrodynamics results as long as

$$x \ll 1/\omega^6. \quad (5.33)$$

Otherwise the continuous spectrum will appear as a boundary layer at infinity at the order (5.33).

We refer to the change of dominance in the point and continuous spectra as "crossover." Therefore, condition (5.33) can be referred to as asymptotic crossover, that is, for $x \leq O(1/\omega^6)$ the continuous spectrum certainly dominates. It seems worthwhile having a more precise criteria for crossover since conceivably this might be measurable in an experiment. The lead term of u_p for the adiabatic model, from (5.16), is

$$u_p(x) \sim \exp[-(\tfrac{3}{5})^{\frac{1}{3}}i\omega x - \tfrac{2}{5}(\tfrac{3}{5})^{\frac{1}{3}}\omega^2 x]. \quad (5.34)$$

The continuous spectrum is calculated from (5.25), (5.26), and we find, keeping all first-order terms,

$$u_c(x) \sim -\frac{x^{\frac{5}{3}}\exp(-\frac{3}{2}x^{\frac{2}{3}})}{3^{\frac{1}{3}}(5+3\omega^2 x^{\frac{4}{3}})}\left(\frac{1}{x^{\frac{1}{3}}}[1+\tfrac{3}{2}i\omega x^{\frac{1}{3}}\alpha_2(0)] - \frac{1}{x^{\frac{1}{3}}}[(\tfrac{3}{5})^{\frac{1}{3}}i\omega x^{\frac{1}{3}}+I]\right). \quad (5.35)$$

To evaluate $\tilde{N}^+(\infty)$, (5.27), in the limit of ω small, we have used the fact that

$$\int_0^\infty \frac{\Omega(t)t}{X(-t,0)}(t^2+2)\,dt = -5, \quad (5.36)$$

which follows by expanding (4.44) for z large and ω small. The explicit crossover is obtained from the match of (5.34) and (5.35). Although $\alpha_2(0)$ is not known, its explicit form is not important since it will be $O(1)$.

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APPENDIX A: THE DISPERSION RELATIONS

Adiabatic Model

The dispersion relation is defined to be $1 - K = 0$ and is of a class that has been exhaustively studied in Refs. 24 and 25. In particular the roots come in pairs. For ω small, we find

$$-ik = \pm(\tfrac{3}{5})^{\frac{1}{2}} i\omega[1 - \tfrac{2}{5}i\omega + \tfrac{7}{25}(i\omega)^2 + O(\omega^2)], \quad \text{(A1)}$$

or, in the z variable,

$$1/z = \mp(\tfrac{3}{5})^{\frac{1}{2}} i\omega[1 - \tfrac{7}{5}i\omega + \tfrac{42}{25}(i\omega)^2 + O(\omega^3)]. \quad \text{(A2)}$$

We denote the root in the fourth quadrant by $+k_0$ (or $+z_0$). Using the methods of Ref. 24, one can show that there are in fact only the two roots as given above. Waves to the right and left are produced, moving at the adiabatic speed to lowest order and decaying in the direction of propagation. It is also known[25] that there exists a $\omega_0 > 0$ such that no roots exists for $\omega > \omega_0$. By arguments similar to (3.8)–(3.10) it is possible to show that there is no root of $\operatorname{Im} k = 0$, $\omega \neq 0$.

Positive Wave Model

The dispersion relation for this model, from (4.34), is

$$1 - \tfrac{1}{30}\int_{-\infty}^{\infty} \Omega(t)[t^4 + 2(15)^{\frac{1}{2}}t^3 + 19t^2 + 4(15)^{\frac{1}{2}}t + 8]\, dt/(1 + i\omega - ikt) = 0, \quad \text{(A3)}$$

or (4.58) in the z variable. For ω small we find the root in the fourth quadrant

$$+ik = \tfrac{3}{5}i\omega[1 - \tfrac{1}{5}i\omega + O(\omega^2)]. \quad \text{(A4)}$$

This dispersion relation lacks the symmetry present in the adiabatic model. We want to show that (A4) is the only root of (A3). To carry this out, we study wave solutions of (3.23), (3.24),

$$(1 + i\omega + s\xi_1)g = (1/\sqrt{2})(\xi_1 + \xi^2/\sqrt{15})w, \quad \text{(A5)}$$

$$w = 1/\sqrt{2}(\xi_1 + \xi^2/\sqrt{15}, g). \quad \text{(A6)}$$

Taking the inner product of (A5) with respect to g^* and separating real and imaginary parts, we find

$$\omega + s_i(g, \xi_1 g) = 0, \quad \text{(A7)}$$

$$1 + s_r(g, \xi_1 g) = \|w\|^2. \quad \text{(A8)}$$

Here s_r and s_i are the real and imaginary parts of s, $(g, g) = \|g\|^2$, and for convenience we have taken $\|g\| = 1$. Hence, in particular $\|w\| \leq 1$. Equations (A7), (A8) give

$$\omega/(1 - \|w\|^2) = s_i/s_r. \quad \text{(A9)}$$

By assuming $\omega \geq 0$ for definiteness, (A9) implies that admissible roots lie in the first or third quadrant. Now consider (A5) for the limiting case $\omega = 0$. The complex conjugate of (A5) is

$$(1 - w)g^* + s^*\xi_1 g^* = (w^*/\sqrt{2})(\xi_1 + \xi^2/\sqrt{15}). \quad \text{(A10)}$$

Then (A10) multiplied by (A5), for $\omega = 0$, gives

$$|g|^2 + |s|^2\,\xi_1^2\,|g|^2 + 2s_r\xi_1\,|g|^2 = |w|^2/2(\xi_1 + \xi^2/\sqrt{15})^2,$$

and, taking the inner product of this with respect to 1, we have

$$1 + |s|^2\,\|\xi_1 g\|^2 + 2s_r(g, \xi_1 g) = \|w\|^2. \quad \text{(A11)}$$

First suppose that $(g, \xi_1 g) = 0$. Then (A11) is satisfied only if $s = 0$ and $\|w\| = 1$ (or, trivially, $\|\xi_1 g\|^2 = 0$, which implies $g = 0$). Secondly, if $(g, \xi_1 g) \neq 0$, by (A7) $s_i = 0$ for $\omega = 0$. It remains to show that $s_r = 0$ in that case. To do this, define

$$f(z) = \int_{-\infty}^{\infty} \frac{\Omega(t)\, dt}{t - z}.$$

For z above and below the real axis ($\pm$ respectively) the representation

$$f^{\pm}(z) = e^{-z^2/2}\left[\pm\frac{\pi i}{\sqrt{2\pi}} - \int_0^z e^{t^2/2}\, dt\right] \quad \text{(A12)}$$

is known.[24] Then the dispersion relation associated with (A5) is just (4.58) in the z variable, setting $s = -ik = (1 + i\omega)/z$. This can be reduced in terms of (A12) to

$$30(1 + i\omega) + z[f^{\pm}(z)\{z^4 + 2(15)^{\frac{1}{2}}z^3 + 19z^2 + 4(15)^{\frac{1}{2}}z + 8\} + z^3 + 2(15)^{\frac{1}{2}}z^2 + 20z + 6(15)^{\frac{1}{2}}] = 0. \quad \text{(A13)}$$

Now as $\omega \to 0$, $z_1 \to s_i/|s|^2$. Thus any root $z(\omega)$ of (A13) approaches a real value since we have shown that $s_i = 0$ when $\omega = 0$, and by continuity this is true in the limit, i.e., $s_i \to 0$ as $\omega \to 0$. By (A12) the imaginary part of (A13), for $\omega = 0$, is found to be

$$\pi/(2\pi)^{\frac{1}{2}}e^{-z^2/2}zP(z), \quad \text{(A14)}$$

where

$$P(z) = z^4 + 2(15)^{\frac{1}{2}}z^3 + 19z^2 + 4(15)^{\frac{1}{2}}z + 8. \quad \text{(A15)}$$

(A14) is zero if $z = 0$, but then the real part of (A13) is nonzero. We must check for zeros of $P(z)$ for z real. From (4.37) and (A3), P is seen to be the integral of a nonnegative function and therefore nonnegative. The stationary points of (A15) are found to be at $-(15)^{\frac{1}{2}}/2$, $-(15)^{\frac{1}{2}}/2 \pm (7)^{\frac{1}{2}}/2$, and at the minima (A15) is positive. Therefore, (A14) is never zero unless $z_r \to \infty$, which implies $s_r = 0$. Hence we conclude that when $\omega = 0$, $s = 0$. Therefore, at least for ω small, (A4) is the only root of (A3).

APPENDIX B: BOUNDEDNESS OF $u'(0)$ FOR THE ADIABATIC MODEL

That $u'(0)$ ought to exist follows from the continuity equation (3.5), since it exists if and only if $\rho(0)$ does, and the latter must be bounded by physical considerations. Differentiating (4.49) and evaluating at $x = 0$, we get

$$u'(0) = -\frac{(1+i\omega)^2}{(i\omega)^2 z_0^2}\frac{\tilde{N}(z_0)}{\tilde{X}(z_0)} + \frac{(1+i\omega)^2}{(i\omega)^2 2\pi i}\int_0^\infty \frac{1}{(z-z_0)}\cdot\frac{1}{z^2}\left\langle\frac{\tilde{N}(z)}{\tilde{X}(z)}\right\rangle dz. \quad \text{(B1)}$$

By (4.50)–(4.52) we see that

$$\langle \tilde{N}(z)/\tilde{X}(z)\rangle = O(z), \quad \text{(B2)}$$

as $z \to 0$. Therefore, the integrand of the integral in (B1) is $O(1/z)$ for z small and the integral does not appear to exist. We demonstrate that (B2) is in fact $O(z^2)$ so that (B1) does exist.

We begin by Fourier-transforming the continuity equation (3.5) in the z variable, (4.38), to give

$$u(k(z)) = -z/(1+i\omega) + [zi\omega/(1+i\omega)]\rho(k(z)). \quad \text{(B3)}$$

By (4.39)

$$u(k(z)) = \frac{z}{(z-z_0)(i\omega)^2}\langle \tilde{N}(z)/\tilde{X}(z)\rangle, \quad \text{(B4)}$$

and in the limit of z small, by (5.2), (B4) or (B3) is

$$u(k(z)) = -z/(1+i\omega) + O(z). \quad \text{(B5)}$$

Therefore, we must have $\rho(k(z)) = O(z)$ for (B3) to be consistent with (B5). This suggests that we write

$$\rho(k(z)) = z[M(z) + R(z)]/(z-z_0)\tilde{X}(z), \quad \text{(B6)}$$

where we suppose

$$M(z) = \int_0^\infty \frac{m(t)}{\tilde{X}(-t)(t+k_0)}\frac{dt}{t-k}. \quad \text{(B7)}$$

$m(t)$ is to be determined, and we require that M be bounded for z small, consistent with (B3). R is analytic in the plane. The form (B6) only says that ρ has the same singular behavior as u which follows from (B3). Therefore, (B3), (B4), and (B6) give

$$\frac{z}{(z-z_0)(i\omega)^2}\frac{\tilde{N}(z)}{\tilde{X}(z)} = -\frac{z}{1+i\omega} + \frac{z^2 i\omega}{1+i\omega}\frac{[M(z)+R(z)]}{(z-z_0)\tilde{X}(z)}. \quad \text{(B8)}$$

Evaluating the jump of (B8) across the positive real axis, one finds that

$$m(t) = \Omega(t)t\left(g_0(t) - \frac{t^2}{1+i\omega}\right)\frac{1+i\omega}{(i\omega)^2}, \quad \text{(B9)}$$

so that by (B2)

$$M(t) = \frac{1+i\omega}{(i\omega)^2}\int_0^\infty \frac{\Omega(t)t}{\tilde{X}(-t)(t+z_0)} \times \left(g_0(t) - \frac{t^2}{1+i\omega}\right)\frac{dt}{t-z}. \quad \text{(B10)}$$

To determine R, observe that in (B8) the left-hand side is $O(1)$ for z large, $(z-z_0)X(z) = O(1)$ so that $R = O(1/z)$. Hence it is zero everywhere. Also note that by (B10), M is bounded for z small. We thus have with this construction of M that

$$\frac{\tilde{N}(z)}{\tilde{X}(z)} = (i\omega)^2\frac{(z-z_0)}{1+i\omega} + (i\omega)^3 z\frac{M(z)}{\tilde{X}(z)}. \quad \text{(B11)}$$

Now the jump in M is $O(z)$ for z small so that (B2) is actually $O(z^2)$. Therefore, the continuous spectrum integral exists and $u'(0)$ is bounded.

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Formulation of the Many-Body Problem for Composite Particles. III. The Projected Hamiltonian*

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A previously developed representation for many-atom problems is extended by incorporation of all effects of interatomic exchange of electrons and nuclei into a "projected Hamiltonian." An expression for the projected Hamiltonian is derived which is exact on the two-atom subspace, and hence incorporates those exchange effects which are important at low densities. By the use of the center-of-mass separation of atomic wavefunctions, this expression for the projected Hamiltonian is transformed into a representation in terms of atomic field operators $\psi_\nu(\mathbf{r})$ and $\psi_\nu^\dagger(\mathbf{r})$, where $\mathbf{r}$ is the center-of-mass position of an atom and ν stands for all of its internal quantum numbers.

1. INTRODUCTION

Consider a system of n identical atoms, each containing l electrons. In cases where real or virtual internal excitation of the atoms is important, it is necessary to use a representation of the states and observables which takes proper account of the internal structure of the atoms. One such representation is a Schrödinger representation in which all nuclear and electronic variables appear explicitly. However, little practical use has been made of this representation, due to the difficulty of simultaneously treating the dynamics responsible for the existence of the atoms and the dynamics of their interactions. An alternative representation in terms of atomic annihilation and creation operators a_α and $a_\alpha^\dagger$ for atoms in orthonormal single-atom states $\varphi_\alpha(Xx_1\cdots x_l)$ has been developed in two previous papers.[1] These operators satisfy Bose or Fermi commutation or anticommutation relations

$$\begin{aligned} a_\alpha a_\beta - (-1)^{2J+l} a_\beta a_\alpha &= 0, \\ a_\alpha a_\beta^\dagger - (-1)^{2J+l} a_\beta^\dagger a_\alpha &= \delta_{\alpha\beta}, \end{aligned} \tag{1}$$

where J is the nuclear spin. All effects of intra-atomic electron exchange are included by using atomic wavefunctions $\varphi_\alpha(Xx_1\cdots x_l)$ which are antisymmetric in the electron variables $x_1\cdots x_l$, whereas the effects of interatomic exchange of electrons and nuclei are incorporated by requiring that all allowed n-atom state vectors $|\psi\rangle$ satisfy the exchange subsidiary conditions

$$\begin{aligned} I_{\text{nuc}}|\psi\rangle &= (-1)^{2J}\tfrac{1}{2}n(n-1)|\psi\rangle, \\ I_{\text{elec}}|\psi\rangle &= -\tfrac{1}{2}n(n-1)|\psi\rangle. \end{aligned} \tag{2}$$

Here the exchange operators I_{nuc} and I_{elec} are

$$\begin{aligned} I_{\text{nuc}} &= \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\, I_{\text{nuc}}\,|\gamma\delta)a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \\ I_{\text{elec}} &= \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\, I_{\text{elec}}\,|\gamma\delta)a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \end{aligned} \tag{3}$$

and the exchange matrix elements are

$$\begin{aligned} &(\alpha\beta|\, I_{\text{nuc}}\,|\gamma\delta) \\ &= \int \varphi_\alpha^*(Xx_1\cdots x_l)\varphi_\beta^*(X'x_1'\cdots x_l')\varphi_\gamma(X'x_1\cdots x_l) \\ &\quad\times \varphi_\delta(Xx_1'\cdots x_l')\,dX\,dx_1\cdots dx_l\,dX'\,dx_1'\cdots dx_l', \\ &(\alpha\beta|\, I_{\text{elec}}\,|\gamma\delta) \\ &= \int \varphi_\alpha^*(Xx_1\cdots x_l)\varphi_\beta^*(X'x_1'\cdots x_l')\varphi_\gamma(Xx_1'x_2\cdots x_l) \\ &\quad\times \varphi_\delta(X'x_1x_2'\cdots x_l')\,dX\,dx_1\cdots dx_l\,dX'\,dx_1'\cdots dx_l'. \end{aligned} \tag{4}$$

Each x_j stands for both the position $\mathbf{r}_j$ and spin (z-component) variable σ_j of an electron, and $\int dx_j$ implies integration over $\mathbf{r}_j$ and summation over σ_j. Similarly, X_j stands for the position $\mathbf{R}_j$ of a nucleus, and also includes its spin variable in case $J \neq 0$. The space of simultaneous eigenstates of the Hamiltonian H, of I_{nuc} and I_{elec} with the proper eigenvalues (2), and of the total atom-number operator

$$N = \sum_\alpha a_\alpha^\dagger a_\alpha \tag{5}$$

with eigenvalue n is physically and mathematically equivalent to the space of Schrödinger wavefunctions $\psi(X_1\cdots X_n x_1\cdots x_{ln})$ which are antisymmetric in the electron variables $x_1\cdots x_{ln}$ and symmetric ($2J$ even) or antisymmetric ($2J$ odd) in the nuclear variables $X_1\cdots X_n$.

The many-atom Hamiltonian H is

$$\begin{gathered} H = H_0 + V', \\ H_0 = T + V_0, \\ T = \sum_{\alpha\beta} (\alpha|\, T\,|\beta) a_\alpha^\dagger a_\beta, \quad V_0 = \sum_{\alpha\beta} (\alpha|\, V\,|\beta) a_\alpha^\dagger a_\beta, \\ V' = \tfrac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|\, V\,|\gamma\delta) a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \end{gathered} \tag{6}$$

where

$$\begin{aligned} (\alpha|\, T\,|\beta) &= \int \varphi_\alpha^*(X x_1 \cdots x_l) \Big(T(X) + \sum_{j=1}^{l} T(x_j) \Big) \\ &\quad \times \varphi_\beta(X x_1 \cdots x_l)\, dX\, dx_1 \cdots dx_l, \\ (\alpha|\, V\,|\beta) &= \int \varphi_\alpha^*(X x_1 \cdots x_l) \Big(\sum_{j=1}^{l} V(X x_j) + \sum_{j<k}^{l} V(x_j x_k) \Big) \\ &\quad \times \varphi_\beta(X x_1 \cdots x_l)\, dX\, dx_1 \cdots dx_l, \\ (\alpha\beta|\, V\,|\gamma\delta) &= \int \varphi_\alpha^*(X x_1 \cdots x_l) \varphi_\beta^*(X' x_1' \cdots x_l') \\ &\quad \times \Big(V(XX') + \sum_{j=1}^{l} V(X x_j') + \sum_{j=1}^{l} V(X' x_j) \\ &\quad + \sum_{j=1}^{l} \sum_{k=1}^{l} V(x_j x_k') \Big) \varphi_\gamma(X x_1 \cdots x_l) \\ &\quad \times \varphi_\delta(X' x_1' \cdots x_l')\, dX\, dx_1 \cdots dx_l\, dX'\, dx_1' \cdots dx_l'. \end{aligned} \tag{7}$$

Here $T(X)$ and $T(x)$ are the single-nucleus and single-electron kinetic energy operators, and $V(XX')$, $V(Xx)$, and $V(xx')$ are the nucleus–nucleus, nucleus–electron, and electron–electron Coulomb interaction potentials. If the φ_α are chosen to be the single-atom energy eigenstates, i.e.,

$$\begin{aligned} &\Big(T(X) + \sum_{j=1}^{l} T(x_j) + \sum_{j=1}^{l} V(X x_j) + \sum_{j<k}^{l} V(x_j x_k) \Big) \\ &\qquad \times \varphi_\alpha(X x_1 \cdots x_l) = \epsilon_\alpha \varphi_\alpha(X x_1 \cdots x_l), \end{aligned} \tag{8}$$

then H_0 takes on the diagonal form

$$H_0 = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha. \tag{9}$$

Since the operators I_{nuc} and I_{elec} have the same general structure as the interatomic interaction Hamiltonian V', satisfying the subsidiary conditions (2) exactly would be as difficult as treating interatomic interactions exactly. However, by use of projection operators for the subsidiary conditions, it is possible to define a "projected Hamiltonian" in which the subsidiary conditions are incorporated as additional effective interatomic exchange interactions, which can then be treated approximately along with the interatomic Coulomb interactions V'. The formal definition of the projected Hamiltonian is given in Sec. 2. As a preliminary to construction of an explicit expression, the algebraic properties of the exchange matrices and exchange operators (3) are investigated in Sec. 3. With the aid of these algebraic properties, expressions for the projection operators and projected Hamiltonian are obtained in Sec. 4 which are explicit and exact on the subspace of two-atom states. By the use of the center-of-mass separation of the atomic wavefunctions, an alternative representation of the projected Hamiltonian in terms of atomic field operators $\psi_\nu(\mathbf{r})$ and $\psi_\nu^\dagger(\mathbf{r})$ is constructed in Sec. 5, where $\mathbf{r}$ refers to the center-of-mass position of an atom and ν stands for all its internal quantum numbers.

2. PROJECTED HAMILTONIAN

Let $\mathcal{P}_{\text{nuc}}$ be the projection operator which projects onto the subspace of eigenstates of I_{nuc} with eigenvalue $(-1)^{2J} \frac{1}{2} n(n-1)$, and let $\mathcal{P}_{\text{elec}}$ be the projection operator onto the subspace of eigenstates of I_{elec} with eigenvalue $-\frac{1}{2} n(n-1)$. Since $\mathcal{P}_{\text{nuc}}$ and $\mathcal{P}_{\text{elec}}$ are projection operators and I_{nuc}, I_{elec}, and H are mutually commuting,[1] one has

$$\begin{gathered} \mathcal{P}_{\text{nuc}}^2 = \mathcal{P}_{\text{nuc}}, \quad \mathcal{P}_{\text{elec}}^2 = \mathcal{P}_{\text{elec}}, \\ [\mathcal{P}_{\text{nuc}}, \mathcal{P}_{\text{elec}}] = [\mathcal{P}_{\text{nuc}}, H] = [\mathcal{P}_{\text{elec}}, H] = 0. \end{gathered} \tag{10}$$

Let $|\lambda_{\text{nuc}}, \lambda_{\text{elec}}\rangle$ be a simultaneous eigenstate of I_{nuc} and I_{elec} with eigenvalues λ_{nuc} and λ_{elec}. Then by the definition of projection operators

$$\begin{aligned} &\mathcal{P}_{\text{nuc}} |\lambda_{\text{nuc}}, \lambda_{\text{elec}}\rangle \\ &\qquad = \delta(\lambda_{\text{nuc}}, (-1)^{2J} \tfrac{1}{2} n(n-1))\, |\lambda_{\text{nuc}}, \lambda_{\text{elec}}\rangle, \\ &\mathcal{P}_{\text{elec}} |\lambda_{\text{nuc}}, \lambda_{\text{elec}}\rangle \\ &\qquad = \delta(\lambda_{\text{elec}}, -\tfrac{1}{2} n(n-1))\, |\lambda_{\text{nuc}}, \lambda_{\text{elec}}\rangle, \end{aligned} \tag{11}$$

where $\delta(\lambda, \lambda')$ is the Kronecker delta function $\delta_{\lambda\lambda'}$. Conversely, if $|\psi\rangle$ is an n-atom state satisfying

$$\mathcal{P}_{\text{nuc}} |\psi\rangle = |\psi\rangle, \quad \mathcal{P}_{\text{elec}} |\psi\rangle = |\psi\rangle, \tag{12}$$

then $|\psi\rangle$ is a simultaneous eigenstate of I_{nuc} and I_{elec} with eigenvalues $(-1)^{2J} \frac{1}{2} n(n-1)$ and $-\frac{1}{2} n(n-1)$, i.e., $|\psi\rangle$ satisfies the subsidiary conditions (2).

Let H be the Hamiltonian (6) and define the "projected Hamiltonian"

$$\mathcal{H} = \mathcal{P}_{\text{nuc}} \mathcal{P}_{\text{elec}} H. \tag{13}$$

Suppose that $|\psi\rangle$ is an eigenstate of $\mathcal{H}$:

$$\mathcal{H} |\psi\rangle = E |\psi\rangle. \tag{14}$$

Then one has[2] with (10) and (13)

$$\begin{aligned} \mathcal{P}_{\text{nuc}} |\psi\rangle &= E^{-1} \mathcal{P}_{\text{nuc}} \mathcal{H} |\psi\rangle = E^{-1} \mathcal{P}_{\text{nuc}}^2 \mathcal{P}_{\text{elec}} H |\psi\rangle \\ &= E^{-1} \mathcal{P}_{\text{nuc}} \mathcal{P}_{\text{elec}} H |\psi\rangle = E^{-1} \mathcal{H} |\psi\rangle = |\psi\rangle. \end{aligned} \tag{15}$$

Similarly

$$\mathcal{P}_{\text{elec}} |\psi\rangle = |\psi\rangle. \tag{16}$$

It follows that any n-atom eigenstate of $\mathcal{K}$ automatically satisfies the subsidiary conditions (2). Furthermore, such an eigenstate of $\mathcal{K}$ is also an eigenstate of H with the same eigenvalue. To see this, it is merely necessary to note from (10) and (13)–(16) that

$$E|\psi\rangle = \mathcal{K}|\psi\rangle = H\mathcal{S}_{\rm nuc}\mathcal{S}_{\rm elec}|\psi\rangle = H|\psi\rangle. \quad (17)$$

Finally, since $\mathcal{S}_{\rm nuc}$, $\mathcal{S}_{\rm elec}$, and H are Hermitian and mutually commuting, it follows that $\mathcal{K}$ is Hermitian. Its n-atom eigenstates consist of those n-atom eigenstates of H which satisfy the subsidiary conditions (2), and the eigenvalues of $\mathcal{K}$ are equal to the corresponding eigenvalues of H.

3. ALGEBRAIC PROPERTIES OF THE EXCHANGE OPERATORS

Explicit expressions for $\mathcal{S}_{\rm nuc}$ and $\mathcal{S}_{\rm elec}$ correct through two-atom terms can be found by making use of algebraic properties of the exchange matrices (4). It is convenient to define new matrices $(\alpha\beta|\, I'_{\rm nuc}\,|\gamma\delta)$ and $(\alpha\beta|\, I'_{\rm elec}\,|\gamma\delta)$ as follows:

$$\begin{aligned}(\alpha\beta|\, I'_{\rm nuc}\,|\gamma\delta) &= (\alpha\beta|\, I_{\rm nuc}\,|\gamma\delta) - (-1)^{2J}\delta_{\alpha\gamma}\delta_{\beta\delta},\\ (\alpha\beta|\, I'_{\rm elec}\,|\gamma\delta) &= (\alpha\beta|\, I_{\rm elec}\,|\gamma\delta) + \delta_{\alpha\gamma}\delta_{\beta\delta}. \end{aligned} \quad (18)$$

We then define

$$\begin{aligned} I'_{\rm nuc} &= \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\, I'_{\rm nuc}\,|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma,\\ I'_{\rm elec} &= \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\, I'_{\rm elec}\,|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \end{aligned} \quad (19)$$

in analogy with (3). Noting that

$$\sum_{\alpha\beta} a^\dagger_\alpha a^\dagger_\beta a_\beta a_\alpha = N(N-1), \quad (20)$$

where N is the atom-number operator (5), one sees that on the space of n-atom states the subsidiary conditions (2) are equivalent to

$$I'_{\rm nuc}|\psi\rangle = I'_{\rm elec}|\psi\rangle = 0. \quad (21)$$

We shall show that within the two-atom state space the operators $I'_{\rm nuc}$, $I'_{\rm elec}$, and certain other operators related to multiple electron exchange form an algebra, i.e., powers and products of these operators are *linear* combinations of the operators in the set.

Consider first $(I'_{\rm nuc})^2$. Squaring the top Eq. (3) and putting all terms into normal order, one finds with (1)

$$\begin{aligned}(I'_{\rm nuc})^2 = \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}\sum_{\alpha_1\alpha_2}&(\alpha\beta|\, I'_{\rm nuc}\,|\alpha_1\alpha_2)\\ &\times[(\alpha_1\alpha_2|\, I'_{\rm nuc}\,|\gamma\delta) + (-1)^{2J+l}(\alpha_2\alpha_1|\, I'_{\rm nuc}\,|\gamma\delta)]\\ &\times a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + (a^\dagger a^\dagger a^\dagger aaa)\\ &+ (a^\dagger a^\dagger a^\dagger a^\dagger aaaa), \end{aligned} \quad (22)$$

where the abbreviated terms in parentheses stand for sums of terms proportional to products of creation and annihilation operators of the indicated structures (three-atom and four-atom operators), which are identically zero on the space of two-atom states. Now it follows from its definition that

$$(\alpha_2\alpha_1|\, I'_{\rm nuc}\,|\gamma\delta) = (\alpha_1\alpha_2|\, I'_{\rm nuc}\,|\delta\gamma). \quad (23)$$

Then, using (1), one has

$$(I'_{\rm nuc})^2 = \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\,(I'_{\rm nuc})^2\,|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + \cdots, \quad (24)$$

where, here and throughout this paper, the dots stand for terms which vanish identically on the two-atom subspace (three-atom, four-atom, ... terms) and where the matrix product notation

$$(\alpha\beta|\, AB\,|\gamma\delta) \equiv \sum_{\alpha_1\alpha_2}(\alpha\beta|\, A\,|\alpha_1\alpha_2)(\alpha_1\alpha_2|\, B\,|\gamma\delta) \quad (25)$$

has been employed. By (18) and (25)

$$\begin{aligned}(\alpha\beta|\,(I'_{\rm nuc})^2\,|\gamma\delta) = \delta_{\alpha\gamma}\delta_{\beta\delta} &- 2(-1)^{2J}(\alpha\beta|\, I_{\rm nuc}\,|\gamma\delta)\\ &+ (\alpha\beta|\, I^2_{\rm nuc}\,|\gamma\delta). \end{aligned} \quad (26)$$

To evaluate the remaining matrix product in (26), we make use of the orthonormality and completeness relations

$$\begin{aligned}&\int \varphi^*_\alpha(Xx_1\cdots x_l)\varphi_\beta(Xx_1\cdots x_l)\,dX\,dx_1\cdots dx_l = \delta_{\alpha\beta},\\ &\sum_\alpha \varphi_\alpha(Xx_1\cdots x_l)\varphi^*_\alpha(X'x'_1\cdots x'_l)\\ &\quad = (l!)^{-1}\delta(X-X')\\ &\qquad\times\sum_P(-1)^{p(P)}P[\delta(x_1-x'_1)\cdots\delta(x_l-x'_l)], \end{aligned} \quad (27)$$

where $\sum_P$ runs over all $l!$ permutations of $x_1\cdots x_l$, and $(-1)^{p(P)}$ is $+1$ for even and -1 for odd permutations.[3] It then follows with (25) and (4) that[4]

$$(\alpha\beta|\, I^2_{\rm nuc}\,|\gamma\delta) = \delta_{\alpha\gamma}\delta_{\beta\delta}. \quad (28)$$

Hence one has with (18) and (26)

$$(\alpha\beta|\,(I'_{\rm nuc})^2\,|\gamma\delta) = -2(-1)^{2J}(\alpha\beta|\, I'_{\rm nuc}\,|\gamma\delta) \quad (29)$$

so that (24) becomes

$$(I'_{\rm nuc})^2 = -2(-1)^{2J}I'_{\rm nuc} + \cdots. \quad (30)$$

Thus, if we neglect the three-atom and four-atom terms which are identically zero on the two-atom subspace ($n=2$) and small if the number density of atoms is low, then $(I'_{\rm nuc})^2$ is linear in $I'_{\rm nuc}$.

Consider next $(I'_{\rm elec})^2$. One has in analogy with (22)

$$(I'_{\rm elec})^2 = \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\,(I'_{\rm elec})^2\,|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + \cdots. \quad (31)$$

By (18)

$$(\alpha\beta|\,(I'_{\rm elec})^2\,|\gamma\delta) = \delta_{\alpha\gamma}\delta_{\beta\delta} + 2(\alpha\beta|\,I_{\rm elec}\,|\gamma\delta) + (\alpha\beta|\,I^2_{\rm elec}\,|\gamma\delta). \quad (32)$$

It follows from (4), (25), and (27) that

$$\begin{aligned}(\alpha\beta|\,I^2_{\rm elec}\,|\gamma\delta) &= (l!)^{-2}\int \varphi^*_\alpha(Xx_1\cdots x_l)\varphi^*_\beta(X'x'_1\cdots x'_l)\\ &\times \varphi_\gamma(Yy'_1y_2\cdots y_l)\varphi_\delta(Y'y_1y'_2\cdots y'_l)\\ &\times \delta(X-Y)\delta(X'-Y')\\ &\times \sum_P (-1)^{p(P)}P[\delta(y_1-x'_1)\delta(y_2-x_2)\cdots\delta(y_l-x_l)]\\ &\times \sum_{P'}(-1)^{p(P')}P'[\delta(y'_1-x_1)\delta(y'_2-x'_2)\cdots\delta(y'_l-x'_l)]\\ &\times dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l\\ &\times dY\,dy_1\cdots dy_l\,dY'\,dy'_1\cdots dy'_l, \end{aligned} \quad (33)$$

where P is an arbitrary permutation of $y_1\cdots y_l$ and P' is an arbitrary permutation of $y'_1\cdots y'_l$. The set of all P can be decomposed into l disjoint subsets $\mathcal{S}_1\cdots\mathcal{S}_l$, where $\mathcal{S}_j$ consists of those $(l-1)!$ permutations for which $Py_1 = y_j$. Furthermore, $\mathcal{S}_j$ is identical with the set of all $(l-1)!$ permutations of $y_1\cdots y_{j-1}y_{j+1}\cdots y_l$. The set of all P' can be decomposed similarly. Making use of the antisymmetry of φ^*_α and φ^*_β, one then finds eventually

$$(\alpha\beta|\,I^2_{\rm elec}\,|\gamma\delta) = l^{-2}[\delta_{\alpha\gamma}\delta_{\beta\delta} - 2(l-1)(\alpha\beta|\,I_{\rm elec}\,|\gamma\delta) + (l-1)^2(\alpha\beta|\,I_2\,|\gamma\delta)]. \quad (34)$$

Here $(\alpha\beta|\,I_2\,|\gamma\delta)$ is the matrix element of double electron exchange; more generally, we define the j-fold electron exchange matrix as

$$\begin{aligned}(\alpha\beta|\,I_j\,|\gamma\delta) = \int \varphi^*_\alpha(Xx_1\cdots x_l)\varphi^*_\beta(X'x'_1\cdots x'_l)\\ \times \varphi_\gamma(Xx'_1\cdots x'_jx_{j+1}\cdots x_l)\\ \times \varphi_\delta(X'x_1\cdots x_jx'_{j+1}\cdots x'_l)\\ \times dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l \end{aligned} \quad (35)$$

for $1 \le j \le l$. Defining

$$(\alpha\beta|\,I'_j\,|\gamma\delta) = (\alpha\beta|\,I_j\,|\gamma\delta) - (-1)^j\delta_{\alpha\gamma}\delta_{\beta\delta}, \quad (36)$$

one then finds with (18) and (32)

$$(\alpha\beta|\,(I'_{\rm elec})^2\,|\gamma\delta) = 2l^{-2}(l^2-l+1)(\alpha\beta|\,I'_{\rm elec}\,|\gamma\delta) + l^{-2}(l-1)^2(\alpha\beta|\,I'_2\,|\gamma\delta). \quad (37)$$

Then by (31)

$$(I'_{\rm elec})^2 = 2l^{-2}(l^2-l+1)I'_{\rm elec} + l^{-2}(l-1)^2I'_2 + \cdots, \quad (38)$$

where

$$I'_j = \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\,I'_j\,|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma. \quad (39)$$

It follows that within the two-atom state space, $(I'_{\rm elec})^2$ is linear in $I'_{\rm elec}$ and I'_2.

Similar derivations, which we shall omit, show that[5]

$$I'_{\rm nuc}I'_{\rm elec} = I'_{\rm nuc} - (-1)^{2J}I'_{\rm elec} + (-1)^{2J+l}I'_{l-1} + \cdots \quad (40)$$

and more generally

$$I'_{\rm nuc}I'_j = -(-1)^jI'_{\rm nuc} - (-1)^{2J}I'_j + (-1)^{2J+l}I'_{l-j} + \cdots \quad (41)$$

for $1 \le j \le l-1$ and $l \ge 2$.

The results obtained so far suggest that, within the two-atom state space, the operators $I'_{\rm nuc}$, $I'_{\rm elec}$, $I'_2, \cdots, I'_{l-1}$ form an algebra, i.e., all powers and products of these operators are linear combinations of the same l operators. This is indeed the case. To complete the proof, it is necessary to evaluate the squares of the operators I'_j and their products with themselves and with $I'_{\rm elec}$ for $2 \le j \le l-1$. By a derivation paralleling that of (38), one finds

$$\begin{aligned}I'_{\rm elec}I'_j &= I'_jI'_{\rm elec}\\ &= -(-1)^jI'_{\rm elec} + (j/l)^2I'_{j-1}\\ &\quad + l^{-2}(l^2-2jl+2j^2)I'_j\\ &\quad + l^{-2}(l-j)^2I'_{j+1} + \cdots \end{aligned} \quad (42)$$

for $2 \le j \le l-1$ and $l \ge 3$. Because of the identities

$$I'_1 = I'_{\rm elec}, \quad I'_l = (-1)^{2J+l}I'_{\rm nuc}, \quad (43)$$

the cases $j = 2$ and $j = l-1$ are exceptional; in these cases (42) reduces to

$$I'_{\rm elec}I'_2 = -l^{-2}(l^2-4)I'_{\rm elec} + l^{-2}(l^2-4l+8)I'_2 + l^{-2}(l-2)^2I'_3 + \cdots \quad (44)$$

and

$$I'_{\rm elec}I'_{l-1} = (-1)^lI'_{\rm elec} + l^{-2}(l-1)^2I'_{l-2} + l^{-2}(l^2-2l+2)I'_{l-1} + l^{-2}(-1)^{2J+l}I'_{\rm nuc} + \cdots. \quad (45)$$

It is not difficult to see, more generally, that within the two-atom subspace $I'_jI'_k$, for arbitrary j and k, is a linear combination of the I'_m. However, to evaluate the projection operators $\mathcal{P}_{\rm nuc}$ and $\mathcal{P}_{\rm elec}$, it will not be necessary to know the explicit expressions.

4. EXPLICIT EXPRESSIONS FOR PROJECTION OPERATORS AND PROJECTED HAMILTONIAN

We now have sufficient information to obtain explicit expressions for the projection operators and projected Hamiltonian correct up to two-atom terms, i.e., exact on the two-atom state space.

Consider first the projection operator $\mathcal{P}_{\rm nuc}$. It is surely some function of $I'_{\rm nuc}$, and from (30) we know that on the two-atom subspace it is a *linear* function

of $I'_{\rm nuc}$. In fact, we shall show that

$$\mathfrak{F}_{\rm nuc} = 1 + \tfrac{1}{2}(-1)^{2J} I'_{\rm nuc} + \cdots \tag{46}$$

We note first, from (30), that (46) satisfies

$$I'_{\rm nuc}\mathfrak{F}_{\rm nuc}|2\rangle = 0, \quad \mathfrak{F}^2_{\rm nuc}|2\rangle = \mathfrak{F}_{\rm nuc}|2\rangle, \tag{47}$$

where $|2\rangle$ is an arbitrary two-atom state. Equations (47) are necessary, but not sufficient, conditions for the correctness of (46). In fact, if $\mathfrak{F}'$ is any projection operator which commutes with $I'_{\rm nuc}$ and $\mathfrak{F}_{\rm nuc}$, then (47) remains satisfied if $\mathfrak{F}_{\rm nuc}$ is replaced by[6] $\mathfrak{F}'\mathfrak{F}_{\rm nuc}$. In order to see that (46) is nevertheless the correct expression, we note from (30) that on the two-atom state space $I'_{\rm nuc}$ has precisely two eigenvalues, $\lambda'_{\rm nuc} = 0$ corresponding to states satisfying the subsidiary condition and $\lambda'_{\rm nuc} = -2(-1)^{2J}$ corresponding to eigenstates of $I'_{\rm nuc}$ which violate the subsidiary condition. Let $|2'\rangle$ be any two-atom state with the wrong eigenvalue of $I'_{\rm nuc}$, i.e.,

$$I'_{\rm nuc}|2'\rangle = -2(-1)^{2J}|2'\rangle. \tag{48}$$

Then (46) satisfies

$$\mathfrak{F}'_{\rm nuc}|2'\rangle = 0. \tag{49}$$

Conditions (47) and (49) are both necessary and sufficient for the correctness of (46).

Determination of $\mathfrak{F}_{\rm elec}$ is more complicated. We expect that $\mathfrak{F}_{\rm elec}$ is some function of $I'_{\rm elec}$, and hence, from the results of Sec. 3, that it is a *linear* function of the l operators $I'_{\rm nuc}$, $I'_{\rm elec}$, and I'_j for $2 \le j \le l-1$. In fact, it is shown in Appendix A that

$$\mathfrak{F}_{\rm elec} = 1 + c_{\rm nuc} I'_{\rm nuc} + c_{\rm elec} I'_{\rm elec} + \sum_{j=2}^{l-1} c_j I'_j + \cdots, \tag{50}$$

where

$$\begin{aligned} c_{\rm nuc} &= (-1)^{2J} l^{-2} d_l, \\ c_{\rm elec} &= -d_l, \\ c_j &= (-1)^j [(l-1)!/j!\,(l-j)!]^2 d_l, \quad 2 \le j \le l-1 \\ d_l &= l^2 (l!)^2/(2l)!. \end{aligned} \tag{51}$$

The derivation is not valid in the simplest cases $l = 1$, 2, and 3, but the expressions (50) and (51) remain valid in those cases if correctly interpreted. Independent derivations show that

$$\begin{aligned} \mathfrak{F}_{\rm elec} &= 1 - \tfrac{1}{2} I'_{\rm elec} + \cdots \\ &= 1 + \tfrac{1}{2}(-1)^{2J} I'_{\rm nuc} + \cdots, \quad l = 1, \\ \mathfrak{F}_{\rm elec} &= 1 + \tfrac{1}{6}(-1)^{2J} I'_{\rm nuc} \\ &\quad - \tfrac{2}{3} I'_{\rm elec} + \cdots, \quad l = 2, \\ \mathfrak{F}_{\rm elec} &= 1 + \tfrac{1}{20}(-1)^{2J} I'_{\rm nuc} \\ &\quad - \tfrac{9}{20} I'_{\rm elec} + \tfrac{9}{20} I'_2 + \cdots, \quad l = 3. \end{aligned} \tag{52}$$

The derivation of (50) and (51) given in Appendix A shows that furthermore

$$\mathfrak{F}_{\rm nuc}\mathfrak{F}_{\rm elec} = \mathfrak{F}_{\rm elec}. \tag{53}$$

Although this appears remarkable at first sight, on further reflection one realizes that it is to be expected since exchange of nuclei between two atoms is equivalent to exchange of the atoms followed by exchange of all electrons. The proper symmetry under exchange of atoms is ensured by the commutation relations (1), and antisymmetry under single electron exchanges, ensured by the projection operator $\mathfrak{F}_{\rm elec}$ and the antisymmetry of the φ_α, implies antisymmetry under multiple electron exchanges, since any permutation is a product of interchanges. Thus (53) is to be expected.

Defining a total exchange operator

$$I' = \tfrac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|\, I' \,|\gamma\delta) a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma, \tag{54}$$

where

$$\begin{aligned} (\alpha\beta|\, I' \,|\gamma\delta) &= c_{\rm nuc}(\alpha\beta|\, I'_{\rm nuc}\,|\gamma\delta) + c_{\rm elec}(\alpha\beta|\, I'_{\rm elec}\,|\gamma\delta) \\ &\quad + \sum_{j=2}^{l-1} c_j (\alpha\beta|\, I'_j\,|\gamma\delta), \end{aligned} \tag{55}$$

one sees from (50) and (53) that

$$\mathfrak{F}_{\rm nuc}\mathfrak{F}_{\rm elec} = 1 + I' + \cdots. \tag{56}$$

The two-atom operator I' depends on the details of the atomic shell structure via the exchange matrix elements in (55). When the atoms overlap strongly, terms involving multiple electron exchange make the major contribution[7] for a large atom ($l \gg 1$). On the other hand, multiple-exchange effects fall off much more rapidly with increasing atomic separation than does the single-exchange term.

An expression for the projected Hamiltonian which is explicit up to two-atom terms can now be derived by substituting (56) and (6) into (13) and putting all terms into normal order with the aid of (1). The derivation is carried out in Appendix B. The resultant expression for the projected Hamiltonian is

$$\begin{aligned} \mathcal{H} &= H + V_{\rm ex} + \cdots = H_0 + V' + V_{\rm ex} + \cdots, \\ V_{\rm ex} &= \tfrac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|\, V_{\rm ex}\,|\gamma\delta) a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma, \end{aligned} \tag{57}$$

where the matrix elements of the exchange interaction $V_{\rm ex}$ are

$$\begin{aligned} &(\alpha\beta|\, V_{\rm ex}\,|\gamma\delta) \\ &\quad = c_{\rm nuc}(\alpha\beta|\, V_{\rm nuc}\,|\gamma\delta) + c_{\rm elec}(\alpha\beta|\, V_{\rm elec}\,|\gamma\delta) \\ &\qquad + \sum_{j=2}^{l-1} c_j (\alpha\beta|\, V_j\,|\gamma\delta). \end{aligned} \tag{58}$$

Here

$$
\begin{aligned}
&(\alpha\beta|\, V_{\text{nuc}}\,|\gamma\delta) \\
&\quad = \int \varphi_\alpha^*(Xx_1\cdots x_l)\varphi_\beta^*(X'x_1'\cdots x_l') \\
&\qquad \times H(XX'x_1\cdots x_l x_1'\cdots x_l') \\
&\qquad \times [\varphi_\gamma(X'x_1\cdots x_l)\varphi_\delta(Xx_1'\cdots x_l') \\
&\qquad - (-1)^{2J}\varphi_\gamma(Xx_1\cdots x_l)\varphi_\delta(X'x_1'\cdots x_l')] \\
&\qquad \times dX\, dx_1\cdots dx_l\, dX'\, dx_1'\cdots dx_l', \\
&(\alpha\beta|\, V_{\text{elec}}\,|\gamma\delta) \\
&\quad = \int \varphi_\alpha^*(Xx_1\cdots x_l)\varphi_\beta^*(X'x_1'\cdots x_l') \\
&\qquad \times H(XX'x_1\cdots x_l x_1'\cdots x_l') \\
&\qquad \times [\varphi_\gamma(Xx_1'x_2\cdots x_l)\varphi_\delta(X'x_1x_2'\cdots x_l') \\
&\qquad + \varphi_\gamma(Xx_1\cdots x_l)\varphi_\delta(X'x_1'\cdots x_l')] \\
&\qquad \times dX\, dx_1\cdots dx_l\, dX'\, dx_1'\cdots dx_l', \\
&(\alpha\beta|\, V_j\,|\gamma\delta) \\
&\quad = \int \varphi_\alpha^*(Xx_1\cdots x_l)\varphi_\beta^*(X'x_1'\cdots x_l') \\
&\qquad \times H(XX'x_1\cdots x_l x_1'\cdots x_l') \\
&\qquad \times [\varphi_\gamma(Xx_1'\cdots x_j'x_{j+1}\cdots x_l) \\
&\qquad \times \varphi_\delta(X'x_1\cdots x_j x_{j+1}'\cdots x_l') \\
&\qquad - (-1)^j\varphi_\gamma(Xx_1\cdots x_l)\varphi_\delta(X'x_1'\cdots x_l')] \\
&\qquad \times dX\, dx_1\cdots dx_l\, dX'\, dx_1'\cdots dx_l'
\end{aligned}
\tag{59}
$$

and $H(XX'x_1\cdots x_lx_1'\cdots x_l')$ is the total Schrödinger Hamiltonian of all the particles in both atoms, treated on an equal footing:

$$
\begin{aligned}
&H(XX'x_1\cdots x_lx_1'\cdots x_l') \\
&\quad = T(X) + T(X') + V(XX') \\
&\qquad + \sum_{j=1}^{l}[T(x_j) + T(x_j') + V(Xx_j) \\
&\qquad + V(X'x_j') + V(Xx_j') + V(X'x_j)] \\
&\qquad + \sum_{j=1}^{l}\sum_{k=1}^{l}V(x_jx_k') + \sum_{1\le j<k\le l}[V(x_jx_k) + V(x_j'x_k')]
\end{aligned}
\tag{60}
$$

[compare with (6) and (7)].

5. ATOMIC FIELD OPERATORS

The physical significance of the various terms in (57) becomes clearer when one carries out a center-of-mass separation of the atomic wavefunctions φ_α and Fourier transforms the operators a_α and $a_\alpha^\dagger$. The index α of φ_α really stands for a set $\alpha = (\mathbf{k}, \nu)$, where ν is the set of all internal quantum numbers and $\hbar\mathbf{k}$ is the eigenvalue of total linear momentum of the atom. This corresponds to the separation

$$
\varphi_\alpha(Xx_1\cdots x_l) = \Omega^{-\frac{1}{2}}e^{i\mathbf{k}\cdot\mathbf{r}}u_\nu(Xx_1\cdots x_l), \tag{61}
$$

where Ω is the volume of the system, $\mathbf{r}$ is the center-of-mass coordinate

$$
\mathbf{r} = (M + lm)^{-1}[M\mathbf{R} + m(\mathbf{r}_1 + \cdots + \mathbf{r}_l)], \tag{62}
$$

and u_ν, the wavefunction in the center-of-mass system, depends on the nuclear position $\mathbf{R}$ and the electron positions $\mathbf{r}_j$ only in the combinations $\mathbf{R} - \mathbf{r}$, $\mathbf{r}_1 - \mathbf{r}, \cdots, \mathbf{r}_l - \mathbf{r}$. We define the atomic field operator $\psi_\nu(\mathbf{r})$ as

$$
\psi_\nu(\mathbf{r}) = \Omega^{-\frac{1}{2}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}a_{\mathbf{k},\nu}, \tag{63}
$$

where $a_{\mathbf{k},\nu}$ is a_α for the case $\alpha = (\mathbf{k}, \nu)$ and the allowed values of $\mathbf{k}$ are determined by periodic boundary conditions (if Ω is a cube then all components of $\mathbf{k}$ are integral multiples of $2\pi\Omega^{-\frac{1}{3}}$). The operators $\psi_\nu(\mathbf{r})$ and $\psi_\nu^\dagger(\mathbf{r})$ annihilate and create an atom with internal quantum numbers ν (wavefunction u_ν in the center-of-mass system) at position $\mathbf{r}$. The commutation or anticommutation relations

$$
\begin{aligned}
&\psi_\nu(\mathbf{r})\psi_{\nu'}(\mathbf{r}') - (-1)^{2J+l}\psi_{\nu'}(\mathbf{r}')\psi_\nu(\mathbf{r}) = 0, \\
&\psi_\nu(\mathbf{r})\psi_{\nu'}^\dagger(\mathbf{r}') - (-1)^{2J+l}\psi_{\nu'}^\dagger(\mathbf{r}')\psi_\nu(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}')\delta_{\nu\nu'}
\end{aligned}
\tag{64}
$$

follow from (1), (63), and completeness of the exponential. The Dirac delta function $\delta(\mathbf{r} - \mathbf{r}')$ does not imply that the atoms have zero size, but merely that their centers of mass are points.

The projected Hamiltonian can be transformed into the ψ_ν, $\psi_\nu^\dagger$ representation by inserting the inverse of (63),

$$
a_{\mathbf{k},\nu} = \Omega^{-\frac{1}{2}}\int d^3r e^{-i\mathbf{k}\cdot\mathbf{r}}\psi_\nu(\mathbf{r}), \tag{65}
$$

into (57). Consider first the single-atom part H_0 of $\mathcal{H}$. Assume that the φ_α are the single-atom energy eigenstates, so that H_0 has the diagonal form (9). The decomposition (61) of the atomic wavefunctions implies a decomposition

$$
\epsilon_{\mathbf{k}\nu} = \hbar^2k^2/2(M + lm)] + \epsilon_\nu \tag{66}
$$

of the energy eigenvalues ϵ_α [with $\alpha = (\mathbf{k}, \nu)$] into a translational kinetic energy and an internal energy ϵ_ν. Substitution of (66) and (65) into (9) and use of

the completeness relation for the exponential yields

$$H_0 = \sum_\nu \int d^3r \psi_\nu^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2(M+lm)} \nabla^2 + \epsilon_\nu \right) \psi_\nu(\mathbf{r}). \tag{67}$$

This has an obvious physical interpretation as the sum of the translational kinetic energy operator and the internal energy operator $\sum_\nu \epsilon_\nu N_\nu$, where

$$N_\nu = \int d^3r \psi_\nu^\dagger(\mathbf{r}) \psi_\nu(\mathbf{r}) \tag{68}$$

is the number operator for atoms in internal state u_ν.

A similar simplification of the interatomic Coulomb interaction Hamiltonian V' in (57) and (6) arises through the translational invariance[8] of the interaction potentials and the u_ν. For the sake of simplicity and definiteness, we take these potentials to be nonrelativistic Coulomb interactions:

$$V(XX') = (Ze)^2/|\mathbf{R} - \mathbf{R}'|, \quad V(x_j x_k) = e^2/|\mathbf{r}_j - \mathbf{r}_k|,$$
$$V(Xx_j) = -Ze^2/|\mathbf{R} - \mathbf{r}_j|. \tag{69}$$

Then, assuming the atoms to be electrically neutral ($l = Z$), one finds

$$V' = \tfrac{1}{2} \sum_{\nu_1 \cdots \nu_4} \int d^3r d^3r' \psi_{\nu_1}^\dagger(\mathbf{r}) \psi_{\nu_2}^\dagger(\mathbf{r}') \times v_{\nu_1 \cdots \nu}^{\text{Coul}}(\mathbf{r} - \mathbf{r}') \psi_{\nu_4}(\mathbf{r}') \psi_{\nu_3}(\mathbf{r}) \tag{70}$$

with

$$\begin{aligned} v_{\nu_1 \cdots \nu_4}^{\text{Coul}}(\mathbf{r} - \mathbf{r}') &= (Ze)^2 \int u_{\nu_1}^*(X x_1 \cdots x_l) u_{\nu_2}^*(X' x_1' \cdots x_l') \\ &\times (|\mathbf{R} - \mathbf{R}' + \mathbf{r} - \mathbf{r}'|^{-1} + |\mathbf{r}_1 - \mathbf{r}_1' + \mathbf{r} - \mathbf{r}'|^{-1} \\ &- |\mathbf{R} - \mathbf{r}_1' + \mathbf{r} - \mathbf{r}'|^{-1} - |\mathbf{r}_1 - \mathbf{R}' + \mathbf{r} - \mathbf{r}'|^{-1}) \\ &\times u_{\nu_3}(X x_1 \cdots x_l) u_{\nu_4}(X' x_1' \cdots x_l') \\ &\times \delta\left(\frac{M\mathbf{R} + m(\mathbf{r}_1 + \cdots + \mathbf{r}_l)}{M + lm} \right) \\ &\times \delta\left(\frac{M\mathbf{R}' + m(\mathbf{r}_1' + \cdots + \mathbf{r}_l')}{M + lm} \right) \\ &\times dX\, dx_1 \cdots dx_l\, dX'\, dx_1' \cdots dx_l'. \end{aligned} \tag{71}$$

The expression for the interatomic exchange interaction Hamiltonian V_{ex} in (57) is simplified by first making use of the fact that the φ_α are single-atom energy eigenstates, as was done in obtaining (67). One then finds

$$(\alpha\beta|\, V_{\text{ex}}\, |\gamma\delta) = (\epsilon_\alpha + \epsilon_\beta)(\alpha\beta|\, I'\, |\gamma\delta) + (\alpha\beta|\, V^{\text{ex}}\, |\gamma\delta), \tag{72}$$

where $(\alpha\beta|\, I'\, |\gamma\delta)$ is defined by (55) and where $(\alpha\beta|\, V^{\text{ex}}\, |\gamma\delta)$ differs from $(\alpha\beta|\, V_{\text{ex}}\, |\gamma\delta)$ [Eqs. (58) and (59)] only in replacement of

$$H(XX' x_1 \cdots x_l x_1' \cdots x_l')$$

by its interatomic Coulomb interaction part V':

$$\begin{aligned} V'(XX' x_1 \cdots x_l x_1' \cdots x_l') &= (Ze)^2 |\mathbf{R} - \mathbf{R}'|^{-1} \\ &- Ze^2 \sum_{j=1}^{l} (|\mathbf{R} - \mathbf{r}_j'|^{-1} + |\mathbf{R}' - \mathbf{r}_j|^{-1}) \\ &+ e^2 \sum_{j=1}^{l} \sum_{k=1}^{l} |\mathbf{r}_j - \mathbf{r}_k'|^{-1}. \end{aligned} \tag{73}$$

The matrix $(\alpha\beta|\, V_{\text{ex}}\, \gamma\delta)$ is Hermitian; however, the two pieces into which this matrix is decomposed in (72) are not individually Hermitian. One can also write

$$\begin{aligned} (\alpha\beta|\, V_{\text{ex}}\, |\gamma\delta) &= \tfrac{1}{2}(\epsilon_\alpha + \epsilon_\beta + \epsilon_\gamma + \epsilon_\delta)(\alpha\beta|\, I'\, |\gamma\delta) \\ &+ \tfrac{1}{2}[(\alpha\beta|\, V^{\text{ex}}\, |\gamma\delta) + (\gamma\delta|\, V^{\text{ex}}\, |\alpha\beta)^*], \end{aligned} \tag{74}$$

a form in which the two pieces are individually Hermitian. However, we shall use the simpler form (72) in the subsequent development. Then one finds, by substitution of (72) into (57) and use of the center-of-mass separation and translational invariance,

$$\begin{aligned} V_{\text{ex}} = \tfrac{1}{2} \sum_{\nu_1 \cdots \nu_4} \int d^3r d^3r' d^3r'' d^3r''' &\times \Big\{ \mathfrak{J}_{\nu_1 \cdots \nu_4}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') \\ &\times \left[-\frac{\hbar^2}{2(M+lm)} \left(\frac{\partial^2}{\partial r^2} + \frac{\partial^2}{\partial r'^2} \right) + \epsilon_{\nu_1} + \epsilon_{\nu_2} \right] \\ &+ v_{\nu_1 \cdots \nu_4}^{\text{ex}}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') \Big\} \psi_{\nu_1}^\dagger(\mathbf{r}) \psi_{\nu_2}^\dagger(\mathbf{r}') \psi_{\nu_4}(\mathbf{r}''') \psi_{\nu_3}(\mathbf{r}''), \end{aligned} \tag{75}$$

where

$$\begin{aligned} \mathfrak{J}_{\nu_1 \cdots \nu_4}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') &= c_{\text{nuc}} \mathfrak{J}_{\nu_1 \cdots \nu_4}^{\text{nuc}}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') \\ &+ c_{\text{elec}} \mathfrak{J}_{\nu_1 \cdots \nu_4}^{\text{elec}}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') \\ &+ \sum_{j=2}^{l-1} c_j \mathfrak{J}_{\nu_1 \cdots \nu_4}^{j}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') \end{aligned} \tag{76}$$

and

$$\begin{aligned} v_{\nu_1 \cdots \nu_4}^{\text{ex}}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') &= c_{\text{nuc}} v_{\nu_1 \cdots \nu_4}^{\text{nuc}}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') \\ &+ c_{\text{elec}} v_{\nu_1 \cdots \nu_4}^{\text{elec}}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') \\ &+ \sum_{j=2}^{l-1} c_j v_{\nu_1 \cdots \nu_4}^{j}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}'''). \end{aligned} \tag{77}$$

Here the nuclear exchange matrix is

$$\mathfrak{J}^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') = \int u^*_{\nu_1}(Xx_1\cdots x_l)u^*_{\nu_2}(X'x'_1\cdots x'_l)\delta\left(\frac{M\mathbf{R}+m(\mathbf{r}_1+\cdots+\mathbf{r}_l)}{M+lm}\right)$$
$$\times\,\delta\left(\frac{M\mathbf{R}'+m(\mathbf{r}'_1+\cdots+\mathbf{r}'_l)}{M+lm}\right)\Big[u_{\nu_3}(X'+\mathbf{r}'-\mathbf{r},x_1\cdots x_l)u_{\nu_4}(X+\mathbf{r}-\mathbf{r}',x'_1\cdots x'_l)$$
$$\times\,\delta\left(\frac{M(\mathbf{R}'-\mathbf{R}+\mathbf{r}'-\mathbf{r})}{M+lm}+\mathbf{r}-\mathbf{r}''\right)\delta\left(\frac{M(\mathbf{R}-\mathbf{R}'+\mathbf{r}-\mathbf{r}')}{M+lm}+\mathbf{r}'-\mathbf{r}'''\right)$$
$$-(-1)^{2J}u_{\nu_3}(Xx_1\cdots x_l)u_{\nu_4}(X'x'_1\cdots x'_l)\delta(\mathbf{r}-\mathbf{r}'')\delta(\mathbf{r}'-\mathbf{r}''')\Big]dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l, \tag{78}$$

where, e.g., $X+\mathbf{r}-\mathbf{r}'$ is a symbolic expression for $(\mathbf{R}+\mathbf{r}-\mathbf{r}',\sigma)$ with $X=(\mathbf{R},\sigma)$, σ being the nuclear spin variable which is summed over as part of $\int dX$. Similarly, the electron exchange matrices are

$$\mathfrak{J}^{j}_{\nu_1\cdots\nu_4}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''')$$
$$=\int u^*_{\nu_1}(Xx_1\cdots x_l)u^*_{\nu_2}(X'x'_1\cdots x'_l)\delta\left(\frac{M\mathbf{R}+m(\mathbf{r}_1+\cdots+\mathbf{r}_l)}{M+lm}\right)\delta\left(\frac{M\mathbf{R}'+m(\mathbf{r}'_1+\cdots+\mathbf{r}'_l)}{M+lm}\right)$$
$$\times\Big[u_{\nu_3}(X,x'_1+\mathbf{r}'-\mathbf{r},\cdots,x'_j+\mathbf{r}'-\mathbf{r},x_{j+1}\cdots x_l)u_{\nu_4}(X',x_1+\mathbf{r}-\mathbf{r}',\cdots,x_j+\mathbf{r}-\mathbf{r}',x'_{j+1}\cdots x'_l)$$
$$\times\,\delta\left(\frac{m(\mathbf{r}'_1+\cdots+\mathbf{r}'_j-\mathbf{r}_1-\cdots-\mathbf{r}_j)+jm(\mathbf{r}'-\mathbf{r})}{M+lm}+\mathbf{r}-\mathbf{r}''\right)$$
$$\times\,\delta\left(\frac{m(\mathbf{r}_1+\cdots+\mathbf{r}_j-\mathbf{r}'_1-\cdots-\mathbf{r}'_j)+jm(\mathbf{r}-\mathbf{r}')}{M+lm}+\mathbf{r}'-\mathbf{r}'''\right)$$
$$-(-1)^j u_{\nu_3}(Xx_1\cdots x_l)u_{\nu_4}(X'x'_1\cdots x'_j)\delta(\mathbf{r}-\mathbf{r}'')\delta(\mathbf{r}'-\mathbf{r}''')\Big]\,dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l, \tag{79}$$

where $\mathfrak{J}^{\mathrm{elec}}_{\nu_1\cdots\nu_4}$ is the special case $j=1$. The Coulomb-exchange potentials $v^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}$, $v^{\mathrm{elec}}_{\nu_1\cdots\nu_4}$, and $v^{j}_{\nu_1\cdots\nu_4}$ are similarly found to be

$$v^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''')$$
$$=(Ze)^2\int u^*_{\nu_1}(Xx_1\cdots x_l)u^*_{\nu_2}(X'x'_1\cdots x'_l)\delta\left(\frac{M\mathbf{R}+m(\mathbf{r}_1+\cdots+\mathbf{r}_l)}{M+lm}\right)\delta\left(\frac{M\mathbf{R}'+m(\mathbf{r}'_1+\cdots+\mathbf{r}'_l)}{M+lm}\right)$$
$$\times\,(|\mathbf{R}-\mathbf{R}'+\mathbf{r}-\mathbf{r}'|^{-1}-|\mathbf{R}-\mathbf{r}'_1+\mathbf{r}-\mathbf{r}'|^{-1}-|\mathbf{R}'-\mathbf{r}_1+\mathbf{r}'-\mathbf{r}|^{-1}+|\mathbf{r}_1-\mathbf{r}'_1+\mathbf{r}-\mathbf{r}'|^{-1})$$
$$\times\Big[u_{\nu_3}(X'+\mathbf{r}'-\mathbf{r},x_1\cdots x_l)u_{\nu_4}(X+\mathbf{r}-\mathbf{r}',x'_1\cdots x'_l)$$
$$\times\,\delta\left(\frac{M(\mathbf{R}'-\mathbf{R}+\mathbf{r}'-\mathbf{r})}{M+lm}+\mathbf{r}-\mathbf{r}''\right)\delta\left(\frac{M(\mathbf{R}-\mathbf{R}'+\mathbf{r}-\mathbf{r}')}{M+lm}+\mathbf{r}'-\mathbf{r}'''\right)$$
$$-(-1)^{2J}u_{\nu_3}(Xx_1\cdots x_l)u_{\nu_4}(X'x'_1\cdots x'_l)\delta(\mathbf{r}-\mathbf{r}'')\delta(\mathbf{r}'-\mathbf{r}''')\Big]\,dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l \tag{80}$$

and

$$
\begin{aligned}
&v^{j}_{\nu_1\cdots\nu_4}(\mathbf{r}\mathbf{r}'\mathbf{r}''\mathbf{r}''') \\
&= \int u^*_{\nu_1}(Xx_1\cdots x_l)u^*_{\nu_2}(X'x'_1\cdots x'_l)\delta\left(\frac{M\mathbf{R}+m(\mathbf{r}_1+\cdots+\mathbf{r}_l)}{M+lm}\right)\delta\left(\frac{M\mathbf{R}'+m(\mathbf{r}'_1+\cdots+\mathbf{r}'_l)}{M+lm}\right) \\
&\quad\times\left(\frac{(Ze)^2}{|\mathbf{R}-\mathbf{R}'+\mathbf{r}-\mathbf{r}'|}-\frac{jZe^2}{|\mathbf{R}-\mathbf{r}'_1+\mathbf{r}-\mathbf{r}'|}-\frac{jZe^2}{|\mathbf{R}'-\mathbf{r}_1+\mathbf{r}'-\mathbf{r}|}\right. \\
&\quad-\frac{Z(Z-j)e^2}{|\mathbf{R}-\mathbf{r}'_{j+1}+\mathbf{r}-\mathbf{r}'|}-\frac{Z(Z-j)e^2}{|\mathbf{R}'-\mathbf{r}_{j+1}+\mathbf{r}'-\mathbf{r}|}+\frac{j^2e^2}{|\mathbf{r}_1-\mathbf{r}'_1+\mathbf{r}-\mathbf{r}'|} \\
&\quad\left.+\frac{j(Z-j)e^2}{|\mathbf{r}_1-\mathbf{r}'_{j+1}+\mathbf{r}-\mathbf{r}'|}+\frac{j(Z-j)e^2}{|\mathbf{r}_{j+1}-\mathbf{r}'_1+\mathbf{r}-\mathbf{r}'|}+\frac{(Z-j)^2e^2}{|\mathbf{r}_{j+1}-\mathbf{r}_{j+1}+\mathbf{r}-\mathbf{r}'|}\right) \\
&\quad\times\Big[u_{\nu_3}(X,x'_1+\mathbf{r}'-\mathbf{r},\cdots,x'_j+\mathbf{r}'-\mathbf{r},x_{j+1}\cdots x_l)u_{\nu_4}(X',x_1+\mathbf{r}-\mathbf{r}',\cdots,x_j+\mathbf{r}-\mathbf{r}',x'_{j+1}\cdots x'_l) \\
&\quad\times\delta\left(\frac{m(\mathbf{r}'_1+\cdots+\mathbf{r}'_j-\mathbf{r}_1-\cdots-\mathbf{r}_j)+jm(\mathbf{r}'-\mathbf{r})}{M+lm}+\mathbf{r}-\mathbf{r}''\right) \\
&\quad\times\delta\left(\frac{m(\mathbf{r}_1+\cdots+\mathbf{r}_j-\mathbf{r}'_1-\cdots-\mathbf{r}'_j)+jm(\mathbf{r}-\mathbf{r}')}{M+lm}+\mathbf{r}'-\mathbf{r}'''\right) \\
&\quad-(-1)^j u_{\nu_3}(Xx_1\cdots x_l)u_{\nu_4}(X'x'_1\cdots x'_l)\delta(\mathbf{r}-\mathbf{r}'')\delta(\mathbf{r}'-\mathbf{r}''')\Big]\,dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l, \qquad (81)
\end{aligned}
$$

where $v^{\mathrm{elec}}_{\nu_1\cdots\nu_4}$ is the case $j=1$.

The expressions for V' and V_{ex} simplify if one takes advantage of the smallness of lm/M and makes the usual approximation of identifying the center of mass with the nuclear position. Then the Dirac delta functions in (71) reduce to $\delta(\mathbf{R})$ and $\delta(\mathbf{R}')$, so that

$$
\begin{aligned}
&v^{\mathrm{Coul}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') \\
&= (Ze)^2\sum_{\sigma\sigma'}\int u^*_{\nu_1}(0,\sigma,x_1\cdots x_l)u^*_{\nu_2}(0,\sigma',x'_1\cdots x'_l) \\
&\quad\times(|\mathbf{r}-\mathbf{r}'|^{-1}+|\mathbf{r}_1-\mathbf{r}'_1+\mathbf{r}-\mathbf{r}'|^{-1} \\
&\quad-|\mathbf{r}'_1-\mathbf{r}+\mathbf{r}'|^{-1}-|\mathbf{r}_1+\mathbf{r}-\mathbf{r}'|^{-1}) \\
&\quad\times u_{\nu_3}(0,\sigma,x_1\cdots x_l)u_{\nu_4}(0,\sigma',x'_1\cdots x'_l) \\
&\quad\times dx_1\cdots dx_l\,dx'_1\cdots dx'_l, \qquad (82)
\end{aligned}
$$

where σ and σ' are the nuclear spin variables (for spin-zero nuclei these arguments and the sum over them are to be omitted). $u_\nu(0,\sigma,x_1\cdots x_l)$ is just the usual form for the internal wavefunction, in which the electron positions are measured in a coordinate system centered on the nucleus. Similarly, (75)–(81) reduce to

$$
\begin{aligned}
V_{\mathrm{ex}} &= \tfrac{1}{2}\sum_{\nu_1\cdots\nu_4}\int d^3r\,d^3r'\,\psi^\dagger_{\nu_1}(\mathbf{r})\psi^\dagger_{\nu_2}(\mathbf{r}')v^{\mathrm{ex}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}',\mathbf{p},\mathbf{p}') \\
&\quad\times\psi_{\nu_4}(\mathbf{r}')\psi_{\nu_3}(\mathbf{r}), \qquad (83)
\end{aligned}
$$

where $\mathbf{p}=(\hbar/i)\nabla$, $\mathbf{p}'=(\hbar/i)\nabla'$, and

$$
\begin{aligned}
&v^{\mathrm{ex}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}',\mathbf{p},\mathbf{p}') \\
&\quad=\mathfrak{J}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}')\left(\frac{p^2}{2M}+\frac{(p')^2}{2M}+\epsilon_{\nu_1}+\epsilon_{\nu_2}\right) \\
&\qquad+v^{\mathrm{ex}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') \qquad (84)
\end{aligned}
$$

with

$$
\begin{aligned}
\mathfrak{J}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') &= c_{\mathrm{nuc}}\mathfrak{J}^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') \\
&\quad+\sum_{j=1}^{l-1}c_j\mathfrak{J}^{j}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}'), \\
v^{\mathrm{ex}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') &= c_{\mathrm{nuc}}v^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') \\
&\quad+\sum_{j=1}^{l-1}c_j v^{j}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}'). \qquad (85)
\end{aligned}
$$

The nuclear and electron exchange matrices are

$$
\begin{aligned}
\mathfrak{J}^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') &= (-1)^{2J}\sum_{\sigma\sigma'}\int u^*_{\nu_1}(0,\sigma,x_1\cdots x_l)u^*_{\nu_2}(0,\sigma',x'_1\cdots x'_l) \\
&\quad\times[(-1)^l u_{\nu_4}(\mathbf{r}'-\mathbf{r},\sigma',x_1\cdots x_l)u_{\nu_3}(\mathbf{r}-\mathbf{r}',\sigma,x'_1\cdots x'_l) \\
&\quad-u_{\nu_3}(0,\sigma,x_1\cdots x_l)u_{\nu_4}(0,\sigma',x'_1\cdots x'_l)]\,dx_1\cdots dx_l\,dx'_1\cdots dx'_l \qquad (86)
\end{aligned}
$$

and

$$\mathfrak{I}^{j}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') = \sum_{\sigma\sigma'}\int u^*_{\nu_1}(0,\sigma,x_1\cdots x_l)u^*_{\nu_2}(0,\sigma',x_1'\cdots x_l')$$
$$\times\,[u_{\nu_3}(0,\sigma,x_1'+\mathbf{r}'-\mathbf{r},\cdots,x_j'+\mathbf{r}'-\mathbf{r},x_{j+1}\cdots x_l)$$
$$\times\,u_{\nu_4}(0,\sigma',x_1+\mathbf{r}-\mathbf{r}',\cdots,x_j+\mathbf{r}-\mathbf{r}',x_{j+1}'\cdots x_l')$$
$$-(-1)^j u_{\nu_3}(0,\sigma,x_1\cdots x_l)u_{\nu_4}(0,\sigma',x_1'\cdots x_l')]\,dx_1\cdots dx_l\,dx_1'\cdots dx_l'. \tag{87}$$

Similarly, the Coulomb-exchange potentials are

$$v^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') = (-1)^{2J}(Ze)^2\sum_{\sigma\sigma'}\int u^*_{\nu_1}(0,\sigma,x_1\cdots x_l)u^*_{\nu_2}(0,\sigma',x_1'\cdots x_l')$$
$$\times\,(|\mathbf{r}-\mathbf{r}'|^{-1}-|\mathbf{r}_1'-\mathbf{r}+\mathbf{r}'|^{-1}-|\mathbf{r}_1+\mathbf{r}-\mathbf{r}'|^{-1}+|\mathbf{r}_1-\mathbf{r}_1'+\mathbf{r}-\mathbf{r}'|^{-1})$$
$$\times\,[(-1)^l u_{\nu_4}(\mathbf{r}'-\mathbf{r},\sigma',x_1\cdots x_l)u_{\nu_3}(\mathbf{r}-\mathbf{r}',\sigma,x_1'\cdots x_l')$$
$$-u_{\nu_3}(0,\sigma,x_1\cdots x_l)u_{\nu_4}(0,\sigma',x_1'\cdots x_l')]\,dx_1\cdots dx_l\,dx_1'\cdots dx_l' \tag{88}$$

and

$$v^{j}_{\nu_1\cdots\nu_4}(\mathbf{r}-\mathbf{r}') = e^2\sum_{\sigma\sigma'}\int u^*_{\nu_1}(0,\sigma,x_1\cdots x_l)u^*_{\nu_2}(0,\sigma',x_1'\cdots x_l')$$
$$\times\left(\frac{Z^2}{|\mathbf{r}-\mathbf{r}'|}-\frac{jZ}{|\mathbf{r}_1'-\mathbf{r}+\mathbf{r}'|}-\frac{jZ}{|\mathbf{r}_1+\mathbf{r}-\mathbf{r}'|}-\frac{Z(Z-j)}{|\mathbf{r}_{j+1}'-\mathbf{r}+\mathbf{r}'|}-\frac{Z(Z-j)}{|\mathbf{r}_{j+1}+\mathbf{r}-\mathbf{r}'|}\right.$$
$$\left.+\frac{j^2}{|\mathbf{r}_1-\mathbf{r}_1'+\mathbf{r}-\mathbf{r}'|}+\frac{j(Z-j)}{|\mathbf{r}_1-\mathbf{r}_{j+1}'+\mathbf{r}-\mathbf{r}'|}+\frac{j(Z-j)}{|\mathbf{r}_{j+1}-\mathbf{r}_1'+\mathbf{r}-\mathbf{r}'|}+\frac{(Z-j)^2}{|\mathbf{r}_{j+1}-\mathbf{r}_{j+1}'+\mathbf{r}-\mathbf{r}'|}\right)$$
$$\times\,[u_{\nu_3}(0,\sigma,x_1'+\mathbf{r}'-\mathbf{r},\cdots,x_j'+\mathbf{r}'-\mathbf{r},x_{j+1}\cdots x_l)$$
$$\times\,u_{\nu_4}(0,\sigma',x_1+\mathbf{r}-\mathbf{r}',\cdots,x_j+\mathbf{r}-\mathbf{r}',x_{j+1}'\cdots x_l')$$
$$-(-1)^j u_{\nu_3}(0,\sigma,x_1\cdots x_l)u_{\nu_4}(0,\sigma',x_1'\cdots x_l')]\,dx_1\cdots dx_l\,dx_1'\cdots dx_l'. \tag{89}$$

In deriving (83) partial integrations have been performed so as to allow the derivative operators to be sandwiched between $\psi^\dagger\psi^\dagger$ and $\psi\psi$. In some of the terms in $\mathfrak{I}^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}$ and $v^{\mathrm{nuc}}_{\nu_1\cdots\nu_4}$ the names of the summation indices ν_3 and ν_4 have been interchanged and ψ_{ν_3} and ψ_{ν_4} permuted with the aid of (64), so that the $\mathbf{r}$ and $\mathbf{r}'$ arguments of all products $\psi^\dagger\psi^\dagger\psi\psi$ are in the standard order $\psi^\dagger_{\nu_1}(\mathbf{r})\psi^\dagger_{\nu_2}(\mathbf{r}')\psi_{\nu_4}(\mathbf{r}')\psi_{\nu_3}(\mathbf{r})$.

The Coulomb-exchange potential $v^{\mathrm{ex}}_{\nu_1\cdots\nu_4}$ in (84) is a generalization of the exchange integrals of quantum chemistry and the theory of magnetism; it arises through coupling between interatomic Coulomb interactions and interatomic nuclear and electronic exchange. The term $\mathfrak{I}_{\nu_1\cdots\nu_4}(\epsilon_{\nu_1}+\epsilon_{\nu_2})$ arises through coupling between interatomic exchange and internal degrees of freedom of the atoms, whereas the momentum-dependent terms

$$\mathfrak{I}_{\nu_1\cdots\nu_4}\left(\frac{p^2}{2M}+\frac{(p')^2}{2M}\right)$$

represent coupling between interatomic exchange and translational motion of the atoms. The explicit expressions for the various terms in the projected Hamiltonian $\mathfrak{K}$ furnish the basis for calculation of the properties of a system of atoms at low densities, where the three-atom, four-atom, ... terms [denoted by ... in (57)] are unimportant compared to the one-atom terms H_0 and the two-atom terms V' and V_{ex}. For a system of only two atoms, $H_0+V'+V_{\mathrm{ex}}$ is an exact expression for $\mathfrak{K}$, so that the formalism developed here provides the basis for an exact theory of inelastic scattering of atoms. The same approach could be applied to systems of molecules or nuclei.

APPENDIX A: EVALUATION OF $\mathfrak{T}_{\mathrm{elec}}$

We want to verify the expressions (50) and (51). It follows from (21) and the definition of $\mathfrak{T}_{\mathrm{elec}}$ that

$$I'_{\mathrm{elec}}\mathfrak{T}_{\mathrm{elec}} = 0. \tag{A1}$$

Substituting (50) into (A1), making use of the results of Sec. 3, and equating the coefficients of I'_{nuc}, I'_{elec}, and the I'_j to zero, one finds an inhomogeneous set of

l linear equations in the l unknowns c_{nuc}, c_{elec}, and c_j:

$$\begin{aligned} &c_{\text{nuc}} + l^{-2}(-1)^{2J+l}c_{l-1} = 0,\\ &-(-1)^{2J}c_{\text{nuc}} + 2l^{-2}(l^2 - l + 1)c_{\text{elec}} - l^{-2}(l^2 - 4)c_2 \\ &\qquad + \sum_{j=3}^{l-1} -(-1)^j c_j = -1, \\ &l^{-2}(l-1)^2 c_{\text{elec}} + l^{-2}(l^2 - 4l + 8)c_2 + 9l^{-2}c_3 = 0, \\ &l^{-2}(l-j+1)^2 c_{j-1} + l^{-2}(l^2 - 2jl + 2j^2)c_j \\ &\qquad + l^{-2}(j+1)^2 c_{j+1} = 0, \quad 3 \le j \le l-2, \\ &(-1)^{2J+l}c_{\text{nuc}} + 4l^{-2}c_{l-2} + l^{-2}(l^2 - 2l + 2)c_{l-1} = 0. \end{aligned} \tag{A2}$$

The solution can be found by first solving the top equation for c_{nuc} in terms of c_{l-1}, substituting into the last equation to obtain c_{l-2} in terms of c_{l-1}, substituting into the $j = l - 2$ equation to obtain c_{l-3} in terms of c_{l-1}, etc. Finally, substitution into the second equation gives an inhomogeneous equation which is easily solved for c_{l-1}. In this way one finds the expressions (51) for c_{nuc}, c_{elec}, and the c_j, with

$$\begin{aligned} d_l &= [s_l + \tfrac{1}{4}l^{-2}(l^4 - 2l^3 + 5l^2 + 8)]^{-1}, \\ s_l &= \sum_{j=3}^{l-1}\left(\frac{(l-1)!}{j!\,(l-j)!}\right)^2. \end{aligned} \tag{A3}$$

The sum s_l can be evaluated with the aid of the formula

$$\sum_{j=0}^{l}\binom{l}{j}^2 = \binom{2l}{l} = \frac{(2l)!}{(l!)^2}. \tag{A4}$$

The expression (51) for d_l then follows immediately.

It follows trivially from (A1) that the operator (50) satisfies

$$I'_{\text{elec}}\mathfrak{T}_{\text{elec}}|2\rangle = 0, \tag{A5}$$

where $|2\rangle$ is any two-atom state. However, as in the case of $\mathfrak{T}_{\text{nuc}}$, we note that (A5) is only a necessary condition for the correctness of (50). Another necessary condition is

$$\mathfrak{T}^2_{\text{elec}}|2\rangle = \mathfrak{T}_{\text{elec}}|2\rangle. \tag{A6}$$

Furthermore, in order to obtain a set of both necessary and sufficient conditions one must require, in analogy with (49), that

$$\mathfrak{T}_{\text{elec}}|2'\rangle = 0, \tag{A7}$$

where $|2'\rangle$ is any two-atom eigenstate of I'_{elec} with an eigenvalue different from zero. A direct proof of (A6) and (A7) would be complicated.[9] However, it is possible to give an indirect proof which at the same time verifies (53). Let

$$|\lambda'_{\text{nuc}}, \lambda'_{\text{elec}}, \lambda'_2, \cdots, \lambda'_{l-1}\rangle \tag{A8}$$

be a simultaneous eigenstate of the mutually commuting operators I'_{nuc}, I'_{elec}, $I'_2, \cdots, I'_{l-1}$ with the indicated eigenvalues. Suppose, furthermore, that this state is a two-atom state. Then, operating on this state with (38), (44), (42), and (45), one finds that

$$\begin{aligned} (\lambda'_{\text{elec}})^2 &= 2l^{-2}(l^2 - l + 1)\lambda'_{\text{elec}} + l^{-2}(l-1)^2\lambda'_2, \\ \lambda'_{\text{elec}}\lambda'_2 &= -l^{-2}(l^2 - 4)\lambda'_{\text{elec}} \\ &\quad + l^{-2}(l^2 - 4l + 8)\lambda'_2 + l^{-2}(l-2)^2\lambda'_3, \\ \lambda'_{\text{elec}}\lambda'_j &= -(-1)^j\lambda'_{\text{elec}} \\ &\quad + (j/l)^2\lambda'_{j-1} + l^{-2}(l^2 - 2jl + 2j)\lambda'_j \\ &\quad + l^{-2}(l-j)^2\lambda'_{j+1}, \quad 3 \le j \le l-2, \\ \lambda'_{\text{elec}}\lambda'_{l-1} &= (-1)^l\lambda'_{\text{elec}} + l^{-2}(l-1)^2\lambda'_{l-2} \\ &\quad + l^{-2}(l^2 - 2l + 2)\lambda'_{l-1} + l^{-2}(-1)^{2J+l}\lambda'_{\text{nuc}}. \end{aligned} \tag{A9}$$

Suppose that $\lambda'_{\text{elec}} = 0$. Then it is easy to show from (A9) that also $\lambda'_{\text{nuc}} = 0$ and all the $\lambda'_j = 0$, i.e., the only states (A8) with $\lambda'_{\text{elec}} = 0$ are those which also have $\lambda'_{\text{nuc}} = \lambda'_2 = \cdots = \lambda'_{l-1} = 0$. But the coefficients (51) were determined precisely so that any state $\mathfrak{T}_{\text{elec}}|2\rangle$, with $\mathfrak{T}_{\text{elec}}$ given by (50), is an eigenstate of I'_{elec} with eigenvalue $\lambda'_{\text{elec}} = 0$; such states, therefore, also have $\lambda'_{\text{nuc}} = \lambda'_2 = \cdots = \lambda'_{l-1} = 0$. Conversely, let $|\text{phys}\rangle$ be any physical two-atom state, i.e., any two-atom state satisfying the subsidiary conditions (21). Then this state will be of the form (A8) with all eigenvalues equal to zero. It then follows from (50) that

$$\mathfrak{T}_{\text{elec}}|\text{phys}\rangle = |\text{phys}\rangle. \tag{A10}$$

This is just the defining property of $\mathfrak{T}_{\text{nuc}}\mathfrak{T}_{\text{elec}}$. We conclude that, on the two-atom state space, the operator defined by (50) and (51) is indeed both $\mathfrak{T}_{\text{elec}}$ and $\mathfrak{T}_{\text{nuc}}\mathfrak{T}_{\text{elec}}$.

APPENDIX B: EVALUATION OF PROJECTED HAMILTONIAN

Substitution of (56) and (6) into (13) gives

$$\mathcal{H} = T + V_0 + V' + I'(T + V_0 + V') + \cdots, \tag{B1}$$

where the various terms in $I'(T + V_0 + V')$ remain to be normally ordered. Substitution of (54) and the expression (6) for T and normal ordering with the aid of (1) yields

$$\begin{aligned} I'T = \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}\sum_{\alpha_1}&[(\alpha\beta|\,I'\,|\alpha_1\delta)(\alpha_1|\,T\,|\gamma) \\ &+ (\alpha\beta|\,I'\,|\gamma\alpha_1)(\alpha_1|\,T\,|\delta)]a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + \cdots. \end{aligned} \tag{B2}$$

Evaluation of the closure sums on $\varphi_{\alpha_1}\varphi^*_{\alpha_1}$ in the usual way then gives with (55), (18), (36), (4), and (35)

$$I'T = \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|\,I'T\,|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + \cdots, \tag{B3}$$

with

$$(\alpha\beta|\, I'T\,|\gamma\delta) = c_{\rm nuc}(\alpha\beta|\, I'_{\rm nuc}T\,|\gamma\delta) + c_{\rm elec}(\alpha\beta|\, I'_{\rm elec}T\,|\gamma\delta) + \sum_{j=2}^{l-1} c_j(\alpha\beta|\, I'_jT\,|\gamma\delta) \quad \text{(B4)}$$

and

$$\begin{aligned}(\alpha\beta|\, I'_{\rm nuc}T\,|\gamma\delta) &= \int \varphi^*_\alpha(Xx_1\cdots x_l)\varphi^*_\beta(X'x'_1\cdots x'_l)\\ &\times T(XX'x_1\cdots x_lx'_1\cdots x'_l)\\ &\times [\varphi_\gamma(X'x_1\cdots x_l)\varphi_\delta(Xx'_1\cdots x'_l)\\ &- (-1)^{2J}\varphi_\gamma(Xx_1\cdots x_l)\varphi_\delta(X'x'_1\cdots x'_l)]\\ &\times dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l,\end{aligned}$$

$$\begin{aligned}(\alpha\beta|\, I'_{\rm elec}T\,|\gamma\delta) &= \int \varphi^*_\alpha(Xx_1\cdots x_l)\varphi^*_\beta(X'x'_1\cdots x'_l)\\ &\times T(XX'x_1\cdots x_lx'_1\cdots x'_l)\\ &\times [\varphi_\gamma(Xx'_1x_2\cdots x_l)\varphi_\delta(X'x_1x'_2\cdots x'_l) \quad \text{(B5)}\\ &+ \varphi_\gamma(Xx_1\cdots x_l)\varphi_\delta(X'x'_1\cdots x'_l)]\\ &\times dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l,\end{aligned}$$

$$\begin{aligned}(\alpha\beta|\, I'_jT\,|\gamma\delta) &= \int \varphi^*_\alpha(Xx_1\cdots x_l)\varphi^*_\beta(X'x'_1\cdots x'_l)\\ &\times T(XX'x_1\cdots x_lx'_1\cdots x'_l)\\ &\times [\varphi_\gamma(Xx'_1\cdots x'_jx_{j+1}\cdots x_l)\\ &\times \varphi_\delta(X'x_1\cdots x_jx'_{j+1}\cdots x'_l)\\ &- (-1)^j\varphi_\gamma(Xx_1\cdots x_l)\varphi_\delta(X'x'_1\cdots x'_l)]\\ &\times dX\,dx_1\cdots dx_l\,dX'\,dx'_1\cdots dx'_l.\end{aligned}$$

Here $T(XX'x_1\cdots x_lx'_1\cdots x'_l)$ is the total kinetic energy operator for all the particles in both atoms:

$$T(XX'x_1\cdots x_lx'_1\cdots x'_l) = T(X) + T(X') + \sum_{j=1}^{l}[T(x_j) + T(x'_j)]. \quad \text{(B6)}$$

The operator $I'V_0$ can be evaluated up to two-atom terms in a similar fashion, whereas evaluation of $I'V'$ involves two closure sums. Combination of the results gives (57)–(60).

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[1] M. D. Girardeau, J. Math. Phys. **4**, 1096 (1963); **11**, 681 (1970).

[2] This argument fails in the exceptional case $E = 0$. However, this does not cause any difficulty, since we are generally not interested in the case $E = 0$, and, even if we were, the origin of energy could be shifted by redefinition of H. Independently of any shift of origin, the eigenvalue $E = 0$ of $\mathcal{H}$ will always include the entire "completely unphysical" subspace, i.e., the subspace orthogonal to the space of states satisfying (2). Hence eigenstates of $\mathcal{H}$ with eigenvalue zero should be discarded.

[3] The anitsymmetrization on the right side of the completeness relation arises from the fact that the set $\{\varphi_\alpha(Xx_1\cdots x_l)\}$ is complete on the space of functions of $Xx_1\cdots x_l$ *which are antisymmetric in* $x_1\cdots x_l$; as always, the meaning of completeness is not absolute, but relative to the given space of functions.

[4] The physical significance of (28) is that exchanging the same nuclei twice is equivalent to no exchange.

[5] The derivation of (40) is not valid in the trivial case $l = 1$, and it simplifies for $l = 2$. It can be shown that for $l = 1$

$$I'_{\rm nuc}I'_{\rm elec} = 2I'_{\rm nuc} + \cdots = -2(-1)^{2J}I'_{\rm elec} + \cdots$$

and for $l = 2$

$$I'_{\rm nuc}I'_{\rm elec} = I'_{\rm nuc} + \cdots.$$

[6] The point is that the operator (46) might be the projection operator onto a *subspace* of the set of eigenstates of $I'_{\rm nuc}$ with eigenvalue zero.

[7] It follows from the asymptotic formula

$$\binom{2l}{l}_{l\to\infty} (\pi l)^{-\frac{1}{2}}2^{2l}$$

that

$$d_{l_{l\to\infty}} \pi^{\frac{1}{2}}l^{\frac{1}{2}}2^{-2l}.$$

Hence, by (51), $c_{\rm nuc}$ and $c_{\rm elec}$ fall off exponentially for large l. This is not the case, however, for all of the coefficients. In fact, the same asymptotic formula, with l replaced by $\frac{1}{2}l$, shows that the c_j with $j \approx \frac{1}{2}l$ fall off only like $l^{-\frac{1}{2}}$ for large l.

[8] Translational invariance of u_ν implies that it is a momentum eigenstate with eigenvalue zero, i.e.,

$$\frac{\hbar}{i}\left(\frac{\partial}{\partial \mathbf{R}} + \sum_{j=1}^{l}\frac{\partial}{\partial \mathbf{r}_j}\right)u_\nu(Xx_1\cdots x_l) = 0,$$

or equivalently that u_ν depends on $\mathbf{R}$ and the $\mathbf{r}_j$ only in the combinations $\mathbf{R} - \mathbf{r}$, $\mathbf{r}_1 - \mathbf{r}, \cdots, \mathbf{r}_l - \mathbf{r}$, where $\mathbf{r}$ is the center-of-mass position (62).

[9] In this connection it should be noted that the formula for the eigenvalues of $I_{\rm elec}$ in the Appendix of the first paper cited in Ref. 1 is incorrect; these eigenvalues are not all integers. This is the reason that $\mathfrak{I}_{\rm elec}$ involves not only $I'_{\rm elec}$ but also $I'_{\rm nuc}$ and the I'_j.