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Matrix Elements of the Octet Operator of SU_3*

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All the nonvanishing matrix elements of all the components of the tensor operator which belongs to the regular representation (the octet) of SU_3 have been evaluated. Of special interest is the component $\mathcal{Y}$, for it is usual in the broken unitary symmetry theory of strong interactions to assume that the interactions which break exact SU_3 invariance have the same transformation properties as $\mathcal{Y}$. Previously, matrix elements of $\mathcal{Y}$ connecting states of the same irreducible representation of SU_3 have been given by Okubo in the form of the mass formula. Knowledge of all the matrix elements of $\mathcal{Y}$ is essential however if one is to do more than evaluate one-particle matrix elements in the broken unitary symmetry theory. Our method provides such knowledge for all components of the octet tensor operator with little more effort than is needed to treat $\mathcal{Y}$ alone.

1. INTRODUCTION

MOTIVATION for the present work is to be found in the theory of the strong interactions which uses SU_3 not as an exact but as an approximate symmetry group.[1] In such a theory the interactions which perturb exact invariance are supposed to have invariance only under the isospin and hypercharge subgroups of SU_3. The simplest possible assumption that can be made to describe the situation is that the perturbative interactions have the same transformation properties under SU_3 as the generator Y (hypercharge) of SU_3. An equivalent statement is that they have the tensorial character with respect to SU_3 of the $I = Y = 0$ component $\mathcal{Y}$ of the octet or regular tensor operator[2] of SU_3. So far there have been very few[3] attempts to do any more than evaluate single-particle matrix elements in the broken SU_3 theory. The most notable achievement of the theory—the now well-known mass formula of Okubo[1]—is of the latter type. Essentially the formula gives the matrix elements of $\mathcal{Y}$ within a given irreducible representation (IR) of SU_3. However, it has become apparent that a systematic development of the broken SU_3 theory is necessary rather than further investigation of the exact theory. Part of the basic machinery of this development is the computation of all matrix elements of $\mathcal{Y}$, including those which connect different IR's of SU_3. Such formulas are needed as soon as one tries to evaluate matrix elements in the broken theory which involve states of more than one particle. These remarks of course refer to the description of the broken theory in which we consider matrix elements of a strong-interaction Hamiltonian of the form $\alpha + \beta\mathcal{Y}$ where α and β are scalar under SU_3, between states of particles assigned to specific IR's of SU_3. But they are equally valid in the variant of the theory wherein the strong-interaction Hamiltonian is taken (at least, in a first approach) to be SU_3-invariant and the observed deviations from consequences of exact invariance are produced by modifications of the description of particles appropriate to the exact theory. Modification of the desired type can be achieved, for example, by mixing

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[1] M. Gell-Mann, Cal. Tech. Rept. CTSL-20, 1961 (unpublished), and Phys. Rev. **125**, 1067 (1962). S. Okubo, Progr. Theoret. Phys. (Kyoto) **27**, 949; **28**, 24 (1962).

[2] By regular tensor operator, we mean the tensor operator which transforms under the group according to the regular representation of the group. For SU_3, this representation is the octet or the IR (1, 1).

[3] See, for example, C. Dullemond, A. J. Macfarlane, and E. C. G. Sudarshan, Phys. Rev. Letters **10**, 423 (1961); and E. C. G. Sudarshan, Proc. Athens Conference on Recently Discovered Resonant Particles, Ohio University, Athens, Ohio, 1963.

a small amount of an $I = Y = 0$ spurion into the bare-particle states, or more generally by associating particles with states produced by suitable mixing of IR's of SU_3.[4]

Originally, then, the present work was undertaken to derive explicit formulas for all matrix elements of the component $\mathcal{Y}$ of the octet operator of SU_3. In fact, with very little extra effort, we were able to obtain such results for all components of the octet operator of SU_3. In the ensuing sections we describe how we implemented this extended program. In Sec. 2, we review those facts regarding the IR's of SU_3 on which our later developments depend, in a manner which ought to prepare a natural approach to them. Then in Sec. 3, we define the octet operator of SU_3 and determine which of the matrix elements of its components do not vanish. Secs. 4 and 5 are concerned with the technical details of evaluating the allowed matrix elements. For ease of reference, all results are presented in tables.

It will be readily observed that the present approach to the regular tensor operator of SU_3 was suggested by the treatment of the corresponding problem for R_3 (which has the vector operator as regular tensor operator) described, e.g., by Condon and Shortley.[5]

Finally, we point out that the results obtained here will also be useful in discussing electromagnetic effects in the unitary symmetry theory. They will allow an extension of the method previously applied[6] to one-particle matrix elements to more general physical situations, e.g., photoproduction.

2. PROPERTIES OF THE IR's OF SU_3

We begin with a discussion of those properties of the IR's of SU_3 that we shall require later.

In the most usual notation, the eight generators of SU_3 are denoted by

$$H_1, H_2, E_{\pm 1}, E_{\pm 2}, E_{\pm 3}. \tag{2.1}$$

They have CR's[7] given in the Weyl[8] canonical form as Eqs. (II.12), (II.17), and (II.18) of the paper by Behrends *et al.*[9] We also note that the Hermiticity properties

$$\begin{aligned} H_i^{\dagger} &= H_i, \qquad i = 1, 2, \\ E_\alpha^{\dagger} &= E_{-\alpha}, \qquad \alpha = 1, 2, 3 \end{aligned} \tag{2.2}$$

can be imposed on the irreducible matrix representations of the generators (2.1). Contact with strong-interaction physics follows from the identifications

$$I_z = \sqrt{3}\, H_1, \qquad Y = 2H_2, \tag{2.3}$$

$$I_\pm = I_x \pm iI_y = 6^{\frac{1}{2}} E_{\pm 1}, \tag{2.4}$$

where $\mathbf{I}$ and Y are, respectively, the generators of isospin rotations and hypercharge gauge transformations. We shall also introduce quantities $F_\pm$ and $G_\pm$ by

$$\begin{aligned} F_+ &= 6^{\frac{1}{2}} E_2, \qquad F_- = 6^{\frac{1}{2}} E_3, \\ G_+ &= -6^{\frac{1}{2}} E_{-3}, \qquad G_- = 6^{\frac{1}{2}} E_{-2}. \end{aligned} \tag{2.5}$$

The motivation for this becomes clear later on in this section. In terms of the set

$$I_z, Y, I_\pm, F_\pm, G_\pm, \tag{2.6}$$

of eight elements, the Weyl CR's of SU_3 are as follows:

$$[I_z, Y] = 0, \tag{A1}$$

$$[I_z, I_\pm] = \pm I_\pm, \tag{A2}$$

$$[I_z, F_\pm] = \pm \tfrac{1}{2} F_\pm, \tag{A3}$$

$$[I_z, G_\pm] = \pm \tfrac{1}{2} G_\pm, \tag{A4}$$

$$[Y, I_\pm] = 0, \tag{A5}$$

$$[Y, F_\pm] = F_\pm, \tag{A6}$$

$$[Y, G_\pm] = -G_\pm, \tag{A7}$$

$$[I_+, I_-] = 2I_z, \tag{A8}$$

$$[F_\pm, G_\mp] = I_z \pm \tfrac{3}{2} Y, \tag{A9}$$

$$[I_\pm, F_\pm] = 0, \tag{A10}$$

$$[I_\pm, G_\pm] = 0, \tag{A11}$$

[4] Particle mixtures in a theory with charge-independent, strong interactions and electromagnetic interaction have been considered by various authors, e. g., S. Okubo, Nuovo Cimento **16**, 963 (1960); S. L. Glashow, Phys. Rev. Letters **7**, 469 (1961). Use of the ϕ–ω mixing to break exact SU_3 invariance has been studied by J. J. Sakurai, Phys. Rev. Letters **9**, 472 (1962); S. Okubo, Phys. Letters **5**, 165 (1962); S. L. Glashow, Phys. Rev. Letters **11**, 48 (1963).

[5] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, Cambridge, England, 1955), p. 61. See also E. Feenberg and G. E. Pake, *Notes on the Quantum Theory of Angular Momentum* (Addison-Wesley Publishing Company, Inc., Cambridge, Massachusetts, 1953), p. 29. The original treatment appears in M. Born and P. Jordan, *Elementare Quantenmechanik* (Springer-Verlag, Leipzig, 1930).

[6] A. J. Macfarlane and E. C. G. Sudarshan, Proc. Stanford Conference on Nucleon Structure, Stanford, California, 1963 (to be published), and Electromagnetic Properties of Stable Particles and Resonances in the Unitary Symmetry Theory (to be published). See also S. P. Rosen, Phys. Rev. Letters **11**, 100 (1963) and C. A. Levinson, H. J. Lipkin and S. Meshkow, Phys. Letters (to be published).

[7] It will be convenient to abbreviate commutation rule and irreducible representation to CR and IR.

[8] See G. Racah, Princeton lectures, 1951 (unpublished).

[9] R. E. Behrends, J. Dreitlein, C. Fronsdal, and B. W. Lee, Rev. Mod. Phys. **34**, 1 (1962).

$$[F_+, F_-] = 0, \tag{A12}$$

$$[G_+, G_-] = 0, \tag{A13}$$

$$[I_\pm, F_\mp] = F_\pm, \tag{A14}$$

$$[I_\pm, G_\mp] = G_\pm, \tag{A15}$$

$$[F_\pm, G_\pm] = \mp I_\pm. \tag{A16}$$

Also, the Hermiticity conditions (2.2) become

$$\begin{aligned} I_z^\dagger &= I_z, \qquad Y^\dagger = Y, \\ I_+^\dagger &= I_-, \quad F_+^\dagger = G_-, \quad F_-^\dagger = -G_+. \end{aligned} \tag{2.7}$$

For the IR's of SU_3 we shall use the highest weight notation (λ, μ), whose significance was explained in a previous paper.[10] In the representation space of the IR (λ, μ), we can introduce a system $|\lambda\ \mu\ I\ \nu\ Y\rangle$ of basic vectors, where $I(I+1)$, ν, and Y are, respectively, the eigenvalues of the commutative operators $\mathbf{I}^2$ (total isospin), I_z (its z component) and Y (hypercharge). In what follows, we shall frequently need explicit formulas for the nonvanishing matrix elements of the nondiagonal elements of the set (2.6) of generators. For $I_\pm$, the relevant results are

$$\langle \lambda\ \mu\ I\ \nu \pm 1\ Y | I_\pm | \lambda\ \mu\ I\ \nu\ Y\rangle = [(I \mp \nu)(I \pm \nu + 1)]^{\frac{1}{2}}. \tag{B.1}$$

The nonvanishing matrix elements of $F_\pm$ and $G_\pm$ have been computed by Biedenharn[11] and others.[12] Here we use Biedenharn's results, mentioning also the fact that the other cited authors have disposed of the existing arbitrariness of phases in a different fashion. We wish to present the results in a very specific manner, which exhibits clearly the relationship of $F_\pm$ and $G_\pm$ to the isospin subgroup $R_3(I)$ of SU_3.

From Eqs. (A3), (A10), and (A14), we note that $F_\pm$ have exactly[13] the CR's with $\mathbf{I}$ necessary for us to regard them as, respectively, the $\nu = \pm\frac{1}{2}$ components of a spherical tensor operator of rank $\frac{1}{2}$ with respect to $R_3(I)$. Accordingly, we expect to find that F_+ obeys the selection rules $I \to I \pm \frac{1}{2}$ and $\nu \to \nu + \frac{1}{2}$, and that F_- obeys $I \to I \pm \frac{1}{2}$ and $\nu \to \nu - \frac{1}{2}$. Also the dependence of the corresponding nonvanishing matrix elements of $F_\pm$ can be written down directly from the Wigner–Eckart theorem for $R_3(I)$. Further, from Eq. (A6), it follows that both $F_\pm$ obey the selection rule $Y \to Y + 1$. All this information can be seen to be present in the following transcription of Biedenharn's formulas:

$$\langle \lambda\ \mu\ I + \tfrac{1}{2}\ \nu + \tfrac{1}{2}\ Y + 1 | F_+ | \lambda\ \mu\ I\ \nu\ Y\rangle = C(I\ \tfrac{1}{2}\ I + \tfrac{1}{2}\ \nu\ \tfrac{1}{2}\ \nu + \tfrac{1}{2}) A(\lambda\ \mu\ I + \tfrac{1}{2} Y)(2I+2)^{-\frac{1}{2}}, \tag{B.2}$$

$$\langle \lambda\ \mu\ I - \tfrac{1}{2}\ \nu + \tfrac{1}{2}\ Y + 1 | F_+ | \lambda\ \mu\ I\ \nu\ Y\rangle = C(I\ \tfrac{1}{2}\ I - \tfrac{1}{2}\ \nu\ \tfrac{1}{2}\ \nu + \tfrac{1}{2}) B(\lambda\ \mu\ I - \tfrac{1}{2} Y)(2I)^{-\frac{1}{2}}, \tag{B.3}$$

$$\langle \lambda\ \mu\ I + \tfrac{1}{2}\ \nu - \tfrac{1}{2}\ Y + 1 | F_- | \lambda\ \mu\ I\ \nu\ Y\rangle = C(I\ \tfrac{1}{2}\ I + \tfrac{1}{2}\ \nu\ -\tfrac{1}{2}\ \nu - \tfrac{1}{2}) A(\lambda\ \mu\ I + \tfrac{1}{2} Y)(2I+2)^{-\frac{1}{2}}, \tag{B.4}$$

$$\langle \lambda\ \mu\ I - \tfrac{1}{2}\ \nu - \tfrac{1}{2}\ Y + 1 | F_- | \lambda\ \mu\ I\ \nu\ Y\rangle = C(I\ \tfrac{1}{2}\ I - \tfrac{1}{2}\ \nu\ -\tfrac{1}{2}\ \nu - \tfrac{1}{2}) B(\lambda\ \mu\ I - \tfrac{1}{2} Y)(2I)^{-\frac{1}{2}}. \tag{B.5}$$

Herein, we have used the notation of Rose[13] for the CG coefficients of $R_3(I)$. The explicit formulas for them are too well known to need repetition here. The functions A and B are given by

$$A(\lambda\mu x) = \big[[\tfrac{1}{3}(\lambda - \mu) + x + 1] \times [\tfrac{1}{3}(\lambda + 2\mu) + x + 2][\tfrac{1}{3}(2\lambda + \mu) - x]\big]^{\frac{1}{2}}, \tag{B.6}$$

$$B(\lambda\mu x) = \big[[\tfrac{1}{3}(\mu - \lambda) + x] \times [\tfrac{1}{3}(\lambda + 2\mu) - x + 1][\tfrac{1}{3}(2\lambda + \mu) + x + 1]\big]^{\frac{1}{2}}. \tag{B.7}$$

We note that the same sets of factors multiply the CG coefficients of $R_3(I)$ in each of the pairs (B2) and (B4), (B3) and (B5). This is a consequence of the Wigner–Eckart theorem for $R_3(I)$, the sets of factors in question being the reduced with respect to $R_3(I)$ matrix elements of F and for the $I \to I \pm \frac{1}{2}$ cases.

Likewise, Eqs. (A4), (A11), and (A15) show that $G_\pm$ also are the $\nu = \pm\frac{1}{2}$ components of a spherical tensor of rank $\frac{1}{2}$ with respect to $R_3(I)$. In fact, this rank-$\frac{1}{2}$ spherical tensor is exactly the Hermitian adjoint in the sense of Edmonds[14] of that which has $F_\pm$ as its $\nu = \pm\frac{1}{2}$ components. This can be seen directly by comparing

$$G_\pm = \mp F_\mp^\dagger, \tag{2.8}$$

with the cited equation.[14] From (B2)–(B5) and Eq. (2.8), we obtain the results:

$$\langle \lambda\ \mu\ I + \tfrac{1}{2}\ \nu + \tfrac{1}{2}\ Y - 1 | G_+ | \lambda\ \mu\ I\ \nu\ Y\rangle = C(I\ \tfrac{1}{2}\ I + \tfrac{1}{2}\ \nu\ \tfrac{1}{2}\ \nu + \tfrac{1}{2})(-) \times B(\lambda\ \mu\ I - \tfrac{1}{2} Y + 1)(2I+2)^{-\frac{1}{2}}, \tag{B.8}$$

[10] A. J. Macfarlane, E. C. G. Sudarshan, and C. Dullemond, Nuovo Cimento **30**, 845 (1963).

[11] L. C. Biedenharn, Phys. Letters **3**, 69 (1962).

[12] M. Harvey and J. P. Elliott, Proc. Roy. Soc. London **A 272**, 557 (1963). K. T. Hecht, SU_3 "Reduction Coefficients and Fractional Parentage Coefficients," (University of Michigan preprint, 1963).

[13] See, e. g., M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957), Eqs. (3.16a) and (3.17a).

[14] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957), Eq. (5.5.3).

$$\langle \lambda\ \mu\ I-\tfrac{1}{2}\ \nu+\tfrac{1}{2}\ Y-1|\ G_+\ |\lambda\ \mu\ I\ \nu\ Y\rangle$$
$$= C(I\ \tfrac{1}{2}\ I-\tfrac{1}{2}\ \nu\ \tfrac{1}{2}\ \nu+\tfrac{1}{2})A(\lambda\ \mu\ I+\tfrac{1}{2}Y-1)(2I)^{-\frac{1}{2}}, \tag{B.9}$$

$$\langle \lambda\ \mu\ I+\tfrac{1}{2}\ \nu-\tfrac{1}{2}\ Y-1|\ G_-\ |\lambda\ \mu\ I\ \nu\ Y\rangle$$
$$= C(I\ \tfrac{1}{2}\ I+\tfrac{1}{2}\ \nu\ -\tfrac{1}{2}\ \nu-\tfrac{1}{2})(-)$$
$$\times B(\lambda\ \mu\ I-\tfrac{1}{2}Y+1)(2I+2)^{-\frac{1}{2}}, \tag{B.10}$$

$$\langle \lambda\ \mu\ I-\tfrac{1}{2}\ \nu-\tfrac{1}{2}\ Y-1|\ G_-\ |\lambda\ \mu\ I\ \nu\ Y\rangle$$
$$= C(I\ \tfrac{1}{2}\ I-\tfrac{1}{2}\ \nu\ -\tfrac{1}{2}\ \nu-\tfrac{1}{2})A(\lambda\ \mu\ I+\tfrac{1}{2}Y-1)(2I)^{-\frac{1}{2}}, \tag{B.11}$$

which completes the catalog, Eq. (B), of the non-vanishing matrix elements of the nondiagonal members of the set (2.6) of generators of SU_3.

It should now be clear that the quantities $F_\pm$ and $G_\pm$ were introduced in Eq. (2.5) so that the crucial importance of the role of the subgroup $R_3(I)$ of SU_3 in the theory of SU_3 could be brought clearly into focus. Of course, the separation of the set (2.6) into a triplet, a singlet and two doublets reflects the by-now-well-known structure of octets in the Ne'eman–Gell-Mann theory.[15]

3. THE OCTET OPERATORS OF SU_3

In this section we define the octet operator of SU_3 and derive the selection rules which determine which of its matrix elements do not vanish identically.

We begin with a general definition of regular tensor operator. Let X_ρ $(1 \leq \rho \leq r)$ be the (Hermitian) generators of a compact Lie group L of order r. It is well known[8] that L is defined uniquely up to local isomorphism by their CR's:

$$[\mathrm{X}_\rho, \mathrm{X}_\sigma] = c_{\rho\sigma}{}^\tau \mathrm{X}_\tau. \tag{3.1}$$

Herein the $c_{\rho\sigma}{}^\tau$ are the structure constants of L which satisfy the antisymmetry property

$$c_{\rho\sigma}{}^\tau + c_{\sigma\rho}{}^\tau = 0, \tag{3.2}$$

and the Jacobi identity. The components $\mathrm{T}_\rho (1 \leq \rho \leq r)$ of the regular tensor operator of L are now defined according to[16]

$$[\mathrm{X}_\rho, \mathrm{T}_\sigma] = c_{\rho\sigma}{}^\tau \mathrm{T}_\tau. \tag{3.3}$$

We observe that Eqs. (3.2) and (3.3) imply the equations

$$[\mathrm{T}_\rho, \mathrm{X}_\sigma] = c_{\rho\sigma}{}^\tau \mathrm{T}_\tau. \tag{3.4}$$

From the fact that $\mathrm{T}_\rho = \mathrm{X}_\rho$ satisfies the definition (3.3), we conclude that the set of generators of L is a special case of the regular tensor operator. Also, by comparison of Eq. (3.3) with (3.1), we may say the set T_ρ transform under L exactly as do the set X_ρ of generators. In the familiar context of the rotation group in three dimensions, the regular tensor operator is just the vector operator. It is readily verified that the CR's of its components with the rotation generators agrees with Eqs. (3.3) and (3.4).

We now introduce the regular tensor operator of SU_3. Since the regular representation of SU_3 is the IR (1, 1) or octet, we normally speak of the octet operator of SU_3. The octet operator of SU_3 is the set of eight quantities

$$\mathcal{I}_z, \mathcal{Y}, \mathcal{I}_\pm, \mathcal{F}_\pm, \mathcal{G}_\pm, \tag{3.5}$$

which transform under SU_3 exactly as do the set (2.6) of generators. The CR's of the components (3.5) of the octet operator with the generators (2.6) bear the same relation to Eq. (A) as does the general definition (3.3) of regular tensor operator to Eq. (3.1). Hence we have

$$[I_z, \mathcal{Y}] = [\mathcal{I}_z, Y] = 0, \qquad \text{(C1), (D1)}$$
$$[I_z, \mathcal{I}_\pm] = [\mathcal{I}_z, I_\pm] = \pm\mathcal{I}_\pm, \qquad \text{(C2), (D2)}$$
$$[I_z, \mathcal{F}_\pm] = [\mathcal{I}_z, F_\pm] = \pm\tfrac{1}{2}\mathcal{F}_\pm, \qquad \text{(C3), (D3)}$$
$$[I_z, \mathcal{G}_\pm] = [\mathcal{I}_z, G_\pm] = \pm\tfrac{1}{2}\mathcal{G}_\pm, \qquad \text{(C4), (D4)}$$
$$[Y, \mathcal{I}_\pm] = [\mathcal{Y}, I_\pm] = 0, \qquad \text{(C5), (D5)}$$
$$[Y, \mathcal{F}_\pm] = [\mathcal{Y}, F_\pm] = \mathcal{F}_\pm, \qquad \text{(C6), (D6)}$$
$$[Y, \mathcal{G}_\pm] = [\mathcal{Y}, G_\pm] = -\mathcal{G}_\pm, \qquad \text{(C7), (D7)}$$
$$[I_-, \mathcal{I}_+] = [\mathcal{I}_-, I_+] = 2\mathcal{I}_z, \qquad \text{(C8), (D8)}$$
$$[F_\pm, \mathcal{G}_\mp] = [\mathcal{F}_\pm, G_\mp] = \mathcal{I}_z \pm \tfrac{3}{2}\mathcal{Y}, \qquad \text{(C9), (D9)}$$
$$[I_\pm, \mathcal{F}_\pm] = [\mathcal{I}_\pm, F_\pm] = 0, \qquad \text{(C10), (D10)}$$
$$[I_\pm, \mathcal{G}_\pm] = [\mathcal{I}_\pm, G_\pm] = 0, \qquad \text{(C11), (D11)}$$
$$[F_+, \mathcal{F}_-] = [\mathcal{F}_+, F_-] = 0, \qquad \text{(C12), (D12)}$$
$$[G_+, \mathcal{G}_-] = [\mathcal{G}_+, G_-] = 0, \qquad \text{(C13), (D13)}$$
$$[I_\pm, \mathcal{F}_\mp] = [\mathcal{I}_\pm, F_\mp] = \mathcal{F}_\pm, \qquad \text{(C14), (D14)}$$
$$[I_\pm, \mathcal{G}_\mp] = [\mathcal{I}_\pm, G_\mp] = \mathcal{G}_\pm, \qquad \text{(C15), (D15)}$$
$$[F_\pm, \mathcal{G}_\pm] = [\mathcal{F}_\pm, G_\pm] = \mp\mathcal{I}_\pm, \qquad \text{(C16), (D16)}$$
$$[I_z, \mathcal{I}_z] = 0, \qquad \text{(E1)}$$
$$[Y, \mathcal{Y}] = 0, \qquad \text{(E2)}$$
$$[I_\pm, \mathcal{I}_\pm] = 0, \qquad \text{(E3)}$$
$$[F_\pm, \mathcal{F}_\pm] = 0, \qquad \text{(E4)}$$
$$[G_\pm, \mathcal{G}_\pm] = 0. \qquad \text{(E5)}$$

[15] Y. Ne'eman, Nucl. Phys. **26**, 222 (1961); M. Gell-Mann, footnote 1.

[16] J. Ginibre, J. Math. Phys. **4**, 720 (1963).

It is our intention to use Eqs. (C), (D), and (E), along with the known formulas (B) for the nonvanishing matrix elements of the generators (2.6), to evaluate all the nonvanishing matrix elements of the components (3.5) of the octet operator. We first must determine what are the nonvanishing matrix elements of the type

$$\langle \lambda' \mu' I' \nu' Y' | \ \mathfrak{M} \ | \lambda \mu I \nu Y \rangle \tag{3.6}$$

where $\mathfrak{M}$ belongs to the set (3.5).

We consider first the selection rules $(\lambda, \mu) \to (\lambda', \mu')$. Since $\mathfrak{M}$ is a component of the octet tensor operator, it is evident that the allowed (λ', μ') are those that are contained as irreducible constituents of the Kronecker product

$$(\lambda, \mu) \otimes (1, 1). \tag{3.7}$$

This is the analog of the statement for the three-dimensional rotation group that the vector operator connects j to $j + 1$, j and $j - 1$. In the present case, the reduction of (2.16) can be effected by exploiting the correspondence of IR's of SU_3 to Young tableaux in the manner of Edmonds[17] or else by the method of Speiser.[18] The result we find is that the product (3.7) contains[19]

(I)	$(\lambda + 2, \mu - 1)$	once unless	$\mu = 0$;
(II)	$(\lambda - 1, \mu - 1)$	once unless	$\mu = 0$ or $\lambda = 0$;
(III)	$(\lambda - 2, \mu + 1)$	once unless	$\lambda = 0$ or 1;
(IV)	$(\lambda + 1, \mu + 1)$	once;	
(V)	$(\lambda - 1, \mu + 2)$	once unless	$\lambda = 0$;
(VI)	$(\lambda + 1, \mu - 2)$	once unless	$\mu = 0$ or 1;
(VII)	(λ, μ)	twice if	$\lambda, \mu \neq 0$,
		once if	$\lambda = 0, \mu \neq 0$ or $\mu = 0, \lambda \neq 0$,
		not at all if	$\lambda = \mu = 0$.

We shall have to treat all seven cases separately. Case (VII) is surely the most complicated since the possible double appearance of (λ, μ) itself means that there are two independent (SU_3) reduced matrix elements involved. Fortunately, Okubo[1] has already treated this case. Okubo derived a formula[20] which shows that the components of the octet operator can be regarded as certain functions of the generators of SU_3 as far as their matrix elements within a given IR of SU_3 are concerned. Hence Eq. (B) allows the nonvanishing matrix elements of the octet operator under Case (VII) to be directly computed. The fact that Okubo's method does not appear to be applicable to Cases (I)–(VI) may be contrasted with the fact that our approach to these cases may also be applied to Case (VII). Our method consists in manipulation of CR's. It will turn out however that we really need apply it only to two suitably chosen cases, e.g., Cases (I) and (II). Then Cases (III) and (IV) can be obtained from these respective cases by a process involving Hermitian conjugation. Finally, Cases (V) and (VI) can be obtained from Cases (III) and (I), respectively, by R conjugation,[21] which effects the transformation $(\lambda, \mu) \to (\mu, \lambda)$. These conjugation processes, which are much more economical than the CR manipulation process, are described in Sec. 5.

We consider next the $(I, \nu, Y) \to (I', \nu', Y')$ selection rules. From Eqs. (E2), (D1), (C5), (C6), and (C7), respectively, we see that $\mathcal{Y}$, $\mathcal{I}_z$, $\mathcal{I}_\pm$ conserve Y; $\mathcal{F}_\pm$ raise Y to $Y + 1$; and $\mathcal{G}_\pm$ lower Y to $Y - 1$. From Eqs. (C2), (D2), (C8), (D8), (E1), and (E3), we see that $\mathcal{I}_\pm$ and $\mathcal{I}_z$ have exactly the CR's with I necessary for $(-(1/\sqrt{2})\mathcal{I}_+, \mathcal{I}_z, (1/\sqrt{2})\mathcal{I}_-)$ to be viewed as the $\nu = 1, 0, -1$ components of a spherical vector with respect to $R_3(I)$. It follows that all three have nonvanishing matrix elements for $I' = I + 1, I$, and $I - 1$. Also the ν dependence of the allowed matrix elements is contained [by the Wigner–Eckart theorem of $R_3(I)$] in a CG coefficient of the form $C(I\ 1\ I'\ \nu\ \nu' - \nu\ \nu')$. Next we observe, by comparison of appropriate members of Eqs. (C) and (D) with the corresponding members of Eq. (A), that $\mathcal{F}_\pm$ and $\mathcal{G}_\pm$ have, respectively, the same tensorial character with respect to $R_3(I)$ as have the generators $F_\pm$ and $G_\pm$. Accordingly, the same remarks regarding I and Y selection rules and ν-dependence of allowed matrix elements as were made for the latter in Sec. 2 apply equally to the former.

Finally, on enumerating, it would appear that, within each of the six cases $(\lambda, \mu) \to (\lambda', \mu')$ to be examined, there are 18 matrix elements of the quantities (3.5) to be evaluated. We must, however, consider this statement more precisely in the light of the Wigner–Eckart theorems for SU_3 and $R_3(I)$. In the former case, the theorem tells us that the entire dependence of any of the matrix elements in question on I, ν, and Y is contained within a single CG coefficient of SU_3 defined uniquely up to a phase, there being at most one reduced matrix element in each of the Cases (I) to (VI). In the case of $R_3(I)$, the Wigner–Eckart theorem gives the

[17] A. R. Edmonds, Proc. Roy. Soc. London **A 268**, 567 (1962).

[18] D. R. Speiser, Proc. Istanbul Summer School, Istanbul, 1962 (to be published).

[19] Familiar results can be verified to follow from this.

[20] See Eq. (A.8) of the first of the papers by Okubo cited in footnote 1.

[21] M. Gell-Mann, footnote 1.

entire ν dependence of any of the matrix elements in question in the form of a CG coefficient of $R_3(I)$. The connection between these last two statements is afforded by a theorem, discussed by Racah[22] in a general context, and by Edmonds[17] in the context of SU_3. The theorem informs us that the CG coefficients of SU_3, with respect to a basis like that being used here, each factorize as the product of two factors. One of these factors is a CG coefficient of $R_3(I)$, and the other is an isoscalar factor, dependent on I and Y but not ν. Since, in all the matrix elements in question, the former of these is known, the task ahead essentially is the determination of the latter. To this end, we introduce notations which incorporate a great deal of the knowledge so far accumulated.

$$\langle \lambda' \mu' I' \nu\ Y | \mathcal{I}_z | \lambda \mu I \nu\ Y\rangle = C(I\ 1\ I'\ \nu\ 0\ \nu)\mathcal{I}(\lambda \mu I\ Y; \lambda' \mu' I'\ Y) \langle \lambda' \mu' || (1,1) || \lambda \mu\rangle, \tag{F.1}$$

$$\langle \lambda' \mu' I' \nu\pm 1\ Y | \mathcal{I}_\pm | \lambda \mu I \nu\ Y\rangle = \mp\sqrt{2} C(I\ 1\ I'\ \nu\ \pm 1\ \nu\pm 1)\mathcal{I}(\lambda \mu I\ Y; \lambda' \mu' I'\ Y) \times \langle \lambda' \mu' || (1,1) || \lambda \mu\rangle, \tag{F.2}$$

$$\langle \lambda' \mu' I' \nu\pm\tfrac{1}{2}\ Y+1 | \mathcal{F}_\pm | \lambda \mu I \nu\ Y\rangle = C(I\ \tfrac{1}{2}\ I'\ \nu\ \pm\tfrac{1}{2}\ \nu\pm\tfrac{1}{2})\mathcal{F}(\lambda \mu I\ Y; \lambda' \mu' I'\ Y+1) \times \langle \lambda' \mu' || (1,1) || \lambda \mu\rangle, \tag{F.3}$$

$$\langle \lambda' \mu' I' \nu\pm\tfrac{1}{2}\ Y-1 | \mathcal{G}_\pm | \lambda \mu I \nu\ Y\rangle = C(I\ \tfrac{1}{2}\ I'\ \nu\ \pm\tfrac{1}{2}\ \nu\pm\tfrac{1}{2})\mathcal{G}(\lambda \mu I\ Y; \lambda' \mu' I'\ Y-1) \times \langle \lambda' \mu' || (1,1) || \lambda \mu\rangle, \tag{F.4}$$

$$\langle \lambda' \mu' I \nu\ Y | \mathcal{Y} | \lambda \mu I \nu\ Y\rangle = \mathcal{Y}(\lambda \mu I\ Y; \lambda' \mu' I\ Y) \times \langle \lambda' \mu' || (1,1) || \lambda \mu\rangle. \tag{F.5}$$

The notation (F) applies to Cases (I) to (VI), the allowed I' values having been given above. Within each case there are eight functions to be obtained. It is to be observed that the functions $\mathcal{I}$, $\mathcal{F}$, $\mathcal{G}$, $\mathcal{Y}$, of Eq. (F) are not defined uniquely by Eq. (F). They contain the entire I and Y dependence of the corresponding isoscalar factors, but part or all the factors of the latter independent of I and Y may be absorbed into the reduced matrix element $\langle \lambda'\mu' || (1,1) || \lambda\mu\rangle$ to give formulas of the type (F). The technical discussion of the deduction of functions $\mathcal{I}$, $\mathcal{F}$, $\mathcal{G}$, and $\mathcal{Y}$ to satisfy Eq. (F) in each of Cases (I) to (VI) is taken up in the following sections.

[22] G. Racah, Phys. Rev. **76** 1352 (1949).

4. MANIPULATION OF CR's

In this section, we illustrate a method of deriving explicit expressions for the functions $\mathcal{I}$, $\mathcal{F}$, $\mathcal{G}$, and $\mathcal{Y}$ of Eq. (F) from Eqs. (B) to (E) with reference to Case (I) i.e., $(\lambda', \mu') = (\lambda + 2, \mu - 1)$. It is possible that more economical procedures could be used; the method described is in fact that actually used in treating Cases (I) and (II).

We first approach the $I' = I + 1$ function of the type $\mathcal{I}(\lambda\ \mu\ I\ Y; \lambda{+}2\ \mu{-}1\ I'\ Y)$.

From the

$$\langle \lambda{+}2\ \mu{-}1\ I{+}\tfrac{3}{2}\ \nu{+}\tfrac{3}{2}\ Y{+}1 | \cdots | \lambda\ \mu\ I\ \nu\ Y\rangle$$

matrix element of the upper half of Eq. (D10), i.e., of $[\mathcal{I}_+, F_+] = 0$, we obtain, using also Eqs. (B2) and (F1), the result

$$\begin{aligned}
&[(2I+3)(2I+4)]^{\frac{1}{2}} \\
&\quad\times \mathcal{I}(\lambda\ \mu\ I{+}\tfrac{1}{2}Y{+}1; \lambda{+}2\ \mu{-}1\ I{+}\tfrac{3}{2}\ Y{+}1) \\
&\quad\times \big[[\tfrac{1}{3}(\lambda-\mu) + (I{+}\tfrac{1}{2}Y{+}1) + 1] \\
&\quad\times [\tfrac{1}{3}(\lambda-\mu) + (I{+}\tfrac{1}{2}Y{+}1) + 2] \\
&\quad\times [\tfrac{1}{3}(\lambda+2\mu) + (I{+}\tfrac{1}{2}Y{+}1) + 2]\big]^{-\frac{1}{2}} \\
&= [(2I+2)(2I+3)]^{\frac{1}{2}}\mathcal{I}(\lambda\ \mu\ I\ Y; \lambda{+}2\ \mu{-}1\ I{+}1\ Y) \\
&\quad\times \big[[\tfrac{1}{3}(\lambda-\mu) + (I{+}\tfrac{1}{2}Y) + 1] \\
&\quad\times [\tfrac{1}{3}(\lambda-\mu) + (I{+}\tfrac{1}{2}Y) + 2] \\
&\quad\times [\tfrac{1}{3}(\lambda+2\mu) + (I{+}\tfrac{1}{2}Y) + 2]\big]^{-\frac{1}{2}}.
\end{aligned} \tag{4.1}$$

We note that all ν dependent factors have canceled as consistency requires. We note also that certain factors have been inserted, once on each side of the equation. This has served to leave Eq. (4.1) in the form

$$f(I{+}\tfrac{1}{2}Y{-}1, I{-}\tfrac{1}{2}Y) = f(I{+}\tfrac{1}{2}Y, I{-}\tfrac{1}{2}Y), \tag{4.2}$$

it being understood that the replacement of $2I$ by $(I{+}\frac{1}{2}Y) + (I{-}\frac{1}{2}Y)$ is made where necessary. It then follows that each side of Eq. (4.2) is independent of $(I{+}\frac{1}{2}Y)$. Hence we have a result of the form

$$\begin{aligned}
&[(2I+2)(2I+3)]^{\frac{1}{2}}\mathcal{I}(\lambda\ \mu\ I\ Y; \lambda{+}2\ \mu{-}1\ I{+}1\ Y) \\
&\quad= \big[[\tfrac{1}{3}(\lambda-\mu) + (I{+}\tfrac{1}{2}Y{+}1)] \\
&\qquad\times [\tfrac{1}{3}(\lambda-\mu) + (I{+}\tfrac{1}{2}Y{+}2)] \\
&\qquad\times [\tfrac{1}{3}(\lambda+2\mu) + (I{+}\tfrac{1}{2}Y{+}2)]\big]^{\frac{1}{2}} \\
&\qquad\times \alpha(\lambda\ \mu\ I{-}\tfrac{1}{2}Y),
\end{aligned} \tag{4.3}$$

where α is an unknown function. Let us call the expression inside the heavy brackets of Eq. (4.3) $a(\lambda\ \mu\ I{+}\frac{1}{2}Y)$. Next, we similarly use the

$$\langle \lambda+2\ \mu-1\ I+\tfrac{3}{2}\ \nu+\tfrac{3}{2}\ Y-1| \cdots |\lambda\ \mu\ I\ \nu\ Y\rangle \quad (4.4)$$

matrix element of the upper line of Eq. (D11), i.e., $[g_+, G_+] = 0$ to deduce the existence of a result of the form

$$\begin{aligned}[(2I+2)(2I+3)]^{\frac{1}{2}} &\times g(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I+1\ Y) \\ = [&[\tfrac{1}{3}(\lambda+2\mu) - (I-\tfrac{1}{2}Y)] \\ &\times [\tfrac{1}{3}(2\lambda+\mu) + (I-\tfrac{1}{2}Y+2)] \\ &\times [\tfrac{1}{3}(2\lambda+\mu) + (I-\tfrac{1}{2}Y+3)]]^{\frac{1}{2}} \\ &\times \beta(\lambda\ \mu\ I+\tfrac{1}{2}Y), \end{aligned} \quad (4.5)$$

where β is an unknown factor. Let us call the expression inside the heavy brackets of Eq. (4.5) $b(\lambda\ \mu\ I-\frac{1}{2}Y)$. Equations (4.3) and (4.5) contain the entire dependence on $I \pm \frac{1}{2}Y$, and hence on I and Y, of $g(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I+1\ Y)$. Accordingly, we can set

$$\begin{aligned}[(2I+2)(2I+3)]^{\frac{1}{2}} &g(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I+1\ Y) \\ &= [a(\lambda\ \mu\ I+\tfrac{1}{2}Y)b(\lambda\ \mu\ I-\tfrac{1}{2}Y)]^{\frac{1}{2}}. \end{aligned} \quad (4.6)$$

Equation (F2) with Eq. (4.6) actually defines the reduced matrix element for the Case (I). We can transfer from it into the right side of (4.6) any function of λ and μ without disturbing agreement with (4.3) and (4.5). However, having made a "minimal" definition (4.6) of a function, $g(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I+1\ Y)$ consistent with Eqs. (4.3) and (4.5), we must take care to respect the definition of the reduced matrix element which it implies throughout the rest of our discussion of Case (I).

We may in like manner use the

$$\langle \lambda+2\ \mu-1\ I-\tfrac{3}{2}\ \nu+\tfrac{3}{2}\ Y+1| \cdots |\lambda\ \mu\ I\ \nu\ Y\rangle$$

matrix element of $[g_+, F_+] = 0$, and the

$$\langle \lambda+2\ \mu-1\ I-\tfrac{3}{2}\ \nu+\tfrac{3}{2}\ Y-1| \cdots |\lambda\ \mu\ I\ \nu\ Y\rangle$$

matrix element of $[g_+, G_+] = 0$ to derive the result

$$\begin{aligned}[2I(2I-1)]^{\frac{1}{2}} &g(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I-1\ Y) \\ = [&[\tfrac{1}{3}(\mu-\lambda) + (I-\tfrac{1}{2}Y-1)] \\ &\times [\tfrac{1}{3}(\mu-\lambda) + (I-\tfrac{1}{2}Y)] \\ &\times [\tfrac{1}{3}(\lambda+2\mu) - (I-\tfrac{1}{2}Y-1)]]^{\frac{1}{2}} \\ &\times [[\tfrac{1}{3}(\lambda+2\mu) + (I+\tfrac{1}{2}Y+1)] \\ &\times [\tfrac{1}{3}(2\lambda+\mu) - (I+\tfrac{1}{2}Y-1)] \\ &\times [(\tfrac{1}{3}2\lambda+\mu) - (I+\tfrac{1}{2}Y-2)]]^{\frac{1}{2}}\ \eta(\lambda, \mu) \\ = [&c(\lambda\ \mu\ I-\tfrac{1}{2}Y)]^{\frac{1}{2}} \\ &\times [d(\lambda\ \mu\ I+\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \eta(\lambda, \mu). \end{aligned} \quad (4.7)$$

The presence of the factor $\eta(\lambda, \mu)$ relates to the point in discussion after Eq. (4.6). Essentially the two steps of our procedure so far effected give the I, ν, and Y dependence of the distinct matrix elements $\langle \lambda+2\ \mu-1\ I\pm1\ \nu+1|\ g_+\ |\lambda\ \mu\ I\ \nu\ Y\rangle$. We have no reason to assume that the reduced matrix elements defined by taking out this dependence in the two cases are the same. The factor $\eta(\lambda, \mu)$ is exactly the factor necessary to ensure that the same reduced matrix element occurs in the lower-sign case as was (arbitrarily, perhaps, but definitely) introduced for the upper-sign case. The form of the results (4.6) and (4.7) suggests $\eta(\lambda, \mu) = 1$ or -1. We cannot yet tell which of the two possibilities is required by consistency.

We go on to relate $\mathfrak{F}(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I\pm\frac{1}{2}\ Y+1)$ to $g(\lambda\ \mu\ I\ Y;\ \lambda+2\ \mu-1\ I\pm1\ Y)$, respectively. Take the upper-sign case first. We can use the matrix element $\langle \lambda+2\ \mu-1\ I+1\ \nu\ Y+2| \cdots |\lambda\ \mu\ I\ \nu\ Y\rangle$ of Eq. (D12), $[\mathfrak{F}_+, F_-] = 0$ to derive a result of the form

$$\begin{aligned}(2I+2)^{\frac{1}{2}}&\mathfrak{F}(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I+\tfrac{1}{2}\ Y+1) \\ &= [a(\lambda\ \mu\ I+\tfrac{1}{2}Y)]^{\frac{1}{2}}\gamma(\lambda\ \mu\ I-\tfrac{1}{2}Y), \end{aligned} \quad (4.8)$$

with a as given above [Eq. (4.3)], and γ an unknown function. Then we use Eq. (4.6) and Eq. (4.8) to transform the matrix element

$$\langle \lambda+2\ \mu-1\ I+1\ \nu+1\ Y| \cdots |\lambda\mu I\nu Y\rangle$$

of Eq. (D16), i.e., $[\mathfrak{F}_+, G_+] = -g_+$, into the following recursion formula for γ:

$$\begin{aligned}-\sqrt{2} = &\gamma(\lambda\ \mu\ I-\tfrac{1}{2}Y+1) \\ &\times [\tfrac{1}{3}(\mu-\lambda) + (I-\tfrac{1}{2}Y+1)]^{\frac{1}{2}} \\ &\times [\tfrac{1}{3}(2\lambda+\mu) + (I-\tfrac{1}{2}Y+1) + 2]^{-\frac{1}{2}} \\ &- \gamma(\lambda\ \mu\ I-\tfrac{1}{2}Y)[\tfrac{1}{3}(\mu-\lambda) + (I-\tfrac{1}{2}Y)]^{\frac{1}{2}} \\ &\times [\tfrac{1}{3}(2\lambda+\mu) + (I-\tfrac{1}{2}Y+2)]^{-\frac{1}{2}}. \end{aligned} \quad (4.9)$$

The solution

$$\begin{aligned}\gamma(\lambda\ \mu\ I-\tfrac{1}{2}Y) = &-\sqrt{2}[[\tfrac{1}{3}(\mu-\lambda) + (I-\tfrac{1}{2}Y)] \\ &\times [\tfrac{1}{3}(2\lambda+\mu) + (I-\tfrac{1}{2}\ Y+2)]]^{\frac{1}{2}} \end{aligned} \quad (4.10)$$

can be obtained easily. We note that Eq. (4.8) with (4.10) is exactly in agreement with (4.6) as it stands. This is because we have used an equation, (D16), directly relating

$$\mathfrak{F}(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I+\tfrac{1}{2}\ Y+1)$$

and

$$g(\lambda\ \mu\ I\ Y; \lambda+2\ \mu-1\ I+1\ Y).$$

TABLE I. $(\lambda + 2, \mu - 1)$.

$$[(2I+2)(2I+3)]^{\frac{1}{2}}\, \mathcal{g}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{+}1\ Y) = [a(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)\ b(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)]^{\frac{1}{2}}.$$

$$2[2I(I+1)]^{\frac{1}{2}}\, \mathcal{g}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I\ Y) = \gamma(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)\ \delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)[\tfrac{1}{3}(\lambda+2\mu)+1+\tfrac{1}{2}\ Y].$$

$$[2I(2I-1)]^{\frac{1}{2}}\, \mathcal{g}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{-}1\ Y) = [c(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)\ d(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)]^{\frac{1}{2}}.$$

$$(2I+2)^{\frac{1}{2}}\, \mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{+}\tfrac{1}{2}\ Y{+}1) = [a(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \gamma(\lambda\ \mu\ I{-}\tfrac{1}{2}Y).$$

$$(2I)^{\frac{1}{2}}\, \mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{-}\tfrac{1}{2}\ Y{+}1) = [c(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y).$$

$$(2I+2)^{\frac{1}{2}}\, \mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{+}\tfrac{1}{2}\ Y{-}1) = -\ [b(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y).$$

$$(2I)^{\frac{1}{2}}\, \mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{-}\tfrac{1}{2}\ Y{-}1) = -\ [d(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \gamma(\lambda\ \mu\ I{-}\tfrac{1}{2}Y).$$

$$\sqrt{2}\,\mathcal{y}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I\ Y) = \gamma(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)\ \delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y).$$

$$a(\lambda\mu x) = [\tfrac{1}{3}(\lambda-\mu)+x+1]\cdot[\tfrac{1}{3}(\lambda-\mu)+x+2][\tfrac{1}{3}(\lambda+2\mu)+x+2].$$

$$b(\lambda\mu x) = [\tfrac{1}{3}(\lambda+2\mu)-x][\tfrac{1}{3}(2\lambda+\mu)+x+2][\tfrac{1}{3}(2\lambda+\mu)+x+3].$$

$$c(\lambda\mu x) = [\tfrac{1}{3}(\mu-\lambda)+x-1]\cdot[\tfrac{1}{3}(\mu-\lambda)+x][\tfrac{1}{3}(\lambda+2\mu)-x+1].$$

$$d(\lambda\mu x) = [\tfrac{1}{3}(\lambda+2\mu)+x+1]\cdot[\tfrac{1}{3}(2\lambda+\mu)-x+1][\tfrac{1}{3}(2\lambda+\mu)-x+2].$$

$$\gamma(\lambda\mu x) = -\ [2[\tfrac{1}{3}(\mu-\lambda)+x][\tfrac{1}{3}(2\lambda+\mu)+x+2]]^{\frac{1}{2}}.$$

$$\delta(\lambda\mu x) = -\ [2[\tfrac{1}{3}(\lambda-\mu)+x+1][\tfrac{1}{3}(2\lambda+\mu)-x+1]]^{\frac{1}{2}}.$$

Next we treat the lower-sign case in a parallel manner. We obtain

$$(2I)^{\frac{1}{2}}\mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{-}\tfrac{1}{2}\ Y{+}1) = [c(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)]^{\frac{1}{2}}\,\delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)\eta(\lambda,\mu), \qquad (4.11)$$

with d as in Eq. (4.7), and δ obtained by solution of a recursion formula in the form

$$\delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y) = -\sqrt{2}[[\tfrac{1}{3}(\lambda-\mu)+(I{+}\tfrac{1}{2}Y{+}1)] \times [\tfrac{1}{3}(2\lambda+\mu)-(I{+}\tfrac{1}{2}Y{-}1)]]^{\frac{1}{2}}, \qquad (4.12)$$

and $\eta(\lambda, \mu)$ the same factor as in (4.7). The factor $\eta(\lambda, \mu)$ is present here because (4.11) and (4.12) are in exact agreement with (4.7) just as (4.8) and (4.10) are with (4.6).

We observe that the respective matrix elements

$$\langle\lambda{+}2\ \mu{-}1\ I{\pm}1\ \nu\ Y{+}2|\ \cdots\ |\lambda\ \mu\ I\ \nu\ Y\rangle \quad \text{of} \quad [\mathcal{F}_+, F_-] = 0$$

have been used in the evaluation of $\mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{\pm}\frac{1}{2}\ Y{+}1)$. Both these quantities occur in the corresponding $I \rightarrow I$ matrix element, which therefore can be used to evaluate $\eta(\lambda, \mu)$. Use of Eqs. (4.8) and (4.11) leads to the reduction of the ensuing equation to $\eta(\lambda, \mu) = 1$. The fact that everything else cancels out of the equation affords a check on the consistency of the calculations so far performed. From this point, we can move rapidly to the completion of the treatment of Case (I).

In search of the unknown functions $\mathcal{g}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I\ Y)$ and $\mathcal{y}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I\ Y)$, we next evaluate the $\langle\lambda{+}2\ \mu{-}1\ I\ \nu\ Y|\ \cdots\ |\lambda\ \mu\ I\ Y\rangle$ matrix element of (D9), i.e., $[\mathcal{F}_+, G_-] = \mathcal{g}_s + \frac{3}{2}\mathcal{y}$. Results (4.8) and (4.11) with $\eta = 1$ and Eqs. (B10) and (B11) constitute the input for the left side. CG coefficients of $R_3(I)$ do not cancel out; we obtain a term independent of ν and a term proportional to ν on each side, these being the $\mathcal{y}$ and $\mathcal{g}_s$ terms, respectively, on the right. Putting $\nu = 0$, gives the result

$$\sqrt{2}\,\mathcal{y}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I\ Y) = \gamma(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)\delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y), \qquad (4.13)$$

with γ and δ as given by Eqs. (4.10) and (4.12). Since the terms independent of ν are equal, the coefficients of ν on each side must also be. From this, we find

$$2\sqrt{2}[I(I+1)]^{\frac{1}{2}}\mathcal{g}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I\ Y) = \gamma(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)\delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y) \times [\tfrac{1}{3}(\lambda+2\mu)+1+\tfrac{1}{2}\ Y]. \qquad (4.14)$$

TABLE II. $(\lambda - 1, \mu - 1)$.

$$[(2I+2)(2I+3)]^{\frac{1}{2}}\, \mathcal{g}(\lambda\ \mu\ I\ Y;\ \lambda{-}1\ \mu{-}1\ I{+}1\ Y) = [p(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)\ q(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)]^{\frac{1}{2}}.$$

$$2[2I(I+1)]^{\frac{1}{2}}\, \mathcal{g}(\lambda\ \mu\ I\ Y;\ \lambda{-}1\ \mu{-}1\ I\ Y) = \rho(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)\ \sigma(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)[\tfrac{1}{3}(\mu{-}\lambda)-\tfrac{1}{2}\ Y].$$

$$[2I(2I-1)]^{\frac{1}{2}}\, \mathcal{g}(\lambda\ \mu\ I\ Y;\ \lambda{-}1\ \mu{-}1\ I{-}1\ Y) = -\ [r(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)\ s(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)]^{\frac{1}{2}}.$$

$$(2I+2)^{\frac{1}{2}}\, \mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{-}1\ \mu{-}1\ I{+}\tfrac{1}{2}\ Y{+}1) = [p(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \rho(\lambda\ \mu\ I{-}\tfrac{1}{2}Y).$$

$$(2I)^{\frac{1}{2}}\, \mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{-}1\ \mu{-}1\ I{-}\tfrac{1}{2}\ Y{+}1) = [r(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \sigma(\lambda\ \mu\ I{+}\tfrac{1}{2}Y).$$

$$(2I+2)^{\frac{1}{2}}\, \mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{-}1\ \mu{-}1\ I{+}\tfrac{1}{2}\ Y{-}1) = [q(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \sigma(\lambda\ \mu\ I{+}\tfrac{1}{2}Y).$$

$$(2I)^{\frac{1}{2}}\, \mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{-}1\ \mu{-}1\ I{-}\tfrac{1}{2}\ Y{-}1) = -\ [s(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)]^{\frac{1}{2}}\ \rho(\lambda\ \mu\ I{-}\tfrac{1}{2}Y).$$

$$\sqrt{2}\ \mathcal{y}(\lambda\ \mu\ I\ Y;\ \lambda{-}1\ \mu{-}1\ I\ Y) = -\rho(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)\ \sigma(\lambda\ \mu\ I{+}\tfrac{1}{2}Y).$$

$$p(\lambda\mu x) = [\tfrac{1}{3}(\lambda-\mu)+x+1]\times[\tfrac{1}{3}(2\lambda+\mu)-x][\tfrac{1}{3}(2\lambda+\mu)-x-1].$$

$$q(\lambda\mu x) = [\tfrac{1}{3}(\mu-\lambda)+x+1]\times[\tfrac{1}{3}(\lambda+2\mu)-x][\tfrac{1}{3}(\lambda+2\mu)-x-1].$$

$$r(\lambda\mu x) = [\tfrac{1}{3}(\mu-\lambda)+x]\times[\tfrac{1}{3}(2\lambda+\mu)+x+1][\tfrac{1}{3}(2\lambda+\mu)+x].$$

$$s(\lambda\mu x) = [\tfrac{1}{3}(\lambda-\mu)+x]\times[\tfrac{1}{3}(\lambda+2\mu)+x+1][\tfrac{1}{3}(\lambda+2\mu)+x].$$

$$\rho(\lambda\mu x) = -\ [2[\tfrac{1}{3}(2\lambda+\mu)+x+1][\tfrac{1}{3}(\lambda+2\mu)-x]]^{\frac{1}{2}}.$$

$$\sigma(\lambda\mu x) = -\ [2[\tfrac{1}{3}(2\lambda+\mu)-x][\tfrac{1}{3}(\lambda+2\mu)+x+1]]^{\frac{1}{2}}.$$

The simplest way to obtain $\mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{+}2\ \mu{-}1\ I{\pm}\frac{1}{2}\ Y{-}1)$ is to use Eq. (D7), i.e., $\mathcal{G}_+ = [G_+, \mathcal{Y}]$. We find

$$(2I+2)^{\frac{1}{2}}\mathcal{G}(\lambda\ \mu\ I\ Y;\lambda{+}2\ \mu{-}1\ I{+}\tfrac{1}{2}\ Y{-}1) = -[b(\lambda\ \mu\ I{-}\tfrac{1}{2}Y)]^{\frac{1}{2}}\delta(\lambda\ \mu\ I{+}\tfrac{1}{2}Y), \quad (4.15)$$

$$(2I)^{\frac{1}{2}}\mathcal{G}(\lambda\ \mu\ I\ Y;\lambda{+}2\ \mu{-}1\ I{-}\tfrac{1}{2}\ Y{-}1) = -[d(\lambda\ \mu\ I{+}\tfrac{1}{2}Y)]^{\frac{1}{2}}\gamma(\lambda\ \mu\ I{-}\tfrac{1}{2}Y). \quad (4.16)$$

The results for Case (I) are collected into Table I. We note that there are available a wide variety of checks on them and comment that we took advantage of several of these.

Case (II) is treated in like manner leading to the results displayed in Table II.

5. CONJUGATION PROCEDURES

We start with a remark that is relevant in connection with each of the conjugation procedures.

It can be readily verified, by Hermitian conjugation and rearrangement of Eqs. (C) to (E), that the ordered set of quantities

$$\mathcal{I}_z^\dagger,\ \mathcal{Y}^\dagger,\ \mathcal{I}_\mp^\dagger,\ \pm\mathcal{G}_\mp^\dagger,\ \mp\mathcal{F}_\mp^\dagger \quad (5.1)$$

have the same CR's with the generators of SU_3 as do the ordered set of components (3.5) of the original octet operator. We can therefore say that the set (5.1) are the components of an octet operator adjoint to the given one. It is to be noted that definition of a Hermitian octet operator, one whose components satisfy

$$\mathcal{I}_z^\dagger = \mathcal{I}_z,\ \mathcal{Y}^\dagger = \mathcal{Y},\ \mathcal{I}_+^\dagger = \mathcal{I}_-,\ \mathcal{F}_\pm^\dagger = \pm\mathcal{G}_\mp, \quad (5.2)$$

is possible. For the general octet operator, we have

TABLE III. $(\lambda - 2, \mu + 1)$.

$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda{-}2\ \mu{+}1\ I{+}1\ Y) = -[(2I+1)/(2I+3)]^{\frac{1}{2}}\,\mathcal{I}(\lambda{+}1\ \mu{+}1\ I{+}1\ Y;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda{-}2\ \mu{+}1\ I\ Y) = \mathcal{I}(\lambda{-}2\ \mu{+}1\ I\ Y;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda{-}2\ \mu{+}1\ I{-}1\ Y) = -[(2I+1)/(2I-1)]^{\frac{1}{2}}\,\mathcal{I}(\lambda{-}2\ \mu{+}1\ I{-}1\ Y;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{-}2\ \mu{+}1\ I{+}\tfrac{1}{2}\ Y{+}1) = [(2I+1)/(2I+2)]^{\frac{1}{2}}\,\mathcal{G}(\lambda{-}2\ \mu{+}1\ I{+}\tfrac{1}{2}\ Y{+}1;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{-}2\ \mu{+}1\ I{-}\tfrac{1}{2}\ Y{+}1) = -[(2I+1)/(2I)]^{\frac{1}{2}}\,\mathcal{G}(\lambda{-}2\ \mu{+}1\ I{-}\tfrac{1}{2}\ Y{+}1;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{-}2\ \mu{+}1\ I{+}\tfrac{1}{2}\ Y{-}1) = -[(2I+1)/(2I+2)]^{\frac{1}{2}}\times\mathcal{F}(\lambda{-}2\ \mu{+}1\ I{+}\tfrac{1}{2}\ Y{-}1;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{-}2\ \mu{+}1\ I{-}\tfrac{1}{2}\ Y{-}1) = -[(2I+1)/(2I)]^{\frac{1}{2}}\times\mathcal{F}(\lambda{-}2\ \mu{+}1\ I{-}\tfrac{1}{2}\ Y{-}1;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{Y}(\lambda\ \mu\ I\ Y;\ \lambda{-}2\ \mu{+}1\ I\ Y) = \mathcal{Y}(\lambda{-}2\ \mu{+}1\ I\ Y;\ \lambda\ \mu\ I\ Y)$.

TABLE IV. $(\lambda + 1, \mu + 1)$.

$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda{+}1\ \mu{+}1\ I{+}1\ Y) = -[(2I+1)/(2I+3)]^{\frac{1}{2}}\,\mathcal{I}(\lambda{+}1\ \mu{+}1\ I{+}1\ Y;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda{+}1\ \mu{+}1\ I\ Y) = \mathcal{I}(\lambda{+}1\ \mu{+}1\ I\ Y;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda{+}1\ \mu{+}1\ I{-}1\ Y) = -[(2I+1)/(2I-1)]^{\frac{1}{2}}\,\mathcal{I}(\lambda{+}1\ \mu{+}1\ I{-}1\ Y;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{+}1\ \mu{+}1\ I{+}\tfrac{1}{2}\ Y{+}1) = [(2I+1)/(2I+2)]^{\frac{1}{2}}\,\mathcal{G}(\lambda{+}1\ \mu{+}1\ I{+}\tfrac{1}{2}\ Y{+}1;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda{+}1\ \mu{+}1\ I{-}\tfrac{1}{2}\ Y{+}1) = -[(2I+1)/(2I)]^{\frac{1}{2}}\,\mathcal{G}(\lambda{+}1\ \mu{+}1\ I{-}\tfrac{1}{2}\ Y{+}1;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{+}1\ \mu{+}1\ I{+}\tfrac{1}{2}\ Y{-}1) = -[(2I+1)/(2I+2)]^{\frac{1}{2}}\,\mathcal{F}(\lambda{+}1\ \mu{+}1\ I{+}\tfrac{1}{2}\ Y{-}1;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda{+}1\ \mu{+}1\ I{-}\tfrac{1}{2}\ Y{-}1) = [(2I+1)/(2I)]^{\frac{1}{2}}\,\mathcal{F}(\lambda{+}1\ \mu{+}1\ I{-}\tfrac{1}{2}\ Y{-}1;\ \lambda\ \mu\ I\ Y)$.

$\mathcal{Y}(\lambda\ \mu\ I\ Y;\ \lambda{+}1\ \mu{+}1\ I\ Y) = \mathcal{Y}(\lambda{+}1\ \mu{+}1\ I\ Y;\ \lambda\ \mu\ I\ Y)$.

expressions for nonvanishing matrix elements analogous to those of Eq. (F). For example, using (5.1) and (F3), we get

$$\pm\langle\lambda'\ \mu'\ I'\ \nu{\pm}\tfrac{1}{2}\ Y{+}1|\ \mathcal{G}_\mp^\dagger\ |\lambda\ \mu\ I\ \nu\ Y\rangle = C(I\ \tfrac{1}{2}\ I'\ \nu\ {\pm}\tfrac{1}{2}\ \nu{\pm}\tfrac{1}{2})\mathcal{F}(\lambda\ \mu\ I\ Y;\lambda'\ \mu'\ I'\ Y{+}1) \times\langle\lambda'\ \mu'||\ (1,\ 1)\ ||\lambda\ \mu\rangle', \quad (5.3)$$

where $\langle\lambda'\ \mu'||\ (1,\ 1)\ ||\lambda\ \mu\rangle'$ is a different reduced matrix element to that in (F3). For a Hermitian octet operator it will be the complex conjugate of some $\langle\bar\lambda'\ \bar\mu'||\ (1,\ 1)\ ||\bar\lambda\ \bar\mu\rangle$.

We may now easily deduce the results under Case (III) from those already obtained by manipulation of CR's under Case (I). A single illustration will be more than sufficient to explain the procedure. We treat the $I \to I + 1$ element of $\mathcal{I}_+$ under Case (III) as follows:

$$\begin{aligned}
&\langle\lambda{-}2\ \mu{+}1\ I{+}1\ \nu{+}1\ Y|\ \mathcal{I}_+\ |\lambda\ \mu\ I\ \nu\ Y\rangle\\
&= \langle\lambda\ \mu\ I\ \nu\ Y|\ \mathcal{I}_+^\dagger\ |\lambda{-}2\ \mu{+}1\ I{+}1\ \nu{+}1\ Y\rangle^*\\
&= \langle\bar\lambda{+}2\ \bar\mu{-}1\ \bar I{-}1\ \bar\nu{-}1\ Y|\ \mathcal{I}_+^\dagger\ |\bar\lambda\ \bar\mu\ \bar I\ \bar\nu\ \bar Y\rangle^*\\
&= \sqrt{2}C(\bar I\ 1\ \bar I{-}1\ \bar\nu\ -1\ \bar\nu{-}1)\\
&\qquad\times\mathcal{I}(\bar\lambda\ \bar\mu\ \bar I\ Y;\ \bar\lambda{+}2\ \bar\mu{-}1\ \bar I{-}1\ Y)\\
&\qquad\times\langle\bar\lambda{+}2\ \bar\mu{-}1||\ (1,\ 1)\ ||\bar\lambda\ \bar\mu\rangle'^*\\
&= [2(2\bar I-1)/(2\bar I+1)]^{\frac{1}{2}}C(\bar I{-}1\ 1\ \bar I\ \bar\nu{-}1\ 1\ \bar\nu)\\
&\qquad\times\mathcal{I}(\bar\lambda\ \bar\mu\ \bar I\ Y;\ \bar\lambda{+}_{\mathrm{o}}\ \bar\mu{-}1\ \bar I{-}1\ Y)\\
&\qquad\times\langle\bar\lambda{+}2\ \bar\mu{-}1||\ (1,\ 1)\ ||\bar\lambda\ \bar\mu\rangle'^*\\
&= [2(2I+1)(2I+3)]^{\frac{1}{2}}C(I\ 1\ I{+}1\ \nu\ 1\ \nu{+}1)\\
&\qquad\times\mathcal{I}(\lambda{-}2\ \mu{+}1\ I{+}1\ Y;\lambda\ \mu\ I\ Y)\\
&\qquad\times\langle\lambda{-}2\ \mu{+}1||\ (1,\ 1)\ ||\lambda\ \mu\rangle. \qquad (5.4)
\end{aligned}$$

TABLE V. $(\lambda - 1, \mu + 2)$.

$$\mathcal{S}(\lambda\,\mu\,I\,Y;\lambda{-}1\,\mu{+}2\,I{+}1\,Y) = [(2I+1)/(2I+3)]^{\frac{1}{2}}\,\mathcal{S}(\mu{+}2\,\lambda{-}1\,I{+}1\,-Y;\mu\,\lambda\,I\,-Y).$$

$$\mathcal{S}(\lambda\,\mu\,I\,Y;\lambda{-}1\,\mu{+}2\,I\,Y) = \mathcal{S}(\mu{+}2\,\lambda{-}1\,I\,-Y;\mu\,\lambda\,I\,-Y).$$

$$\mathcal{S}(\lambda\,\mu\,I\,Y;\lambda{-}1\,\mu{+}2\,I{-}1\,Y) = [(2I+1)/(2I-1)]^{\frac{1}{2}}\,\mathcal{S}(\mu{+}2\,\lambda{-}1\,I{-}1\,-Y;\mu\,\lambda\,I\,-Y).$$

$$\mathcal{F}(\lambda\,\mu\,I\,Y;\lambda{-}1\,\mu{+}2\,I{+}\tfrac{1}{2}\,Y{+}1) = [(2I{+}1)/(2I{+}2)]^{\frac{1}{2}}\,\mathcal{F}(\mu{+}2\,\lambda{-}1\,I{+}\tfrac{1}{2}\,-Y{-}1;\mu\,\lambda\,I\,-Y).$$

$$\mathcal{F}(\lambda\,\mu\,I\,Y;\lambda{-}1\,\mu{+}2\,I{-}\tfrac{1}{2}\,Y{+}1) = [(2I+1)/(2I)]^{\frac{1}{2}}\,\mathcal{F}(\mu{+}2\,\lambda{-}1\,I{-}\tfrac{1}{2}\,-Y{-}1;\mu\,\lambda\,I\,-Y).$$

$$\mathcal{G}(\lambda\,\mu\,I\,Y;\lambda{-}1\,\mu{+}2\,I{+}\tfrac{1}{2}\,Y{-}1) = -[(2I+1)/(2I+2)]^{\frac{1}{2}} \times \mathcal{G}(\mu{+}2\,\lambda{-}1\,I{+}\tfrac{1}{2}\,-Y{+}1;\mu\,\lambda\,I\,-Y).$$

$$\mathcal{G}(\lambda\,\mu\,I\,Y;\lambda{-}1\,\mu{+}2\,I{-}\tfrac{1}{2}\,Y{-}1) = -[(2I+1)/(2I)]^{\frac{1}{2}} \times \mathcal{G}(\mu{+}2\,\lambda{-}1\,I{-}\tfrac{1}{2}\,-Y{+}1;\mu\,\lambda\,I\,-Y).$$

$$\mathcal{Y}(\lambda\,\mu\,I\,Y;\lambda{-}1\,\mu{+}2\,I\,Y) = -\mathcal{Y}(\mu{+}2\,\lambda{-}1\,I\,-Y;\mu\,\lambda\,I\,-Y).$$

In step two of the above, we introduced a convenient relabeling of states; in step three, Eqs. (F2) and (5.1); in step four, symmetry properties[13] of the CG coefficient of $R_3(I)$. Finally, in the fifth step, we restored the original labels, and made the definition

$$\langle\lambda\,\mu||\,(1,1)\,||\lambda{-}2\,\mu{+}1\rangle'^{*} = \langle\lambda{-}2\,\mu{+}1||\,(1,1)\,||\lambda\,\mu\rangle, \tag{5.5}$$

which is adhered to throughout the treatment of Case (III). From Eqs. (5.4) and (F2), we immediately deduce the desired result

$$\mathcal{S}(\lambda\,\mu\,I\,Y;\lambda{-}2\,\mu{+}1\,I{+}1\,Y) = -[(2I+1)/(2I+3)]^{\frac{1}{2}} \times \mathcal{S}(\lambda{-}2\,\mu{+}1\,I{+}1\,Y;\lambda\,\mu\,I\,Y), \tag{5.6}$$

the right side being already known. Other entries in Table III arise in like fashion.

We turn now to the deduction of the results of Table V from those of Table III by means of R conjugation. We use the antiunitary operator R to effect the transformation of an IR (λ, μ) of SU_3 into the IR (μ, λ) which is complex conjugate to it but not equivalent to it unless $\lambda = \mu$. A more transparent statement having the same content is that R is the operator which effects the reflection of the weight diagram of an IR of SU_3 in the origin of weight space. The antiunitary operator R satisfies[23]

$$R^2 = 1, \qquad R^\dagger = R. \tag{5.7}$$

Its effect on the basis of the IR (λ, μ) of SU_3 is given by

$$|\lambda\,\mu\,I\,\nu\,Y\rangle \to R\,|\lambda\,\mu\,I\,\nu\,Y\rangle = \omega(\lambda\,\mu\,I\,\nu\,Y)\,|\,\mu\,\lambda\,I\,-\nu\,-Y\rangle, \tag{5.8}$$

where ω is a real phase, dependent possibly on all of the indicated arguments. The effect on the generators of SU_3 is given by

$$M \to M_R = RMR, \tag{5.9}$$

where M is a member of the set (2.6). We must arrange the details of Eqs. (5.8) and (5.9) to satisfy two criteria. The first is that (5.9) should preserve the CR's [Eq. (A)] of SU_3. The second is as follows. Given any IR (λ, μ) of SU_3 and the general formulas (B) for it, we must be able to use Eqs. (5.2) and (5.3) to deduce results in exact agreement with formulas (B) for the IR (μ, λ). These criteria do not, it transpires, fix ω uniquely. Any choice consistent with them however will serve our needs. In virtue of the antiunitary nature of R, we have the condition[24]

$$\langle\lambda\,\mu\,I'\,\nu'\,Y'|\,M\,\,|\lambda\,\mu\,I\,\nu\,Y\rangle = \omega(\lambda\,\mu\,I\,\nu\,Y)\omega(\lambda\,\mu\,I'\,\nu'\,Y')^* \times \langle\mu\,\lambda\,I\,-\nu\,-Y|\,M^\dagger\,|\mu\,\lambda\,I'\,-\nu'\,-Y'\rangle. \tag{5.10}$$

We may use this to prove that if the CR-preserving choice

$$Y_R = -Y, \qquad (I_z)_R = -I_z, \qquad (I_+)_R = -I_-, \qquad (F_\pm)_R = \mp G_\mp \tag{5.11}$$

is made, then

$$\omega = \omega(\lambda, \mu)(-)^{\nu - \frac{1}{2}Y} \tag{5.12}$$

is a permissible choice for ω. We note[25] that $(\nu - \frac{1}{2}Y)$ is necessarily integral for those IR's of present interest [i.e., those which satisfy $\lambda = \mu$ (mod. 3)], so that then $\omega(\lambda, \mu)$ is real. We also observe[26] that R effects an outer automorphism of SU_3.

Given the behavior (5.11) of the generators (2.6) under R conjugation, it is necessary, in order that the definition [Eqs. (C), (D), and (E)] of the components (3.5) of the octet operator be preserved by R conjugation, that the results

[23] For a discussion of antiunitary operators see E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959), p. 325, and A. Messiah, *Quantum Mechanics* (North-Holland Publishing Company, Amsterdam, 1962), Vol. II, p. 633.

[24] Using Eq. (XV. 22) of Messiah (footnote 23), we write the definition of the adjoint $A^\dagger$ of an antilinear operator as $\langle t|\,(A^\dagger\,|u\rangle) = \langle u|\,(A\,|t\rangle)$, where $|u\rangle$ and $|t\rangle$ are any two states. If $|\tilde{u}\rangle = R\,|u\rangle$, $|\tilde{t}\rangle = R\,|t\rangle$, and $|s\rangle = M\,|\tilde{t}\rangle$, with M a linear operator belonging to the set (2.6), we can develop $\langle u|\,RMR\,|t\rangle = \langle u|\,(R\,|s\rangle) = \langle s|\,(R\,|u\rangle) = \langle s\,|\,\tilde{u}\rangle = \langle\tilde{t}|\,M^\dagger\,|\tilde{u}\rangle$. Here we have used $R = R^\dagger$.

[25] See Ref. 10, Sec. 2.

[26] L. C. Biedenharn, J. Math. Phys. 4, 436 (1963), Appendix.

$$\mathcal{Y}_R = -\mathcal{Y}, \qquad (\mathcal{I}_z)_R = -\mathcal{I}_z,$$
$$(\mathcal{I}_+)_R = -\mathcal{I}_-, \qquad (\mathcal{F}_\pm)_R = \mp\mathcal{G}_\mp \tag{5.13}$$

hold. We may now exhibit how the results of Table V can be generated from those of Table I with the aid of a single example. As before, we take the $I \to I + 1$ element of $\mathcal{I}_+$ and develop

$$\begin{aligned}
&\langle \lambda-1\ \mu+2\ I+1\ \nu+1\ Y|\ \mathcal{I}_+\ |\lambda\ \mu\ I\ \nu\ Y\rangle \\
&= -\omega(\lambda\ \mu\ I\ \nu\ Y)\omega(\lambda-1\ \mu+2\ I+1\ \nu+1\ Y)^* \\
&\times \langle \mu\ \lambda\ I\ -\nu\ -Y|\ \mathcal{I}_-^\dagger\ |\mu+2\ \lambda-1\ I+1\ -\nu-1\ -Y\rangle \\
&= -\sqrt{2}C(I+1\ 1\ I\ -\nu-1\ -1\ -\nu) \\
&\times \mathcal{I}(\mu+2\ \lambda-1\ I+1\ -Y;\ \mu\ \lambda\ I\ -Y) \\
&\times \omega(\lambda,\ \mu)\omega(\lambda-1,\ \mu+2)\langle \mu\ \lambda||\ (1,\ 1)\ ||\mu+2\ \lambda-1\rangle' \\
&= -[2(2I+1)/(2I+3)]^{\frac{1}{2}}C(I\ 1\ I+1\ \nu\ 1\ \nu+1) \\
&\times \mathcal{I}(\mu+2\ \lambda-1\ I+1\ -Y;\ \mu\ \lambda\ I\ -Y) \\
&\times \langle \lambda-1\ \mu+2||\ (1,\ 1)\ ||\lambda\ \mu\rangle.
\end{aligned} \tag{5.14}$$

Herein, in the first step, we have used Eq. (5.10), (5.13) and (5.1); in the second step, Eqs. (F2) and (5.12); in the third step, we have used symmetry properties of the *CG* coefficient of $R_3(I)$ and defined a reduced matrix element. We adhere to the definition there made throughout our treatment of Case (V). Equations (F2) and (5.14) now give

$$\begin{aligned}
&\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda-1\ \mu+2\ I+1\ Y) \\
&= [(2I+1)/(2I+3)]^{\frac{1}{2}} \\
&\times \mathcal{I}(\mu+2\ \lambda-1\ I+1\ -Y;\ \mu\ \lambda\ I\ -Y).
\end{aligned} \tag{5.15}$$

The right side is known from Table III. In this manner, Table V arises.

Similarly, from Table II we can generate Table IV by Hermitian conjugation, and from Table I we can generate Table VI by R conjugation.

TABLE VI. $(\lambda + 1, \mu - 2)$.

$$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda+1\ \mu-2\ I+1\ Y) = [(2I+1)/(2I+3)]^{\frac{1}{2}}\ \mathcal{I}(\mu-2\ \lambda+1\ I+1\ -Y;\ \mu\ \lambda\ I\ -Y).$$

$$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda+1\ \mu-2\ I\ Y) = \mathcal{I}(\mu-2\ \lambda+1\ I\ -Y;\ \mu\ \lambda\ I\ -Y).$$

$$\mathcal{I}(\lambda\ \mu\ I\ Y;\ \lambda+1\ \mu-2\ I-1\ Y) = [(2I+1)/(2I-1)]^{\frac{1}{2}}\ \mathcal{I}(\mu-2\ \lambda+1\ I-1\ -Y;\ \mu\ \lambda\ I\ -Y).$$

$$\mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda+1\ \mu-2\ I+\tfrac{1}{2}\ Y+1) = [(2I+1)/(2I+2)]^{\frac{1}{2}} \times \mathcal{F}(\mu-2\ \lambda+1\ I+\tfrac{1}{2}\ -Y-1;\ \mu\ \lambda\ I\ -Y).$$

$$\mathcal{F}(\lambda\ \mu\ I\ Y;\ \lambda+1\ \mu-2\ I-\tfrac{1}{2}\ Y+1) = [(2I+1)/(2I)]^{\frac{1}{2}}\ \mathcal{F}(\mu-2\ \lambda+1\ I-\tfrac{1}{2}\ -Y-1;\ \mu\ \lambda\ I\ -Y).$$

$$\mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda+1\ \mu-2\ I+\tfrac{1}{2}\ Y-1) = -[(2I+1)/(2I+2)]^{\frac{1}{2}} \times \mathcal{G}(\mu-2\ \lambda+1\ I+\tfrac{1}{2}\ -Y+1;\ \mu\ \lambda\ I\ -Y).$$

$$\mathcal{G}(\lambda\ \mu\ I\ Y;\ \lambda+1\ \mu-2\ I-\tfrac{1}{2}\ Y-1) = -[(2I+1)/(2I)]^{\frac{1}{2}}\ \mathcal{G}(\mu-2\ \lambda+1\ I-\tfrac{1}{2}\ -Y+1;\ \mu\ \lambda\ I\ -Y).$$

$$\mathcal{Y}(\lambda\ \mu\ I\ Y;\ \lambda+1\ \mu-2\ I\ Y) = -\mathcal{Y}(\mu-2\ \lambda+1\ I\ -Y;\ \mu\ \lambda\ I\ -Y).$$

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Generalized Shmushkevich Method: Proof of Basic Results*

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We here derive certain orthogonality properties of the Clebsch-Gordan (CG) coefficients of an arbitrary compact group G. Our discussion recognizes the fact that the irreducible representations (IR's) of G need not be equivalent to their complex conjugates and that the same IR can appear more than once in the reduction of the direct product of two IR's of G. The properties obtained allow the development of a generalized Shmushkevich method for directly writing down consequences of the invariance of particle interactions under G. The discussion given is sufficiently general to apply to the currently interesting cases of SU_3 and G_2.

1. INTRODUCTION

THE aim of this work is to exhibit the proofs of certain facts concerning compact groups and their Clebsch–Gordan (CG) coefficients which are used in the development of the generalized Shmushkevich method for writing down consequences of the invariance of the strong interactions with respect to a given compact group. We commence with an explanation of this method.

Shmushkevich[1] originally described the method now known as Shmushkevich's method in connection with the charge-independent theory of the strong interactions. It is a technique for writing down linear relationships among the cross sections for various elementary-particle reactions that exist as a result of the assumption of charge independence or invariance with respect to the isospin rotation group, R_3. Simple expositions of it with examples may be found in recent books on elementary-particle physics.[2] Its notable characteristics are its economy, particularly in complicated physical contexts, and the fact that it proceeds without the use of (and therefore without the need for knowledge of) numerical values of CG coefficients of R_3. Formal proof[3] of the results which underlie the method depends only on certain general properties of CG coefficients of R_3, to be noted below.

In view of the great interest currently surrounding the theories[4,5] which use SU_3 and G_2 as invariance groups of the strong interactions, it is desirable to possess a generalization of Shmushkevich's method for these theories. Provided we assume that those properties of CG coefficients of R_3 which were used in the justification of the method for R_3 generalize to SU_3 and G_2, we can proceed directly to the development of the generalized Shmushkevich methods for SU_3 and G_2. Several illustrations have already been given of how consequences of SU_3 and G_2 invariance may be written down by the method: relationships between decay weights for the decays of certain resonances that exist as a result of SU_3 invariance[6] or G_2 invariance,[7] relationships between meson–baryon scattering cross sections that exist as a result of SU_3 invariance.[8]

The two properties of CG coefficients of R_3[9] used in the justification of Shmushkevich's method for R_3 are the following[3]:

(1) Orthogonality

$$\sum_{m_1 m_2} C(j_1 j_2 j;\, m_1 m_2 m) C(j_1 j_2 j';\, m_1 m_2 m') = \delta(jj')\delta(mm'); \qquad (1.1)$$

(2) Modified orthogonality[10]

$$\sum_{m_2 m} C(j_1 j_2 j;\, m_1 m_2 m) C(j_1' j_2 j;\, m_1' m_2 m) = [(2j+1)/(2j_1+1)]\delta(j_1 j_1')\delta(m_1 m_1'). \qquad (1.2)$$

The modified orthogonality rule arises from the

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‡ On leave of absence during the academic year 1963-4 at Institüt für Theoretische Physik, Universität Bern, Bern, Switzerland.

[1] I. M. Shmushkevich, Dokl. Akad. Nauk SSSR **103**, 235 (1955).

[2] R. E. Marshak and E. C. G. Sudarshan, *Introduction to Elementary Particle Physics* (Interscience Publishers, Inc., New York, 1961), p. 185; P. Roman, *Theory of Elementary Particles* (North-Holland Publishing Company, Amsterdam, 1960), p. 443.

[3] Such a proof is given in a forthcoming paper, A. J. Macfarlane and E. C. G. Sudarshan, "Shmushkevich's Method for a Charge Independent Theory: Nucleon–Anti-Nucleon Annihilation" (to be published).

[4] Y. Ne'eman, Nucl. Phys. **26**, 222 (1961); M. Gell-Mann, Phys. Rev. **125**, 1067 (1962); S. Okubo, Progr. Theoret. Phys. (Kyoto) **27**, 944, **28**, 24 (1962).

[5] R. E. Behrends and L. F. Landowitz, Phys. Rev. Letters **11**, 296 (1963).

[6] C. Dullemond, A. J. Macfarlane, and E. C. G. Sudarshan, Phys. Rev. Letters **10**, 423 (1963).

[7] A. J. Macfarlane, N. Mukunda, and E. C. G. Sudarshan, Phys. Rev. **133**, B. 475, (1964).

[8] E. C. G. Sudarshan, *Proceedings of the Athens Conference on Newly Discovered Resonant Particles*, edited by B. A. Munir and L. J. Gallaher (Ohio University, Athens, Ohio, 1963).

[9] We use the notation of M. E. Rose, *Elementary Theory of Angular Momentum* (John Wiley & Sons, Inc., New York, 1957).

[10] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952), p. 791.

ordinary orthogonality rule by means of the symmetry property

$$C(j_1 j_2 j; m_1 m_2 m) = (-)^{j_2+m_2}[(2j+1)/(2j_1+1)]^{\frac{1}{2}} \times C(j j_2 j_1; -m\ m_2\ -m_1). \quad (1.3)$$

In this paper, we define CG coefficients for an arbitrary compact group, and establish that results analogous to Eqs. (1.1) and (1.2) obtain, so that a generalized Shmushkevich method may indeed justifiably be used to write down consequences of invariance with respect to any compact group, in particular with respect to SU_3 or G_2. That an orthogonality rule like (1.1) obtains is to be expected. It is not obvious although true, however, that a natural generalization of (1.2) exists. Indeed the opposite might be expected since a natural generalization of (1.3) does not exist—e.g., (1.3) for R_3 has to be replaced by a complicated crossing relation for an arbitrary compact group. The reason for this stems from the fact that the representation theory of R_3 is simpler than that of an arbitrary compact group in two important respects. These are as follows:

(A) An irreducible representation of an arbitrary compact group need not be equivalent to its complex conjugate.

(B) The direct product of two irreducible representations of an arbitrary compact group may contain the same irreducible representation more than once in its reduction.

For R_3 neither (A) nor (B) can occur. Since for SU_3 both (A) and (B) can occur[11] and do in practically interesting cases, the relevance of the present discussion becomes clear.

Among previous literature on the subject, we note that Wigner[14] has discussed CG coefficients of finite groups which do not allow either (A) or (B), and that Sharp[15] has discussed the same problem for compact groups and also for compact groups for which (A) but not (B) can occur. On the other hand, Hamermesh[16] has discussed groups which allow (B) but not (A). We here use the notation used by Hamermesh and refer to his book for many of the general properties of irreducible representations of groups used in the ensuing sections.

The material of the paper is presented as follows. In Sec. 2, we mention various facts regarding the representation theory of an arbitrary compact group and define its CG coefficients. In Sec. 3, we derive the desired generalizations of Eqs. (1.1) and (1.2). Sec. 4 contains an illustrative example.

2. SIMPLE PROPERTIES OF IR's AND CG COEFFICIENTS

We consider an arbitrary compact group G with general element R. Since G is compact, each of the IR's is of finite dimension and equivalent to a unitary IR. Thus we may confine attention to unitary IR's of G, i.e., to $D^{\mu}(R)$ which satisfy

$$D^{\mu}(R)^{\dagger} = D^{\mu}(R)^{-1}. \quad (2.1)$$

Here we use as a labeling of the IR's of G a single lower-case Greek letter $\mu, \nu, \rho \cdots$, which may in fact stand for several labels. For example, we may write

$$\mu = (\mu_1, \mu_2, \cdots \mu_l)$$

in the case of the IR of highest weight μ of l components if G is of rank l.

We do not assume that the IR $D^{\mu}(R)$ is equivalent to its complex conjugate $D^{\mu}(R)^*$, which is still however an IR of G, but set

$$D^{\mu}(R)^* = J(\mu', \mu)^{-1} D^{\mu'}(R) J(\mu', \mu), \quad (2.2)$$

where J is unitary and independent of R.[17] We shall apply primes to lower-case Greek letters always exactly in this sense and never at all to other letters. It is obvious that passage from $D^{\mu}(R)$ to $D^{\mu'}(R)$ is an involution, so that $D^{\mu''}(R) = D^{\mu}(R)$. Also,

$$J(\mu, \mu') = \tilde{J}(\mu', \mu), \quad (2.3)$$

where the tilde denotes transposition. We may summarize the situation by saying that the set $\{\cdots \mu, \nu, \rho \cdots\}$ of all IR's of G is the same as the set $\{\cdots \mu', \nu', \rho' \cdots\}$, possibly in a different order.

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[11] In the currently popular form of unitary symmetry theory[4,12] the baryons, pseudoscalar and vector mesons, are classified according to the octet or IR (1, 1) of SU_3, and the spin-$\frac{3}{2}$ baryon resonances are classified according to the decuplet or IR (3,0). The direct product of two octets contains an octet twice—a fact which reflects the possibility of constructing two independent Yukawa-type meson–baryon interactions. The IR (3,0) is not equivalent to its complex conjugate, but to the complex conjugate of the IR (0,3). The notation used here for IR's of SU_3 is explained in Ref. 13.

[12] S. L. Glashow and J. J. Sakurai, Nuovo Cimento **26**, 622 (1962).

[13] A. J. Macfarlane, E. C. G. Sudarshan, and C. Dullemond, Nuovo Cimento **30**, 845 (1963).

[14] E. P. Wigner, Am. J. Math **63**, 57 (1941), and "On the Matrices Which Reduce the Kronecker Product of Representations of Simply Reducible Groups" (unpublished).

[15] W. T. Sharp, "Racah Algebra and the Contraction of Groups," CRT-935, Chalk River, Canada, 1960.

[16] M. Hamermesh, *Group Theory* (Addison Wesley Publishing Company, Inc., Reading, Massachusetts, 1962). See especially Chap. 5 and Sec. 7–14.

[17] The matrix J plays a role for the general compact group analogous to that played by the "$1-j$ symbol" for R_3.

We go on to consider the direct product

$$D^{\mu}(R) \otimes D^{\nu}(R) \tag{2.4}$$

of a pair of IR's of G. Since G is compact, we know that this is equivalent to a direct sum of IR's of G, possibly containing several IR's more than once. We may use

$$D^{\mu}(R) \otimes D^{\nu}(R) \cong \sum_{\rho} (\mu\nu\rho) D^{\rho}(R) \tag{2.5}$$

to define $(\mu\nu\rho)$ as the number of times $D^{\rho}(R)$ occurs as a direct summand in the reduction of (2.4). Allowed values of $(\mu\nu\rho)$ are 0, 1, 2 $\cdots$. We have

$$(\mu\nu\rho) = (\nu\mu\rho). \tag{2.6}$$

If $D^{\mu}(R)$ has character $\chi^{\mu}(R)$, Eq. (2.5) implies

$$\chi^{\mu}(R)\chi^{\nu}(R) = \sum_{\rho} (\mu\nu\rho)\chi^{\rho}(R). \tag{2.7}$$

We may use the orthogonality relation for characters

$$\int \chi^{\mu}(R)\chi^{\nu}(R)^{*}\, dR = A\,\delta(\mu\nu), \tag{2.8}$$

where A is a normalization constant and the integration is the usual left- and right-invariant integration over the group manifold of G, to give

$$(\mu\nu\rho) = A^{-1} \int \chi^{\mu}(R)\chi^{\nu}(R)\chi^{\rho}(R)^{*}\, dR. \tag{2.9}$$

Hence using the consequence

$$\chi^{\mu}(R)^{*} = \chi^{\mu'}(R) \tag{2.10}$$

of Eq. (2.2), we may deduce the important result

$$(\mu\nu\rho) = (\rho'\nu\mu'). \tag{2.11}$$

We now define the CG coefficients of G for the direct product (2.4) and show that they are the elements of the unitary matrix which generates the similarity transformation that brings the direct sum on the left side of (2.5) into equivalence with the right side. If n_{μ} is the dimension of $D^{\mu}(R)$, suppose $\psi^{\mu}{}_{j}$ with j standing for a set of labels which take on n_{μ} distinct sets of values is an orthonormal basis in the representation space of the IR μ. Under R, we have

$$\psi^{\mu}{}_{i} \underset{R}{\rightarrow} O_R \psi^{\mu}{}_{i} = \psi^{\mu}{}_{k} D^{\mu}(R)_{ki}. \tag{2.12}$$

Here we are using summation convention for Latin indices but not Greek ones. Similarly, $\psi^{\nu}{}_{k}$ is an orthonormal basis for the representation space of the IR ν, so that the products $\psi^{\mu}{}_{i}\psi^{\nu}{}_{k}$ are the basis functions for the product (2.4). Reduction of this product into a direct sum of IR's $D^{\rho}(R)$, various ρ, involves a unitary change of basis wherein we replace the products $\psi^{\mu}{}_{i}\psi^{\nu}{}_{k}$ by sets of basis functions $\psi^{\rho}{}_{l}$ which transform according to $D^{\rho}(R)$,

$$\psi^{\rho}{}_{l} \underset{R}{\rightarrow} O_R \psi^{\rho}{}_{l} = \psi^{\rho}{}_{m} D^{\rho}(R)_{ml}. \tag{2.13}$$

Since $(\mu\nu\rho) > 1$ is possible for a given ρ appearing in the reduction, there can be more than one independent set of n_{ρ} basis functions $\psi^{\rho}{}_{l}$. To distinguish these we add a Latin capital label (to which summation convention does not apply) to the basis functions, e.g., $\psi^{\rho A}{}_{l}$, there being $(\mu\nu\rho)$ allowed (sets of) values for the (perhaps composite) label A. We demand that basis functions $\psi^{\rho A}{}_{l}$ for different A be orthogonal. Also we arrange[18] to have

$$\psi^{\rho A}{}_{l} \underset{R}{\rightarrow} O_R \psi^{\rho A}{}_{l} = \psi^{\rho A}{}_{m} D^{\rho}(R)_{ml}, \tag{2.14}$$

with $D^{\rho}(R)_{ml}$ independent of A. We may define $\psi^{\rho A}{}_{l}$ explicitly by setting

$$\psi^{\rho A}{}_{l} = \psi^{\mu}{}_{j}\psi^{\nu}{}_{k}(\mu j, \nu k \mid \rho A l), \tag{2.15}$$

where

$$(\mu j, \nu k \mid \rho A l) \tag{2.16}$$

is the generalized CG coefficient of G for the product (2.4). We may also give an inverse to Eq. (2.15) in the form

$$\psi^{\mu}{}_{j}\psi^{\nu}{}_{k} = \sum_{\rho A} \psi^{\rho A}{}_{l}(\rho A l \mid \mu j, \nu k), \tag{2.17}$$

where the quantities

$$(\rho A l \mid \mu j, \nu k)$$

are elements of the matrix inverse to that with the CG coefficients (2.16) as elements, i.e.,[19]

$$(\mu j, \nu k \mid \rho A l)(\sigma B m \mid \mu j, \nu k) = \delta(\rho\sigma)\delta(AB)\delta(lm), \tag{2.18}$$

$$\sum_{\rho A} (\mu j, \nu k \mid \rho A l)(\rho A l \mid \mu p, \nu q) = \delta(jp)\delta(kq). \tag{2.19}$$

We can now exhibit that the CG coefficients (2.16) are the elements of the

$$n_{\mu}n_{\nu} = \sum_{\rho} (\mu\nu\rho) n_{\rho} \tag{2.20}$$

-dimensional matrix of the similarity transformation which brings the direct sum on the right of Eq. (2.5) into equivalence with the direct product on the left. We apply O_R to (2.17), use (2.15) and cancel the product basis functions, as they are linearly independent, obtaining

$$D^{\mu}(R)_{pi} D^{\nu}(R)_{qk} = \sum_{\rho A} (\mu p, \nu q \mid \rho A l) D^{\rho}(R)_{lm} (\rho A m \mid \mu j, \nu k), \tag{2.21}$$

which demonstrates the equivalence.

[18] Ref. 16, p. 150.
[19] Ref. 16, p. 149.

We should stress the fact that there is a great deal of arbitrariness[20] in the definition of the CG coefficient of G for the product (2.4) if for given ρ, $(\mu\nu\rho) > 1$, so that there are several orthogonal sets of basis functions $\psi^{\rho A}{}_l$. This is because we can make unitary transformations with respect to A for fixed ρ without disturbing the explicit reduction of the product (2.4) or the orthogonality of the sets $\psi^{\rho A}{}_l$ with different A. Fortunately, we do not have to dwell on this arbitrariness in our work.

We now proceed to obtain analogs of Eqs. (1.1)–(1.3) in terms of the quantities (2.16).

3. GENERALIZATION OF EQS. (1.1)–(1.3).

The generalization of (1.1) is immediate. As the matrix of CG coefficients is unitary, we have

$$(\mu j, \nu k \mid \rho A l)^* = (\rho A l \mid \mu j, \nu k), \tag{3.1}$$

so that (2.18) becomes

$$(\mu j, \nu k \mid \rho A l)(\mu j, \nu k \mid \sigma B m)^* = \delta(\rho\sigma)\delta(AB)\delta(lm), \tag{3.2}$$

which is the required generalization of (1.1).

To generalize (1.3), we need a lemma.

Lemma. The direct-product representation $D^\mu(R) \otimes D^\nu(R)$ contains the identity representation O only if $\nu = \mu'$, and then only once.

The corresponding normalized wavefunction is

$$(n_\mu)^{\frac{1}{2}}\psi^{(\rho=0)} = J(\mu, \mu')_{jk}\psi^\mu{}_j\psi^{\mu'}{}_k. \tag{3.3}$$

The first part of the lemma follows (2.9) and (2.8) on setting $\rho = 0$ and $\chi^0(R) = 1$. To verify the statement that the $\psi^{(0)}$ as given by (3.3) is the correct invariant basis function, we use Eqs. (2.1), (2.2), and (2.14) as well as the fact that $J(\mu, \mu')$ is unitary, in the following way:

$$\begin{aligned}
\psi^{(0)} &= J(\mu, \mu')_{jk}\psi^\mu{}_j\psi^{\mu'}{}_k \\
&\underset{R}{\rightarrow} J(\mu, \mu')_{jk}D^\mu(R)_{mj}D^{\mu'}(R)_{lk}\psi^\mu{}_m\psi^{\mu'}{}_l \\
&= J(\mu', \mu)_{kj}D^\mu(R)_{mj}J(\mu', \mu)_{ln} \\
&\quad \times D^\mu(R)^*_{np}J(\mu', \mu)^\dagger_{pk}\psi^\mu{}_m\psi^{\mu'}{}_l \\
&= D^\mu(R)_{mp}D^\mu(R)^*_{np}J(\mu, \mu')_{nl}\psi^\mu{}_m\psi^{\mu'}{}_l \\
&= J(\mu, \mu')_{nl}\psi^\mu{}_n\psi^{\mu'}{}_l = \psi^{(0)}.
\end{aligned}$$

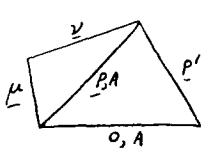

FIG. 1. The $(\mu\nu)\,\rho' \rightarrow \rho\,\rho' \rightarrow 0$ coupling.

[20] Ref. 16, p. 261.

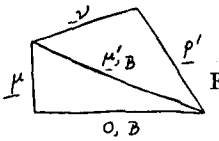

FIG. 2. The $\mu\,(\nu\rho') \rightarrow \mu\,\mu' \rightarrow 0$ coupling.

The normalization of $\psi^{(0)}$ follows from the unitarity of $J(\mu, \mu')$. Thus the proof of the lemma is complete.

Suppose now we have three sets of basis functions $\psi^\mu{}_j$, $\psi^\nu{}_k$ and $\psi^{\rho'}{}_l$ together with their associated matrices $D^\mu(R)$, $D^\nu(R)$, $D^{\rho'}(R)$. We seek combinations of the product functions $\psi^\mu{}_j\psi^\nu{}_k\psi^{\rho'}{}_l$ that are invariant under G. In general, a whole subspace of such combinations exists. We can build a basis for this subspace in the following manner. From the lemma it is clear that in an invariant linear combination of products, whatever multiplies the $\psi^{\rho'}{}_l$, must be a quantity of the type $\psi^\rho{}_m$. That is, we must first combine the products $\psi^\mu{}_j\psi^\nu{}_k$ to a wavefunction of type ρ, and then combine that with the $\psi^{\rho'}{}_l$ to get an invariant. Thus we arrive at a set of $(\mu\nu\rho)$ orthonormal invariant states labeled by a letter A,

$$(n_\rho)^{\frac{1}{2}}\psi^{\rho A} = J(\rho, \rho')_{ml}(\mu j, \nu k \mid \rho A m)\psi^\mu{}_j\psi^\nu{}_k\psi^{\rho'}{}_l. \tag{3.4}$$

These states form an orthonormal basis for the manifold of invariant states in the triple-product space. We may represent Eq. (3.4) schematically as in Fig. 1.

It is clear however that we must obtain the same manifold if we start by coupling the $\psi^{\rho'}{}_l$ and $\psi^\nu{}_k$ to form states of type $\psi^{\mu' B}{}_m$, and then combine these with $\psi^\mu{}_j$ to form invariant states $\phi^{\rho B}$. In this way, we get

$$(n_\mu)^{\frac{1}{2}}\phi^{\rho B} = J(\mu, \mu')_{jm}\psi^\mu{}_j(\rho' l, \nu k \mid \mu' B m)\psi^{\rho'}{}_l\psi^\nu{}_k. \tag{3.5}$$

This may be represented as in Fig. 2. Since $\psi^{\rho A}$ and $\phi^{\rho B}$ span the same subspace of the triple-product space, there is a unitary transformation connecting them, so that we have

$$\psi^{\rho A} = \sum_B M(\mu\nu\rho)_{AB}\phi^{\rho B}. \tag{3.6}$$

We now insert (3.4) and (3.5) into (3.6) and obtain, after dropping the linearly independent product functions, the relationship[21]

$$\begin{aligned}
&(n_\rho)^{-\frac{1}{2}}J(\rho, \rho')_{ml}(\mu j, \nu k \mid \rho A m) \\
&= \sum_B M(\mu\nu\rho)_{AB}(n_\mu)^{-\frac{1}{2}}J(\mu', \mu)_{nj}(\rho' l, \nu k \mid \mu' B n).
\end{aligned} \tag{3.7}$$

In the absence of multiplicities, i.e., when $(\mu\nu\rho) =$

[21] Following Hamermesh, (Ref. 16, Sec. 7–14), we may show that the arbitrariness in the definition of CG coefficients of G may be disposed of in such a way that $M\,(\mu\nu\rho) = 1$. We can however proceed without effecting this.

$(\rho'\nu\mu') = 1$, Eq. (3.7) reduces to

$$(n_\rho)^{-\frac{1}{2}} J(\rho, \rho')_{ml}(\mu j, \nu k \mid \rho m) = (n_\mu)^{-\frac{1}{2}} J(\mu', \mu)_{nj}(\rho' l, \nu k \mid \mu' n). \quad (3.8)$$

Equations (3.8) and (3.7)[21] exhibit how a crossing relation replaces the simple symmetry property (1.3) when IR's are no longer all equivalent to their complex conjugates and when $(\mu\nu\rho) > 1$ is allowed.

It is now a simple matter to derive from (3.7) the required generalization of Eq. (1.2). To do this, we first obtain from Eq. (3.7)

$$(n_\rho)^{-\frac{1}{2}} J(\rho, \rho')^\dagger_{lq}(\lambda p, \nu k \mid \rho C q)^* = \sum_D M(\lambda\nu\rho)^\dagger_{DC}(n_\lambda)^{-\frac{1}{2}} J(\lambda', \lambda)^\dagger_{ps}(\rho' l, \nu k \mid \lambda' D s)^* \quad (3.9)$$

by complex conjugation and relabeling. Then we multiply corresponding sides of Eqs. (3.7) and (3.9) and sum over k and l. First, we note that the unitarity of $J(\rho, \rho')$ simplifies the left side to

$$(n_\rho)^{-1}(\mu j, \nu k \mid \rho A m)(\lambda p, \nu k \mid \rho C m)^*;$$

summation over k and m implied here as always. On the right side, we first use (3.2) to obtain a factor

$$\delta(\mu\lambda)\delta(BD)\delta(ns).$$

Now the M's on the right refer to the same triples of IR's, and the J's to the same pair of complex conjugates of IR's, so that their unitarity reduces the right side to

$$(n_\lambda)^{-1}\delta(\mu\lambda)\delta(jp)\delta(AC).$$

We thus obtain

$$(\mu j, \nu k \mid \rho A m)(\lambda p, \nu k \mid \rho C m)^* = (n_\rho/n_\mu)\delta(\mu\lambda)\delta(jp)\delta(AC) \quad (3.10)$$

as the required generalization of (1.2).

4. ILLUSTRATIVE EXAMPLE

Justification of the application of Shmushkevich's method to SU_3 is here provided in a simple case on the basis of the work of the previous sections.

We use the notation (μ_1, μ_2) for an IR of SU_3, the integers μ_1 and μ_2 being the components of its highest weight. Basis states for any IR $\mu = (\mu_1, \mu_2)$ are obtained as simultaneous eigenstates of operators which may be identified with $\mathbf{I}^2$, total isospin; I_z its z component; and Y, hypercharge. Thus in place of $\psi^\mu{}_i$ we have $|\mu_1\mu_2; II_zY\rangle$. It is customary[4,12] to associate sets of particles of the same spins and parities, "approximately" the same masses, and appropriate I and Y with such IR's of SU_3 in order to set up a unitary symmetry theory. For the purpose of illustration let us consider all the allowed decays of a particle belonging to the IR $\rho = (\rho_1, \rho_2)$ into two particles belonging to μ and ν. Such decays have matrix elements

$$\langle \mu I_1 I_{1z} Y_1; \nu I_2 I_{2z} Y_2 \mid T \mid \rho I I_z Y\rangle = \sum_A (\mu I_1 I_{1z} Y_1, \nu I_2 I_{2z} Y_2 \mid \rho A I I_z Y)\langle \rho A \mid\mid T \mid\mid \rho\rangle. \quad (4.1)$$

In order to derive the results which correspond to the Shmushkevich tables used in Refs. 6 and 8, we must consider the following sums over the squared moduli of matrix elements (4.1). These are $Q(II_zY)$, the sum over I_1, I_{1z}, Y_1, and I_2, I_{2z}, Y_2 at fixed I, I_z, Y; and $R(I_1, I_{1z}, Y_1)$, the sum over I_2, I_{2z}, Y_2 and I, I_z, Y at fixed I_1, I_{1z}, Y_1.

We get

$$\begin{aligned} Q(II_zY) &= \sum\sum_A (\mu I_1 I_{1z} Y_1, \nu I_2 I_{2z} Y_2 \mid \rho A I I_z Y)\langle \rho A \mid\mid T \mid\mid \rho\rangle \\ &\quad \times \sum_B (\mu I_1 I_{1z} Y_1, \nu I_2 I_{2z} Y_2 \mid \rho B I I_z Y)^* \langle \rho B \mid\mid T \mid\mid \rho\rangle^* \\ &= \sum_{AB} \delta(AB)\langle \rho A \mid\mid T \mid\mid \rho\rangle\langle \rho B \mid\mid T \mid\mid \rho\rangle^* \\ &= \sum_A |\langle \rho A \mid\mid T \mid\mid \rho\rangle|^2. \end{aligned} \quad (4.2)$$

The sum set first in the first line is by definition over I_1, I_{1z}, Y_1, I_2, I_{2z}, Y_2 at fixed I, I_z, Y—just that required to allow the use of Eq. (3.2). The result (4.2)—$Q(II_zY)$ independent of I, I_z and Y—states the equality of the total widths for all decays for different members of the unitary multiplet ρ.

Likewise, we get

$$R(I_1, I_{1z}, Y_1) = (n_\rho/n_\mu) \sum_A |\langle \rho A \mid\mid T \mid\mid \rho\rangle|^2, \quad (4.3)$$

the summation involved in the derivation being, by definition, just that required to allow the use of Eq. (3.10). Thus $R(I_1, I_{1z}, Y_1)$ is independent of I_1, I_{1z}, and Y_1, which is just what has been called[6] a Shmushkevich theorem for the decay situation.

No further information than is provided by Eqs. (3.2), (3.10) is required for the writing down of Shmushkevich theorems for more complex situations.

Intensive Observables in Quantum Theory*

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The notion of strictly intensive observables is introduced in a theory of local observables (such as that of R. Haag). If $\mathcal{O}_1$, $\mathcal{O}_2$ are two disjoint regions, then the value of a strictly intensive observable in $\mathcal{O}_1 \cup \mathcal{O}_2$ is the sum of its values in $\mathcal{O}_1$ and $\mathcal{O}_2$. It is shown that energy–momentum can never be strictly intensive. This result is used to prove that the algebras of observables is not of Type I for some regions. By analogy with the energy–momentum tensor density for the free field, the definition is weakened, so that an intensive observable in a region $\mathcal{O}$ is only "approximately" in $\mathfrak{A}(\mathcal{O})$. This leads to the introduction of germs of intensive observables. It is proved that the unitary intensive operators form a sheaf $\mathfrak{F}$ of groups, and the Hermitian intensive operators form a sheaf $\mathfrak{G}$ of Abelian groups with operators in $\mathfrak{F}$, and on which the inner derivative $Y \to i(XY - YX)$ is defined.

I. INTRODUCTION

QUANTUM field theory describes local systems by means of local observables, which are self-adjoint operators and can be determined by an experiment performed in a finite region of space and completed in a finite time. The smaller the region of space–time, the less scope there is for maneuver by the experimenter, and so the fewer are the observables which can be measured. In a field theory the field itself (suitably integrated with a test function) is an unbounded operator and may be an observable, but is not necessarily so. In general, then, some local observables may be unbounded operators. For mathematical convenience we shall work with the algebras of bounded observables, introduced by Haag.[1] The connection with field theory is very close, but has not yet been rigorously established. The following axioms will be used; they have been extensively developed by Araki.[2]

Axiom 1. To every open set $\mathcal{O}$ of space–time is associated an algebra $\mathfrak{A}(\mathcal{O})$ of bounded operators on a Hilbert space $\mathfrak{H}$. The algebra is generated from the bounded observables by taking sums and products with complex coefficients. All weakly convergent limits of sequences of such operators are also included in the algebra. In other words, the algebra $\mathfrak{A}(\mathcal{O})$ is the W^* algebra generated by the bounded observables in $\mathcal{O}$.

Axiom 2. If $\mathcal{O}$ is an open set of $\mathbf{R}^4$, define $\mathfrak{A}'(\mathcal{O})$ to be the set of bounded operators on $\mathfrak{H}$ which commute with all the operators of $\mathfrak{A}(\mathcal{O})$. A theorem of von Neumann[3] states that $\mathfrak{A}'(\mathcal{O})$ is a W^* algebra, called the *commutant* of $\mathfrak{A}(\mathcal{O})$, and $\mathfrak{A}'' = \mathfrak{A}$. To any open set $\mathcal{O}$ we define the *causally independent* set to be the interior set $\mathcal{O}'$ where

$$\bar{\mathcal{O}}' = \{x \in \mathbf{R}^4 / (x - y)^2 < 0 \quad \text{for all} \quad y \in \mathcal{O}\}.$$

Then axiom 2 states

(a) $\mathfrak{A}'(\mathcal{O}) = \mathfrak{A}(\mathcal{O}')$;
(b) $\mathfrak{A}'(\mathcal{O}) \cap \mathfrak{A}(\mathcal{O})$ contains only scalars;
(c) $\mathfrak{A}(\mathbf{R}^4) = \mathfrak{B}(\mathfrak{H})$, i.e., the algebra of *all* bounded observables on $\mathfrak{H}$.

In other words, $\mathfrak{A}(\mathcal{O})$ is a *direct factor*, whose commutant is $\mathfrak{A}(\mathcal{O}')$.

These properties have been discussed in connection with the time-slice axiom.[4] We do not expect $\mathfrak{A}(\mathcal{O})$ to be a factor if there are superselection rules in the theory,[5] for then there are some operators which commute with all the observables in $\mathcal{O}$ and all the observables in $\mathcal{O}'$. The charge is an example of such an operator. Physically interesting cases are covered if we assume that all operators defining superselection rules commute with each other.[5] The modifications in the axioms necessary to allow for this do not change the conclusions of this paper.

Axiom 3. The theory is relativistically covariant; this means, there exists a unitary representation[6] of the inhomogeneous $SL(2, C)$, say $\{a, A\} \to$

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[1] R. Haag in *Colloques sur les problèmes mathématiques de la théorie quantique des champs* (Centre National de la Recherche Scientifique, Paris, 1959).

[2] H. Araki, J. Math. Phys. 4, 1343 (1963).

[3] J. Dixmier, *Les algèbres d'opérateurs dans l'espace hilbertien* (Gauthier-Villars, Paris, 1957), p. 42, *et seq.*

[4] R. Haag and B. Schroer, J. Math. Phys. 3, 248 (1962).

[5] A. S. Wightman, Nuovo Cimento Suppl. 14, 81 (1959).

[6] For the basic properties of quantum field theory see a forthcoming book: R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics and all That* (W. A. Benjamin Company, Inc., New York).

$U(a, A)$, where $U(a, A)$ is a unitary operator continuous in the parameters a and A.

Axiom 4. If $U(a) = \exp(iP_\mu a^\mu)$, then $P^\mu P_\mu \geq 0$, $P^0 \geq 0$, and $P^0 = 0$ only for the vacuum state Ψ_0. It follows that Ψ_0 is the only normalizable eigenstate of P^0 or $\mathbf{P}$ or P^1.

Axiom 5. If $\{\mathcal{O}_i\}$ is a collection of open sets in $\mathbf{R}^4$, then

$$\mathfrak{A}(\cup_i \mathcal{O}_i) = [\cup_i (\mathfrak{A}_i)]'',$$

that is, the algebra associated with the open set $\cup_i \mathcal{O}_i$ is that generated by the operators of the individual algebras $\mathfrak{A}(\mathcal{O}_i)$.

Axioms (1)–(5) correspond closely to those of local field theory.[6,7] It remains an unsolved program to prove that there exist local *bounded* observables in a general Wightman theory of quantized fields. We might begin such a program as follows.

Suppose $\varphi(x)$ is a local field, $\mathcal{O}$ is an open set, and $f(x)$ is a real test function—zero outside $\mathcal{O}$—so that

$$\varphi(f) = \int \varphi(x) f(x)\, dx$$

is an unbounded Hermitian operator defined on the domain D_0 (of Ref. 7) of vectors in $\mathfrak{H}$. It has not been proved that $\varphi(f)$ so defined is essentially self-adjoint. Let us add this as an axiom. The spectral resolutions $E_f(\lambda)$ of $\varphi(f)$ generate a W^* algebra as f varies over the set of all test functions zero outside $\mathcal{O}$; call this algebra $\mathfrak{A}(\mathcal{O})$. The main remaining problem is to prove that the commutativity axiom holds, namely, if $\varphi(f)$ and $\varphi(g)$ commute, so do their spectral resolutions. It can be shown[8] that a sufficient condition is that $\varphi(f)\varphi(g)$ be essentially self-adjoint. In the present paper we bypass this problem by working directly from the axioms.

It is worth remarking that if $f(x) = 0$ outside $\mathcal{O}$, then $\varphi(f)$ should commute with the operators of $\mathfrak{A}(\mathcal{O}')$. We say that an unbounded operator X is *affiliated*[9] to $\mathfrak{A}(\mathcal{O})$, and write $X \eta \mathfrak{A}(\mathcal{O})$, if X commutes with $\mathfrak{A}'(\mathcal{O})$. Thus we should expect all the fields in the Borchers class of $\varphi(x)$ to be affiliated to $\mathfrak{A}(\mathcal{O})$, if they are integrated with test functions zero outside $\mathcal{O}$. Any unbounded self-adjoint operator affiliated to $\mathfrak{A}(\mathcal{O})$ may be regarded as a local observable. In the next section we discuss the observables associated with a symmetry, such as the Lorentz group. We shall show that the translation operator cannot be localized in the sense defined here. This is used to prove that a W^* algebra associated with a translation-invariant region is not of Type I. The question of type was raised by Haag and Schroer[5]; W* algebras fall into five main classes[10] which, in increasing order of complexity, are I_n, I_∞, II_1, II_∞, and III. Algebras of Type I are isomorphic to the algebra of all bounded operators on some Hilbert space $\mathfrak{K}$; the algebras of Types II and III are not. In Sec. 3 intensive observables in local field theory are briefly discussed. This suggests the definition of intensive observables used in Sec. 4, where unitary and Hermitian intensive observables are defined as germs. Here the basic group properties are established. In Sec. 5 we prove that the germs of intensive operators form a sheaf.

The interpretation of the mathematical operators in physical terms is often a problem as difficult as fixing the dynamics. If $X \in \mathfrak{A}(\mathcal{O})$ is an operator with a certain physical interpretation, then $U(a, \Lambda)XU(a, \Lambda)^{-1}$ is the observable whose interpretation is the Lorentz transform of X. This means, in particular, that $U(a, \Lambda)\mathfrak{A}(\mathcal{O})U(a, \Lambda)^{-1} = \mathfrak{A}(\mathcal{O}_{a,\Lambda})$, where $\mathcal{O}_{a,\Lambda}$ is the set of points

$$\mathcal{O}_{a,\Lambda} = \{x/\Lambda^{-1}(x - a) \in \mathcal{O}\}.$$

It is easy to find the physical interpretation of the infinitesimal generators of a symmetry group; these observables are conserved in time, and, in their study, it suffices to discuss a spacelike surface $\sigma(t)$, say the plane $t = 0$.

In Axiom 2 we defined the "causally independent" set of a given set $\mathcal{O}$ to be the set $\mathcal{O}'$. We call $\mathcal{O}'' = (\mathcal{O}')'$ the *causally dependent* set. Then Axiom 2 implies that $\mathfrak{A}(\mathcal{O}'') = \mathfrak{A}(\mathcal{O})''$, which in turn means that $\mathfrak{A}(\mathcal{O})$ is defined by an open set, $\mathcal{O}^*$ say, in $\mathbf{R}^3$, lying on a spacelike surface σ, such that $\mathcal{O}^{*\prime\prime\prime} = \mathcal{O}''$. In the following, $\mathcal{O}$ will mean an open set in $\mathbf{R}^3$ located at $t = 0$, and $\mathfrak{A}(\mathcal{O})$ will mean $\mathfrak{A}(\mathcal{O}'')$.

II. STRICTLY INTENSIVE OBSERVABLES

If an observable X is conserved in time, we might expect that for each subdivision of space (at the given time $t = 0$) into open sets $\mathcal{O}_i$ such that $\mathbf{R}^3 = \cup_i(\bar{\mathcal{O}}_i)$, we have

$$X = \sum_i X_i, \tag{1}$$

[7] A. S. Wightman, Lectures at the Seminar on Theoretical Physics, Palazzino Miramare, Trieste, 1962; *Theoretical Physics* (International Atomic Energy Agency, Vienna, 1963).

[8] A. Devinatz, J. von Neumann, and A. E. Nussbaum, Ann. Math **62**, 199 (1955).

[9] Ref. 3, p. 17, example 10C.

[10] J. Dixmier, *Les algèbres d' opérateurs dans l'espace hilbertien* (Gauthier-Villars, Paris, 1957).

where

$$X_i \in \mathfrak{A}(\mathcal{O}_i). \tag{2}$$

If X is an unbounded operator, we may postulate instead of (2)

$$X_i \eta \mathfrak{A}(\mathcal{O}_i). \tag{3}$$

An operator X with these properties is said to be *strictly intensive* provided that the X_i have the physical interpretation of a measurement of X in region $\mathcal{O}_i$. In the case of observables defined by a symmetry, the physical interpretation is clear, and we are able to give the following

Definition: If U is a unitary symmetry operator defining an observable X, we say U(or X) is *strictly intensive* if for every local algebra $\mathfrak{A}(\mathcal{O})$ invariant under U there exists a local operator $U(\mathcal{O}) \in \mathfrak{A}(\mathcal{O})$ such that

$$USU^{-1} = U(\mathcal{O})SU(\mathcal{O})^{-1} \tag{4}$$

for all $S \in \mathfrak{A}(\mathcal{O})$.

The physical interpretation of $U(\mathcal{O})$ as the local value of U is fixed by (4).

We remark that symmetries defined by anti-unitary transformations cannot be included in this way. These symmetries are anyway less interesting because they do not give rise to conserved Hermitian observables.

Theorem 1. If a unitary operator U has a local value $U(\mathcal{O})$, then $U(\mathcal{O})$ is unique up to a factor. Further, U commutes with $U(\mathcal{O})$, and, if $\mathcal{O}_1$ and $\mathcal{O}_2$ are disjoint and the factor is suitably chosen,

$$U(\mathcal{O}_1 \cup \mathcal{O}_2) = U(\mathcal{O}_1)U(\mathcal{O}_2).$$

Proof: Putting $S = U(\mathcal{O})$ in (4) proves that U commutes with $U(\mathcal{O})$. Suppose, if possible, two operators $U_1(\mathcal{O})$, $U_2(\mathcal{O})$ satisfy the conditions. Then

$$U_1(\mathcal{O})SU_1(\mathcal{O})^{-1} = U_2(\mathcal{O})SU_2(\mathcal{O})^{-1},$$

$S \in \mathfrak{A}(\mathcal{O})$, i.e., $U_2^{-1}U_1$ commutes with S, and so lies in $\mathfrak{A}'$ as well as $\mathfrak{A}$. By Axiom 2, $U_2^{-1}U_1$ must be a scalar. Now suppose $S_1 \in \mathfrak{A}(\mathcal{O}_1)$, $S_2 \in \mathfrak{A}(\mathcal{O}_2)$, and let $U_1 = U(\mathcal{O}_1)$, $U_2 = U(\mathcal{O}_2)$ be the values of U in $\mathcal{O}_1$, $\mathcal{O}_2$. Then

$$U_1U_2S_1U_2^{-1}U_1^{-1} = U_1S_1U_1^{-1} = US_1U^{-1},$$

$$U_1U_2S_2U_2^{-1}U_1^{-1} = U_2S_2U_2^{-1} = US_2U^{-1}.$$

Therefore, for any polynomial T_n in S_1 and S_2,

$$U_1U_2T_nU_2^{-1}U_1^{-1} = UT_nU^{-1}.$$

Now let $T_n \to T$ weakly. Then $U_1U_2T_nU_2^{-1}U_1^{-1}$ converges weakly to $U_1U_2TU_2^{-1}U_1^{-1}$ and UT_nU^{-1} converges weakly to UTU^{-1}, and $T \in \mathfrak{A}(\mathcal{O}_1 \cup \mathcal{O}_2)$. In fact every $T \in \mathfrak{A}(\mathcal{O}_1 \cup \mathcal{O}_2)$ is such a limit.[10] Clearly $U_1U_2 \in \mathfrak{A}(\mathcal{O}_1 \cup \mathcal{O}_2)$, and satisfies the condition 4 for $\mathcal{O} = \mathcal{O}_1 \cup \mathcal{O}_2$. Since this defines an operator uniquely,

$$U(\mathcal{O}_1 \cup \mathcal{O}_2) = U(\mathcal{O}_1)U(\mathcal{O}_2)$$

up to a factor. Q.E.D.

The additive property of the generator of the unitary transformation is brought out by the remark that if $U = e^{iX}$, $U(\mathcal{O}_1) = e^{iX_1}$, $U(\mathcal{O}_2) = e^{iX_2}$, and $U = U(\mathcal{O}_1)U(\mathcal{O}_2)$, then $X = X_1 + X_2$ on their common domain of definition. The fact that U commutes with U_1 and U_2 means roughly that local measurements of X are compatible with a given total value of X.

Of particular interest[11] is the question of whether we can define local energy–momentum and angular momentum operators. For the free field ϕ^0 there exists a spin-2 field in the Borchers class[12] of ϕ^0 given by

$$T^{\mu\nu} = 2{:}\phi^\mu\phi^\nu{:} - g_{\mu\nu}(\phi^\lambda\phi^\lambda - \mu^2\phi^2,$$

where $\phi^\mu = \partial\phi^0(x)/\partial x^\mu$, with the properties

$$T^{\mu\nu}(x) = T^{\nu\mu}(x), \tag{5}$$

$$\partial_\mu T^{\mu\nu}(x) = 0, \tag{6}$$

$$\int d^3x T^{0\mu}(x) = P^\mu. \tag{7}$$

These properties indicate that $T^{\mu\nu}(x)$ can be interpreted as the energy–momentum tensor density. The properties of $T^{\mu\nu}(x)$, (5), (6), (7), together with being in the Borchers class of ϕ^0, determine it up to a c-number spin-2 tensor field. Unfortunately, the "momentum inside a region $\mathcal{O}$" cannot be defined as

$$P^\mu(\mathcal{O}) = \int_{\mathcal{O}} T^{0\mu}(x)\, d^3x, \tag{8}$$

even for the free field, since (8), as it stands, takes the vacuum to a nonnormalizable state. The field $T^{\mu\nu}(x)$ is integrable over $\mathcal{O}$ only if it is multiplied by a test function which vanishes at the boundary of $\mathcal{O}$.

The question as to whether the energy operator is strictly intensive in our sense is a trivial one, since we have defined the "local value" of the time-

[11] J. Schwinger, Phys. Rev. **130**, 402, 406, 800(1963).

[12] H. J. Borchers, Nuovo Cimento **15**, 784 (1960); Ref. 6, Chap. 4 or Sect. 6.

translation operator so far only for algebras invariant under time translation; a theorem of Borchers[13] says that such algebras consist of all bounded operators. The next theorem shows that it is not possible to define a space-translation operator (in regions invariant under space translation). The uniqueness of the vacuum plays an important part in the proof.

Theorem 2. Let $\mathcal{O}$ be such that $U(a)\mathcal{O}U(a)^{-1} = \mathcal{O}$ for all spacelike translations $a = \lambda \mathbf{b}$, where $\mathbf{b}$ is fixed and $-\infty < \lambda < \infty$. Then there does not exist $V(a) \in \mathfrak{A}(\mathcal{O})$ with

$$V(a)SV(a)^{-1} = U(a)SU(a)^{-1} \tag{9}$$

for all $S \in \mathfrak{A}(\mathcal{O})$, unless $\mathcal{O}'$ is empty.

Proof: Suppose $\mathcal{O}'$ contains an open set and $V(a)$ exists satisfying (9). Then

$$S = V(b)^{-1}V(a)V(b)V(a)^{-1}SV(a)V(b)^{-1}V(a)^{-1}V(b)$$

for all $S \in \mathfrak{A}(\mathcal{O})$, i.e., $V(b)^{-1}V(a)V(b)V(a)^{-1}$ is in $\mathfrak{A}'$ as well as $\mathfrak{A}$, and so, by Axiom 2, there exists $\lambda(a, b)$ such that

$$\begin{aligned} V(b) &= \lambda(a, b)V(a)V(b)V(a)^{-1} \\ &= \lambda(a, b)U(a)V(b)U(a)^{-1} \quad \text{by} \quad (9), \end{aligned}$$

which leads to

$$V(b)\Psi_0 = \lambda(a, b)U(a)(V(b)\Psi_0).$$

Now, Ψ_0 is the only normalizable ray which changes only by a phase under $U(a)$, so $V(b)\Psi_0 = \alpha\Psi_0$. Thus $V(b) - \alpha\mathbf{1} \in \mathfrak{A}(\mathcal{O})$ and annihilates the vacuum, impossible if $\mathcal{O}'$ contains an open set.[14] This contradiction proves the result.

Corollary (first proved in Ref. 2). If $\mathcal{O}$ is invariant under a spacelike translation group, then $\mathfrak{A}(\mathcal{O})$ is not of Type I.

Note added in proof: This result is proved by the same method by R. V. Kadison, J. Math. Phys. **4**, 1511 (1963).

Proof: Suppose $U(a)\ \mathfrak{A}(\mathcal{O})U(a)^{-1} = \mathfrak{A}(\mathcal{O})$. Then the transformation

$$S \to U(a)SU(a)^{-1} = \Phi(S)$$

defines an automorphism for the * algebra $\mathfrak{A}$, i.e., a 1 : 1 map of $\mathfrak{A}$ onto $\mathfrak{A}$ preserving the algebraic structure. Therefore if $\mathfrak{A}$ is of Type I, Φ is an inner automorphism, i.e., $\Phi(S) = V(a)SV(a)^{-1}$ for some $V \in \mathfrak{A}$ and all $S \in \mathfrak{A}$.[15] This contradicts Theorem 2.

[13] H. J. Borchers, Nuovo Cimento **19**, 787 (1961).
[14] H. Reeh and S. Schlieder, Nuovo Cimento **22**, 1051 (1961); Ref. 6, Chap. 4.
[15] Ref. 3, p. 256, Corollary.

III. INTENSIVE OBSERVABLES IN LOCAL FIELD THEORY

We have seen that, in the theory of the free field, the energy–momentum tensor $T^{\mu\nu}(x)$ does not satisfy the definition we gave of "strictly intensive". It is easy to see that other "densities" defined in the usual way for the free field, such as isospin and charge density, are not operators when integrated over a finite region, unless they are smoothed with a test function. Since these local fields (the densities) are undoubtedly very useful objects, there is an indication that the definition given was too restrictive. We therefore weaken it to

Definition: A conserved quantity X in a field theory of a field is said to be *intensive* if there exists a field $X(x)$ in the Borchers class of φ such that, for any $\mathcal{O} \subset \mathbf{R}^3$,

$$[X(f), \varphi(x)] = [X, \varphi(x)], \qquad x \in \mathcal{O},$$

where f is a test function $= 1$ in $\mathcal{O}$. The definition implies that $X(x)$ can be restricted to a spacelike surface. This could be avoided by smoothing both sides in the time, so as to read

$$\left[\int \rho(t)f(\mathbf{x}')X(\mathbf{x}', t)\, d\mathbf{x}'\, dt, \varphi(x)\right] = \left(\int \rho\, dt\right)[X, \varphi(x)].$$

The definition means that, to measure an intensive quantity in $\mathcal{O}$ we need a region $\mathcal{O}^*$ slightly larger all around, but which can be made arbitrarily small. With this definition, $T^{\mu\nu}(x)$ for the free field is an intensive field.

For the free field, $T^{\mu\nu}(x)$ is a reducible field, since it commutes with the projections onto even- and odd-particle states. It is conceivable that field theories exist in which $T^{\mu\nu}(x)$ is irreducible. We will call such theories purely *gravitational.* If a collection of intensive fields such as $T^{\mu\nu}(x)$, $j^{\mu}(x)$, etc. form an irreducible set, we will call the theory an *intensive field theory:* it is a theory purely involving the given conserved quantities. In a sense we may regard every field as a local density. The problem is, to find under what conditions a field is the local value of the intensive operator, and, if so, how do we physically interpret the conserved operator?

Unlike strictly intensive operators, we do not expect intensive fields to commute with the operator they represent. There is always some overlap outside the region $\mathcal{O}$ under discussion. Since the enveloping region $\mathcal{O}_1$ can be made as small as we like, we should expect $T^{0\mu}(x)$ and P^{μ} to commute "in some

limiting sense". To see how this might be made rigorous we return to the bounded observables $\mathfrak{A}(\mathcal{O})$.

IV. GERMS OF LOCAL OBSERVABLES

Let $\mathcal{O} \subset \mathbf{R}^3$ be a bounded open set, and U, V two unitary operators $\in \mathfrak{B}(\mathfrak{H})$. The operators U, V define symmetries, and induce transformations USU^{-1}, VSV^{-1} on any $S \in \mathfrak{A}(\mathcal{O})$. We say two unitary operators are *physically equivalent in* $\mathcal{O}$ if

$$\left.\begin{aligned} &USU^{-1} = VSV^{-1} \\ &\text{and} \\ &U^{-1}SU = V^{-1}SV \end{aligned}\right\} \quad \text{for all} \quad S \in \mathfrak{A}(\mathcal{O}).$$

We then write $U \equiv V$ in $\mathcal{O}$. Obviously $\equiv$ is an equivalence relation, and $U^{-1}V \in \mathfrak{A}'(\mathcal{O})$, $UV^{-1} \in \mathfrak{A}'(\mathcal{O})$ if and only if $U \equiv V$ in $\mathcal{O}$. For Hermitian operators the commutator is the physically significant thing. We say two Hermitian operators X_1, X_2 *are physically equivalent in* $\mathcal{O}$ if

$$[X_1, S] = [X_2, S] \quad \text{for all} \quad S \in \mathfrak{A}(\mathcal{O});$$

clearly this is equivalent to $(X_1 - X_2) \in \mathfrak{A}'(\mathcal{O})$ and we write $X_1 \equiv X_2$ in $\mathcal{O}$. Obviously $\equiv$ is an equivalence relation. If X_1, X_2 are unbounded self-adjoint operators, we say $X_1 \equiv X_2$ in $\mathcal{O}$ if $(X_1 - X_2)\eta\mathfrak{A}'(\mathcal{O})$. This requires that the domain of definition of $X_1 - X_2$ is mapped into itself by $\mathfrak{A}'(\mathcal{O})$. We are now in a position to give a suitable

Definition: A unitary operator $U \in \mathfrak{B}(\mathfrak{H})$ is said to be *intensive* if to any open set $\mathcal{O}$ invariant under U, and to every open set $\mathcal{O}_1$ containing the closure $\bar{\mathcal{O}}$ of $\mathcal{O}$, there exists a unitary operator $U(\mathcal{O}, \mathcal{O}_1) \in \mathfrak{A}(\mathcal{O}_1)$ such that $U \equiv U(\mathcal{O}, \mathcal{O}_1)$ on $\mathcal{O}$. A similar definition can be given for an intensive Hermitian operator, but in this case $\mathcal{O}$ may be any open set whatever. It is clear that if $U \equiv V$ on $\mathcal{O}$ then $U \equiv V$ on any open subset of $\mathcal{O}$. The set of pairs $\{\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1)\}$ for all $\mathcal{O}_1 \supset \bar{\mathcal{O}}$ we will denote by $U(\mathcal{O})$, and call it the restriction of U to $\mathcal{O}$.

More generally, we can define a *section over* $\mathcal{O}$ without reference to an outside operator U as follows.

To every open set $\mathcal{O}$ and $\mathcal{O}_1 \supset \bar{\mathcal{O}}$ is given a unitary operator $U(\mathcal{O}, \mathcal{O}_1) \in \mathfrak{A}(\mathcal{O}_1)$. The pairs $(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))$ have the following property $P(\mathcal{O})$: given $\mathcal{O}_1$ and $\mathcal{O}_2$ both containing $\bar{\mathcal{O}}$, there is to exist an $\mathcal{O}_3$ such that

$$\mathcal{O}_3 \subset \mathcal{O}_1 \cap \mathcal{O}_2, \qquad \mathcal{O}_3 \supset \bar{\mathcal{O}},$$

and

$$U(\mathcal{O}, \mathcal{O}_1) \equiv U(\mathcal{O}, \mathcal{O}_2) \quad \text{on} \quad \mathcal{O}_3.$$

The sets of pairs $\{(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))\}$ is said to be equivalent to the set of pairs $\{(\mathcal{O}_1', U'(\mathcal{O}, \mathcal{O}_1'))\}$, if to any $\mathcal{O}_1$, $\mathcal{O}_1'$ there exists an open set $\mathcal{O}_3$ in $\mathcal{O}_1 \cap \mathcal{O}_1'$ such that

$$U(\mathcal{O}, \mathcal{O}_1) \equiv U'(\mathcal{O}, \mathcal{O}_1') \quad \text{in} \quad \mathcal{O}_3$$

and $\mathcal{O}_3 \supset \bar{\mathcal{O}}$.

The next theorem proves that this is an equivalence relation; we write

$$\{(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))\} \equiv \{(\mathcal{O}_1', U'(\mathcal{O}, \mathcal{O}_1'))\}.$$

Before proving the theorem let us define these objects more explicitly. Let $\Omega(\bar{\mathcal{O}})$ be the collection of all open sets in $\mathbf{R}^3$ containing $\bar{\mathcal{O}}$, and $\Omega(x)$ the set of all open sets containing x. Then the pairs $(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))$ with the property P define a mapping

$$\Omega \overset{U(\mathcal{O})}{\longrightarrow} \mathfrak{B}(\mathfrak{H})$$

as $\mathcal{O}_1$ varies over $\Omega(\bar{\mathcal{O}})$. Let $\mu(\Omega)$ be set of all mappings from Ω to $\mathfrak{B}(\mathfrak{H})$. Then the equivalence relation $\equiv$ is defined between elements of $\mu(\Omega)$, which therefore fall into equivalence classes.

Theorem 3. The relation $\equiv$ between elements of $\mu(\Omega)$ is an equivalence relation.

Proof: Since $U \in \mu(\Omega)$ is a collection of pairs $(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))$ with the property P, the relation is by definition reflexive. It is also obviously symmetric, since $\equiv$ is a symmetric relation in $\mathfrak{B}(\mathfrak{H})$. To prove transitivity, suppose

$$\{(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))\} \equiv \{(\mathcal{O}_1', U'(\mathcal{O}, \mathcal{O}_1'))\},$$

and

$$\{(\mathcal{O}_1', U'(\mathcal{O}, \mathcal{O}_1'))\} \equiv \{(\mathcal{O}_1'', U''(\mathcal{O}, \mathcal{O}_1''))\}.$$

Then by definition for given $\mathcal{O}_1$, $\mathcal{O}_1'$, $\mathcal{O}_1''$ there exist open sets $\mathcal{O}_3$ and $\mathcal{O}_3'$ such that

$$\mathcal{O}_3 \subset \mathcal{O}_1 \cap \mathcal{O}_1', \quad \mathcal{O}_3' \subset \mathcal{O}_1' \cap \mathcal{O}_1'', \quad \mathcal{O}_3 \supset \bar{\mathcal{O}}, \quad \mathcal{O}_3' \supset \bar{\mathcal{O}},$$

and

$$U(\mathcal{O}, \mathcal{O}_1) \equiv U'(\mathcal{O}, \mathcal{O}_1') \text{ on } \mathcal{O}_3,$$

$$U'(\mathcal{O}, \mathcal{O}_1') \equiv U''(\mathcal{O}, \mathcal{O}_1'') \quad \text{on} \quad \mathcal{O}_3'.$$

Since the relation $\equiv$ is transitive we have

$$U(\mathcal{O}, \mathcal{O}_1) \equiv U''(\mathcal{O}, \mathcal{O}_1'') \quad \text{on} \quad \mathcal{O}_3 \cap \mathcal{O}_3',$$

and $\mathcal{O}_3 \cap \mathcal{O}_3' \supset \bar{\mathcal{O}}$. Therefore by definition

$$\{(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))\} \equiv \{(\mathcal{O}_1'', U''(\mathcal{O}, \mathcal{O}_1''))\},$$

and the relation $\equiv$ is an equivalence relation.

Definition: An equivalence class in $\mu(\Omega)$ with respect to the relation $\equiv$ is called a *unitary section over* $\mathcal{O}$ written $U(\mathcal{O})$. In the same way we define a *Hermitian section over* $\mathcal{O}$, $X(\mathcal{O})$, by replacing $U(\mathcal{O}, \mathcal{O}_1) \in \mathfrak{A}(\mathcal{O}_1)$ by $X(\mathcal{O}, \mathcal{O}_1) \in \mathfrak{A}(\mathcal{O}_1)$, where X is Hermitian; with no extra trouble we can include the case where X is unbounded.

The usual axioms do not say that every Hermitian operator is intensive; we note that a unitary operator such as $U(a, \Lambda)$ which moves the region $\mathcal{O}$ around cannot be intensive in our sense, except in regions invariant under the subgroup of $L(\mathbf{R})$ generated by the element (a, Λ). We can, however, consider infinitesimal Lorentz transformations. This means, that given $\mathcal{O}$ and $\mathcal{O}_1 \supset \bar{\mathcal{O}}$ we consider those $U(a, \Lambda)$ sufficiently close to the identity, such that $U(a, \Lambda)\, \bar{\mathcal{O}} \subset \mathcal{O}_1$. We might add the axiom that certain "important" operators are intensive. This idea works for the free field. Another point is not covered by the usual axioms. There is no proof that every section over $\mathcal{O}$ is the restriction to $\mathcal{O}$ of some global operator. We can either postulate that it is true (thus restricting the class of theories under discussion), or consider only those sections which are restrictions of global intensive observables.

If U is an intensive unitary operator in $\mathfrak{B}(\mathfrak{H})$, we can define a thing called the *germ of U at x*, written $U(x)$, in the same way as we defined $U(\mathcal{O})$ for an open set; choose $x \in \mathbf{R}^3$ and U, a section over $\mathbf{R}^3$, and consider that set $U(x)$ of all sections of U over open sets containing x. Given any two such sections, their restrictions to a small enough neighborhood of x are $\equiv$ equivalent. If we regard $U(x)$ as the collection, as $\mathcal{O}$ varies over $\Omega(x)$, of all the pairs $\{(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))\} \in \mu(\Omega)$ in the equivalence class $U(\mathcal{O})$, we see that $U(x)$ is defined as an equivalence class of mappings with the property $P(x)$ from $\Omega(x)$ into $\mathfrak{B}(\mathfrak{H})$, two mappings U, V being equivalent if for any two sets $\mathcal{O}_1$, $\mathcal{O}_2 \in \Omega(x)$ there exists an open set $\mathcal{O}_3 \in \Omega(x)$ such that $U(\mathcal{O}_1) \equiv V(\mathcal{O}_2)$ on $\mathcal{O}_3$. This result brings the definition of germ into line with that of section. The germs $U(x)$ are called *unitary germs* and the germs $X(x)$ (defined similarly for Hermitian operators) are called *Hermitian germs*.

We can define an operation of multiplication among unitary sections, and among unitary germs; we can define addition among Hermitian sections and germs.

Let $U(\mathcal{O})$, $V(\mathcal{O})$ be two unitary sections over $\mathcal{O}$. Let us define $UV(\mathcal{O})$ to be the section defined by the equivalence class defined by the following element of $\mu(\Omega(\bar{\mathcal{O}}))$. To any open set $\mathcal{O}_1 \supset \bar{\mathcal{O}}$, choose the operator $U(\mathcal{O}_1)V(\mathcal{O}_1)$, where $U(\mathcal{O}_1)$ is chosen from among equivalent operators $U(\mathcal{O}, \mathcal{O}_1)$ in the section $U(\mathcal{O})$, and the same for $V(\mathcal{O}_1)$. We must prove two things: first, that this defines a section and secondly, that the section is independent of the representatives $U(\mathcal{O}_1)$, $V(\mathcal{O}_1)$ chosen. To prove the first, suppose we have chosen to the sets $\mathcal{O}'$, $\mathcal{O}''$, the representatives $U(\mathcal{O}')$, $U(\mathcal{O}'')$, and $V(\mathcal{O}')$, $V(\mathcal{O}'')$, respectively. We are given $U(\mathcal{O}')SU(\mathcal{O}')^{-1} = U(\mathcal{O}'')SU(\mathcal{O}'')^{-1}$ if $S \in \mathfrak{A}(\mathcal{O}_3)$, say, and $V(\mathcal{O}')SV(\mathcal{O}')^{-1} = V(\mathcal{O}'')SV(\mathcal{O}'')^{-1}$ if $S \in \mathfrak{A}(\mathcal{O}_4)$, say. Since $(\mathcal{O}_1, U(\mathcal{O}, \mathcal{O}_1))$, $(\mathcal{O}_1, V(\mathcal{O}, \mathcal{O}_1))$ have the property $P(\mathcal{O})$, we may find $U(\mathcal{O}_3 \cap \mathcal{O}_4)$, $V(\mathcal{O}_3 \cap \mathcal{O}_4)$ such that

$$U(\mathcal{O}_3 \cap \mathcal{O}_4)SU^{-1}(\mathcal{O}_3 \cap \mathcal{O}_4) = U(\mathcal{O}')SU^{-1}(\mathcal{O}') \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_5),$$

$$V(\mathcal{O}_3 \cap \mathcal{O}_4)SV^{-1}(\mathcal{O}_3 \cap \mathcal{O}_4) = V(\mathcal{O}')SV^{-1}(\mathcal{O}') \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_6).$$

Let $S \in \mathfrak{A}(\mathcal{O}_5 \cap \mathcal{O}_6)$. Then we have

$$U(\mathcal{O}')(V(\mathcal{O}')SV(\mathcal{O}')^{-1})U(\mathcal{O}')^{-1} = U(\mathcal{O}')(V(\mathcal{O}_3 \cap \mathcal{O}_4)SV^{-1}(\mathcal{O}_3 \cap \mathcal{O}_4))U(\mathcal{O}')^{-1}.$$

Since

$$V(\mathcal{O}_3 \cap \mathcal{O}_4)SV^{-1}(\mathcal{O}_3 \cap \mathcal{O}_4) \in \mathfrak{A}(\mathcal{O}_3),$$

the above line is

$$= U(\mathcal{O}'')(V(\mathcal{O}_3 \cap \mathcal{O}_4)SV^{-1}(\mathcal{O}_3 \cap \mathcal{O}_4))U(\mathcal{O}'')^{-1}$$
$$= U(\mathcal{O}'')(V(\mathcal{O}')SV^{-1}(\mathcal{O}'))U(\mathcal{O}'')^{-1}$$
$$= U(\mathcal{O}'')V(\mathcal{O}'')SV^{-1}(\mathcal{O}'')U(\mathcal{O}'')^{-1},$$

since $S \in \mathfrak{A}(\mathcal{O}_4)$. This proves that $UV(\mathcal{O})$ is a section over $\mathcal{O}$. To prove the second part, suppose that instead of $U(\mathcal{O}')$, $V(\mathcal{O}')$ we had chosen the representatives $U'(\mathcal{O}')$, $V'(\mathcal{O}')$ in the same equivalence class. Thus we are given $\mathcal{O}_1 \in \Omega(\bar{\mathcal{O}})$, $\mathcal{O}_2 \in \Omega(\bar{\mathcal{O}})$ such that

$$U(\mathcal{O}')SU(\mathcal{O}')^{-1} = U'(\mathcal{O}')SU'(\mathcal{O}')^{-1}, \qquad S \in \mathfrak{A}(\mathcal{O}_1),$$
$$V(\mathcal{O}')SV(\mathcal{O}')^{-1} = V'(\mathcal{O}')SV'(\mathcal{O}')^{-1}, \qquad S \in \mathfrak{A}(\mathcal{O}_2).$$

We may also find $U(\mathcal{O}_1 \cap \mathcal{O}_2)$, $V(\mathcal{O}_1 \cap \mathcal{O}_2)$ such that

$$U(\mathcal{O}_1 \cap \mathcal{O}_2)SU^{-1}(\mathcal{O}_1 \cap \mathcal{O}_2) = U'(\mathcal{O}')SU'(\mathcal{O}')^{-1} = U(\mathcal{O}')SU(\mathcal{O}')^{-1} \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_3);$$

$$V(\mathcal{O}_1 \cap \mathcal{O}_2)SV^{-1}(\mathcal{O}_1 \cap \mathcal{O}_2) = V'(\mathcal{O}')SV'(\mathcal{O}')^{-1} = V(\mathcal{O}')SV(\mathcal{O}')^{-1} \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_4),$$

where $\mathcal{O}_3$, $\mathcal{O}_4$, $\in \Omega(\bar{\mathcal{O}})$ and $\mathcal{O}_1 \cap \mathcal{O}_2 \supset \mathcal{O}_3$, $\supset \mathcal{O}_4$. Then choose $S \in \mathfrak{A}(\mathcal{O}_3 \cap \mathcal{O}_4)$. We have

$$U(\mathcal{O}')V(\mathcal{O}')SV^{-1}(\mathcal{O}')U^{-1}(\mathcal{O}') = U(\mathcal{O}')[V(\mathcal{O}_1 \cap \mathcal{O}_2)SV^{-1}(\mathcal{O}_1 \cap \mathcal{O}_2)]U^{-1}(\mathcal{O}')$$
$$= U'(\mathcal{O}')[V(\mathcal{O}_1 \cap \mathcal{O}_2)SV^{-1}(\mathcal{O}_1 \cap \mathcal{O}_2)]U'(\mathcal{O}')^{-1},$$

since

$$V(\mathcal{O}_1 \cap \mathcal{O}_2)SV^{-1}(\mathcal{O}_1 \cap \mathcal{O}_2) \in \mathfrak{A}(\mathcal{O}_1)$$

$$= U'(\mathcal{O}')[V'(\mathcal{O}')SV'(\mathcal{O}')^{-1}]U'(\mathcal{O}')^{-1}, \quad S \in \mathfrak{A}(\mathcal{O}_3 \cap \mathcal{O}_4).$$

Similarly,

$$V^{-1}(\mathfrak{O}'')U^{-1}(\mathfrak{O}'')SU(\mathfrak{O}'')V(\mathfrak{O}'') = V'(\mathfrak{O}'')^{-1}U'(\mathfrak{O}'')^{-1}SU'(\mathfrak{O}'')V'(\mathfrak{O}'').$$

This proves that $U(\mathfrak{O}'')V(\mathfrak{O}'') \equiv U'(\mathfrak{O}'')V'(\mathfrak{O}'')$ on $\mathfrak{O}_3 \cap \mathfrak{O}_4$, i.e., they belong to the same equivalence class, showing that the section defined by $UV(\mathfrak{O})$ is unique. In a similar way we can define the product $U(x)V(x)$ of germs.

To any section $U(\mathfrak{O})$ we can define the *inverse section* $U(\mathfrak{O})^{-1}$ as follows: Given $\mathfrak{O}'' \in \Omega(\bar{\mathfrak{O}})$, choose the representative of $U^{-1}(\mathfrak{O})$ to be $U(\mathfrak{O}'')^{-1}$, i.e., the inverse of some representative. We have to prove that this is a section, and that it is independent of the representatives. To prove the first, suppose $\mathfrak{O}''$ and $\mathfrak{O}'''$ are given. We have to prove that $U(\mathfrak{O}'')^{-1} \equiv U(\mathfrak{O}''')^{-1}$ on some subset $\mathfrak{O}_3 \in \Omega(\bar{\mathfrak{O}})$ of $\mathfrak{O}'' \cap \mathfrak{O}'''$. This follows immediately from the definition of $U(\mathfrak{O}'') \equiv U(\mathfrak{O}''')$. Secondly, we must show that it defines a unique section. Let $U'(\mathfrak{O}'')$ be chosen instead of $U(O'')$. Since $U'(\mathfrak{O}'')$ leads to a section equivalent to $U(\mathfrak{O}'')$, it is clear that $U'(\mathfrak{O}'')^{-1}$ leads to an equivalent section to $U(\mathfrak{O}'')^{-1}$. This proves that the inverse section is unique. We can also check the equation $U(\mathfrak{O})U^{-1}(\mathfrak{O}) = 1(\mathfrak{O})$. Note that the unit operator is an intensive unitary operator. The section over $\mathfrak{O}$ is defined as the map which takes an open set $\mathfrak{O}''$ to any operator in $\mathfrak{A}(\mathfrak{O}'' - \bar{\mathfrak{O}}_3)$, say where $\mathfrak{O}_3$ is any set in $\Omega(\bar{\mathfrak{O}})$. This operator commutes with $\mathfrak{A}(\mathfrak{O}_3)$, i.e., is equivalent to the identity on $\mathfrak{O}_3$. To prove the equation $UU^{-1} = 1(\mathfrak{O})$, it is sufficient to pick any representatives, since as we have shown, multiplication is unique. Picking inverses of each other immediately gives the result. We have therefore proved

Theorem 4. The unitary sections over $\mathfrak{O}$ form a multiplicative group, $\mathfrak{F}(\mathfrak{O})$.

We note that multiplication by a phase does not alter a unitary section, since $e^{i\alpha}U(\mathfrak{O}'') \equiv U(\mathfrak{O}'')$ on $\mathfrak{O}''$. This is in line with Theorem 1, where the strictly intensive unitary operators are unique except for a factor.

If $\bar{\mathfrak{O}}_1$ and $\bar{\mathfrak{O}}_2$ are disjoint sets we can define quite a different type of multiplication of sections: $U(\mathfrak{O}_1) \times U(\mathfrak{O}_2)$. This is a section over $\mathfrak{O}_1 \cup \mathfrak{O}_2$ whose representatives are the products of the representatives of $U(\mathfrak{O}_1)$ and $U(\mathfrak{O}_2)$. This defines a section, since a sufficiently small neighborhood of $\mathfrak{O}_1 \cup \mathfrak{O}_2$ can always be split into open sets $\mathfrak{O}_1'' \supset \bar{\mathfrak{O}}_1$ and $\mathfrak{O}_2'' \supset \bar{\mathfrak{O}}_2$, with $\mathfrak{O}_1'' \cap \mathfrak{O}_2'' = \phi$. Let us choose representatives $U_1(\mathfrak{O}_1'')$, $U_2(\mathfrak{O}_2'')$, and to another pair $\mathfrak{O}_1'''$, $\mathfrak{O}_2'''$ the representatives $U_1(\mathfrak{O}_1''')$, $U_2(\mathfrak{O}_2''')$; we have to show that

$$U_1(\mathfrak{O}_1'')U_2(\mathfrak{O}_2'') \equiv U_1(\mathfrak{O}_1''')U_2(\mathfrak{O}_2''')$$

in a neighborhood of $\mathfrak{O}_1 \cup \mathfrak{O}_2$. There exist open sets

$$\mathfrak{O}_3 \subset \mathfrak{O}_1''' \cap \mathfrak{O}_1'', \qquad \mathfrak{O}_4 \subset \mathfrak{O}_2''' \cap \mathfrak{O}_2''$$

such that

$$\mathfrak{O}_3 \supset \bar{\mathfrak{O}}_1, \qquad \mathfrak{O}_4 \supset \bar{\mathfrak{O}}_2$$

and

$$U_1(\mathfrak{O}_1'') \equiv U_1(\mathfrak{O}_1''') \quad \text{on} \quad \mathfrak{O}_3;$$

$$U_2(\mathfrak{O}_2'') \equiv U_2(\mathfrak{O}_2''') \quad \text{on} \quad \mathfrak{O}_4.$$

Now for $S \in \mathfrak{A}(\mathfrak{O}_3)$, $T \in \mathfrak{A}(\mathfrak{O}_4)$ we have

$$U_1(\mathfrak{O}'')U_2(\mathfrak{O}'')SU_2^{-1}(\mathfrak{O}'')U_1^{-1}(\mathfrak{O}'') = U_1(\mathfrak{O}'')SU_1(\mathfrak{O}'')^{-1} = U_1(\mathfrak{O}''')SU_1^{-1}(\mathfrak{O}''') = U_1(\mathfrak{O}''')U_2(\mathfrak{O}''')SU_2^{-1}(\mathfrak{O}''')U_1^{-1}(\mathfrak{O}'''),$$

and similarly,

$$U_1(\mathfrak{O}'')U_2(\mathfrak{O}'')TU_2^{-1}(\mathfrak{O}'')U_1^{-1}(\mathfrak{O}'') = U_1(\mathfrak{O}''')U_2(\mathfrak{O}''')TU_2^{-1}(\mathfrak{O}''')U_1^{-1}(\mathfrak{O}''').$$

Then, by taking weak limits of polynomials in $S \in \mathfrak{A}(\mathfrak{O}_3)$, $T \in \mathfrak{A}(\mathfrak{O}_4)$, as in the proof of Theorem 1, for any

$$S \in (\mathfrak{A}(\mathfrak{O}_3) \cup \mathfrak{A}(\mathfrak{O}_4))'' = \mathfrak{A}(\mathfrak{O}_3 \cup \mathfrak{O}_4),$$

we have

$$U_1(\mathfrak{O}'')U_2(\mathfrak{O}'')SU_2^{-1}(\mathfrak{O}'')U_1^{-1}(\mathfrak{O}'') = U_1(\mathfrak{O}''')U_2(\mathfrak{O}''')SU_2^{-1}(\mathfrak{O}''')U_1^{-1}(\mathfrak{O}'''),$$

which proves $U(\mathfrak{O}_1) \times U(\mathfrak{O}_2)$ is a section over $\mathfrak{O}_1 \cup \mathfrak{O}_2$.

If we had chosen $U_1'(\mathfrak{O}_1'')$, $U_2'(\mathfrak{O}_2'')$ instead of $U_1(\mathfrak{O}_1'')$, $U_2(\mathfrak{O}_2'')$, similar arguments show that

$$U_1'(\mathfrak{O}_1'')U_2'(\mathfrak{O}_2'') \equiv U_1(\mathfrak{O}_1'')U_2(\mathfrak{O}_2'')$$

on some neighborhood of $\mathfrak{O}_1 \cup \mathfrak{O}_2$. This proves that the $\times$ product is unique. Now, we may write $U(\mathfrak{O}_1 \cup \mathfrak{O}_2)$ for $U(\mathfrak{O}_1) \times U(\mathfrak{O}_2)$ if $\bar{\mathfrak{O}}_1$ and $\bar{\mathfrak{O}}_2$ are disjoint, since the restrictions of $U(\mathfrak{O}_1) \times U(\mathfrak{O}_2)$ to $\mathfrak{O}_i$ are clearly $U(\mathfrak{O}_i)$. Therefore we have the generalization of Theorem 1 to sections:

Theorem 5. If $U(\mathbf{R}^3)$ is a section over $\mathbf{R}^3$ then $U(\mathbf{R}^3)$ commutes with its local values, and if $\bar{\mathfrak{O}}_1$ and $\bar{\mathfrak{O}}_2$ are disjoint, then $U(\mathfrak{O}_1 \cup \mathfrak{O}_2) = U(\mathfrak{O}_1) \times U(\mathfrak{O}_2)$.

Proof: It remains to prove that $U(\mathbf{R}^3)$ commutes with its local values, or, rather, to define $U(\mathfrak{O}_1)V(\mathfrak{O}_2)$

when $\mathcal{O}_1 \neq \mathcal{O}_2$ and they are not disjoint. We define $U(\mathcal{O}_1)V(\mathcal{O}_2)$ to be $U(\mathcal{O}_1 \cap \mathcal{O}_2)V(\mathcal{O}_1 \cap \mathcal{O}_2)$, i.e., the product of the restrictions, and it is a section over $\mathcal{O}_1 \cap \mathcal{O}_2$. Since the restriction of $U(\mathbf{R}^3)$ to $\mathcal{O}$ is just $U(\mathcal{O})$, it is trivial that $U(\mathbf{R}^3)$ commutes with $U(\mathcal{O})$. Q.E.D.

We note that if $\mathcal{O}_1$ and $\mathcal{O}_2$ are disjoint but have common boundaries, then neither $\times$ nor ordinary multiplication can be defined for general sections. However, for sections which are restrictions of global operators we may simply define

$$U(\mathcal{O}_1) \times U(\mathcal{O}_2) = U(\mathcal{O}_1 \cup \mathcal{O}_2) \quad \text{if} \quad \mathcal{O}_1 \cap \mathcal{O}_2 = \phi,$$

bringing Theorem 5 (by definition!) into line with Theorem 1. The problem of dealing with the boundary of $\mathcal{O}$ in defining $\times$ will turn up again later.

We can define multiplication on the set of Hermitian sections as follows: If $X(\mathcal{O}')$ is a representative of X, then $\lambda X(\mathcal{O}')$ is a representative of λX. We can also define addition of Hermitian sections over $\mathcal{O}$. Choose, for a given set $\mathcal{O}' \supset \mathcal{O}$, representatives $X(\mathcal{O}')$, $Y(\mathcal{O}')$ and define the representative of $X(\mathcal{O}) + Y(\mathcal{O})$ to be $X(\mathcal{O}') + Y(\mathcal{O}')$. To prove this is a section, we have, for any $\mathcal{O}'$, $\mathcal{O}''$, a set $\mathcal{O}_3$ with $\mathcal{O}_3 \supset \bar{\mathcal{O}}$ and

$$[X(\mathcal{O}'), S] = [X(\mathcal{O}''), S] \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_3),$$

and a set $\mathcal{O}_4$ with

$$[Y(\mathcal{O}'), S] = [Y(\mathcal{O}''), S] \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_4).$$

Choose $S \in \mathfrak{A}(\mathcal{O}_3 \cap \mathcal{O}_4)$. Then

$$\begin{aligned}[X(\mathcal{O}') + Y(\mathcal{O}'), S] &= [X(\mathcal{O}'), S] + [Y(\mathcal{O}'), S] \\ &= [X(\mathcal{O}''), S] + [Y(\mathcal{O}''), S] \\ &= [X(\mathcal{O}'') + Y(\mathcal{O}''), S] \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_3 \cap \mathcal{O}_4).\end{aligned}$$

This proves that the addition of two sections is a section. To show it is unique, suppose that instead of these we had chosen other representatives $X'(\mathcal{O}')$, $Y'(\mathcal{O}')$. Then a simple argument shows that $X(\mathcal{O}') + Y(\mathcal{O}') \equiv X'(\mathcal{O}') + Y'(\mathcal{O}')$ on some $\mathcal{O}_3 \supset \bar{\mathcal{O}}$. Thus we have proved

Theorem 6. The Hermitian sections form an Abelian group $\mathcal{G}(\mathcal{O})$. We note that the zero of the group is the section containing multiples of the identity.

With no extra trouble we can define the addition of two Hermitian germs at the same point in the same way, and the addition of two Hermitian sections over different intersecting sets as the sum of their restrictions. If $\bar{\mathcal{O}}_1 \cap \bar{\mathcal{O}}_2 = \phi$ we can also define the $\dotplus$ sum of $X(\mathcal{O}_1)$, $Y(\mathcal{O}_2)$ as a section over $\mathcal{O} = \mathcal{O}_1 \cup \mathcal{O}_2$, whose representatives are just sums, i.e.,

$$(X \dotplus Y)(\mathcal{O}') = X(\mathcal{O}_1') + Y(\mathcal{O}_2').$$

It is obvious that this is a well defined section, *provided X and Y are bounded,* for the argument analogous to that before Theorem 5 goes through. If $X(\mathcal{O}_1)Y(\mathcal{O}_2)$ are the restrictions to $\mathcal{O}_1$, $\mathcal{O}_2$ of a global section $X(\mathbf{R}^3)$, we may define $X(\mathcal{O}_1) \dotplus X(\mathcal{O}_2)$ as $X(\mathcal{O}_1 \cup \mathcal{O}_2)$ if $\mathcal{O}_1 \cap \mathcal{O}_2 = \phi$ but $\mathcal{O}_1$ and $\mathcal{O}_2$ have a boundary in common.

We cannot in general define multiplication of Hermitian sections (or addition of unitary sections) because the production of two Hermitian operators is not general Hermitian, and we have no good definition of "physical equivalence" for arbitrary operators. Thus our formalism does not allow us to define things like $(X(x))^2$, and so we cannot write equations of motion, etc. We can define the $\times$ product of two Hermitian sections $X(\mathcal{O}_1)$, $Y(\mathcal{O}_2)$ if all the representatives of one commute with all those of the other (in the usual sense) in some neighborhood of $\mathcal{O} = \mathcal{O}_1 \times \mathcal{O}_2 \subset \mathbf{R}^6$, for then all the products are Hermitian. It is obvious that this defines a unique section over $\mathcal{O}$. In particular we can define the product of two germs $X(x)$, $Y(y)$ at different points of $\mathbf{R}^3$. The analogy with field theory is very strong.

There are two further operations which are possible on the sections $U(\mathcal{O})$ and $X(\mathcal{O})$. We can define a *derivation* for each $X(\mathcal{O})$ as follows. Let $X(\mathcal{O})$ be a Hermitian section. Then, to every Hermitian section $Y(\mathcal{O})$ we define the derivative

$$Y(\mathcal{O}) \to i[X(\mathcal{O}), Y(\mathcal{O})] \equiv \frac{\partial Y}{\partial(\partial/\partial X)}.$$

We now prove that this a Hermitian section. The expression means, of course, that the representative of the deriviative is

$$i[X(\mathcal{O}'), Y(\mathcal{O}')] \quad \text{if} \quad \mathcal{O}' \supset \bar{\mathcal{O}}.$$

Suppose now $\mathcal{O}'$, $\mathcal{O}''$ are given. Then we know that there exist sets $\mathcal{O}_1$, $\mathcal{O}_2$ such that

$$[X(\mathcal{O}'), S] = [X(\mathcal{O}''), S], \qquad S \in \mathfrak{A}(\mathcal{O}_1)$$

and

$$[Y(\mathcal{O}'), S] = [Y(\mathcal{O}''), S], \qquad S \in \mathfrak{A}(\mathcal{O}_2).$$

There also exist sections $X(\mathcal{O}_1 \cap \mathcal{O}_2)$, $Y(\mathcal{O}_1 \cap \mathcal{O}_2)$ with the property that, for some sets $\mathcal{O}_3$, $\mathcal{O}_4 \supset \bar{\mathcal{O}}$,

$$[X(\mathcal{O}_1 \cap \mathcal{O}_2), S] = [X(\mathcal{O}'), S] = [X(\mathcal{O}''), S], \qquad S \in \mathfrak{A}(\mathcal{O}_3),$$

$$[Y(\mathcal{O}_1 \cap \mathcal{O}_2), S] = [Y(\mathcal{O}'), S] = [Y(\mathcal{O}''), S], \qquad S \in \mathfrak{A}(\mathcal{O}_4).$$

Let $S \in \mathfrak{A}(\mathcal{O}_3 \cap \mathcal{O}_4)$. Then by the Jacobi identity,

$$\begin{aligned}[[X(\mathcal{O}'), Y(\mathcal{O}')], S] &= [[X(\mathcal{O}'), S], Y(\mathcal{O}')] \\ &\quad + [[S, Y(\mathcal{O}')], X(\mathcal{O}')] \\ &= [[X(\mathcal{O}_1 \cap \mathcal{O}_2), S], Y(\mathcal{O}')] \\ &\quad + [[S, Y(\mathcal{O}_1 \cap \mathcal{O}_2)], X(\mathcal{O}')] \\ &= [[X(\mathcal{O}_1 \cap \mathcal{O}_2), S], Y(\mathcal{O}'')] \\ &\quad + [[S, Y(\mathcal{O}_1 \cap \mathcal{O}_2)], X(\mathcal{O}'')],\end{aligned}$$

since

$$[X(\mathcal{O}_1 \cap \mathcal{O}_2), S] \in \mathfrak{A}(\mathcal{O}_2)$$

and

$$[Y(\mathcal{O}_1 \cap \mathcal{O}_2), S] \in \mathfrak{A}(\mathcal{O}_1).$$

Proceeding, we see that

$$\begin{aligned}&[[X(\mathcal{O}'), Y(\mathcal{O}')], S] \\ &\quad = [[X(\mathcal{O}''), S], Y(\mathcal{O}'')] + [[S, Y(\mathcal{O}'')], X(\mathcal{O}'')] \\ &\quad = [[X(\mathcal{O}''), Y(\mathcal{O}'')], S] \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_3 \cap \mathcal{O}_4).\end{aligned}$$

This proves that $i[X(\mathcal{O}), Y(\mathcal{O})]$ is a Hermitian section. To prove it is unique, let representatives $X(\mathcal{O}')$, $Y(\mathcal{O}')$ and $X'(\mathcal{O}')$, $Y'(\mathcal{O}')$ be given. We know that there are sets $\mathcal{O}_1$, $\mathcal{O}_2$ such that

$$\begin{aligned}&[X(\mathcal{O}'), S] = [X'(\mathcal{O}'), S], \qquad S \in \mathfrak{A}(\mathcal{O}_1), \\ &[Y(\mathcal{O}'), S] = [Y'(\mathcal{O}'), S] \quad \text{if} \quad S \in \mathfrak{A}(\mathcal{O}_2), \\ &\qquad \mathcal{O}_1 \supset \bar{\mathcal{O}}, \qquad \mathcal{O}_2 \supset \bar{\mathcal{O}}.\end{aligned}$$

There also exist $X(\mathcal{O}_1 \cap \mathcal{O}_2)$, $Y(\mathcal{O}_1 \cap \mathcal{O}_2)$ such that, for some sets $\mathcal{O}_3$, $\mathcal{O}_4 \supset \bar{\mathcal{O}}$,

$$[X(\mathcal{O}'), S] = [X'(\mathcal{O}'), S] = [X(\mathcal{O}_1 \cap \mathcal{O}_2), S], \qquad S \in \mathfrak{A}(\mathcal{O}_3),$$

$$[Y(\mathcal{O}'), S] = [Y'(\mathcal{O}'), S] = [Y(\mathcal{O}_1 \cap \mathcal{O}_2), S], \qquad S \in \mathfrak{A}(\mathcal{O}_4).$$

We now proceed as above, with $X'(\mathcal{O}')$ replacing $X(\mathcal{O}'')$, and $Y'(\mathcal{O}')$ replacing $Y(\mathcal{O}'')$, to prove

$$[[X(\mathcal{O}'), Y(\mathcal{O}')], S] \equiv [[X'(\mathcal{O}'), Y'(\mathcal{O}')], S],$$

in some neighborhood of $\mathcal{O}$, proving that $\partial Y/\partial(\partial/\partial X)$ is a unique section.

The other elementary operation on the group of $X(\mathcal{O})$ is the unitary transformation $X(\mathcal{O}) \to U(\mathcal{O})X(\mathcal{O})U(\mathcal{O})^{-1}$ for a fixed $U(\mathcal{O})$, as $X(\mathcal{O})$ varies over $\mathcal{G}(\mathcal{O})$. To prove it defines a section, suppose $\mathcal{O}'$, $\mathcal{O}'' \supset \bar{\mathcal{O}}$ are given. Combining together all the properties, there exists $\mathcal{O}_1 \supset \bar{\mathcal{O}}$ such that

$$\left.\begin{aligned}&[X(\mathcal{O}'), S] = [X(\mathcal{O}''), S], \\ &U(\mathcal{O}')SU(\mathcal{O}')^{-1} = U(\mathcal{O}'')SU(\mathcal{O}'')^{-1}, \\ &U(\mathcal{O}')^{-1}SU(\mathcal{O}') = U(\mathcal{O}'')^{-1}SU(\mathcal{O}''),\end{aligned}\right\} \text{ for } S \in \mathfrak{A}(\mathcal{O}_1).$$

Then there exist $X(\mathcal{O}_1)$ and $U(\mathcal{O}_1)$ such that, for some set $\mathcal{O}_2 \subset \mathcal{O}_1$, $\mathcal{O}_2 \supset \bar{\mathcal{O}}$,

$$\begin{aligned}&[X(\mathcal{O}'), S] = [X(\mathcal{O}''), S] = [X(\mathcal{O}_1), S], \\ &U(\mathcal{O}_1)SU(\mathcal{O}_1)^{-1} = U(\mathcal{O}')SU(\mathcal{O}')^{-1} = U(\mathcal{O}'')SU(\mathcal{O}'')^{-1}, \\ &U^{-1}(\mathcal{O}_1)SU(\mathcal{O}_1) = U^{-1}(\mathcal{O}')SU(\mathcal{O}') = U^{-1}(\mathcal{O}'')SU(\mathcal{O}''),\end{aligned}$$

for all $S \in \mathfrak{A}(\mathcal{O}_1)$. Further, there exists an operator $U(\mathcal{O}_2)$, say, where $\mathcal{O}_2 \supset \mathcal{O}_3 \supset \bar{\mathcal{O}}$, such that $U(\mathcal{O}_2)^{-1}SU(\mathcal{O}_2) = U(\mathcal{O}')^{-1}SU(\mathcal{O}') = U^{-1}(\mathcal{O}'')SU(\mathcal{O}'')$ for $S \in \mathfrak{A}(\mathcal{O}_3)$. Let $S \in \mathfrak{A}(\mathcal{O}_3)$. then

$$\begin{aligned}&[U(\mathcal{O}')X(\mathcal{O}')U(\mathcal{O}')^{-1}, S] \\ &\quad = U(\mathcal{O}')[X(\mathcal{O}'), U(\mathcal{O}')^{-1}SU(\mathcal{O}')]U(\mathcal{O}')^{-1} \\ &\quad = U(\mathcal{O}')[X(\mathcal{O}'), U(\mathcal{O}_2)^{-1}SU(\mathcal{O}_2)]U(\mathcal{O}')^{-1} \\ &\quad = U(\mathcal{O}')[X(\mathcal{O}_1), U(\mathcal{O}_2)^{-1}SU(\mathcal{O}_2)]U(\mathcal{O}')^{-1} \\ &\quad = U(\mathcal{O}'')[X(\mathcal{O}_1), U(\mathcal{O}_2)^{-1}SU(\mathcal{O}_2)]U(\mathcal{O}'')^{-1} \\ &\quad = U(\mathcal{O}'')[X(\mathcal{O}''), U(\mathcal{O}_2)^{-1}SU(\mathcal{O}_2)]U(\mathcal{O}'')^{-1} \\ &\quad = U(\mathcal{O}'')[X(\mathcal{O}''), U(\mathcal{O}'')^{-1}SU(\mathcal{O}'')]U(\mathcal{O}'')^{-1} \\ &\quad = [U(\mathcal{O}'')X(\mathcal{O}'')U(\mathcal{O}'')^{-1}, S] \quad \text{for} \quad S \in \mathfrak{A}(\mathcal{O}_3).\end{aligned}$$

This proves that

$$U(\mathcal{O}')X(\mathcal{O}')U(\mathcal{O}')^{-1} \equiv U(\mathcal{O}'')X(\mathcal{O}'')U(\mathcal{O}'')^{-1} \tag{10}$$

on $\mathcal{O}_3$, i.e., we have defined a section. To prove it is unique, suppose $U'(\mathcal{O}')$, $X'(\mathcal{O}')$ were chosen instead of $U(\mathcal{O}')$, $X(\mathcal{O}')$. Then following exactly the above proof of (10), just replacing everywhere $U(\mathcal{O}'')$ by $U'(\mathcal{O}')$ and $X(\mathcal{O}'')$ by $X'(\mathcal{O}')$, we prove that there exists a set $\mathcal{O}_3 \supset \bar{\mathcal{O}}$ such that

$$U(\mathcal{O}')X(\mathcal{O}')U(\mathcal{O})^{-1} \equiv U'(\mathcal{O}')X'(\mathcal{O}')U'(\mathcal{O}')^{-1}$$

on $\mathcal{O}_3$, proving that the definition is unique, Therefore we have

Theorem 7. The group $\mathcal{G}(\mathcal{O})$ has an endomorphism

$$Y(\mathcal{O}) \to \partial Y/\partial(\partial/\partial X) = i[X(\mathcal{O}), Y(\mathcal{O})],$$

and has operators in $\mathfrak{F}(\mathcal{O})$, $X(\mathcal{O}) \to U(\mathcal{O})X(\mathcal{O})U(\mathcal{O})^{-1}$.

There are many as yet hidden and unused properties of the theory; for example, the existence of $U(a, \Lambda)$ and its effect on local observables; the mass spectrum of the theory; that $\mathfrak{A}(\mathcal{O})$ are factors and have separating and cyclic vectors, etc. We

have lost touch with the original Hilbert space, and some of our sections are not operators. A section X will be an operator X if $X(\mathcal{O})$ is strictly intensive, i.e., if we can extend the map $\mu(\Omega) \to \mathfrak{B}(\mathfrak{H})$ to all sets in $\Omega(\mathcal{O})$, i.e., to the set $\mathcal{O}$ itself. Conversely, if X is strictly intensive, we pick all representatives to be $X(\mathcal{O})$ and get a section $X(\mathcal{O})$. Thus

Theorem 8. Let $\mathfrak{A}_h(\mathcal{O})$ be the set of all Hermitian operators (modulo scalars), and $\mathfrak{A}_u(\mathcal{O})$ the set of all unitary operations (modulo phases) in $\mathfrak{A}(\mathcal{O})$. We can regard the strictly intensive elements of $\mathfrak{A}_h(\mathcal{O})$, $\mathfrak{A}_u(\mathcal{O})$ as subsets of $\mathcal{G}(\mathcal{O})$, $\mathcal{F}(\mathcal{O})$ given by the condition that $U(\mathcal{O}) \in \mathfrak{A}_u(\mathcal{O})$ if and only if the map $\Omega(\bar{\mathcal{O}}) \xrightarrow{U} \mathfrak{B}(\mathfrak{H})$ can be extended to $\Omega(\mathcal{O}) \xrightarrow{U} \mathfrak{B}(\mathfrak{H})$, and similarly for $\mathfrak{A}_h(\mathcal{O})$. The formulation of "intensive observables" presented here shows that a meaning can be given to the commutation relations suggested by Gell-Mann and Schwinger, and used in calculations in Ref. 16.

V. SHEAFS OF INTENSIVE OBSERVABLES

We have defined sections over bounded sets $\mathcal{O}$; these form the groups $\mathcal{F}(\mathcal{O})$, $\mathcal{G}(\mathcal{O})$ of unitary and Hermitian sections. If $\mathcal{O}_1 \subset \mathcal{O}$ we can define the *restriction map* $\rho^{\mathcal{O}}_{\mathcal{O}_1}$ from $\mathcal{F}(\mathcal{O})$ to $\mathcal{F}(\mathcal{O}_1)$ as follows: we map $U(\mathcal{O})$ onto $U_1(\mathcal{O}_1)$ if their representatives coincide in all sufficiently small neighborhoods of $\bar{\mathcal{O}}_1$. [This is possible only if $U(\mathcal{O})$ is intensive, not for general operators in $\mathfrak{A}(\mathcal{O})$]. This map is obviously well defined since any two representatives of $U_1(\mathcal{O}_1)$ are equivalent in some neighborhood of $\bar{\mathcal{O}}_1$. The mapping defines a group homomorphism, because if $U(\mathcal{O})$, $V(\mathcal{O})$ separately coincide with $U_1(\mathcal{O}_1)$, $V_1(\mathcal{O}_1)$, then the product $U(\mathcal{O})V(\mathcal{O})$ coincides with $U_1(\mathcal{O}_1)V_1(\mathcal{O}_1)$. It is also obvious that if $\mathcal{O}_2 \subset \mathcal{O}_1 \subset \mathcal{O}$, then

$$\rho^{\mathcal{O}_1}_{\mathcal{O}_2}\rho^{\mathcal{O}}_{\mathcal{O}_1} = \rho^{\mathcal{O}}_{\mathcal{O}_2}.$$

Therefore the sets $\mathcal{F}(\mathcal{O})$ satisfy the axioms making them form a *presheaf* of groups. Similarly the $\mathcal{G}(\mathcal{O})$ form a presheaf of Abelian groups. The elements of $\mathcal{F}(\mathcal{O})$, $\mathcal{G}(\mathcal{O})$ are called the sections of $\mathcal{F}$, $\mathcal{G}$ over $\mathcal{O}$.

If a presheaf is to be a sheaf, two further axioms must hold. First, suppose $\mathcal{O}_i$ is a collection of open sets with union $\mathcal{O}$, and suppose $U(\mathcal{O})$, $V(\mathcal{O})$ are two sections whose restrictions to each $\mathcal{O}_i$ are equal. We have to prove $U = V$. We can prove this if $\mathcal{O}$ is bounded. We are given $U(\mathcal{O}_i) = V(\mathcal{O}_i)$, which means, for all $\mathcal{O}' \supset \bar{\mathcal{O}}$ there exists $\mathcal{O}_i'' \supset \mathcal{O}_i$ such that

$$U(\mathcal{O}_i, \mathcal{O}_i'')SU(\mathcal{O}_i, \mathcal{O}_i'')^{-1} = V(\mathcal{O}_i, \mathcal{O}_i'')SV(\mathcal{O}_i, \mathcal{O}_i'')^{-1},$$
$$\text{for} \quad S \in \mathfrak{A}(\mathcal{O}_i'').$$

But $U(\mathcal{O}_i)$ is the restriction of $U(\mathcal{O})$ which means that to any $\mathcal{O}' \supset \bar{\mathcal{O}}$ and representatives $U(\mathcal{O}_i, \mathcal{O}_i')$, $U(\mathcal{O}, \mathcal{O}')$ there exists an $\mathcal{O}_3^{(i)} \supset \bar{\mathcal{O}}$ on which

$$U(\mathcal{O}_i, \mathcal{O}_i') \equiv U(\mathcal{O}, \mathcal{O}').$$

Similarly there exists an $\mathcal{O}_4^{(i)} \supset \mathcal{O}_i$ on which, for a given $\hat{\mathcal{O}} \supset \bar{\mathcal{O}}$,

$$V(\mathcal{O}_i, \mathcal{O}_i') \equiv V(\mathcal{O}, \hat{\mathcal{O}}).$$

Since $\mathcal{O}$ is finite we may assume that there are a finite number of $\mathcal{O}_i$. Choosing $\mathcal{O}_5^{(i)} \supset \bar{\mathcal{O}}_i$ small enough we have

$$U(\mathcal{O}, \mathcal{O}')SU(\mathcal{O}, \mathcal{O}')^{-1} = V(\mathcal{O}, \hat{\mathcal{O}})SV(\mathcal{O}, \hat{\mathcal{O}})^{-1},$$
$$\text{for} \quad S \in \mathfrak{A}(\mathcal{O}_5^{(i)}).$$

For any $T \in \mathfrak{A}(U_i\mathcal{O}_5^{(i)})$, let $S \to T$ weakly where

$$S \in U_i(\mathfrak{A}(\mathcal{O}_5^{i})).$$

Therefore

$$V(\mathcal{O}, \hat{\mathcal{O}}) \equiv U(\mathcal{O}, \mathcal{O}') \quad \text{on} \quad U_i\mathcal{O}_5^{(i)}, \quad \text{i.e.,} \quad U = V.$$

The second axiom is: if $\mathcal{O}_i$ is a (finite) family of open sets with union $\mathcal{O}$, and for each i we are given a section $U(\mathcal{O}_i)$ of $\mathcal{F}$ over $\mathcal{O}_i$ in such a way that for all i, j the restrictions of $U(\mathcal{O}_i)$, $U(\mathcal{O}_j)$ to $\mathcal{O}_i \cap \mathcal{O}_j$ are equal, then there exists a section $U(\mathcal{O})$ over $\mathcal{O}$ whose restriction to each $\mathcal{O}_i$ is just $U(\mathcal{O}_i)$.

It is obvious that if we consider only those $U(\mathcal{O}_i)$ which are restrictions of some U over $\mathcal{O}$, then there is nothing to prove. But the axiom does raise the question, is it possible for $\mathcal{F}(\mathcal{O}_i)$ to be sheaves without there being an $\mathcal{F}(\mathcal{O})$? If $\bar{\mathcal{O}}_i$ and $\bar{\mathcal{O}}_j$ are disjoint sets, we can form $\mathcal{F}(\mathcal{O}_i \cup \mathcal{O}_j)$ as the product $\mathcal{F}(\mathcal{O}_i) \times \mathcal{F}(\mathcal{O}_j)$ [or the sum $\mathcal{G}(\mathcal{O}_i) \dotplus \mathcal{G}(\mathcal{O}_j)$ for $\mathcal{G}$]. The only question to be settled is, what is the effect of the boundary if $\mathcal{O}_i \cap \mathcal{O}_j = \phi$ but $\bar{\mathcal{O}}_i \cap \bar{\mathcal{O}}_j \neq \phi$. This surface effect can hardly have physical importance, unless there are superselection rules. Such questions can be investigated by means of the technique of "exact sequences" common in algebraic topology.

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[16] A. P. Balachandran and H. Pietschmann, Acta. Phys. Austraica **16**, 362 (1963).

Coulomb Green's Functions and the Furry Approximation*†

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The Coulomb Green's function for the nonrelativistic Schrödinger equation is obtained in closed form starting from the partial-wave expansion and using an integral representation for a product of two Whittaker functions with different arguments. The Neumann's series for $J_\nu(kz)$ is required in evaluating the sum on states. Using the same methods, the Coulomb Green's functions for the Klein–Gordon and iterated Dirac equations are obtained in closed form in the "Furry approximation," $a^2/(J+\frac{1}{2})^2 \ll 1$, $a = Ze^2/4\pi\hbar c$. The Klein–Gordon Green's function in this approximation is shown to be at the same time the exact Green's function for the Klein–Gordon equation without the potential squared term. An alternate and very simple derivation of the approximate Green's function for the iterated Dirac equation is given using perturbation theory. From this Green's function, an approximate Coulomb Green's function in closed form for the Dirac equation itself is constructed. Certain known results for Coulomb wavefunctions with modified plane-wave behavior at large distances are rederived using the foregoing methods and results.

INTRODUCTION

IN the following we study the Green's function for a particle moving in a Coulomb field and obeying either the nonrelativistic Schrödinger equation, the Klein–Gordon equation, or the Dirac equation. The "physical" Green's function as defined here is the Fourier transform in time of the propagator of quantum field theory, and it is from this fact that the Green's function derives much of its physical interest. Of course, the Coulomb Green's function is also of interest from the point of view of "one-particle" (relativistic or nonrelativistic) quantum mechanics.

There are not many previous attempts to obtain the Coulomb Green's function in closed form. Meixner[1] in 1933 obtained the nonrelativistic Coulomb Green's function for a one-dimensional system, but he obtained the three-dimensional Green's function in closed form only in the two special cases $r_2 \to \infty$ and $r_1 = 0$. In 1937[2] he outlined a perturbation treatment of the Dirac Coulomb Green's function which connected the Dirac Coulomb Green's function with the Coulomb Green's function of the Klein–Gordon equation without the potential squared term (which however was known only in the special case that $r_1 = 0$). More recently, Martin and Glauber[3] have obtained the exact expression for the Dirac Coulomb Green's function in the special case that $r_1 = 0$. Mapleton[4] and Mano[5] have shown how to go from the partial-wave expansion to the eigenfunction expansion of the nonrelativistic Coulomb Green's function, and Wichmann and Woo[6] have given a double integral representation for the nonrelativistic Coulomb Green's function.

The results to be presented here will complete the work of Meixner. We obtain the exact three-dimensional nonrelativistic Coulomb Green's function in closed form, and also the exact Green's function for the Klein–Gordon equation without the potential squared term. Thus we are able to carry out Meixner's perturbation approach to the Dirac Coulomb Green's function. However, we are still unable to give the exact expression in closed form for either the Klein–Gordon or the Dirac Coulomb Green's function.

Our plan of attack is to obtain for the Green's function results paralleling known results for the Coulomb wavefunctions with modified plane-wave behavior at large distances due to Gordon,[7] Furry,[8] and Sommerfeld and Maue[9] (see also Bethe and Maximon[10]).

Paralleling these results for the wavefunction, we obtain in Sec. I an expression in closed form [Eq. (1.18)] for the exact nonrelativistic Coulomb Green's function, working from the partial-wave

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† A more complete account of this work is given in Levere Hostler, "Coulomb Green's Functions," Ph.D. thesis, Stanford University, 1963.
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[1] J. Meixner, Math. Z. **36**, 677 (1933).
[2] J. Meixner, Ann. Physik **29**, 97 (1937).
[3] P. C. Martin and R. J. Glauber, Phys. Rev. **109**, 1307 (1958).
[4] R. A. Mapleton, J. Math. Phys. **2**, 478 (1961).
[5] K. Mano, J. Math. Phys. **4**, 522 (1963).
[6] E. H. Wichmann and C.-H. Woo, J. Math. Phys. **2**, 178 (1961).
[7] W. Gordon, Z. Physik **48**, 180 (1928).
[8] W. H. Furry, Phys. Rev. **46**, 391 (1934).
[9] A. Sommerfeld and A. W. Maue, Ann. Physik **22**, 629 (1935).
[10] H. A. Bethe and L. C. Maximon, Phys. Rev. **93**, 768 (1954).

expansion of the Green's function. The partial-wave expansion is summed using an integral representation [Eq. (1.9)] for a product of two Whittaker functions with different arguments. The Neumann's series for the Bessel function $I_\nu(kz)$ [Eq. (1.11)] is used to perform the sum on states.

In Sec. II we obtain the exact Green's function for the Klein–Gordon equation without the potential squared term. This Green's function is then shown to be at the same time the Green's function in the "Furry approximation," $a^2/(l+\frac{1}{2})^2 \ll 1$, $a = Ze^2/4\pi\hbar c$, for the Klein–Gordon equation itself. The derivation of the "eigenfunction" expansion for the Klein–Gordon Green's function poses a special problem due to the fact that we are now dealing with a wave equation which is second order in the time derivative rather than only first order, as in the nonrelativistic case.

In Sec. III we are really interested in the Dirac Coulomb Green's function. However, the Dirac Green's function is first expressed in terms of the Green's function of the iterated Dirac equation [see Eqs. (3.5a), (3.5b)] and the remainder of Sec. III concerns the Green's function of the iterated Dirac equation. An approximate expression in closed form [Eq. (3.16)] for this Green's function is derived using perturbation theory (along the lines of Meixner[2]). Here the approximate Klein–Gordon Green's function developed in Sec. II is required. We show that the approximate Green's function obtained by perturbation theory is at the same time the Green's function of the iterated Dirac equation in the Furry approximation, $a^2/(J+\frac{1}{2})^2 \ll 1$. In order to give the proof of this, we derive the partial-wave expansion of the exact Green's function of the iterated Dirac equation. It is then shown how the Green's function in the Furry approximation can be obtained directly from this partial-wave expansion, by using the methods developed in Sec. I. At the end of Sec. III we obtain certain properties of the exact Green's function of the iterated Dirac equation, including a formula [Eq. (3.49)] exhibiting the γ dependence of the Green's function.

In Sec. IV we study the Coulomb wavefunctions with modified plane-wave behavior at large distances using the preceding methods and results. Here a result due to Johnson and Deck[11] is rederived using the standpoint of the Green's function to advantage, and a derivation of the Furry wavefunction is given in which the only sum formula needed is the Neumann's series (above). Also, the Furry or Sommerfeld–Maue wavefunction is obtained from our approximate Green's function by looking at the asymptotic behavior as $r_1 \to \infty$.

[11] W. R. Johnson and R. T. Deck, J. Math. Phys. 3, 319 (1962).

I. NONRELATIVISTIC COULOMB GREEN'S FUNCTION

The Green's function $G(\mathbf{r}_2, \mathbf{r}_1, \omega)$ will be defined as in Meixner[1] as the solution of the differential equation

$$[\nabla_2^2 + (2k\nu)/r_2 + k^2]G(\mathbf{r}_2, \mathbf{r}_1, \omega) = \delta^3(\mathbf{r}_2 - \mathbf{r}_1), \quad (1.1)$$
$$\nu = (ka_1)^{-1}; \qquad a_1 = 4\pi\hbar^2/mZe^2;$$
$$k = (2m\omega/\hbar)^{\frac{1}{2}}, \qquad \mathrm{Im}\,(k) > 0,$$

which satisfies the following boundary conditions at the origin and at infinity:

$$\left.\begin{aligned} r_2^{\frac{1}{2}}G(\mathbf{r}_2, \mathbf{r}_1, \omega) &\to 0 \\ r_2^{\frac{1}{2}}\mathbf{r}_2 \cdot \nabla_2 G(\mathbf{r}_2, \mathbf{r}_1, \omega) &\to 0 \end{aligned}\right\} \text{ as } r_2 \to 0,$$
$$\left.\begin{aligned} r_2 G(\mathbf{r}_2, \mathbf{r}_1, \omega) &\to 0 \\ \mathbf{r}_2 \cdot \nabla_2 G(\mathbf{r}_2, \mathbf{r}_1, \omega) &\to 0 \end{aligned}\right\} \text{ for } r_2 \to \infty. \quad (1.2)$$

Here $\hbar\omega$ is a complex number not in the eigenvalue spectrum, discrete and continuous, of the Hamiltonian H of the system. The Green's function as defined by (1.1) and (1.2) is unique and symmetric, $G(\mathbf{r}_2, \mathbf{r}_1, \omega) = G(\mathbf{r}_1, \mathbf{r}_2, \omega)$.[1] The Green's function is an analytic function of $\hbar\omega$ on the complex $\hbar\omega$ plane cut along the positive real axis (the continuous spectrum, $0 \leq \hbar\omega < +\infty$), except for simple poles at the distinct bound-state energy eigenvalues of the system. The retarded (advanced) "physical" Green's function, defined for real $\hbar\omega$, is obtained from $G(\mathbf{r}_2, \mathbf{r}_1, \omega)$ by taking the limit as $\hbar\omega$ approaches the real axis from above (below). For $\hbar\omega > 0$, the physical Green's functions so obtained have an oscillatory behavior as $r_2 \to \infty$; at large distances the retarded Green's function consists of only outgoing spherical waves and the advanced Green's function consists of only incoming spherical waves. For $\hbar\omega < 0$, the retarded and advanced Green's functions coincide and both agree with the "general" Green's function as defined by (1.1) and (1.2). These $\hbar\omega$ values are "nonpropagating" in the sense that the Green's functions decay exponentially as $r_2 \to \infty$.

The solution of (1.1) and (1.2) can be written down in the form of an eigenfunction expansion:

$$G(\mathbf{r}_2, \mathbf{r}_1, \omega) = -\frac{\hbar^2}{2m}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_0^\infty dk\,\frac{\phi_{lm}(k;\mathbf{r}_2)\phi_{lm}^*(k;\mathbf{r}_1)}{(\hbar^2k^2/2m) - \hbar\omega}$$
$$-\frac{\hbar^2}{2m}\sum_{n=1}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{\phi_{nlm}(\mathbf{r}_2)\phi_{nlm}^*(\mathbf{r}_1)}{E_{nl} - \hbar\omega}. \quad (1.3)$$

The eigenfunctions here are the simultaneous eigenfunctions of the Hamiltonian and of $\mathbf{L}\cdot\mathbf{L}$ and L_z, where $\mathbf{L}$ = the orbital angular momentum operator of the particle. In the first term of (1.3) we have a summation and integration over the continuous spectrum of H; in the second a summation over the discrete spectrum. Inserting the explicit expressions for the wavefunctions and doing the integration over the continuous spectrum,[12] we obtain

$$G(\mathbf{r}_2, \mathbf{r}_1, \omega) = (8\pi ikr_1r_2)^{-1} \sum_{l=0}^{\infty} (2l+1)P_l \times \Gamma(1+l-i\nu)W_{i\nu;l+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{i\nu;l+\frac{1}{2}}(-2ikr_1) \tag{1.4}$$

$$r_2 > r_1, \quad k = (2m\omega/\hbar)^{\frac{1}{2}}, \quad \mathrm{Im}\,(k) > 0, \quad \nu = (ka_1)^{-1}.$$

Here P_l denotes the Legendre polynomial[13] $P_l(\cos\theta)$. θ is the angle between $\mathbf{r}_2$ and $\mathbf{r}_1$. The functions W and $\mathfrak{M}$ are Whittaker functions as defined in Buchholz,[14]

$$\mathfrak{M}_{k;\frac{1}{2}\mu}(z) = \frac{z^{\frac{1}{2}(1+\mu)}e^{\mp z/2}}{\Gamma(1+\mu)} \times {}_1F_1(\tfrac{1}{2}(1+\mu) \mp k; 1+\mu; \pm z) \tag{1.5}$$

$$W_{k;\frac{1}{2}\mu}(z) = \frac{\pi}{\sin\pi\mu}\left\{-\frac{\mathfrak{M}_{k;\frac{1}{2}\mu}(z)}{\Gamma(\frac{1}{2}(1-\mu)-k)} + \frac{\mathfrak{M}_{k;-\frac{1}{2}\mu}(z)}{\Gamma(\frac{1}{2}(1+\mu)-k)}\right\}. \tag{1.6}$$

[For $\mu = 2l+1$ the right-hand side of (1.6) is to be interpreted as the limiting value as $\mu \to 2l+1$ (cf. Ref. 14 p. 20).]

Both the expansions (1.3) and (1.4) for the Green's function are quite standard. Now we want to go a step further and sum the series (1.4). The key formula for this prupose will be the integral representation[15,16]

$$W_{k;\frac{1}{2}\mu}(bt)\mathfrak{M}_{k;\frac{1}{2}\mu}(at) = \frac{t(ab)^{\frac{1}{2}}}{\Gamma(-k+\frac{1}{2}(1+\mu))} \times \int_0^{\infty} ds\left(\coth\frac{s}{2}\right)^{2k} e^{-\frac{1}{2}(a+b)t\cosh s} I_\mu(t(ab)^{\frac{1}{2}}\sinh s) \tag{1.7}$$

$$\mathrm{Re}\,(-k+\tfrac{1}{2}(1+\mu)) > 0, \qquad b > a > 0,$$

$$\mathrm{Re}\,(t) > 0, \qquad |\mathrm{arc}\,(t)| < \pi,$$

expressing a product of two Whittaker functions with different arguments as an integral involving a Bessel function of imaginary argument. If we want to apply (1.7) to the products of Whittaker functions occurring in (1.4), we are lead to make the following identification of the parameters:

	k	μ	b	a	t
Eq. (1.7)					
Eq. (1.4)	$i\nu$	$2l+1$	$2r_2$	$2r_1$	$-ik$

(1.8)

The condition $\mathrm{Re}\,(t) > 0$ follows from $\mathrm{Im}\,(k) > 0$. The condition $b > a > 0$ holds for $r_2 > r_1 > 0$. We find, however, that the condition $\mathrm{Re}\,(-k + \frac{1}{2}(1+\mu)) > 0$ is not satisfied for all $\hbar\omega$ in the cut plane. For this reason, Eq. (1.7) is not quite general enough for our purposes. There is a standard trick however by which we can generalize (1.7) so as to eliminate the condition $\mathrm{Re}\,(-k+\frac{1}{2}(1+\mu)) > 0$. In (1.7) this condition is required to make the integral converge at the lower limit $s = 0$. By going over from a real to a contour integral, we can go around rather than through the origin, thereby avoiding a possible singularity of the integrand at the origin. By an analytic continuation argument, we find that the resulting integral representation holds without the restriction $\mathrm{Re}\,(-k+\frac{1}{2}(1+\mu)) > 0$. Using this method (but first making the change of variables $\zeta = \cosh s$) we obtain the following generalization of Eq. (1.7)[17]:

$$W_{k;\frac{1}{2}\mu}(bt)\mathfrak{M}_{k;\frac{1}{2}\mu}(at) = -t(ab)^{\frac{1}{2}}e^{\pi i(k+\frac{1}{2}(1-\mu))}\Gamma(k+\tfrac{1}{2}(1-\mu)) \tag{1.9}$$

$$(2\pi i)^{-1}\int_{+\infty\,\mathrm{arc}\,(\zeta\pm1)=0}^{(1+)} d\zeta(\zeta+1)^{k-\frac{1}{2}}(\zeta-1)^{-k-\frac{1}{2}} \times e^{-\frac{1}{2}(a+b)t\zeta}I_\mu(t(ab)^{\frac{1}{2}}(\zeta^2-1)^{\frac{1}{2}}),$$

$$b > a > 0, \qquad \mathrm{Re}\,(t) > 0, \qquad |\mathrm{arc}\,(t)| < \pi,$$

$$-k+\tfrac{1}{2}(1+\mu) \neq 1, 2, 3, \cdots.$$

This integral representation is still subject to a condition on the quantity $(-k+\frac{1}{2}(1+\mu))$, but this condition is now much milder than before. Because of this condition, there are still exceptional points in the complex $\hbar\omega$ plane for which the integral representation breaks down for one or more terms of (1.4). However these exceptional points are now just the bound-state energy eigenvalues of the system, and are not in the domain of definition

[12] See, for example, Ref. 4, or see Sec. II of this work for the analogous calculation for the Klein–Gordon problem.

[13] For Legendre functions and spherical harmonics, we use the definitions of A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

[14] H. Bucholz, *Die Konfluente Hypergeometrische Funktion* (Springer-Verlag, Berlin, 1953).

[15] Ref. 14, p. 86, Eq. (5c). The condition $\mathrm{Re}(\mu) > 0$ stated there is a misprint and should read $\mathrm{Re}(t) > 0$ as in Eq. (1.7).

[16] W. T. Howell, Phil. Mag. **28**, 493 (1939). Also, for a more detailed proof of (1.7) based on Howell's paper, see the author's thesis (see footnote to title of this article), Appendix I.

[17] The integration contour begins at $\zeta = +\infty$, runs down the positive real axis to a point on the right of $\zeta = +1$, circles the point $\zeta = +1$ in the positive (counter clockwise) sense, and then returns along the positive real axis to $\zeta = +\infty$. The angles of $(\zeta \pm 1)$ are determined along the contour by continuity, their initial values at $\zeta = +\infty$ being $\mathrm{arc}(\zeta \pm 1) = 0$.

of the Green's function. Thus (1.9) may be applied to the terms of (1.4) for any $\hbar\omega$ value in the domain of definition of the Green's function. Using the identification (1.8) of the parameters as before, we find from (1.4) and (1.9)

$$G(\mathbf{r}_2, \mathbf{r}_1, \omega) = \frac{1}{4i(r_1r_2)^{\frac{1}{2}}} \frac{e^{-\pi\nu}}{\sinh \pi\nu} \frac{1}{2\pi i} \times \int_{+\infty \text{ arc } (\zeta\pm1)=0}^{(1+)} d\zeta(\zeta+1)^{i\nu-\frac{1}{2}}(\zeta-1)^{-i\nu-\frac{1}{2}} e^{ik(r_1+r_2)\zeta} \times \sum_{l=0}^{\infty} (2l+1)P_l I_{2l+1}(-2ik(r_1r_2)^{\frac{1}{2}}(\zeta^2-1)^{\frac{1}{2}}). \quad (1.10)$$

The condition $r_2 > r_1$, which applies to (1.4), can now be dropped, since $\mathbf{r}_2$ and $\mathbf{r}_2$ enter on the right-hand side of (1.10) on equal footing and the Green's function is known to be symmetric in $\mathbf{r}_1$ and $\mathbf{r}_2$. The integral representation (1.9) is seen to "extract the Z dependence" of the sum in the sense that the sum which we end up with in (1.10) no longer has anything to do with the presence of the Coulomb field. This sum is just a special case of the Neumann's series[18]

$$(\tfrac{1}{2}kz)^{\mu-\nu} I_\nu(kz) = k^\mu \sum_{l=0}^{\infty} \frac{\Gamma(\mu+l)}{l!\,\Gamma(\nu+1)} (2l+\mu) \times {}_2F_1(-l, l+\mu, \nu+1; k^2)(-1)^l I_{2l+\mu}(z), \quad \mu, \nu, \mu-\nu \neq -1, -2, -3, \cdots. \quad (1.11)$$

From the relation[19]

$$P_l(z) = (-1)^l\, {}_2F_1(-l, l+1, 1; \tfrac{1}{2}(1+z)), \quad (1.12)$$

we see that the series occurring in (1.10) can be summed using (1.11). We then obtain an integral representation of the Green's function in the form

$$G(\mathbf{r}_2, \mathbf{r}_1, \omega) = \frac{ik}{8\pi} \frac{e^{-\pi\nu}}{\sinh \pi\nu} \int_{+\infty \text{ arc } (\zeta\pm1)=0}^{(1+)} d\zeta[(\zeta+1)/(\zeta-1)]^{i\nu} \times e^{ik(r_1+r_2)\zeta} I_0(-2ik(r_1r_2)^{\frac{1}{2}} \cos\tfrac{1}{2}\theta(\zeta^2-1)^{\frac{1}{2}}), \quad (1.13)$$

$$k = (2m\omega/\hbar)^{\frac{1}{2}}, \quad \text{Im}\,(k) > 0, \quad \nu = (ka_1)^{-1}, \quad a_1 = 4\pi\hbar^2/mZe^2.$$

Note that the nuclear charge occurs in the integrand of (1.13) only in the factor $[(\zeta+1)/(\zeta-1)]^{i\nu}$. The remaining factors of the integrand, containing the $\mathbf{r}_1$ and $\mathbf{r}_2$ dependence, are the same factors we would have in the case of a free particle. We refer to this property of the integral representation as "extracting" the Z dependence of the Green's function. Because of this property of extracting the Z dependence the integral representation (1.13) may prove to be convenient for calculations involving the Green's function.[20]

The final integration in (1.13) can be performed by another application of the integral representation (1.9) for a product of two Whittaker functions with different arguments. First we transform (1.13) as follows:

$$G(\mathbf{r}_2, \mathbf{r}_1, \omega) = -\frac{1}{u}\frac{\partial}{\partial u} u \frac{1}{8\pi} \frac{e^{-\pi\nu}}{\sinh \pi\nu} \int_{+\infty \text{ arc } (\zeta\pm1)=0}^{(1+)} d\zeta(\zeta+1)^{i\nu-\frac{1}{2}} \times (\zeta-1)^{-i\nu-\frac{1}{2}} e^{iku\zeta} I_1(-iku(\zeta^2-1)^{\frac{1}{2}}), \quad (1.14)$$

$$u = 2(r_1r_2)^{\frac{1}{2}} \cos\tfrac{1}{2}\theta, \qquad v = r_1 + r_2.$$

We can now apply (1.9). For this purpose we need two real quantities α_1 and α_2 such that $\alpha_2 > \alpha_1 > 0$ and

$$\tfrac{1}{2}(\alpha_1+\alpha_2) = v, \qquad (\alpha_1\alpha_2)^{\frac{1}{2}} = u. \quad (1.15)$$

In terms of α_1 and α_2 we find

$$G(\mathbf{r}_2, \mathbf{r}_1, \omega) = \frac{\Gamma(1-iv)}{4\pi iku} \frac{\partial}{\partial u} W_{iv;\frac{1}{2}}(-ik\alpha_2)\mathfrak{M}_{i\nu;\frac{1}{2}}(-ik\alpha_1). \quad (1.16)$$

The solution of (1.15) for α_1 and α_2 is

$$\alpha_2 = v + (v^2-u^2)^{\frac{1}{2}} = r_1 + r_2 + |\mathbf{r}_2 - \mathbf{r}_1|, \qquad \alpha_1 = v - (v^2-u^2)^{\frac{1}{2}} = r_1 + r_2 - |\mathbf{r}_2 - \mathbf{r}_1|, \quad (1.17)$$

and the final expression for the Green's function is found to be[21]

$$G(\mathbf{r}_2, \mathbf{r}_1, \omega) = -\frac{\Gamma(1-iv)}{4\pi\,|\mathbf{r}_2-\mathbf{r}_1|} \times \det\begin{bmatrix} W_{iv;\frac{1}{2}}(-ik\alpha_2) & \mathfrak{M}_{i\nu;\frac{1}{2}}(-ik\alpha_1) \\ \dot{W}_{iv;\frac{1}{2}}(-ik\alpha_2) & \dot{\mathfrak{M}}_{i\nu;\frac{1}{2}}(-ik\alpha_1) \end{bmatrix}, \quad (1.18)$$

$$\alpha_2 = r_2 + r_1 + |\mathbf{r}_2 - \mathbf{r}_1|, \quad k = (2m\omega/\hbar)^{\frac{1}{2}}, \quad \text{Im}\,(k) > 0,$$
$$\alpha_1 = r_2 + r_1 - |\mathbf{r}_2 - \mathbf{r}_1|, \quad \nu = (ka_1)^{-1},$$
$$a_1 = 4\pi\hbar^2/mZe^2.$$

Here the dots over the Whittaker functions denote differentiation with respect to the arguments of the

[18] G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, Cambridge, England, 1962), 2nd ed. Equation (1.11) results from Watson's formula (3) p. 140 (Sec. 5.21) after making the replacement $z \to ze^{\frac{1}{2}\pi i}$ and using the formulas in Watson (p. 77) relating J_ν and I_ν.

[19] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis*, (Cambridge University Press, Cambridge, England, 1958), 4th ed. p. 312 (Sec. 15.22).

[20] An integral representation for the nonrelativistic Coulomb Green's function involving a double integral (and also having the property of extracting the Z dependence) has been given by Wichmann and Woo. (Ref. 6).

[21] For an *a posteriori* derivation of (1.18), which makes no use of infinite series, see L. Hostler and R. H. Pratt, Phys. Rev. Letters 10, 469 (1963).

Whittaker functions. The determinant here has the form of a Wronskian except that the two arguments are different.

It may be of interest to look at (1.18) in various special cases. The free-particle Green's function $(-4\pi\ |\mathbf{r}_2 - \mathbf{r}_1|)^{-1}e^{ik|\mathbf{r}_2-\mathbf{r}_1|}$ is obtained from (1.18) on setting the nuclear charge Z equal to zero, whereby the Whittaker functions go over essentially into spherical Bessel or Hankel functions.[22] Another special case of (1.18) which may be obtained quite easily is

$$G(\mathbf{r}_2, 0, \omega) = -(4\pi r_2)^{-1}\Gamma(1 - i\nu)W_{i\nu;\frac{1}{2}}(-2ikr_2). \quad (1.19)$$

This is in agreement with the expression previously obtained by Meixner[1] for this special case. Also, in Sec. IV [see Eq. (4.1)] we give the asymptotic form of (1.18) for $r_1 \to \infty$ in a definite direction $\mathbf{u}_1$.

II. APPROXIMATE KLEIN-GORDON COULOMB GREEN'S FUNCTION

We will here give two derivations of an approximate Klein–Gordon Coulomb Green's function. In order to show the equivalence of the two approximation methods, we start out working not with the Klein–Gordon equation itself but with the "generalized" Klein–Gordon equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \frac{2ib}{cr}\frac{\partial}{\partial t} + \frac{a^2}{r^2} - \frac{m^2c^2}{\hbar^2}\right)\psi = 0, \quad (2.1)$$

where b and a are regarded as independent real parameters. Here and subsequently, the formulas may be specialized to the Klien–Gordon case by choosing $b = a = Ze^2/4\pi\hbar c$. We assume $b > 0$ and $-\frac{1}{2} < a < +\frac{1}{2}$. The condition $b > 0$ is imposed for definiteness in order to make the bound states of (2.1) lie in the positive frequency spectrum rather than in the negative frequency spectrum. The condition $-\frac{1}{2} < a < +\frac{1}{2}$ ensures that the stationary-state solutions of (2.1) with a definite angular momentum will meet the boundary conditions

$$\left.\begin{aligned} r^{\frac{1}{2}}\psi &\to 0 \\ r^{\frac{1}{2}}\mathbf{u}_r\cdot\nabla\psi &\to 0 \end{aligned}\right\} \quad \text{as} \quad r \to 0 \quad (2.2)$$

at the origin for each l value $l = 0, 1, 2, \cdots$. The boundary conditions (2.2) at the origin are in turn required to ensure that the stationary-state solutions of (2.1) belonging to different frequencies be "orthogonal," and that the net particle flux out of a sphere with center at the origin will approach zero as the radius of that sphere approaches zero. "Orthogonal" in connection with (2.1) means with respect to the (not positive-definite) inner product

$$\langle\phi|\psi\rangle = i\int d^3r \times \left(\phi^*\frac{1}{c}\frac{\partial\psi}{\partial t} - \frac{1}{c}\frac{\partial\phi^*}{\partial t}\psi - \frac{2ib}{r}\phi^*\psi\right). \quad (2.3)$$

The Green's function $\mathcal{G}_{KG}(\mathbf{r}_2, \mathbf{r}_1, \omega)$ corresponding to the wave equation (2.1) is the solution of the differential equation

$$[\nabla_2^2 + (2k\nu)/r_2 + k^2 + a^2/r_2^2] \times \mathcal{G}_{KG}(\mathbf{r}_2, \mathbf{r}_1, \omega) = \delta^3(\mathbf{r}_2 - \mathbf{r}_1), \quad (2.4)$$

$$\nu = b\omega/kc, \quad k = ((\omega/c)^2 - (mc/\hbar)^2)^{\frac{1}{2}}, \quad \mathrm{Im}\,(k) > 0,$$

subject to the boundary conditions (1.2) at the origin and at infinity. Here ω is a complex number not equal to one of the frequencies, positive or negative, of the stationary-state solutions of (2.1). As in the nonrelativistic problem, we can show that the Green's function defined by (2.4) and (1.2) is unique and symmetric.

Green's Function for the Klein–Gordon Equation without the Potential Squared Term

If we neglect the potential squared term in the differential equation (2.4), then (2.4) goes over into the equation of the nonrelativistic Green's function, excepting only that the meanings of the parameters k and ν are different. Denoting by G_0 the Green's function so defined, we have

$$[\nabla_2^2 + (2k\nu)/r_2 + k^2]G_0(\mathbf{r}_2, \mathbf{r}_1, \omega) = \delta^3(\mathbf{r}_2 - \mathbf{r}_1), \quad (2.5)$$

$$\nu = b\omega/kc, \quad k = ((\omega/c)^2 - (mc/\hbar)^2)^{\frac{1}{2}}, \quad \mathrm{Im}\,(k) > 0.$$

Equation (2.5) together with the boundary conditions (1.2) can be solved exactly using the preceding methods. G_0 as defined by (2.5) and (1.2) is the exact Green's function for the Klein–Gordon equation without the potential squared term:

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \frac{2ib}{cr}\frac{\partial}{\partial t} - \frac{m^2c^2}{\hbar^2}\right)\psi = 0. \quad (2.6)$$

An "eigenfunction" expansion similar to (1.3) can be derived using the space parts of the stationary-state solutions of (2.6) as basis functions.[23] As in

[22] Ref. 14, p. 24, Eq. (29a), and p. 13, Eq. (11a):

$$W_{0;\frac{1}{2}\mu}(z) = (z/\pi)^{\frac{1}{2}}K_{\frac{1}{2}\mu}(\tfrac{1}{2}z),$$

$$\mathfrak{M}_{0;\frac{1}{2}\mu}(z) = (z\pi)^{\frac{1}{2}}\{I_{\frac{1}{2}\mu}(\tfrac{1}{2}z)/\Gamma(\tfrac{1}{2}(1+\mu))\}.$$

(Here K denotes the Hankel function of imaginary argument, as defined in Ref. 18.)

[23] See the treatment of the almost identical problem in connection with the Green's function (2.4).

the nonrelativistic case, the integration over the continuous spectrum can be performed, leading to a series similar to (1.4), which can then be summed using the integral representation (1.9) for a product of two Whittaker functions with different arguments. As one would expect from the similarity of equations (2.5) and (1.1), the expression obtained for G_0 is the same as the expression (1.18) for the nonrelativistic Green's function, excepting only that k and ν are replaced by their values as defined in (2.5). The integral representation (1.13) also applies to G_0 when k and ν are as defined in (2.5).[24]

Equation (2.4) of the generalized Klein–Gordon Green's function can be converted into the integral equation

$$\mathcal{G}_{KG}(2,1) = G_0(2,1) - \int d^3r_3 G_0(2,3)(a^2/r_3^2)\mathcal{G}_{KG}(3,1), \qquad (2.7)$$

with the help of the Green's function G_0 of the Klein–Gordon equation without the potential squared term. By iteration, the integral equation (2.7) will give $\mathcal{G}_{KG}$ in the form of a perturbation expansion, the potential squared term being treated as a small perturbation. The Green's function of the Klein–Gordon equation without the potential squared term is the first term in this perturbation expansion. Since the parameter a does not enter in G_0, the perturbation expansion for $\mathcal{G}_{KG}$ will be just the Taylor expansion of $\mathcal{G}_{KG}$ in ascending powers of a, with only even powers of a occurring in the expansion.

We can obtain the same power series expansion of $\mathcal{G}_{KG}$ working from the partial-wave expansion of $\mathcal{G}_{KG}$, by expanding each partial wave of $\mathcal{G}_{KG}$ in powers of a and then combining the contributions from all partial waves to like powers of a. Now we find that the parameter a enters the lth partial wave of the partial-wave expansion of $\mathcal{G}_{KG}$ only through the parameter γ defined by $\gamma + \frac{1}{2} = (l + \frac{1}{2})(1 - a^2/(l + \frac{1}{2})^2)^{\frac{1}{2}}$. Consequently, the Taylor expansion of the lth partial wave in powers of a is at the same time effectively an expansion in powers of the parameter $a/(l + \frac{1}{2})$, considered small in comparison to unity. It follows that the perturbation expansion of $\mathcal{G}_{KG}$ treating the potential squared term as a small perturbation is identical, term by term, with the result of expanding each partial wave of $\mathcal{G}_{KG}$ in powers of the parameter $a/(l + \frac{1}{2})$ considered small in comparison to unity and collecting together terms belonging to like powers of $a/(l+\frac{1}{2})$. In particular, the approximation $\mathcal{G}_{KG} \approx G_0$, being the first term in the perturbation expansion, is identical with the result of collecting together the constant terms in the Taylor expansion of the partial waves, neglecting all terms of order $a^2/(l + \frac{1}{2})^2$ [25] in comparison to unity. This neglect of terms of order $a^2/(l + \frac{1}{2})^2$ in comparison to unity is strictly analogous to the approximation introduced by Furry[8,26] in connection with the Dirac Coulomb continuum states. Hence we call the resulting expression for $\mathcal{G}_{KG}$ the Green's function in the "Furry approximation." By the foregoing discussion, the Green's function of the generalized Klein–Gordon equation in the Furry approximation is the first (zero-order) term in an ordinary perturbation expansion of $\mathcal{G}_{KG}$ treating the potential squared term as a small perturbation, and is identical with the exact Green's function for the Klein–Gordon equation without the potential squared term.

Of course, we are not primarily interested in $\mathcal{G}_{KG}$ but in the Green's function of the Klein–Gordon equation itself, obtained from $\mathcal{G}_{KG}$ by specializing the values of the parameters b and a to $b = a = Ze^2/4\pi\hbar c$. But by working with $\mathcal{G}_{KG}$ we are able to show the equivalence to all orders of the two approximation methods—one treating the potential squared term as a small perturbation, the other involving an expansion in powers of $a/(l + \frac{1}{2})$ occurring in the parameter γ in the partial-wave expansion. The equivalence of the two approximation methods for the Klein–Gordon case itself is thereby also established.

$\mathcal{G}_{KG}$ in the Furry Approximation

We will here obtain the partial wave expansion of $\mathcal{G}_{KG}$, and show that the parameter a enters only through the quantity γ. We write the stationary-state solutions of (2.1) in the form

$$\psi^\rho(\mathbf{r}, t) = \phi^\rho(\mathbf{r})e^{-(i/\hbar)\epsilon_\rho E t},$$
$$\epsilon_\rho = +1 \quad \rho = 1, \quad \epsilon_\rho = -1 \quad \rho = 2. \qquad (2.8)$$

Here $E \geq 0$. The quantum number ρ distinguishes between positive and negative frequency states.

[24] In this case the exceptional points for the integral representation (1.13) are $\omega = 0$, and $\omega = \pm$ one of the frequencies of the bound-state solutions of (2.6).

[25] There being no terms linear in $a/(l + \frac{1}{2})$.

[26] Actually, Furry made a high-energy approximation in addition to the high angular momentum approximation, corresponding to $a^2/(l + \frac{1}{2})^2 \ll 1$. However, we here do not include the high-energy approximation under the term "Furry approximation," whether in connection with the Green's functions or the wavefunctions. (It was shown later[10] that the high-energy approximation is not required to obtain an expression in closed form for the wavefunction, and that making the high angular momentum approximation alone leads to the Sommerfeld–Maue wavefunction.[9])

The solutions for $\phi^\rho(\mathbf{r})$ corresponding to sharp $\mathbf{L}\cdot\mathbf{L}$ and L_z are

Continuum States:

$$\phi^1_{lm}(k;\mathbf{r}) = R^1_l(k;r)Y_{lm}(\mathbf{u}_r),$$
$$\phi^2_{lm}(k;\mathbf{r}) = R^2_l(k;r)Y^*_{lm}(\mathbf{u}_r), \tag{2.9}$$
$$R^\rho_l(k;r) = k(\hbar c/\pi E)^{\frac{1}{2}}\Gamma(1+\gamma+iv)e^{\epsilon_\rho\frac{1}{2}(\pi\nu)} \times(-2ikr\epsilon_\rho)^{-1}\mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr\epsilon_\rho).$$

The quantum number k runs over the continuous spectrum $0 \le k < +\infty$; $E = +\hbar c(k^2 + (mc/\hbar)^2)^{\frac{1}{2}}$. γ is defined by $\gamma + \frac{1}{2} = ((l+\frac{1}{2})^2 - a^2)^{\frac{1}{2}}$, $\nu = bE/\hbar ck$. $Y_{lm}(\mathbf{u}_r)$ denotes the spherical harmonic [13]of the polar angles of the unit vector $\mathbf{u}_r$ in the direction of $\mathbf{r}$.

Bound States:

$$\phi_{nlm}(\mathbf{r}) = R_{nl}(r)Y_{lm}(\mathbf{u}_r) \tag{2.10}$$
$$R_{nl}(r) = \frac{\hbar}{mc}\eta^2\left[\frac{2}{b}\frac{(n-1)!}{\Gamma(n+2\gamma+1)}\right]^{\frac{1}{2}} \times(2\eta r)^\gamma e^{-\eta r}L^{2\gamma+1}_{n-1}(2\eta r);$$

γ is defined as in (2.9). $\eta = +((mc/\hbar)^2 - (E_{nl}/\hbar c)^2)^{\frac{1}{2}}$, $E_{nl} = mc^2/[1 + b^2/(\gamma+n)^2]^{\frac{1}{2}}$. The quantum number n takes the values $n = 1, 2, 3, \cdots$, independently of the quantum number l. $L^{2\gamma+1}_{n-1}(2\eta r)$ are the Laguerre polynomials as defined in Ref. 14.

The wavefunctions are normalized with respect to the metric (2.3) such that

$$\langle\phi^{\rho'}_{l'm'}(k') \mid \phi^\rho_{lm}(k)\rangle = \epsilon_\rho\delta_{\rho\rho'}\delta_{ll'}\delta_{mm'}\delta(k-k'),$$
$$\langle\phi_{n'l'm'} \mid \phi_{nlm}\rangle = \delta_{nn'}\delta_{ll'}\delta_{mm'}, \tag{2.11}$$
$$\langle\phi^{\rho'}_{l'm'}(k') \mid \phi_{nlm}\rangle = 0.$$

We expect to be able to obtain an expansion of the Green's function $\mathcal{G}_{\mathrm{KG}}$ in a form similar to the eigenfunction expansion (1.3) of the nonrelativistic problem, using the space parts ϕ^ρ [Eqs. (2.9), (2.10)] of the stationary-state solutions ψ^ρ of the wave equation (2.1) as basis functions. However, we have as yet no expansion theorem using the functions ϕ^ρ as basis functions. We do have an expansion theorem for the full time-dependent functions ψ^ρ. This expansion theorem states that any physically admissible solution $f(\mathbf{r}, t)$ of the wave equation (2.1) can be expressed as a linear combination of the stationary-state solutions ψ^ρ:

$$f(\mathbf{r},t) = \sum_{\rho=1}^{2}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_0^\infty dk\, a^\rho_{lm}(k)\psi^\rho_{lm}(k;\mathbf{r},t) + \sum_{n=1}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}a_{nlm}\psi_{nlm}(\mathbf{r},t). \tag{2.12}$$

The expansion coefficients are found to be

$$a^\rho_{lm}(k) = \epsilon_\rho\langle\psi^\rho_{lm}(k;\mathbf{r},t) \mid f(\mathbf{r},t)\rangle,$$
$$a_{nlm} = \langle\psi_{nlm}(\mathbf{r},t) \mid f(\mathbf{r},t)\rangle. \tag{2.13}$$

But we are looking for an expansion theorem for a function ($\mathcal{G}_{\mathrm{KG}}$) which does not have anything to do with the time. We find that we can obtain such an expansion theorem from (2.12) by specializing to the case $t = 0$. When we do this we find certain striking differences between this and the nonrelativistic problem. These differences are due to the fact that we are now dealing with a wave equation which is second order in the time derivative rather than first order.

Writing out the expressions for the coefficients (2.13), substituting in (2.12), and letting $t = 0$, we obtain

$$f(\mathbf{r}_2,0) = \sum_{\rho=1}^{2}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_0^\infty dk\,\epsilon_\rho i \times\int d^3r_1\phi^\rho_{lm}(k;\mathbf{r}_2)\phi^{\rho*}_{lm}(k;\mathbf{r}_1) \times\{\dot f(\mathbf{r}_1,0)/c - ((i\epsilon_\rho E/\hbar c) + (2ib/r_1))f(\mathbf{r}_1,0)\}$$
$$+\sum_{n=1}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i\int d^3r_1\phi_{nlm}(\mathbf{r}_2)\phi^*_{nlm}(\mathbf{r}_1) \times\{\dot f(\mathbf{r}_1,0)/c - ((iE_{nl}/\hbar c) + (2ib/r_1))f(\mathbf{r}_1,0)\}. \tag{2.14}$$

Equation (2.14) is beginning to look like the desired expansion theorem expressing a space function $f(\mathbf{r}_2, 0)$ as a linear combination of the functions ϕ^ρ. Since the initial value $f(\mathbf{r}, 0)$ of a solution $f(\mathbf{r}, t)$ of the wave equation (2.1) may be arbitrarily prescribed, this expansion is indeed applicable to an arbitrary space function $f(\mathbf{r}_2, 0)$. However, in (2.14) we notice a striking difference from the nonrelativistic problem. The right-hand side of (2.14) seems to depend on $\dot f(\mathbf{r}, 0)$ in addition to $f(\mathbf{r}, 0)$. Now since we are dealing with a wave equation which is second order in the time derivative, $\dot f(\mathbf{r}, 0)$ can be arbitrarily prescribed as well as $f(\mathbf{r}, 0)$. Hence $\dot f(\mathbf{r}_1, 0)$ must somehow disappear from the expansion (2.14) of $f(\mathbf{r}_2, 0)$. How this happens can be seen in the following way. In (2.14) we can substitute $f(\mathbf{r}_2, 0) = f(\mathbf{r}_1, 0) = 0$. From the fact that $\dot f(\mathbf{r}, 0)$ may still be arbitrarily prescribed, there follows the identity

$$0 = \sum_{\rho=1}^{2}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\epsilon_\rho\int_0^\infty dk\phi^\rho_{lm}(k;\mathbf{r}_2)\phi^{\rho*}_{lm}(k;\mathbf{r}_1) + \sum_{n=1}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\phi_{nlm}(\mathbf{r}_2)\phi^*_{nlm}(\mathbf{r}_1). \tag{2.15}$$

This shows that the functions ϕ^ρ are linearly dependent. In fact, (2.15) contains infinitely many linear dependency relations between the functions $\phi^\rho(\mathbf{r}_2)$, there being one such relation for each point

$\mathbf{r}_1$ in space. The functions ϕ^ρ still form a complete set however—i.e., we do obtain an expansion theorem. As a consequence of (2.15) not only the terms of (2.14) involving $\dot{f}(\mathbf{r}_1, 0)$ but also the terms involving the potential b/r_1 drop out. Using the fact that $f(\mathbf{r}, 0)$ can be arbitrarily prescribed, we find[27]

$$\delta^3(\mathbf{r}_2 - \mathbf{r}_1) = \sum_{\rho=1}^{2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int_0^\infty dk\, (E/\hbar c)\phi^\rho_{lm}(k; \mathbf{r}_2)\phi^{\rho *}_{lm}(k; \mathbf{r}_1) + \sum_{n=1}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (E_{nl}/\hbar c)\phi_{nlm}(\mathbf{r}_2)\phi_{nlm}(\mathbf{r}_1). \tag{2.16}$$

Equation (2.16) is the completeness relation that we are looking for.

We now want to use these relations to obtain the expansion of the Green's function $\mathcal{G}_{KG}$ using the functions ϕ^ρ as basis functions. From the differential equations satisfied by $\mathcal{G}_{KG}$ and ϕ^ρ we obtain the identity

$$\int d^3r_3 \phi^{\rho *}(\mathbf{r}_3)[(\hbar\omega + \epsilon_\rho E)/\hbar c + 2b/r_3] \times \mathcal{G}_{KG}(\mathbf{r}_3, \mathbf{r}_1, \omega) = \hbar c \phi^{\rho *}(\mathbf{r}_1)/(\hbar\omega - \epsilon_\rho E). \tag{2.17}$$

Multiplying on the left by $\epsilon_\rho \phi^\rho(\mathbf{r}_2)$, summing and integrating over all states, and using (2.15) and (2.16) now gives the desired expansion of $\mathcal{G}_{KG}$:

$$\mathcal{G}_{KG}(\mathbf{r}_2, \mathbf{r}_1, \omega) = \sum_{\rho=1}^{2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \epsilon_\rho \hbar c \int_0^\infty dk\, \frac{\phi^\rho_{lm}(k; \mathbf{r}_2)\phi^{\rho *}_{lm}(k; \mathbf{r}_1)}{\hbar\omega - \epsilon_\rho E} + \sum_{n=1}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \hbar c \frac{\phi_{nlm}(\mathbf{r}_2)\phi^*_{nlm}(\mathbf{r}_1)}{\hbar\omega - E_{nl}}. \tag{2.18}$$

As in the nonrelativistic case, we can do the the integration over the continuous spectrum. Defining

$$J_l = \sum_{\rho=1}^{2} \epsilon_\rho \hbar c \int_0^\infty dk\, \frac{R^\rho_l(k; r_2)R^{\rho *}_l(k; r_1)}{\hbar\omega - \epsilon_\rho E}, \tag{2.19}$$

we have

$$\mathcal{G}_{KG}(\mathbf{r}_2, \mathbf{r}_1, \omega) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l J_l + \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l \sum_{n=1}^{\infty} \hbar c \frac{R_{nlm}(r_2)R^*_{nlm}(r_1)}{\hbar\omega - E_{nl}}, \tag{2.20}$$

where P_l denotes P_l (cos θ), θ being the angle between $\mathbf{r}_2$ and $\mathbf{r}_1$. Substituting the explicit expressions (2.9) for the radial functions R^ρ_l and using the identity[28]

$$\mathfrak{M}_{k;\frac{1}{2}\mu}(z) = \frac{e^{\pm\pi ik} W_{-k;\frac{1}{2}\mu}(ze^{\pm\pi i})}{\Gamma(\frac{1}{2}(1+\mu) - k)} + \frac{e^{\pm\pi i(k-\frac{1}{2}(1+\mu))} W_{k;\frac{1}{2}\mu}(z)}{\Gamma(\frac{1}{2}(1+\mu) + k)}, \tag{2.21}$$

(2.19) can be written out in the form[29]

$$J_l = \hbar^2c^2/4\pi r_1 r_2 \Big[\int_0^\infty \frac{dk}{E} \Gamma(1+\gamma-i\nu) \frac{W_{i\nu;\gamma+\frac{1}{2}}(-2ikr_2)e^{-\pi i(\gamma+1)}\mathfrak{M}_{-i\nu;\gamma+\frac{1}{2}}(2ikr_1)}{\hbar\omega - E} + \int_0^\infty \frac{dk}{E} \Gamma(1+\gamma+i\nu) \frac{W_{-i\nu;\gamma+\frac{1}{2}}(2ikr_2)\mathfrak{M}_{-i\nu;\gamma+\frac{1}{2}}(2ikr_1)}{\hbar\omega - E} - \int_0^\infty \frac{dk}{E} \Gamma(1+\gamma+i\nu) \frac{W_{-i\nu;\gamma+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{-i\nu;\gamma+\frac{1}{2}}(-2ikr_1)}{\hbar\omega + E} - \int_0^\infty \frac{dk}{E} \Gamma(1+\gamma-i\nu) \frac{W_{i\nu;\gamma+\frac{1}{2}}(2ikr_2)e^{\pi i(\gamma+1)}\mathfrak{M}_{-i\nu;\gamma+\frac{1}{2}}(-2ikr_1)}{\hbar\omega + E} \Big], \tag{2.22}$$

$$E = +\hbar c(k^2 + (mc/\hbar)^2)^{\frac{1}{2}}.$$

Using the identity[30]

$$\mathfrak{M}_{-k;\frac{1}{2}\mu}(z) = e^{\mp\pi i(1+\frac{1}{2}\mu)}\mathfrak{M}_{k;\frac{1}{2}\mu}(ze^{\pm\pi i}), \tag{2.23}$$

the phase factors $e^{\pm\pi i(\gamma+1)}$ occurring in the 1st and 4th terms of (2.22) can be absorbed in the $\mathfrak{M}$ functions. Changing the integration variable from k to $E = +\hbar c(k^2 + (mc/\hbar)^2)^{\frac{1}{2}}$ in the first two integrals and to $E = -\hbar c(k^2 + (mc/\hbar)^2)^{\frac{1}{2}}$ in the last two, we obtain

[27] Considering the time derivative of (2.12) rather than (2.12) itself leads to the additional relation

$$\frac{2b}{r_2}\delta^3(\mathbf{r}_2 - \mathbf{r}_1) = -\sum_{\rho=1}^{2} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \epsilon_\rho \int_0^\infty dk(E/\hbar c)^2 \phi^\rho_{lm}(k; \mathbf{r}_2)\phi^{\rho *}_{lm}(k; \mathbf{r}_1) - \sum_{n=1}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (E_{nl}/\hbar c)^2 \phi_{nlm}(\mathbf{r}_2)\phi^*_{nlm}(\mathbf{r}_1).$$

[28] Ref. 14 p. 19, Eq. (20a).

[29] We use the upper or lower signs in (2.21) as required to stay on one branch of the Whittaker functions.

[30] Ref. 14, p. 11, Eq. (5a).

$$J_l = (4\pi r_1 r_2)^{-1}\Bigg[\int_{+\infty}^{+mc^2} \frac{dE}{k}\,\Gamma(1+\gamma-i\nu)\,\frac{W_{i\nu;\gamma+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr_1)}{E-\hbar\omega}$$
$$-\int_{+mc^2}^{+\infty} \frac{dE}{k}\,\Gamma(1+\gamma+i\nu)\,\frac{W_{-i\nu;\gamma+\frac{1}{2}}(2ikr_2)\mathfrak{M}_{-i\nu;\gamma+\frac{1}{2}}(2ikr_1)}{E-\hbar\omega}$$
$$+\int_{-\infty}^{-mc^2} \frac{dE}{k}\,\Gamma(1+\gamma-i\nu)\,\frac{W_{i\nu;\gamma+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr_1)}{E-\hbar\omega}$$
$$-\int_{-mc^2}^{-\infty} \frac{dE}{k}\,\Gamma(1+\gamma+i\nu)\,\frac{W_{-i\nu;\gamma+\frac{1}{2}}(2ikr_2)\mathfrak{M}_{-i\nu;\gamma+\frac{1}{2}}(2ikr_1)}{E-\hbar\omega}\Bigg], \tag{2.24}$$
$$k = +((E/\hbar c)^2 - (mc/\hbar)^2)^{\frac{1}{2}}.$$

We now define k for general values of E on the complex plane less the two branch cuts $-\infty < E \leq -mc^2$ and $+mc^2 \leq E < +\infty$. This definition is

$$k = ((E/\hbar c)^2 - (mc/\hbar)^2)^{\frac{1}{2}}, \quad 0 < \arg(k) < \pi. \tag{2.25}$$

It is seen that $\mathrm{Im}\,(k) > 0$ for all E on the cut plane. The function

$$\frac{1}{4\pi k r_1 r_2}\,\Gamma(1+\gamma-i\nu)$$
$$\times \frac{W_{i\nu;\gamma+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr_1)}{E-\hbar\omega} \tag{2.26}$$

with k defined by (2.25) is seen to reduce to the integrands of (2.24) when evaluated above or below the positive or negative energy branch cut. Thus the terms (2.24) can be interpreted as the contributions to a contour integral of a single function (2.26), the contour consisting of two disjoint parts running along the positive and negative frequency branch cuts so as to circle the branch points $E = \pm mc^2$ in the counterclockwise sense. Using the equations[31]

$$W_{k;\frac{1}{2}\mu}(z) \sim z^k e^{-\frac{1}{2}z}, \quad |z| \to \infty, \quad |\arg(z)| < \tfrac{3}{2}\pi, \tag{2.27}$$

$$\mathfrak{M}_{k;\frac{1}{2}\mu}(z) \sim \frac{z^{-k}e^{+\frac{1}{2}z}}{\Gamma(\frac{1}{2}(1+\mu)-k)}$$
$$+\frac{z^k e^{-z/2}}{\Gamma(\frac{1}{2}(1+\mu)+k)}\,e^{\pm\pi i[k-\frac{1}{2}(1+\mu)]}, \tag{2.28}$$
$$|z| \to \infty;\quad \text{upper sign: } -\tfrac{3}{2}\pi < \arg(z) < +\tfrac{1}{2}\pi,$$
$$\text{lower sign: } -\tfrac{1}{2}\pi < \arg(z) < +\tfrac{3}{2}\pi$$

for the asymptotic behavior of the Whittaker functions W and $\mathfrak{M}$, we can compute the asymptotic behavior as $|E| \to \infty$ of the integrand [the function (2.26)] of this contour integral. For $r_2 > r_1$ we find that the contour may be closed by semicircles "at infinity" in the upper and lower half-planes [here we require the condition $\mathrm{Re}\,(k) > 0$]:

$$J_l = \oint \frac{dE}{4\pi k r_1 r_2}\,\Gamma(1+\gamma-i\nu)$$
$$\times \frac{W_{i\nu;\gamma+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr_1)}{E-\hbar\omega}, \tag{2.29}$$
$$r_2 > r_1.$$

The contour is now a closed loop enclosing the entire cut plane. The integral $J_l = -2\pi i$ times the sum of the residues of the integrand on the cut plane (the contour circles the plane in the negative (clockwise) sense). The poles of the integrand are the poles of the Gamma function $\Gamma(1+\gamma-i\nu)$, and the pole at $E = \hbar\omega$. The poles of the Gamma function occur at precisely the bound-state energy levels of the system. The residues at the poles of the Gamma function can be evaluated explicitly in terms of Laguerre polynomials.[32] The residue at the pole $E = \hbar\omega$ is simply the integrand [less the factor $(E-\hbar\omega)^{-1}$] evaluated at $E = \hbar\omega$. When the resulting expression for J_l is substituted into (2.20) it is found, as in the nonrelativistic problem,[4] that the contribution to the first sum of (2.20) coming from the residues at the poles of the Gamma function exactly cancels the contribution to $\mathcal{G}_{KG}$ from the sum on bound states [the second sum of (2.20)]. The only surviving terms after substitution into (2.20) are the contributions to the first sum coming from the residues at the pole $E = \hbar\omega$. Thus,

[31] Ref. 14, p. 91, Eqs. (1a) and (3). For $-\frac{1}{2}\pi < \arg(z) < +\frac{1}{2}\pi$, both the upper and lower signs apply in (2.28), and there appears to be a contradiction. However, for these values of $\arg(z)$ the ambiguous term is of smaller order of magnitude than the other, and is to be neglected (cf. "Stoke's phenomenon" in Ref. 18).

[32] Ref. 14, p. 135, Eq. (1):

$$L_n^{\mu}(z) = \frac{\Gamma(n+\mu+1)}{n!}\,z^{-\frac{1}{2}(1+\mu)}e^{+\frac{1}{2}z}\mathfrak{M}_{n+\frac{1}{2}(1+\mu);\frac{1}{2}\mu}(z)$$
$$= \frac{(-1)^n}{n!}\,z^{-\frac{1}{2}(1+\mu)}e^{+\frac{1}{2}z}W_{n+\frac{1}{2}(1+\mu);\frac{1}{2}\mu}(z).$$

$$\mathcal{G}_{KG}(\mathbf{r}_2, \mathbf{r}_1, \omega) = (8\pi ikr_1r_2)^{-1} \sum_{l=0}^{\infty} (2l+1)P_l$$
$$\times \Gamma(1+\gamma-i\nu)W_{i\nu;\gamma+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr_1)$$
$$r_2 > r_1, \quad k = ((\omega/c)^2 - (mc/\hbar)^2)^{\frac{1}{2}}, \quad \mathrm{Im}\,(k) > 0,$$
$$\nu = b\omega/kc, \quad (\gamma + \tfrac{1}{2}) = ((l+\tfrac{1}{2})^2 - a^2)^{\frac{1}{2}}.$$

a is seen to occur in the partial-wave expansion (2.30) only through the parameter γ, as previously stated. This justifies our earlier statement that the perturbation expansion of $\mathcal{G}_{KG}$ treating the potential squared term as a small perturbation is equivalent to the expansion of the lth partial waves of (2.30) in powers of the parameter $a/(l+\frac{1}{2})$.

Except for the difference in the meanings of the parameters k and ν, the expansion (2.30) of $\mathcal{G}_{KG}$ only differs from the corresponding expansion (1.4) of the nonrelativistic case in the replacement of l in (1.4) by γ in (2.30). This replacement of l by γ is the most serious obstacle in trying to sum the series (2.30) exactly. In the Furry approximation, where we neglect the $a^2/(l+\frac{1}{2})^2$ term in comparison to unity in the expression for γ, γ goes over into l and the series (2.30) becomes essentially identical with the series (1.4). It can then be summed using the same method as in the nonrelativistic case, and its sum is given by the same expression (1.13) or (1.18) as before, except that k and ν are as defined in (2.30). This expression is just the Green's function G_0 of the Klein–Gordon equation without the potential squared term, as we know it must be.

III. APPROXIMATE DIRAC COULOMB GREEN'S FUNCTION

The Dirac Coulomb Green's function $K(\mathbf{r}_2, \mathbf{r}_1, \omega)$ is defined as the solution of the differential equation[33,34]

$$\left[\gamma^0\left(\frac{\omega}{c} + \frac{a}{r_2}\right) + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2 - \frac{mc}{\hbar}\right]K(\mathbf{r}_2, \mathbf{r}_1, \omega) = \delta^3(\mathbf{r}_2 - \mathbf{r}_1) \qquad (3.1)$$

[33] A Note on notation: We use the metric

$$g^{\mu\nu} = \begin{bmatrix} +1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{bmatrix}, \qquad \mu, \nu = 0, 1, 2, 3.$$

We define $\gamma^0 = \beta$ and $\gamma^{1,2,3} = \beta\alpha_{1,2,3}$. β and α are the 4 by 4 matrics $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}$. Here 0 and 1 denote the 2 by 2 null, and unit matrices, respectively, and the σ are the usual Pauli matrices. Subsequently, σ will denote either the 4 by 4 matrix $\begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$ made up of the Pauli matrices or the Pauli matrices themselves, depending upon the context.

[34] The delta function on the right-hand side of (3.1) is understood to be multiplied by the 4 by 4 unit matrix.

$$a = Ze^2/4\pi\hbar c,$$

subject to the following boundary conditions at the origin and at infinity:

$$r_2K(\mathbf{r}_2, \mathbf{r}_1, \omega) \to 0 \quad \text{as} \quad \begin{cases} r_2 \to 0 \\ \text{or} \\ r_2 \to \infty. \end{cases} \qquad (3.2)$$

As before, $\hbar\omega$ is a possibly complex number not in the eigenvalue spectrum of the Hamiltonian of the system. By use of Green's theorem it can be shown quite straightforwardly that the Green's function as defined by (3.1) and (3.2) is unique and possesses the following symmetry property:

$$K(\mathbf{r}_2, \mathbf{r}_1, \omega) = T\tilde{K}(\mathbf{r}_1, \mathbf{r}_2, \omega)T. \qquad (3.3)$$

The matrix $T = i\gamma^3\gamma^0\gamma^1$ is both Hermitian and unitary. The wavy line over K in (3.3) denotes the ordinary transpose of the 4 by 4 matrix K. Applying (3.3) in (3.1) leads to an alternate form of the differential equation of the Dirac Green's function,

$$K(\mathbf{r}_2, \mathbf{r}_1, \omega)\left[\gamma^0\left(\frac{\omega}{c} + \frac{a}{r_1}\right) - i\boldsymbol{\gamma}\cdot\overleftarrow{\boldsymbol{\nabla}}_1 - \frac{mc}{\hbar}\right] = \delta^3(\mathbf{r}_2 - \mathbf{r}_1). \qquad (3.4)$$

The Green's function K can be expressed in the form

$$K(\mathbf{r}_2, \mathbf{r}_1, \omega) = \left[\gamma^0\left(\frac{\omega}{c} + \frac{a}{r_2}\right) + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2 + \frac{mc}{\hbar}\right]G_I(\mathbf{r}_2, \mathbf{r}_1, \omega) \qquad (3.5a)$$

$$= G_I(\mathbf{r}_2, \mathbf{r}_1, \omega)\left[\gamma^0\left(\frac{\omega}{c} + \frac{a}{r_1}\right) - i\boldsymbol{\gamma}\cdot\overleftarrow{\boldsymbol{\nabla}}_1 + \frac{mc}{\hbar}\right], \qquad (3.5b)$$

where G_I is the Green's function of the iterated Dirac equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2} + \frac{2ia}{cr}\frac{\partial}{\partial t} + \frac{a^2 + ia\boldsymbol{\alpha}\cdot\mathbf{u}_r}{r^2}\right)\varphi = 0. \qquad (3.6)$$

This is explained as follows. If G_I satisfies the differential equation (3.9) (with $b = a = Ze^2/4\pi\hbar c$) for the Green's function of the iterated Dirac equation, then the expression on the right-hand side of (3.5a) satisfies the differential equation (3.1) of the Dirac Green's function. One can check that if G_I is taken to be the Green's function of the iterated Dirac equation then the expression on the right-hand side of (3.5a) also satisfies the boundary conditions of the Dirac Green's function. That the expression

(3.5a) gives the Dirac Green's function when G_I is taken to be the Green's function of the iterated Dirac equation now follows, by uniqueness. Similarly, the expression on the right-hand side of (3.5b) will satisfy the differential equation (3.4) of the Dirac Green's function if G_I satisfies the alternate form (3.10) (with $b = a = Ze^2/4\pi\hbar c$) of the differential equation of the Green's function of the iterated Dirac equation. Again checking the boundary conditions, it follows that the Dirac Green's function is also given in the form (3.5b) where G_I is the Green's function of the iterated Dirac equation. It can be shown that the frequency spectrum of the iterated Dirac equation is the same as the frequency spectrum of the Dirac equation itself,[35] as it must be for relations like (3.5) to be meaningful.

We will give two derivations of an approximate expression for G_I, entirely analogous to the two derivations of the approximate Klein–Gordon Green's function considered in Sec. II. As in Sec. II, to show the equivalence of the two approximation methods involved we will be working not with the iterated Dirac equation itself, but with the "generalized" equation

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \frac{2ib}{cr}\frac{\partial}{\partial t} - \frac{m^2c^2}{\hbar^2} + \frac{a^2 + ia\boldsymbol{\alpha}\cdot\mathbf{u}_r}{r^2}\right)\varphi = 0, \qquad (3.7)$$

where b and a are independent real parameters with $b > 0$ and $a^2 < \frac{3}{4}$.[36] The physically admissable solutions of (3.7) must remain bounded as $r \to \infty$ and must satisfy the boundary conditions (2.2) at the origin. The inner product associated with (3.7) is given by

$$\langle\phi \mid \varphi\rangle = i\int d^3r\left(\bar{\phi}\frac{1}{c}\frac{\partial\varphi}{\partial t} - \frac{1}{c}\frac{\partial\bar{\phi}}{\partial t}\varphi - \frac{2ib}{r}\bar{\phi}\varphi\right), \quad \bar{\phi} = \phi^\dagger\beta. \qquad (3.8)$$

The Green's function $\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega)$ associated with (3.7) is the solution of the differential equation

$$\left(\nabla_2^2 + \frac{2k\nu}{r_2} + k^2 + \frac{a^2 + ia\boldsymbol{\alpha}\cdot\mathbf{u}_2}{r_2^2}\right) \times \mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = \delta^3(\mathbf{r}_2 - \mathbf{r}_1), \qquad (3.9)$$

$\nu = (b\omega/kc)$, $k = ((\omega/c)^2 - (mc/\hbar)^2)^{\frac{1}{2}}$, $\mathrm{Im}\,(k) > 0$,

subject to the boundary conditions (1.2). $\mathcal{G}_I$ as defined by (3.9) and (1.2) can be shown to be unique and to possess the same symmetry property (3.3) as the Dirac Green's function. Using this symmetry property, we obtain the differential equation of the Green's function in the alternate form

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega)\left(\overleftarrow{\nabla}_1^2 + \frac{2k\nu}{r_1} + k^2 + \frac{a^2 + ia\boldsymbol{\alpha}\cdot\mathbf{u}_1}{r_1^2}\right) = \delta^3(\mathbf{r}_2 - \mathbf{r}_1). \qquad (3.10)$$

Solution by Perturbation Theory

An approximate expression in closed form for $\mathcal{G}_I$ can be obtained using perturbation theory (along the lines of Meixner[2]). This method is entirely analogous to the corresponding treatment of the (generalized) Klein–Gordon case given in Sec. II. The differential equation (3.9) can be converted into the integral equation

$$\mathcal{G}_I(2, 1) = G_0(2, 1) - \int d^3r_3 G_0(2, 3)\frac{a^2 + ia\boldsymbol{\alpha}\cdot\mathbf{u}_3}{r_3^2}\mathcal{G}_I(3, 1), \qquad (3.11)$$

with the help of the Green's function G_0 of the Klein–Gordon equation without the potential squared term. By iteration, the integral equation (3.11) will give $\mathcal{G}_I$ in the form of a perturbation expansion. Since a does not enter into G_0, this perturbation expansion will be just the Taylor expansion of $\mathcal{G}_I$ in ascending powers of a. Keeping only the first two terms, constant and linear, in this expansion gives the following approximate expression for $\mathcal{G}_I$:

$$\mathcal{G}_I(2, 1) \approx G_0(2, 1) - \int d^3r_3 G_0(2, 3)(ia\boldsymbol{\alpha}\cdot\mathbf{u}_3/r_3^2)G_0(3, 1). \qquad (3.12)$$

The integral in (3.12) for the "spin correction" term can be evaluated quite simply working with the differential equation (2.5) satisfied by G_0. Changing $\mathbf{r}_2$ to $\mathbf{r}_3$ in (2.5) and applying the gradient operator ∇_3 to both sides of the equation, we find

$$[\nabla_3^2 + (2k\nu/r_3) + k^2]\nabla_3 G_0(3, 1) - (2k\nu/r_3^2)\mathbf{u}_3 G_0(3, 1) = \nabla_3\delta^3(\mathbf{r}_3 - \mathbf{r}_1). \qquad (3.13)$$

We now multiply on the left by $G_0(2, 3)$ and integrate over all $\mathbf{r}_3$. After performing a number of integrations by parts—which are permissable, since $G_0(2, 3)$ and $G_0(3, 1)$ decay exponentially as $r_3 \to \infty$—we find

[35] For a discussion of the relation between the two equations, see R. P. Feynman and M. Gell-Mann, Phys. Rev. 109, 193 (1958).

[36] We do not consider the case $a^2 \geq \frac{3}{4}$. If $a^2 > \frac{3}{4}$ there will be a finite number of J values for which the "regular" and "irregular" solutions corresponding to $l = J - \frac{1}{2}$ [see Eqs. (3.23) and (3.26)] change roles. For a given a, J values (if they exist) such that $J(J+1) = a^2$ appear to be exceptional in that neither (the "regular" nor "irregular") solution meets the boundary conditions (2.2) at the origin.

$$\int d^3r_3 G_0(2,3)[\overleftarrow{\nabla_3^2} + (2kv/r_3) + k^2]\nabla_3 G_0(3,1)$$
$$- \int d^3r_3 G_0(2,3)(2kv/r_3^2)\mathbf{u}_3 G_0(3,1)$$
$$= -\int d^3r_3 \delta^3(\mathbf{r}_3 - \mathbf{r}_1)\nabla_3 G_0(2,3). \tag{3.14}$$

Using (2.5) again and carrying out the integrations over delta functions, find

$$\int d^3r_3 G_0(2,3)(2kv/r_3^2)\mathbf{u}_3 G_0(3,1)$$
$$= (\nabla_2 + \nabla_1)G_0(2,1). \tag{3.15}$$

With this result, our approximate Green's function (3.12) can be written in the form

$$\mathcal{G}_I(2,1)$$
$$\approx \{1 - (ia/2kv)\boldsymbol{\alpha}\cdot(\nabla_2 + \nabla_1)\}G_0(2,1). \tag{3.16}$$

The result (3.16) (for $b = a = Ze^2/4\pi\hbar c$) is in agreement, except for terms of order a^2, with the exact result obtained for the special case $\mathbf{r}_1 = 0$ by Martin and Glauber.[3]

When used in conjunction with (3.5a) or (3.5b), the result (3.16) leads to an approximate Dirac Coulomb Green's function. However, the resulting expressions for $K(\mathbf{r}_2, \mathbf{r}_1, \omega)$ obtained from (3.5a) and (3.5b) are not quite the same, the difference consisting of the product of the potential terms of (3.5a, b) times the spin-correction term of (3.16).

The approximation method by which we arrived at (3.16) parallels closely the derivation by Sommerfeld and Maue[9] of an approximate Dirac Coulomb wavefunction with modified plane-wave behavior at infinity. They too worked from the iterated Dirac equation and used perturbation theory, treating the $(a^2 + ia\boldsymbol{\alpha}\cdot\mathbf{u}_r)/r^2$ term as a small perturbation. The "Sommerfeld–Maue" wavefunction was obtained by neglecting the potential squared term and keeping only the first correction due to the spin term—the same approximation involved in (3.16). Now it is known that, for the wavefunction, the Sommerfeld–Maue approximation is equivalent to the Furry approximation.[26] We will show that the same is true of the Green's function: the expression (3.16) for $\mathcal{G}_I$ is identical to the expression obtained by neglecting terms of order $a^2/(J+\frac{1}{2})^2$ in comparison to unity in the (lJ)th partial wave of the partial-wave expansion of the exact Green's function $\mathcal{G}_I$. We find in fact, in complete analogy to the Klein–Gordon case, that when the power-series expansion of $\mathcal{G}_I$ in ascending powers of a is obtained by working from the partial-wave expansion of the Green's function, then the expansion parameter for the (lJ)th partial wave is effectively $a/(J+\frac{1}{2})$. This is the reason why our perturbation calculation of $\mathcal{G}_I$, keeping only the constant and linear terms in a, is equivalent to the neglect of terms of order $a^2/(J+\frac{1}{2})^2$ in the (lJ)th partial wave of $\mathcal{G}_I$. Before we can show this, however, we require the explicit expression for the partial-wave expansion of the exact Green's function $\mathcal{G}_I$.

Derivation of the Partial-Wave Expansion of $\mathcal{G}_I$

We write the stationary-state solutions of (3.7) in the form due to Biedenharn[37] and Martin and Glauber.[3] We define

$$\psi^\rho(\mathbf{r}, t) = \phi^\rho(\mathbf{r})e^{-i(\epsilon_\rho E t/\hbar)}, \tag{3.17}$$
$$\epsilon_\rho = +1, \quad \rho = 1, \quad \epsilon_\rho = -1, \quad \rho = 2.$$

Here we have $E \geq 0$. The positive and negative frequency solutions are distinguished by the quantum number ρ. $\phi^\rho(\mathbf{r})$ is written in the form

$$\phi^\rho(\mathbf{r}) = S\chi^\rho(\mathbf{r}), \tag{3.18}$$

where[38]

$$S = \cosh(\tfrac{1}{2}\theta) + i\boldsymbol{\alpha}\cdot\mathbf{u}_r \sinh(\tfrac{1}{2}\theta), \tag{3.19}$$
$$\theta = \tanh^{-1}(a/K), \tag{3.20}$$
$$K = \boldsymbol{\sigma}\cdot\mathbf{L} + 1. \tag{3.21}$$

$\boldsymbol{\alpha}\cdot\mathbf{u}_r$ commutes with any even function of K and anticommutes with any odd function of K. The functions $\chi^\rho(\mathbf{r})$ can be taken to be simultaneous eigenfunctions of $\mathbf{L}\cdot\mathbf{L}$, $\mathbf{J}\cdot\mathbf{J}$, J_z, and β. Here $\mathbf{L}$ and $\mathbf{J} = \mathbf{L} + \frac{1}{2}\boldsymbol{\sigma}$ are the orbital and total angular momentum operators, respectively, of the particle, measured in units of $\hbar$. The simultaneous eigenfunctions of $\mathbf{J}\cdot\mathbf{J}$ and $\mathbf{L}\cdot\mathbf{L}$ are at the same time eigenfunctions of K, the eigenvalues being

$$K = \begin{cases} +(J+\frac{1}{2}) = l+1 & \text{for } l = J - \frac{1}{2}, \\ -(J+\frac{1}{2}) = -l & \text{for } l = J + \frac{1}{2}. \end{cases} \tag{3.22}$$

The expressions for $\chi^\rho(\mathbf{r})$ are

Continuum-State Solutions:

$$\chi^{1\rho}_{lJM}(k;\mathbf{r}) = \begin{bmatrix} R^\rho_{lJ}(k;r)\Omega_{lJM}(\mathbf{u}_r) \\ 0 \end{bmatrix}, \tag{3.23}$$

$$\chi^{2\rho}_{lJM}(k;\mathbf{r}) = \begin{bmatrix} 0 \\ R^\rho_{lJ}(k;r)\Omega_{lJM}(\mathbf{u}_r) \end{bmatrix},$$

$$R^\rho_{lJ}(k;r) = k(\hbar c/\pi E)^{\frac{1}{2}}\Gamma(1+\gamma+i\nu)e^{(\epsilon_\rho \frac{1}{2}\pi\nu)} \times (-2ikr\epsilon_\rho)^{-1}\mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr\epsilon_\rho).$$

The quantum number k runs over the continuous

[37] L. C. Biedenharn, Phys. Rev. **126**, 845 (1962).
[38] Our K differs from that of Biedenharn and of Martin and Glauber by a factor β.

spectrum $0 \leq k < +\infty$. $E = +\hbar c(k^2 + (mc/\hbar)^2)^{\frac{1}{2}}$, $\nu = (bE/\hbar ck)$ (as before). The γ values are given by

$$\gamma = \begin{cases} -1 + ((l+1)^2 - a^2)^{\frac{1}{2}} = \\ -1 + ((J+\frac{1}{2})^2 - a^2)^{\frac{1}{2}}, \quad l = J - \frac{1}{2}, \\ (l^2 - a^2)^{\frac{1}{2}} = ((J+\frac{1}{2})^2 - a^2)^{\frac{1}{2}}, \\ \qquad\qquad l = J + \frac{1}{2}. \end{cases} \tag{3.24}$$

The states are normalized with respect to the metric (3.8) such that

$$\langle \psi^{s'\rho'}_{l'J'M'}(k'; \mathbf{r}t) \mid \psi^{s\rho}_{lJM}(k; \mathbf{r}t)\rangle = \epsilon_s \delta_{ss'} \epsilon_\rho \delta_{\rho\rho'} \delta_{ll'} \delta_{JJ'} \delta_{MM'} \delta(k - k'), \tag{3.25}$$

$$\epsilon_s = +1, \quad s = 1; \quad \epsilon_s = -1, \quad s = 2.$$

The first superscript here, s, is the quantum number indicating the eigenvalue of β: for $s = 1$ $\beta = +1$ and for $s = 2$ $\beta = -1$,

Bound-State Solutions:

$$\chi^1_{nlJM}(\mathbf{r}) = \begin{bmatrix} R_{nlJ}(r)\Omega_{lJM}(\mathbf{u}_r) \\ 0 \end{bmatrix}, \tag{3.26}$$

$$\chi^2_{nlJM}(\mathbf{r}) = \begin{bmatrix} 0 \\ R_{nlJ}(r)\Omega_{lJM}(\mathbf{u}_r) \end{bmatrix},$$

$$R_{nlJ}(r) = \frac{\hbar}{mc}\eta^2\left[\frac{2}{b}\frac{(n-1)!}{\Gamma(n+2\gamma+1)}\right]^{\frac{1}{2}} \times (2\eta r)^\gamma e^{-\eta r} L^{2\gamma+1}_{n-1}(2\eta r).$$

γ is defined as in (3.24), $\eta = +((mc/\hbar)^2 - (E_{nlJ}/\hbar c)^2)^{\frac{1}{2}}$, $E_{nlJ} = +mc^2/(1 + b^2/(\gamma + n)^2)^{\frac{1}{2}}$. The quantum number n runs over the values $n = 1, 2, 3, \cdots$, independently of the quantum numbers l and J. Since there are no negative frequency bound states, the quantum number ρ has been omitted here. The normalization is

$$\langle \psi^{s'}_{n'l'J'M'}(\mathbf{r}, t) \mid \psi^s_{nlJM}(\mathbf{r}, t)\rangle = \epsilon_s \delta_{ss'} \delta_{nn'} \delta_{ll'} \delta_{JJ'} \delta_{MM'}. \tag{3.27}$$

Also, each bound-state wavefunction is orthogonal to each continuum-state wavefunction.

The angular functions $\Omega_{lJM}(\mathbf{u}_r)$ in (3.23) and (3.26) are the simultaneous eigenfunctions of $\mathbf{L}\cdot\mathbf{L}$, $\mathbf{J}\cdot\mathbf{J}$, and J_z where $\mathbf{J} = \mathbf{L} + \frac{1}{2}\boldsymbol{\delta}$, $\boldsymbol{\delta}$ now denoting the Pauli matrices. They have the explicit representations

$$\Omega_{J-\frac{1}{2}JM}(\mathbf{u}_r) = \begin{bmatrix} [(J+M)/2J]^{\frac{1}{2}} Y_{J-\frac{1}{2}M-\frac{1}{2}}(\mathbf{u}_r) \\ [(J-M)/2J]^{\frac{1}{2}} Y_{J-\frac{1}{2}M+\frac{1}{2}}(\mathbf{u}_r) \end{bmatrix}, \tag{3.28}$$

$$\Omega_{J+\frac{1}{2}JM}(\mathbf{u}_r) = \begin{bmatrix} [(J+1-M)/(2J+2)]^{\frac{1}{2}} Y_{J+\frac{1}{2}M-\frac{1}{2}}(\mathbf{u}_r) \\ -[(J+1+M)/(2J+2)]^{\frac{1}{2}} Y_{J+\frac{1}{2}M+\frac{1}{2}}(\mathbf{u}_r) \end{bmatrix},$$

and they have the important property

$$\boldsymbol{\delta}\cdot\mathbf{u}_r \Omega_{lJM}(\mathbf{u}_r) = \Omega_{l'JM}(\mathbf{u}_r), \quad l + l' = 2J. \tag{3.29}$$

An "eigenfunction" expansion for $\mathcal{G}_I$, similar to the expansion (2.18) of the generalized Klein–Gordon Green's function, can be derived using the functions $\phi^{s\rho}_{lJM}(k; \mathbf{r})$, $\phi^s_{nlJM}(\mathbf{r})$ as basis functions. The expansion is

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = \sum_{s=1}^{2}\sum_{\rho=1}^{2}\sum_{lJM} \hbar c\epsilon_s\epsilon_\rho \times \int_0^\infty dk \frac{\phi^{s\rho}_{lJM}(k; \mathbf{r}_2)\bar{\phi}^{s\rho}_{lJM}(k; \mathbf{r}_1)}{\hbar\omega - \epsilon_\rho E} + \sum_{s=1}^{2}\sum_{n=1}^{\infty}\sum_{lJM} \hbar c\epsilon_s \frac{\phi^s_{nlJM}(\mathbf{r}_2)\bar{\phi}^s_{nlJM}(\mathbf{r}_1)}{\hbar\omega - E_{nlJ}}. \tag{3.30}$$

We omit the derivation of this expansion, since it is practically the same as the derivation given in Sec. II of the corresponding expansion for the Klein–Gordon problem. Define

$$T_{1,2} = \cosh\tfrac{1}{2}\psi + i\boldsymbol{\alpha}\cdot\mathbf{u}_{1,2}\sinh\tfrac{1}{2}\psi, \tag{3.31}$$

where ψ denotes the eigenvalue (depending upon l and J) of θ associated with the functions χ. By (3.18) and (3.19), we have $\phi = T\chi$, $\bar{\phi} = \chi^\dagger T^\dagger\beta = \chi^\dagger\beta\beta T^\dagger\beta$. Now $\beta T^\dagger\beta = T$, whence $\bar{\phi} = \chi^\dagger\beta T$. Each function χ is an eigenfunction of β, the eigenvalue being ϵ_s. Thus $\bar{\phi} = \epsilon_s\chi^\dagger T$. Inserting this expression for the functions $\bar{\phi}(\mathbf{r}_1)$ occurring in (3.30) and using the fact that $\epsilon_s^2 = +1$, (3.30) becomes

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = \sum_{s=1}^{2}\sum_{\rho=1}^{2}\sum_{lJM} \hbar c\epsilon_\rho \times \int_0^\infty dk T_2 \frac{\chi^{s\rho}_{lJM}(k; \mathbf{r}_2)\chi^{s\rho\dagger}_{lJM}(k; \mathbf{r}_1)}{\hbar\omega - \epsilon_\rho E} T_1 + \sum_{s=1}^{2}\sum_{n=1}^{\infty}\sum_{lJM} \hbar c T_2 \frac{\chi^s_{nlJM}(\mathbf{r}_2)\chi^{s\dagger}_{nlJM}(\mathbf{r}_1)}{\hbar\omega - E_{nlJ}} T_1. \tag{3.32}$$

The sums on s and M here can be worked out explicitly. Referring to the expressions (3.23) and (3.26) for the functions χ, we obtain

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = \sum_{\rho=1}^{2}\sum_{lJ} \hbar c\epsilon_\rho \times \int_0^\infty dk \frac{R^\rho_{lJ}(k; r_2)R^{\rho *}_{lJ}(k; r_1)}{\hbar\omega - \epsilon_\rho E} T_2\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)T_1 + \sum_{n=1}^{\infty}\sum_{lJ} \hbar c \frac{R_{nlJ}(r_2)R^*_{nlJ}(r_1)}{\hbar\omega - E_{nlJ}} T_2\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)T_1, \tag{3.33}$$

where

$$\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1) = \begin{bmatrix} \sum_M \Omega_{lJM}(\mathbf{u}_2)\Omega^\dagger_{lJM}(\mathbf{u}_1) & 0 \\ 0 & \sum_M \Omega_{lJM}(\mathbf{u}_2)\Omega^\dagger_{lJM}(\mathbf{u}_1) \end{bmatrix}. \tag{3.34}$$

Defining

$$J_{lJ} = \sum_{\rho=1}^{2} \hbar c\epsilon_\rho \int_0^\infty dk \frac{R^\rho_{lJ}(k; r_2)R^{\rho *}_{lJ}(k; r_1)}{\hbar\omega - \epsilon_\rho E}, \qquad (3.35)$$

we find

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = \sum_{lJ} J_{lJ}T_2\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)T_1$$
$$+ \sum_{lJ}\sum_{n=1}^{\infty} \hbar c \frac{R_{nlJ}(r_2)R^*_{nlJ}(r_1)}{\hbar\omega - E_{nlJ}} T_2\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)T_1. \quad (3.36)$$

The integration over k in (3.35) can be performed by residues, just as in the Klein–Gordon case. In fact, when we write out the integral (3.35) using the explicit expressions (3.23) for the radial functions $R^\rho_{lJ}(k; r)$, we find that the integrand is identical to the integrand of (2.19) excepting only that the parameter γ is defined differently. The evaluation of J_{lJ} is the same, step by step, as the evaluation of J_l given in Sec. II for the Klein–Gordon case, and the final expression for J_{lJ} is the same as for J_l except that γ is defined as in (3.24). As in the Klein–Gordon case, we find that the contribution to the first sum of (3.36) coming from the poles of the Gamma function $\Gamma(1 + \gamma - i\nu)$ exactly cancels the contribution to $\mathcal{G}_I$ coming from the sum on bound states. Thus $\mathcal{G}_I$ equals the contribution to the first sum of (3.36) coming from the pole at $E = \hbar\omega$:

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = (2ikr_1r_2)^{-1}$$
$$\times \sum_{lJ} \Gamma(1 + \gamma - i\nu)W_{i\nu;\gamma+\frac{1}{2}}(-2ikr_2)$$
$$\times \mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr_1)T_2\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)T_1, \qquad (3.37)$$

$r_2 > r_1$, $k = ((\omega/c)^2 - (mc/\hbar)^2)^{\frac{1}{2}}$, $\mathrm{Im}\,(k) > 0$,

$\nu = (b\omega/kc)$, γ is defined by (3.24).

We find the following simple explicit expressions for the angular functions $\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)$[39]:

$$\Lambda_{ll+\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1) = (4\pi)^{-1}[(l + 1)P_l$$
$$- i\boldsymbol{\sigma}\cdot(\mathbf{u}_2 \times \mathbf{u}_1)\dot{P}_l], \quad l = 0, 1, 2, \cdots, \qquad (3.38a)$$

$$\Lambda_{ll-\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1) = (4\pi)^{-1}[lP_l$$
$$+ i\boldsymbol{\sigma}\cdot(\mathbf{u}_2 \times \mathbf{u}_1)\dot{P}_l], \quad l = 1, 2, 3, \cdots. \qquad (3.38b)$$

$\mathcal{G}_I$ in the Furry Approximation

The parameter a enters (3.37) only through γ and through $\psi = \tanh^{-1} a/(J + \frac{1}{2})$ for $l = J - \frac{1}{2}$, and $\psi = -\tanh^{-1} a/(J + \frac{1}{2})$ for $l = J + \frac{1}{2}$. The expressions (3.24) for γ can be written $\gamma = -1 + (J + \frac{1}{2})(1 - a^2/(J + \frac{1}{2})^2)^{\frac{1}{2}}$ for $l = J - \frac{1}{2}$, and $\gamma = (J + \frac{1}{2})(1 - a^2/(J + \frac{1}{2})^2)^{\frac{1}{2}}$ for $l = J + \frac{1}{2}$. From these expressions for ψ and γ it is apparent that the Taylor expansion of the (lJ)th partial wave of (3.37) in ascending powers of a is, at the same time, effectively an expansion in powers of the parameter $a/(J + \frac{1}{2})$. Now the Taylor expansion of $\mathcal{G}_I$ in powers of a coincides with the perturbation expansion discussed before. This is the justification of the statement made earlier: that the perturbation expansion of $\mathcal{G}_I$ in powers of a obtained by treating the term $(a^2 + ia\boldsymbol{\alpha}\cdot\mathbf{u}_2)/r_2^2$ in the differential equation of the Green's function as a small perturbation coincides, term by term, with the expansion of $\mathcal{G}_I$, obtained by working with the partial-wave series for $\mathcal{G}_I$ and expanding the (lJ)th partial wave in powers of the parameter $a/(J + \frac{1}{2})$. In particular, the same expression (3.16) for $\mathcal{G}_I$ as before must result by expanding the (lJ)th partial wave of (3.37) in powers of $a/(J + \frac{1}{2})$, keeping only the constant and linear terms (Furry approximation), and summing the resulting series. We will here rederive (3.16) using this method. We find that the sum for the spin-correction term of (3.16) can be obtained in closed form by the same method as the sum for the main term G_0—by using the integral representation (1.9) for a product of two Whittaker functions with different arguments.

In the Furry approximation we can make the replacements

$$\gamma \approx l,$$
$$\psi \approx \begin{cases} a/(l + 1), & J = l + \frac{1}{2} \\ -a/l, & J = l - \frac{1}{2}. \end{cases} \qquad (3.39)$$

From (3.37) and (3.31) we find for the first two terms in the expansion in powers of $a/(J + \frac{1}{2})$

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) \approx (2ikr_1r_2)^{-1} \sum_{l=1}^{\infty} \Gamma(1 + l - i\nu)$$
$$\times W_{i\nu;l+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{i\nu;l+\frac{1}{2}}(-2ikr_1)$$
$$\times [\Lambda_{ll-\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1) - (ia/2l)\boldsymbol{\alpha}\cdot\mathbf{u}_2\Lambda_{ll-\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1)$$
$$- \Lambda_{ll-\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1)(ia/2l)\boldsymbol{\alpha}\cdot\mathbf{u}_1]$$
$$+ (2ikr_1r_2)^{-1} \sum_{l=0}^{\infty} \Gamma(1 + l - i\nu)$$
$$\times W_{i\nu;l+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{i\nu;l+\frac{1}{2}}(-2ikr_1)[\Lambda_{ll+\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1)$$
$$+ (ia/2(l + 1))\boldsymbol{\alpha}\cdot\mathbf{u}_2\Lambda_{ll+\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1)$$
$$+ \Lambda_{ll+\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1)(ia/2(l + 1))\boldsymbol{\alpha}\cdot\mathbf{u}_1]. \qquad (3.40)$$

We write the $l = 0$ term of the second sum separately

[39] From (3.34) and (3.28) we obtain by direct calculation

$$\sum_{J=|l-\frac{1}{2}|}^{l+\frac{1}{2}} \sum_{M=-J}^{+J} \Omega_{lJM}(\mathbf{u}_2)\Omega^\dagger_{lJM}(\mathbf{u}_1) = \frac{(2l + 1)}{4\pi} P_l.$$

Applying the projection operator $(2l + 1)^{-1}(l + 1 + \boldsymbol{\sigma}\cdot\mathbf{L}_2)$ or $(2l + 1)^{-1}(l - \boldsymbol{\sigma}\cdot\mathbf{L}_2)$ to both sides of this relation then leads to (3.38a) or (3.38b), respectively.

and then combine the remaining terms of the second sum with corresponding terms of the first sum. Using the relations

$$\Lambda_{ll+\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1) + \Lambda_{ll-\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1) = [(2l+1)/4\pi]\cdot P_l, \tag{3.41}$$

$$(l+1)^{-1}\Lambda_{ll+\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1) - l^{-1}\Lambda_{ll-\frac{1}{2}}(\mathbf{u}_2, \mathbf{u}_1) = -\dot{P}_l i\boldsymbol{\partial}\cdot(\mathbf{u}_2 \times \mathbf{u}_1)[(2l+1)/4\pi l(l+1)],$$

which may be obtained from (3.38a, b), find

$$\begin{aligned}\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) &\approx (8\pi ikr_1r_2)^{-1}\Gamma(1-iv)W_{iv;\frac{1}{2}}(-2ikr_2)\\ &\times \mathfrak{M}_{iv;\frac{1}{2}}(-2ikr_1)\cdot[1 + (ia/2)\boldsymbol{\alpha}\cdot(\mathbf{u}_2+\mathbf{u}_1)]\\ &+ (8\pi ikr_1r_2)^{-1}\sum_{l=1}^{\infty}\Gamma(1+l-iv)W_{iv;l+\frac{1}{2}}(-2ikr_2)\\ &\times \mathfrak{M}_{iv;l+\frac{1}{2}}(-2ikr_1)(2l+1)[P_l - ia\{\dot{P}_l/2l(l+1)\}\\ &\times \{\boldsymbol{\alpha}\cdot\mathbf{u}_2 i\boldsymbol{\partial}\cdot(\mathbf{u}_2\times\mathbf{u}_1) + i\boldsymbol{\partial}\cdot(\mathbf{u}_2\times\mathbf{u}_1)\boldsymbol{\alpha}\cdot\mathbf{u}_1\}].\end{aligned} \tag{3.42}$$

This expression can be simplified using the identity

$$\boldsymbol{\alpha}\cdot\mathbf{u}_2 i\boldsymbol{\partial}\cdot(\mathbf{u}_2\times\mathbf{u}_1) + i\boldsymbol{\partial}\cdot(\mathbf{u}_2\times\mathbf{u}_1)\boldsymbol{\alpha}\cdot\mathbf{u}_1 = (1-\cos\theta)\boldsymbol{\alpha}\cdot(\mathbf{u}_2+\mathbf{u}_1).$$

Using the further identities (1.12) and[40]

$$\dot{P}_l(z)\cdot(1-z)/l(l+1) = (-1)^{l+1}\,{}_2F_1(-l, l+1, 2; \tfrac{1}{2}(1+z)) \qquad l = 1, 2, 3, \cdots, \tag{3.43}$$

we can then include the separate term of (3.42) in the sum over l:

$$\begin{aligned}\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) &\approx (8\pi ikr_1r_2)^{-1}\sum_{l=0}^{\infty}(2l+1)(-1)^l\\ &\times \Gamma(1+l-iv)W_{iv;l+\frac{1}{2}}(-2ikr_2)\mathfrak{M}_{iv;l+\frac{1}{2}}(-2ikr_1)\\ &\times [{}_2F_1(-l, l+1, 1; \cos^2\tfrac{1}{2}\theta) + (ia/2)\boldsymbol{\alpha}\cdot(\mathbf{u}_2+\mathbf{u}_1)\\ &\times {}_2F_1(-l, l+1, 2; \cos^2\tfrac{1}{2}\theta)].\end{aligned} \tag{3.44}$$

The first term in the bracket here is seen to produce precisely the series for our approximate Klein–Gordon Green's function G_0 [Eq. (2.30) with $\gamma \to l$, or Eq. (1.4) with k and ν defined as in (2.5)]. Separating out this term and applying the integral representation (1.9), find

$$\begin{aligned}\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) &\approx G_0(\mathbf{r}_2, \mathbf{r}_1, \omega)\\ &+ [a/16\pi i(r_1r_2)^{\frac{1}{2}}]\boldsymbol{\alpha}\cdot(\mathbf{u}_2+\mathbf{u}_1)e^{-\pi\nu}(\sinh\pi\nu)^{-1}\\ &\times \int_{+\infty,\arg(\zeta\pm1)=0}^{(1+)} d\zeta(\zeta+1)^{i\nu-\frac{1}{2}}(\zeta-1)^{-i\nu-\frac{1}{2}}e^{ik(r_1+r_2)\zeta}\\ &\times \sum_{l=0}^{\infty}(2l+1)(-1)^l\,{}_2F_1(-l, l+1, 2; \cos^2\tfrac{1}{2}\theta)\\ &\times I_{2l+1}(-2ik(r_1r_2)^{\frac{1}{2}}(\zeta^2-1)^{\frac{1}{2}}).\end{aligned} \tag{3.45}$$

As before, the use of the integral representation has led to a special case of the Neumann's series (1.11). By (1.11), the sum of the series in (3.45) is found to be

$$(\cos\tfrac{1}{2}\theta)^{-1}I_1(-2ik\cos\tfrac{1}{2}\theta(r_1r_2)^{\frac{1}{2}}(\zeta^2-1)^{\frac{1}{2}}).$$

Substituting into (3.45), the final integration is seen to be essentially identical with the integral (1.14) encountered in connection with the nonrelativistic problem. Thus we find the following closed-form expression for $\mathcal{G}_I$ in the Furry approximation:

$$\begin{aligned}\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) &\approx G_0(\mathbf{r}_2, \mathbf{r}_1, \omega)\\ &+ a(4\pi k\alpha_1\alpha_2)^{-1}\boldsymbol{\alpha}\cdot(\mathbf{u}_2+\mathbf{u}_1)\Gamma(1-iv)\\ &\times W_{iv;\frac{1}{2}}(-ik\alpha_2)\mathfrak{M}_{iv;\frac{1}{2}}(-ik\alpha_1)\end{aligned} \tag{3.46}$$

$$\alpha_2 = r_1 + r_2 + |\mathbf{r}_2 - \mathbf{r}_1|, \quad k = ((\omega/c)^2 - (mc/\hbar)^2)^{\frac{1}{2}},$$

$$\alpha_1 = r_1 + r_2 - |\mathbf{r}_2 - \mathbf{r}_1|, \quad \operatorname{Im}(k) > 0, \quad \nu = b\omega/kc.$$

Although this has only been proved for $r_2 > r_1$, it is valid for general values of $\mathbf{r}_2$ and $\mathbf{r}_1$. This follows from the symmetry property (3.3) satisfied by $\mathcal{G}_I$.[41] One can check by direct calculation[42] that this expression for $\mathcal{G}_I$ is the same as the expression (3.16) obtained before using perturbation theory.

Properties of the Exact Green's Function $\mathcal{G}_I$

Using the identity

$$\boldsymbol{\alpha}\cdot\mathbf{u}_2\,\boldsymbol{\alpha}\cdot\mathbf{u}_1 = \mathbf{u}_2\cdot\mathbf{u}_1 + i\boldsymbol{\partial}\cdot(\mathbf{u}_2\times\mathbf{u}_1), \tag{3.47}$$

we can rewrite (3.38a, b) in the form[43]

[40] Equation (3.43) can be verified by direct calculation, working with the power-series expansions of both sides of the equation in powers of $(1+z)$. In obtaining the expansion of the left-hand side of the equation, Rodrigues's formula for the Legendre function is found to be a convenient starting point.

[41] Since T in (3.3) is independent of a, it follows that the Taylor expansion of $\mathcal{G}_I$ in powers of a must satisfy the symmetry property (3.3), term by term. In particular, the Furry approximation (since it consists in the first two terms of this Taylor expansion) must have this symmetry property. The validity of (3.46) for general values of $\mathbf{r}_2$ and $\mathbf{r}_1$ now follows from the fact that the right-hand side of (3.46) is actually invariant under the symmetry operation (3.3). [Equation (3.46) is also invariant under interchange of $\mathbf{r}_1$ and $\mathbf{r}_2$ alone—without taking the transpose and multiplying on the left and right by T. This is a property not enjoyed by the exact Green's function $\mathcal{G}_I$.]

[42] For example, by carrying out the differentiations in (3.16) and comparing with (3.46); in doing this, the differential equation [Ref. 14, p. 10, Eq. (2)]

$$f''(z) + (-\tfrac{1}{4} + k/z + (1-\mu^2)/4z^2)f(z) = 0,$$

satisfied by the Whittaker functions $W_{k;\frac{1}{2}\mu}(z)$ and $\mathfrak{M}_{k;\frac{1}{2}\mu}(z)$, is required.

[43] The occurrence of the same coefficients A and B in connection with both angular functions $\Lambda_{J\pm\frac{1}{2}J}$ follows quite nicely from (3.29) (and the reality of A and B).

$$\Lambda_{J+\frac{1}{2}J}(\mathbf{u}_2, \mathbf{u}_1) = A + B\boldsymbol{\alpha}\cdot\mathbf{u}_2\,\boldsymbol{\alpha}\cdot\mathbf{u}_1,$$
$$\Lambda_{J-\frac{1}{2}J}(\mathbf{u}_2, \mathbf{u}_1) = B + A\boldsymbol{\alpha}\cdot\mathbf{u}_2\,\boldsymbol{\alpha}\cdot\mathbf{u}_1, \qquad (3.48)$$
$$A = -(4\pi)^{-1}\dot{P}_{J-\frac{1}{2}}, \qquad B = +(4\pi)^{-1}\dot{P}_{J+\frac{1}{2}}.$$

After forming $T_2\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)T_1$ using (3.48) and (3.31) and multiplying out, we find only terms proportional to 1, $\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1)$, and $\boldsymbol{\alpha}\cdot\mathbf{u}_2\boldsymbol{\alpha}\cdot\mathbf{u}_1$. By (3.37), $\mathcal{G}_I$ itself is a linear combination of terms of this form. Using (3.47) again, it follows that $\mathcal{G}_I$ can also be expressed as a linear combination of 1, $\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1)$, and $\boldsymbol{\delta}\cdot(\mathbf{u}_2 \times \mathbf{u}_1)$:

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = U + V\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1) + W\boldsymbol{\delta}\cdot(\mathbf{u}_2 \times \mathbf{u}_1). \qquad (3.49)$$

Although (3.49) has been obtained only for $r_2 > r_1$, using the symmetry property (3.3) it can be shown that (3.49) holds for general values of $\mathbf{r}_2$ and $\mathbf{r}_1$. At the same time we find that U, V, and W are symmetric; $U(\mathbf{r}_2, \mathbf{r}_1) = U(\mathbf{r}_1, \mathbf{r}_2)$ and similarly for V and W. The functions $U(\mathbf{r}_2, \mathbf{r}_1)$, $V(\mathbf{r}_2, \mathbf{r}_1)$, $W(\mathbf{r}_2, \mathbf{r}_1)$ (since they depend on $\mathbf{r}_2$ and $\mathbf{r}_1$ only through the quantities r_2, r_1, cos θ) are rotationally invariant. Equation (3.49) exhibits the general structure of the Green's function $\mathcal{G}_I$, especially as regards its γ dependence.

Substituting (3.49) into the differential equation (3.9) for the Green's function leads to a system of three coupled equations for the scalar functions U, V, W. Two equations of this system are vector equations, but when the rotational invariance and symmetry of the functions U, V, W are taken into account, the vector equations each lead to only one independent scalar equation. We obtain the following pair of equations for U and V:

$$\mathfrak{D}_2 U + (ia/r_2^2)(1 + \mathbf{u}_1\cdot\mathbf{u}_2)V = \delta^3(\mathbf{r}_2 - \mathbf{r}_1),$$
$$\mathfrak{D}_2 V + (ia/r_2^2)(1 + \mathbf{u}_1\cdot\mathbf{u}_2)^{-1}U = 0, \qquad (3.50)$$
$$\mathfrak{D}_2 = \left(\nabla_2^2 + \frac{2k\nu}{r_2} + k^2 + \frac{a^2}{r_2^2}\right).$$

The scalar function W can be determined quite simply once V is known [see the identities (3.52)].

$\mathcal{G}_I$ satisfies the identity

$$\left[\gamma^0\left(\frac{\omega}{c}\frac{b}{a} + \frac{a}{r_2}\right) + i\boldsymbol{\gamma}\cdot\nabla_2 + \frac{mc}{\hbar}\right]\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = \mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega)\left[\gamma^0\left(\frac{\omega}{c}\frac{b}{a} + \frac{a}{r_1}\right) - i\boldsymbol{\gamma}\cdot\overleftarrow{\nabla}_1 + \frac{mc}{\hbar}\right]. \qquad (3.51)$$

For the special case that $b = a = Ze^2/4\pi\hbar c$, (3.51) becomes just the statement of the equivalence of the two representations (3.5a, b) of the Dirac Green's function. The proof of (3.51) for general values of a and b can be based on the partial-wave expansion (3.37) of $\mathcal{G}_I$. This proof, however, involves a great deal of algebra. In an Appendix we indicate the main points in the proof.

When we use (3.51) in conjunction with (3.49), a number of identities satisfied by the functions U, V, and W are obtained. These are

$$(a/r_2 - a/r_1)U + i(\nabla_2 - \nabla_1)\cdot\mathbf{V} = 0,$$
$$((2\omega b/ca) + a/r_2 + a/r_1)\mathbf{V} + i(\nabla_2 + \nabla_1)U - (\nabla_2 - \nabla_1)\times\mathbf{W} = 0,$$
$$(a/r_2 - a/r_1)\mathbf{W} - (\nabla_2 + \nabla_1)\times\mathbf{V} = 0, \qquad (3.52)$$
$$(\nabla_2 + \nabla_1)\cdot\mathbf{W} = 0,$$

where $\mathbf{V} = V(\mathbf{u}_2 + \mathbf{u}_1)$ and $\mathbf{W} = W(\mathbf{u}_2 \times \mathbf{u}_1)$.

One might use these identities, for example, to solve for U and $\mathbf{W}$ in terms of $\mathbf{V}$, whereby all our ignorance about $\mathcal{G}_I$ is put into the single scalar function V. When we do this a rather interesting expression results for $\mathcal{G}_I$:

$$\mathcal{G}_I(\mathbf{r}_2, \mathbf{r}_1, \omega) = (a/r_2 - a/r_1)^{-1}[(a/r_2 - i\boldsymbol{\alpha}\cdot\nabla_2)\boldsymbol{\alpha}\cdot\mathbf{V} - \boldsymbol{\alpha}\cdot\mathbf{V}(-i\boldsymbol{\alpha}\cdot\overleftarrow{\nabla}_1 + a/r_1)], \qquad (3.53)$$
$$\mathbf{V} = V(\mathbf{u}_2 + \mathbf{u}_1).$$

(The operator $\overleftarrow{\nabla}_1$ here does not act on the factor $(a/r_2 - a/r_1)^{-1}$ outside the parentheses.) Note that the second term of (3.53) is obtained from the first upon symmetrizing in the sense of (3.3). The first of the identities (3.52) can be used to eliminate U from the second of the equations (3.50). In this way a differential equation for the scalar function V is obtained:

$$\left(\nabla_2^2 + \frac{2k\nu}{r_2} + k^2 + \frac{a^2}{r_2^2}\right)V + \frac{r_1}{r_2}\frac{(\mathbf{u}_2 + \mathbf{u}_1)\cdot(\nabla_2 - \nabla_1)V}{(r_1 - r_2)(1 + \mathbf{u}_1\cdot\mathbf{u}_2)} = 0. \qquad (3.54)$$

This equation involves ∇_1 as well as ∇_2. However, consideration of rotational invariance and symmetry shows that V may be expressed in terms of three functionally independent and symmetric combinations of r_2, r_1, cos θ, and then ∇_2 and ∇_1 can both be expressed in terms of derivatives with respect to the same three independent variables.

IV. COULOMB WAVEFUNCTIONS

Derivation from the Green's Function

Considering the nonrelativistic case, the physical retarded (advanced) Green's function $G(\mathbf{r}_2, \mathbf{r}_1, \omega)$

regarded as a function of $\mathbf{r}_2$ can be interpreted as the Schrödinger wavefunction corresponding to a source (sink) point located at $\mathbf{r}_1$ of particles of frequency ω. When $\hbar\omega$ lies in the continuous spectrum, we obtain the Coulomb wavefunctions with modified plane-wave behavior at large distances by taking the source point (or sink point) $\mathbf{r}_1$ infinitely remote from the origin in a definite direction $\mathbf{u}_1$. This derivation of the Coulomb wavefunctions with modified plane-wave behavior at large distances has been given by Meixner[1] working with the eigenfunction expansion (in parabolic coordinates) of the Green's function. The same result can also be obtained from our closed-form expression (1.18) for the Green's function. Using the formula (2.27) for the asymptotic behavior of the Whittaker function $W_{k;\frac{1}{2}\mu}(z)$, we obtain the following expression for the Green's function (1.18) in the limit $r_1 \to \infty$[44]:

$$\begin{aligned} G(\mathbf{r}_2, \mathbf{r}_1, \omega) \sim & -(4\pi r_1)^{-1} e^{ikr_1}(-2ikr_1)^{i\nu}\Gamma(1 - i\nu) \\ & \times e^{-ik\mathbf{u}_1\cdot\mathbf{r}_2}\, {}_1F_1(i\nu, 1, ik(r_2 + \mathbf{r}_2\cdot\mathbf{u}_1)) \\ & \times [1 + O(r_2/r_1) + O(1/|k|\, r_1)] \qquad (4.1) \\ & r_1 \to \infty, \qquad |\arg(-2ikr_1)| < \pi. \end{aligned}$$

Discarding factors independent of $\mathbf{r}_2$ gives the desired wavefunctions in the form

$$\phi(\mathbf{r}_2) = e^{-ik\mathbf{u}_1\cdot\mathbf{r}_2}\, {}_1F_1(i\nu, 1, ik(r_2 + \mathbf{r}_2\cdot\mathbf{u}_1)). \qquad (4.2)$$

Here $\hbar\omega$ is to be evaluated at a point $E \geq 0$ above or below the continuous spectrum, corresponding to a point source or sink, respectively, of particles at infinity in the direction $\mathbf{u}_1$. k in (4.2) is interpreted as the corresponding limiting value of k defined by $k = (2m\omega/\hbar)^{\frac{1}{2}}$ and $\mathrm{Im}\,(k) > 0$. In the former case, k approaches $+(2mE/\hbar^2)^{\frac{1}{2}}$; in the latter case k approaches $-(2mE/\hbar^2)^{\frac{1}{2}}$. In either case the exponential in (4.2) gives the "asymptotic momentum" of the particles associated with the wavefunction (4.2). This momentum is $\mathbf{p} = -k\mathbf{u}_1$. We can check that this momentum is in agreement with our interpretation of the wavefunction (4.2) as corresponding to a source or sink point of particles at infinity in the direction $\mathbf{u}_1$. Indeed, when $\hbar\omega$ is evaluated above the continuous spectrum, k is positive and $\mathbf{p}$ is in the direction $-\mathbf{u}_1$ corresponding to particles coming in from the point $\mathbf{r}_1$ at infinity. On the other hand, when $\hbar\omega$ is evaluated below the continuous spectrum, k is negative and $\mathbf{p}$ is in the direction $+\mathbf{u}_1$, corresponding to particle motion toward the point $\mathbf{r}_1$ at infinity.

A similar construction of the relativistic Coulomb continuum states as a limiting case of the physical Green's function is possible. We here find four types of wavefunctions corresponding to allowing ω approach the positive or negative frequency continuous spectrum from above or below. For negative ω the charge conjugate of the wavefunction obtained is interpreted as the ordinary Schrödinger wavefunction of the antiparticle. In considering the Dirac problem or the iterated Dirac problem, there is an additional complication due to spin. The Green's function is now a 4 by 4 matrix and cannot be interpreted directly as a wavefunction. However, multiplication on the right by an arbitrary constant spinor Φ converts the physical Green's function into a spinor field satisfying an inhomogeneous Schrödinger equation with source term $\delta^3(\mathbf{r}_2 - \mathbf{r}_1)\Phi$. This spinor field can be interpreted as the Schrödinger wavefunction generated by the point source (sink) $\delta^3(\mathbf{r}_2 - \mathbf{r}_1)\Phi$ located at the point $\mathbf{r}_1$. The Coulomb wavefunctions with modified plane-wave behavior at large distances due to a point source (sink) proportional to Φ at infinity in a definite direction $\mathbf{u}_1$ are then obtained from this spinor field by looking at the asymptotic behavior as $r_1 \to \infty$.

Applying this method to the Green's function of the iterated Dirac equation, we are lead to seek the asymptotic behavior as $r_1 \to \infty$ of the spinor field $G_I(\mathbf{r}_2, \mathbf{r}_1, \omega)\Phi$. This is the same as the asymptotic behavior, as $r_1 \to \infty$, of $T\tilde{G}_I(1, 2)T$ computed using (3.37) with $\mathbf{r}_2$ and $\mathbf{r}_1$ interchanged and with $b = a = Ze^2/4\pi\hbar c$. We find the desired wavefunctions in the form

$$\phi(\mathbf{r}_2) = \mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega)\Phi, \qquad \Phi \text{ arbitrary}, \qquad (4.3)$$

and

$$\begin{aligned} \mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega) = & -\sum_{lJ} \Gamma(1 + \gamma - i\nu)(-2ikr_2)^{-1} \\ & \times \mathfrak{M}_{i\nu;\gamma+\frac{1}{2}}(-2ikr_2)T_2\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)T_1. \qquad (4.4) \end{aligned}$$

Here ω is to be evaluated at a point above or below the positive or negative frequency continuous spectrum. k is interpreted as the limiting value approached by the quantity $k = ((\omega/c)^2 - (mc/\hbar)^2)^{\frac{1}{2}}$, $\mathrm{Im}\,(k) > 0$. The same expressions (4.3), (4.4) for the wavefunction(s) could also be obtained without reference to the Green's function, as follows. $\phi(\mathbf{r}_2)$ could be expanded in a series of the stationary-state solutions $S\chi^{\rho}_{lJM}(k; \mathbf{r}_2)$ to the same frequency of the iterated Dirac equation, with the expansion co-

[44] In deriving (4.1), we also require the identity

$$\mathfrak{M}_{i\nu;\frac{1}{2}}(z) + \tfrac{1}{2}\mathfrak{M}_{i\nu;\frac{1}{2}}(z) = e^{\frac{1}{2}z}\, {}_1F_1(i\nu, 1, -z).$$

This identity may be obtained by combining Eqs. (38b) (with the lower sign) and (39b) in Ref. 14, p. 81, and using the defining equation (1.5) of the Whittaker function $\mathfrak{M}_{k;\frac{1}{2}\mu}(z)$.

efficients choosen to correspond to an incoming or outgoing modified plane wave at large distances.

We can write the actual physical energy of the particle or antiparticle associated with the state (4.3) in the form

$$E = \epsilon_\rho \hbar\omega. \tag{4.5}$$

Here, as before, the quantum number $\rho = 1, 2$ distinguishes between positive and negative frequency states. $\epsilon_\rho = +1$ for $\rho = 1$ and $\epsilon_\rho = -1$ for $\rho = 2$. When $\hbar\omega$ approaches the continuous spectrum from above, the wavefunction obtained describes a particle or antiparticle coming in from the source point $\mathbf{r}_1$ at infinity in the direction $\mathbf{u}_1$. Hence the actual physical particle or antiparticle "asymptotic" momentum $\mathbf{p}$ is in the direction $-\mathbf{u}_1$: $\mathbf{p} = -\hbar\,|k|\,\mathbf{u}_1$. Now above the continuous spectrum $k = \epsilon_\rho\,|k|$, so the relation

$$\mathbf{p} = -\epsilon_\rho \hbar k \mathbf{u}_1 \tag{4.6}$$

holds for either positive or negative frequencies. When $\hbar\omega$ approaches the continuous spectrum from below, the wavefunction obtained describes a particle or antiparticle destined to be absorbed at the point $\mathbf{r}_1$ at infinity in the direction $\mathbf{u}_1$. In this case the asymptotic momentum of the particle or antiparticle is in the direction $+\mathbf{u}_1$: $\mathbf{p} = +\hbar\,|k|\,\mathbf{u}_1$. But below the continuous spectrum $k = -\epsilon_\rho\,|k|$, whence $\mathbf{p} = -\epsilon_\rho\hbar k\mathbf{u}_1$ as before. Thus (4.6) holds for positive or negative frequencies and above or below the continuous spectrum.

Just as for the Green's function, $\mathcal{O}$ has the general form

$$\mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega) = u + v\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1) + w\boldsymbol{\delta}\cdot(\mathbf{u}_2 \times \mathbf{u}_1). \tag{4.7}$$

This can be regarded as a consequence of the general structure (3.49) of the Green's function, obtained from (3.49) by looking at the asymptotic behavior as $r_1 \to \infty$.[45] Looking at the asymptotic behavior as $r_1 \to \infty$ of (3.51) (with $b = a = Ze^2/4\pi\hbar c$), we deduce the identity

$$\left[\gamma^0\left(\frac{\omega}{c} + \frac{a}{r_2}\right) + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2 + \frac{mc}{\hbar}\right]\mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega) = \mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega)\,\frac{\epsilon_\rho \mathfrak{p} + mc}{\hbar}, \tag{4.8}$$

$$\mathfrak{p} = \gamma^0(E/c) - \boldsymbol{\gamma}\cdot\mathbf{p}.$$

Here E and $\mathbf{p}$ are as defined in (4.5) and (4.6).

[45] It also, of course, follows immediately from the series expansion (4.4) by the same observation which originally led to (3.49).

The identity (4.8) could also be established directly, working from the series expansion (4.4) of $\mathcal{O}$. This derivation would be similar in detail to the derivation of (3.51) outlined in the Appendix. Again, using (4.8) in conjunction with (4.7) leads to a number of identities satisfied by the functions u, v, and w. They may be obtained from the corresponding identities (3.52) by making the replacements $U \to u$, $V \to v$, $W \to w$, $\boldsymbol{\nabla}_1 \to -i\epsilon_\rho\mathbf{p}/\hbar$, and of course $b = a = Ze^2/4\pi\hbar c$.

When we apply the foregoing method to the Dirac wavefunction we find an easy derivation of a result previously obtained by Johnson and Deck[11]: that the exact Dirac Coulomb continuum state with modified plane-wave behavior at large distances has the form[46]

$$\psi^{\pm}(\mathbf{r}) = \{u_\pm + v_\pm\boldsymbol{\alpha}\cdot(\mathbf{u}_r \mp \mathbf{u}_p) + w_\pm\boldsymbol{\delta}\cdot(\mathbf{u}_r \times \mathbf{u}_p)\}U^\rho(\mathbf{p}), \tag{4.9}$$

where $U^\rho(\mathbf{p})$ is the Dirac free-particle plane-wave spinor associated with the asymptotic expression for $\psi^{\pm}(\mathbf{r})$. We multiply Eqs. (3.5) on the right by an arbitrary constant spinor Φ, and seek the asymptotic behavior as $r_1 \to \infty$. This leads to the Dirac wavefunction $\psi(\mathbf{r})$ in the form

$$\psi(\mathbf{r}_2) = \left[\gamma^0\left(\frac{\omega}{c} + \frac{a}{r_2}\right) + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2 + \frac{mc}{\hbar}\right]\mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega)\Phi \tag{4.10a}$$

$$= \mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega)\,\frac{\epsilon_\rho \mathfrak{p} + mc}{\hbar}\,\Phi. \tag{4.10b}$$

Here the notation is the same as in connection with the wavefunction of the iterated Dirac equation. We have here the identity (4.8) again, but multiplied on the right by an arbitrary constant spinor Φ. The result of Johnson and Deck is contained in (4.10b). The factor $(\epsilon_\rho\mathfrak{p} + mc)/\hbar$ is proportional to the Dirac free-particle positive or negative frequency projection operator, and adjusts the arbitrary constant spinor Φ to a Dirac positive or negative frequency plane-wave spinor according as the Coulomb wavefunction $\psi(\mathbf{r}_2)$ belongs to positive or negative frequency. Two degrees of freedom in the arbitrary constant spinor Φ are in effect projected out. We can replace $(\mathfrak{p} + mc)\Phi$ with Φ arbitrary by simply $U^\rho(\mathbf{p})$ where $U^\rho(\mathbf{p})$ is a general Dirac positive frequency plane-wave spinor, and similarly for $(-\mathfrak{p} + mc)\Phi$. Thus (4.10b) can be written

$$\psi(\mathbf{r}_2) = \mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega)U^\rho(\mathbf{p}). \tag{4.11}$$

[46] The superscripts $\pm$ in $\psi^{\pm}(\mathbf{r})$ refer to incoming/outgoing modified plane-wave behavior at large distances.

The result (4.9) of Johnson and Deck now follows by observing that $\mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega)$ has the general structure (4.7) and that $\mathbf{u}_1 = \mp\mathbf{u}_p$ according as we consider incoming/outgoing wave boundary conditions at large distances. From the point of view of the Green's function, the result (4.9) of Johnson and Deck is seen to have a very simple explanation: it is a consequence of the representation (3.5b) of the Dirac Green's function and of the general structure (3.49) of the Green's function of the iterated Dirac equation.

Use of the Neumann's Series in Connection with the Wavefunction[47]

The Neumann's series (1.11), by which we were able to sum the series for the Green's function, can also be used to sum the partial-wave expansions for the Coulomb wavefunctions with modified plane-wave behavior at large distances, exactly in the nonrelativistic case and in the Furry approximation in the Klein–Gordon and Dirac cases. To accomplish this, we require the integral representation[48]

$$a^{-\frac{1}{2}}\Gamma(k + \tfrac{1}{2}(1 + \mu))e^{-(a/2)}\mathfrak{M}_{k;\frac{1}{2}\mu}(a) = \int_0^\infty dx e^{-x}x^{k-\frac{1}{2}}J_\mu(2(ax)^{\frac{1}{2}})$$

$$\operatorname{Re}(k + \tfrac{1}{2}(1 + \mu)) > 0, \qquad (4.12)$$

expressing the Whittaker function $\mathfrak{M}_{k;\frac{1}{2}\mu}(a)$ as an integral involving a Bessel function. The derivation of Gordon[7] for the nonrelativistic case has been redone in this way. Here we will outline the derivation by this method of the Furry wavefunction.

The result follows quite nicely from the representation (4.11) of the Dirac wavefunction. We obtain $\mathcal{O}(\mathbf{r}_2, \mathbf{u}_1, \omega)$ in the Furry approximation from the expansion (4.4) by making the substitution (3.39) and the substitution

$$T_2\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)T_1 \approx [\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1) + (i\tfrac{1}{2}\psi)\boldsymbol{\alpha}\cdot\mathbf{u}_2 \times \Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1) + \Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)(i\tfrac{1}{2}\psi)\boldsymbol{\alpha}\cdot\mathbf{u}_1].$$

The resulting expression for $\psi(\mathbf{r}_2)$ can be simplified exactly as in the case of the Green's function, by combining the two angular momentum sums and using the explicit expressions (3.38a, b) for the angular sums. We find

$$\psi(\mathbf{r}_2) \approx \sum_{l=0}^{\infty}[(2l + 1)/4\pi](-1)^{l+1}\Gamma(1 + l - i\nu) \times (-2ikr_2)^{-1}\mathfrak{M}_{i\nu;l+\frac{1}{2}}(-2ikr_2) \times [{}_2F_1(-l, l + 1, 1; \cos^2\tfrac{1}{2}\theta) + {}_2F_1(-l, l + 1, 2; \cos^2\tfrac{1}{2}\theta) \times (ia/2)\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1)]U^p(\mathbf{p}). \qquad (4.13)$$

If in the Neumann's series (1.11) we replace k by q and z by $2(ax)^{\frac{1}{2}}e^{-i\frac{1}{2}\pi}$, multiply through by $e^{-x}x^{k-\frac{1}{2}}$, and integrate on x from 0 to ∞, then we obtain by (4.12)[49]

$$a^{\frac{1}{2}(1+\mu)}e^{a\frac{1}{2}(1-e^{i\pi})}\mathfrak{M}_{k+\frac{1}{2}(\mu-\nu);\frac{1}{2}\nu}(aq^2) = (q^2a)^{\frac{1}{2}(1+\nu)}\sum_{l=0}^{\infty}\frac{\Gamma(\mu + l)}{l!\,\Gamma(\nu + 1)}\frac{\Gamma(k + \frac{1}{2}(1 + \mu) + l)}{\Gamma(k + \frac{1}{2}(1 + \mu))} \times (2l + \mu)\,{}_2F_1(-l, \mu + l, \nu + 1; q^2) \times \mathfrak{M}_{k;\frac{1}{2}(2l+\mu)}(a); \quad \mu, \nu \neq -1, -2, \cdots. \qquad (4.14)$$

The sums occurring in (4.13) are just special cases of the general formula (4.14). After summing these series, we obtain

$$\psi(\mathbf{r}_2) \approx -\Gamma(1 - i\nu)(4\pi)^{-1}e^{-ikr_2\cdot u_1} \times {}_1F_1(i\nu, 1; ik(r_2 + \mathbf{r}_2\cdot\mathbf{u}_1))U^p(\mathbf{p}) - \Gamma(1 - i\nu)(4\pi)^{-1}e^{-ikr_2\cdot u_1} \times {}_1F_1(i\nu + 1, 2; ik(r_2 + \mathbf{r}_2\cdot\mathbf{u}_1)) \times (ia/2)\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1)U^p(\mathbf{p}). \qquad (4.15)$$

[Here we have used (1.5).] Now using the identity[50]

$$d/dz\,{}_1F_1(a, b, z) = (a/b)\,{}_1F_1(a + 1, b + 1; z), \qquad (4.16)$$

the Furry or Sommerfeld–Maue wavefunction results:

$$\psi(\mathbf{r}_2) \approx -(4\pi)^{-1}\Gamma(1 - i\nu)e^{-ikr_2\cdot u_1}[1 - (i\hbar/2\omega)\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}_2] \times {}_1F_1i(\nu, 1; ik(r_2 + \mathbf{r}_2\cdot\mathbf{u}_1))U^p(\mathbf{p}). \qquad (4.17)$$

Note that both positive and negative frequency states and both incoming and outgoing wave boundary conditions are contained in the single expression (4.17).

The Furry wavefunction can also be derived from our approximate Dirac Green's function as obtained from (3.5b) by looking at the asymptotic behavior as $r_1 \to \infty$. The expression for this approximate Green's function is

$$K(\mathbf{r}_2, \mathbf{r}_1, \omega) \approx [G_0(\mathbf{r}_2, \mathbf{r}_1, \omega) - (ic/2\omega)\boldsymbol{\alpha}\cdot(\boldsymbol{\nabla}_2 + \boldsymbol{\nabla}_1)G_0(\mathbf{r}_2, \mathbf{r}_1, \omega)] \times [\gamma^0(\omega/c + a/r_1) - i\boldsymbol{\gamma}\cdot\overleftarrow{\boldsymbol{\nabla}}_1 + mc/\hbar], \qquad (4.18)$$

where G_0 is the Green's function of the Klein–Gordon equation without the potential squared term. The

[47] See also B. Rosen, J. Math. Phys. 4, 392 (1963).

[48] Ref. 14, p. 14, Eq. (13a). The angle arc(a) may be arbitrary, but it must be the same on both sides of the equation.

[49] Ref. 14, p. 130, Eq. (16).

[50] Ref. 14, p. 5, Eq. (10).

asymptotic behavior as $r_1 \to \infty$ of G_0 is given by Eq. (4.1), but with k and ν defined as in (2.5). Using (4.1), we find the asymptotic expansion of (4.18), and multiply on the right by an arbitrary constant spinor Φ. This gives the approximate Dirac wavefunction

$$\psi(\mathbf{r}_2) \approx [1 - (ic/2\omega)\boldsymbol{\alpha}\cdot(\boldsymbol{\nabla}_2 + ik\mathbf{u}_1)]e^{-ikr_2\cdot u_1} \times {}_1F_1(i\nu, 1; ik(r_2 + \mathbf{r}_2\cdot\mathbf{u}_1))(\epsilon_p\mathfrak{p} + mc)/\hbar\cdot\Phi. \quad (4.19)$$

Here E, $\mathbf{p}$, and $\mathfrak{p}$ are as defined previously [Eqs. (4.5), (4.6), and (4.8)]. As before, $(\mathfrak{p} + mc)/\hbar\cdot\Phi$ here with Φ arbitrary can be replaced by simply $U^\rho(\mathbf{p})$ where $U^\rho(\mathbf{p})$ is a general positive frequency free-particle Dirac plane-wave spinor, and similarly for $(-\mathfrak{p} + mc)/\hbar\cdot\Phi$. Also, by using the operator identity

$$(\boldsymbol{\nabla}_2 + ik\mathbf{u}_1)e^{-ikr_2\cdot u_1} = e^{-ikr_2\cdot u_1}\boldsymbol{\nabla}_2, \quad (4.20)$$

the exponential factor in (4.19) can be moved to the left. Making these changes, we find the Furry or Sommerfeld–Maue wavefunction (4.17) again.

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APPENDIX

Here we will indicate the main points in the proof of the identity (3.51) for general values of b and a. $\mathcal{G}_I$ is written in the form

$$\mathcal{G}_I(2, 1) = \theta(r_2 - r_1)\mathcal{G}_2(2, 1) + \theta(r_1 - r_2)\mathcal{G}_1(2, 1),$$
$$\theta(x) = +1, \quad x > 0; \quad \theta(x) = 0, \quad x < 0.$$

The function $\mathcal{G}_2(2, 1)$ is defined for $r_2 < r_1$ as well as for $r_2 > r_1$ by the series (3.37). $\mathcal{G}_1(2, 1)$ is obtained from $\mathcal{G}_2(2, 1)$ by application of the symmetry operation (3.3): $\mathcal{G}_1(2, 1) = T\bar{\mathcal{G}}_2(1, 2)T$. The problem can be reduced to showing that $\mathcal{G}_2(2, 1)$ satisfies (3.51). To show that $\mathcal{G}_2(2, 1)$ satisfies (3.51) we write out (3.37) as two sums on J, one sum containing the $l = J - \frac{1}{2}$ terms and the other the $l = J + \frac{1}{2}$ terms. The ψ and γ values belonging to these two types of terms are expressed in terms of the same parameters $\eta = \tanh^{-1}(a/(J + \frac{1}{2}))$ and $\tau = ((J + \frac{1}{2})^2 - a^2)^{\frac{1}{2}}$, respectively. The representation (3.48) of the angular functions is used. Also the relations $\cosh^2\frac{1}{2}\eta = \frac{1}{2} + (J + \frac{1}{2})/2\tau$, $\sinh^2\frac{1}{2}\eta = -\frac{1}{2} + (J + \frac{1}{2})/2\tau$, and $\sinh\frac{1}{2}\eta \times \cosh\frac{1}{2}\eta = a/2\tau$ are used. There results

$$\begin{aligned}\mathcal{G}_2(2, 1) = {} & \sum_J (2ikr_1r_2)^{-1}\Gamma(1 + \tau - i\nu)W_{i\nu;\tau+\frac{1}{2}}(-2ikr_2) \\ & \times \mathfrak{M}_{i\nu;\tau+\frac{1}{2}}(-2ikr_1)[P + D(J + \tfrac{1}{2})/\tau - (ia/\tau) \\ & \times P\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1) + (P - D(J + \tfrac{1}{2})/\tau)\boldsymbol{\alpha}\cdot\mathbf{u}_2\boldsymbol{\alpha}\cdot\mathbf{u}_1] \\ & + \sum_J (2ikr_1r_2)^{-1}\Gamma(\tau - i\nu)W_{i\nu;\tau-\frac{1}{2}}(-2ikr_2) \\ & \times \mathfrak{M}_{i\nu;\tau-\frac{1}{2}}(-2ikr_1)\cdot[P - D(J + \tfrac{1}{2})/\tau + (ia/\tau) \\ & \times P\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1) + (P + D(J + \tfrac{1}{2})/\tau)\boldsymbol{\alpha}\cdot\mathbf{u}_2\boldsymbol{\alpha}\cdot\mathbf{u}_1]; \\ & P = \tfrac{1}{2}(A + B), \quad D = \tfrac{1}{2}(A - B). \end{aligned} \quad (1)$$

We transform $i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2$ as follows:

$$i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2 = 2k\gamma^0\boldsymbol{\alpha}\cdot\mathbf{u}_2[\partial/\partial z_2 + 1/z_2 - K_2/z_2], \quad (2)$$
$$z_2 = -2ikr_2, \qquad K_2 = (\boldsymbol{\sigma}\cdot\mathbf{L}_2 + 1).$$

The derivative $\partial/\partial z_2$ of (1) is evaluated using the identities[51]

$$\begin{aligned}\left(\frac{\partial}{\partial z_2} + \frac{1}{z_2}\right)z_2^{-1}W_{i\nu;\tau+\frac{1}{2}}(z_2) &= \left(-\frac{\gamma}{z_2^2} + \frac{i\nu}{2\gamma z_2}\right) \\ &\times W_{i\nu;\tau+\frac{1}{2}}(z_2) - \frac{\gamma + i\nu}{2\gamma z_2}W_{i\nu;\tau-\frac{1}{2}}(z_2), \\ \left(\frac{\partial}{\partial z_2} + \frac{1}{z_2}\right)z_2^{-1}W_{i\nu;\tau-\frac{1}{2}}(z_2) &= \left(\frac{\gamma}{z_2^2} - \frac{i\nu}{2\gamma z_2}\right) \\ &\times W_{i\nu;\tau-\frac{1}{2}}(z_2) - \frac{\gamma - i\nu}{2\gamma z_2}W_{i\nu;\tau+\frac{1}{2}}(z_2).\end{aligned} \quad (3)$$

To evaluate $K_2\mathcal{G}_2$ we go back to (3.37). K_2 is anticommuted through the $\boldsymbol{\alpha}\cdot\mathbf{u}_2$ of T_2, and the fact that the angular functions $\Lambda_{lJ}(\mathbf{u}_2, \mathbf{u}_1)$ are eigenfunctions of K_2 is used. The resulting expression can then be put into the form

$$\begin{aligned}-(i\gamma^0/r_2)\boldsymbol{\alpha}\cdot\mathbf{u}_2K_2\mathcal{G}_2(2, 1) &= (\gamma^0/r_2)(r_1z_2)^{-1}\sum_J \Gamma(1 + \tau - i\nu)W_{i\nu;\tau+\frac{1}{2}}\mathfrak{M}_{i\nu;\tau+\frac{1}{2}} \\ &\times [aD(J + \tfrac{1}{2})/\tau - aD\boldsymbol{\alpha}\cdot\mathbf{u}_2\boldsymbol{\alpha}\cdot\mathbf{u}_1(J + \tfrac{1}{2})/\tau \\ &\quad - i\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1)P(\tau^2 + a^2)/\tau \\ &\quad - i\boldsymbol{\alpha}\cdot(\mathbf{u}_2 - \mathbf{u}_1)\tau D(J + \tfrac{1}{2})/\tau] \\ &+ (\gamma^0/r_2)(r_1z_2)^{-1}\sum_J \Gamma(\tau - i\nu)W_{i\nu;\tau-\frac{1}{2}}\mathfrak{M}_{i\nu;\tau-\frac{1}{2}} \\ &\times [-aD(J + \tfrac{1}{2})/\tau + aD\boldsymbol{\alpha}\cdot\mathbf{u}_2\boldsymbol{\alpha}\cdot\mathbf{u}_1(J + \tfrac{1}{2})/\tau \\ &\quad + i\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1)(\tau^2 + a^2)P/\tau \\ &\quad - i\boldsymbol{\alpha}\cdot(\mathbf{u}_2 - \mathbf{u}_1)\tau D(J + \tfrac{1}{2})/\tau].\end{aligned} \quad (4)$$

When (4) is added to the expression obtained for

[51] Ref. 14, p. 82, Eq. (42a).

$2k\gamma^0\boldsymbol{\alpha}\cdot\mathbf{u}_2(\partial/\partial z_2 + 1/z_2)\,\mathcal{G}_2(2, 1)$, there results

$$
\begin{aligned}
&(\gamma^0 a/r_2 + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2)\mathcal{G}_2(2, 1)\\
&= \sum_J -2k\gamma^0(-2ikr_1r_2)^{-1}\Gamma(\tau - i\nu)\mathfrak{M}_{i\nu;\tau+\frac{1}{2}}(z_1)\\
&\times (\tau - i\nu)\cdot[(i\nu/2\tau)W_{i\nu;\tau+\frac{1}{2}}(z_2)\\
&- W_{i\nu;\tau-\frac{1}{2}}(z_2)\cdot(\tau + i\nu)/2\tau]\\
&\times [(P + D(J + \tfrac{1}{2})/\tau)\boldsymbol{\alpha}\cdot\mathbf{u}_2 + (P - D(J + \tfrac{1}{2})/\tau)\\
&\qquad \times \boldsymbol{\alpha}\cdot\mathbf{u}_1 - (ia/\tau)P(1 + \boldsymbol{\alpha}\cdot\mathbf{u}_2\boldsymbol{\alpha}\cdot\mathbf{u}_1)]\\
&+ \sum_J -2k\gamma^0(-2ikr_1r_2)^{-1}\Gamma(\tau - i\nu)\mathfrak{M}_{i\nu;\tau-\frac{1}{2}}(z_1)\\
&\times [-(i\nu/2\tau)W_{i\nu;\tau-\frac{1}{2}}(z_2) - W_{i\nu;\tau+\frac{1}{2}}(z_2)\cdot(\tau - i\nu)/2\tau]\\
&\times [(P - D(J + \tfrac{1}{2})/\tau)\boldsymbol{\alpha}\cdot\mathbf{u}_2 + (P + D(J + \tfrac{1}{2})/\tau)\\
&\qquad \times \boldsymbol{\alpha}\cdot\mathbf{u}_1 + (ia/\tau)P(1 + \boldsymbol{\alpha}\cdot\mathbf{u}_2\boldsymbol{\alpha}\cdot\mathbf{u}_1)]. \qquad (5)
\end{aligned}
$$

The expression for $(\gamma^0 a/r_2 + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2)\mathcal{G}_1(2, 1)$ can be obtained from (5) by making the replacements

$$
\begin{aligned}
&W_{i\nu;\tau+\frac{1}{2}}(z_2) \to -(\tau + i\nu)\mathfrak{M}_{i\nu;\tau+\frac{1}{2}}(z_2)\\
&W_{i\nu;\tau-\frac{1}{2}}(z_2) \to \mathfrak{M}_{i\nu;\tau-\frac{1}{2}}(z_2)\\
&\mathfrak{M}_{i\nu;\tau+\frac{1}{2}}(z_1) \to -(\tau + i\nu)^{-1}W_{i\nu;\tau+\frac{1}{2}}(z_1)\\
&\mathfrak{M}_{i\nu;\tau-\frac{1}{2}}(z_1) \to W_{i\nu;\tau-\frac{1}{2}}(z_1).
\end{aligned} \qquad (6)
$$

[Making these replacements changes $\mathcal{G}_2(2, 1)$ into $\mathcal{G}_1(2, 1)$, while at the same time the relations (3) are transformed into valid relations for the functions $\mathfrak{M}_{i\nu;\tau\pm\frac{1}{2}}(z_2)$.[52]] If in the expression so obtained for $(\gamma^0 a/r_2 + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2)\mathcal{G}_1(2, 1)$, we interchange $\mathbf{r}_2$ and $\mathbf{r}_1$, take the transpose, and multiply on the left and right by $T = i\gamma^3\gamma^0\gamma^1$, we obtain an expression for $\mathcal{G}_2(2, 1)(-i\boldsymbol{\gamma}\cdot\overleftarrow{\boldsymbol{\nabla}}_1 + \gamma^0 a/r_1)$ similar to (5). When this expression is subtracted from (5), there results

$$
\begin{aligned}
&(\gamma^0 a/r_2 + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_2)\mathcal{G}_2(2, 1)\\
&- \mathcal{G}_2(2, 1)(-i\boldsymbol{\gamma}\cdot\overleftarrow{\boldsymbol{\nabla}}_1 + \gamma^0 a/r_1) = 2k\sum_J (2ikr_1r_2)^{-1}\\
&\times \gamma^0\Gamma(1 + \tau - i\nu)W_{i\nu;\tau+\frac{1}{2}}(z_2)\mathfrak{M}_{i\nu;\tau+\frac{1}{2}}(z_1)\\
&\times (i\nu/\tau)P\boldsymbol{\alpha}\cdot(\mathbf{u}_2 + \mathbf{u}_1)\\
&- 2k\sum_J (2ikr_1r_2)^{-1}\gamma^0\Gamma(\tau - i\nu)W_{i\nu;\tau-\frac{1}{2}}(z_2)\\
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But by (1), the right-hand side of (7) is just $(\omega/c)\cdot(b/a)\cdot[\mathcal{G}_2(2, 1)\gamma^0 - \gamma^0\mathcal{G}_2(2, 1)]$, whence it follows that $\mathcal{G}_2(2, 1)$ satisfies (3.51).

[52] Ref. 14, p. 82, Eq. (42b).

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(Received 10 January 1964)

In a recent paper Zabusky has given an accurate estimate of the time interval in which solutions of the nonlinear string equation $y_{tt} = c^2(1 + \epsilon y_x)y_{xx}$ exist. A previous numerical study of solutions of this equation disclosed an anomaly in the partition of energy among the various modes; Zabusky's estimate shows that at the time when the anomaly was observed the solution does not exist. The proof of Zabusky uses the hodograph method; in this note we give a much simpler derivation of the same result based on an estimate given some years ago by the author.

1. PRELIMINARY LEMMAS ABOUT ORDINARY DIFFERENTIAL EQUATIONS

OUR estimates are based on two simple and well-known results concerning solutions of quadratic ordinary differential equations:

Theorem 1. Let $z(t)$ be the solution of the initial-value problem

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and suppose that m is positive; then

$$T < (mA)^{-1}. \qquad (1.2)$$

Theorem 2. Suppose that $a(t)$ satisfies the inequality

$$|a(t)| < B;$$

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$2k\gamma^0\boldsymbol{\alpha}\cdot\mathbf{u}_2(\partial/\partial z_2 + 1/z_2)\,\mathcal{G}_2(2, 1)$, there results

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Theorem 2. Suppose that $a(t)$ satisfies the inequality

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then the initial value problem (1) *has a solution for* $|t| < |mB|^{-1}$.

Proof: Let $z_0(t)$ be the solution of the comparison equation

$$dz_0/dt = Az_0^2, \qquad z_0(0) = m.$$

Since A is a lower bound for $a(t)$, it follows easily that $z_0(t)$ is a lower bound for $z(t)$ for all positive t. Since $z_0 = m/(1 - mAt) \to \infty$ at $t = (mA)^{-1}$, it follows that $z(t)$ cannot exist beyond this time.

The proof of Theorem 2 is similar: we note that the solution z_1 of

$$dz_1/dt = Bz_1^2, \qquad z_1(0) = |m|$$

is an upper bound for $|z(t)|$ for all positive t.

2. QUASILINEAR SYSTEMS FOR TWO UNKNOWNS

The following estimates were derived in Ref. 1.

Consider a system of two first-order partial differential equations:

$$\begin{aligned} u_t + au_x + bv_x &= 0, \\ v_t + cu_x + dv_x &= 0, \end{aligned} \tag{2.1}$$

a, b, c, d being functions of u and v. Suppose that this system is hyperbolic, i.e., that the matrix

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

has real and distinct eigenvalues λ and μ for all relevant values of u and v.

Let (l_1, l_2) be the left eigenvector of the above matrix corresponding to the eigenvalue λ. Multiply the first equation in (2.1) by l_1, the second by l_2 and add; we obtain the characteristic equation

$$l_1u' + l_2v' = 0, \tag{2.2}$$

where

$$' = \partial/\partial t + \lambda(\partial/\partial x).$$

Let ϕ be an integrating factor for (2.2), i.e., a function ϕ of u and v such that ϕl_1 and ϕl_2 become the u and v derivatives, respectively, of some function $r(u, v)$. Multiply (2.2) by ϕ; we get

$$r' = r_t + \lambda r_x = 0. \tag{2.3}$$

For the other eigenvalue we get a similar equation

$$\grave{s} = 0, \tag{2.4}$$

where

$$\grave{} = \partial/\partial t + \mu(\partial/\partial x). \tag{2.5}$$

The functions r and s are called Riemann invariants; Eqs. (2.3) and (2.4) express the fact that they remain constant along their respective characteristics.

Differentiate (2.3) with respect to x:

$$r_{tx} + \lambda r_{xx} + \lambda_r r_x^2 + \lambda_s s_x r_x = 0. \tag{2.6}$$

From (2.4) and (2.5) we have

$$0 = \grave{s} = s' - (\lambda - \mu)s_x,$$

so

$$s_x = s'/(\lambda - \mu). \tag{2.7}$$

Substitute (2.7) into (2.6) and abbreviate r_x by w; we get

$$w' + \lambda_r w^2 + [\lambda_s/(\lambda - \mu)]s'w = 0. \tag{2.8}$$

Denote by h a function of r and s which satisfies

$$h_s = \lambda_s/(\lambda - \mu).$$

Using (2.3) we have

$$h' = h_r r' + h_s s' = [\lambda_s/(\lambda - \mu)]s'.$$

Substituting this into (2.8) gives

$$w' + \lambda_r w^2 + h'w = 0.$$

Multiplying by e^h and abbreviating $e^h w$ by z gives

$$z' + e^{-h}\lambda_r z^2 = 0, \tag{2.9}$$

an equation of the form (1.1), with

$$a = -e^{-h}\lambda_r.$$

We make now the additional assumption that λ_r *is nonzero* for the relevant values of r and s; this amounts to requiring that the system (2.1) is genuinely nonlinear.

Consider bounded initial values for r and s; since r and s are constant along characteristics, it follows that r and s stay between the same bounds for all time. The quantity $|\lambda_r e^{-h}|$ has then a lower bound A for the relevant values of r and s. Suppose that λ_r is negative, and denote by m the maximum of the initial value of z. Then, according to Theorem 1, solutions with such initial values cannot exist beyond $t = (Am)^{-1}$.

Denote by B the supremum of $|\lambda_r e^{-h}|$, and by m the maximum of $|z|$. According to the proof of Theorem 2 we can place an *a priori* limitation on $|z|$ valid for all values of t less than $(Bm)^{-1}$; this gives an *a priori* estimate for $|r_x|$. We can get a similar estimate for $|s_x|$ in a similar time interval. According to the theory of first-order quasilinear hyperbolic equations[2], solutions to initial-value

[1] Unpublished note.

[2] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1962), Vol. II, Chap. V.

problems exist as long as one can place an *a priori* limitation on the magnitude of their first derivatives.

To summarize: Using theorems 1 and 2 we can place upper and lower bounds on the time interval in which the solution of a given initial-value problem for (2.1) exists.

For arbitrary initial values, these bounds are far from sharp. There is, however, one case in which these bounds are asymptotically correct; when the initial values differ little from a constant r_0, s_0. It follows then that r and s are nearly constant for all time, and so we have the following bounds:

$$e^{-h(0)}\lambda_r(0) - \epsilon < e^{-h}\lambda_r < e^{-h(0)}\lambda_r(0) + \epsilon,$$

$$(e^{h(0)} - \epsilon) \max r_x(0) < \max z(0) < [e^{h(0)} + \epsilon] \max r_x(0),$$

where $a(0)$ denotes the value of $a(r, s)$ at r_0, s_0, and $r_x(0)$ the initial value of r_x. So according to Theorems 1 and 2, the time T_{crit} beyond which a solution cannot be continued is given asymptotically by the smaller of the two numbers

$$[-\lambda_r(0) \max r_x(0)]^{-1}, \quad [-\mu_s(0) \max s_x(0)]^{-1}. \tag{2.10}$$

(Here the sign of r and s is so chosen that λ_r and μ_s are both negative.

It would be interesting and useful to derive such estimates for solutions of systems of equations for more than two variables.

3. NONLINEAR SECOND-ORDER HYPERBOLIC EQUATIONS

In this section we shall rederive the result of Zabusky[3] about the equation studied by Fermi, Pasta and Ulam.[4]

We shall apply now the foregoing theory to the second-order equation

$$y_{tt} = K^2(y_x)y_{xx}. \tag{3.1}$$

We prescribe initial values in the interval $(0, L)$:

$$y(x, 0) = y_0(x), \qquad y_t(x, 0) = 0, \qquad 0 \le x \le L.$$

At the end points we require y to be fixed:

$$y(0, t) = y(L, t) = 0.$$

This mixed initial-boundary-value problem can be converted into a pure initial-value problem by extending y_0 to be an odd function in $(-L, L)$ and further extending it periodically with period $2L$.

We make a first-order system out of (3.1) by introducing

$$y_x = u, \qquad y_t = v$$

as unknowns.,

$$u_t = v_x,$$
$$v_t = K^2u_x.$$

Multiply the first equation by K and add to (subtract from) the second. We get

$$v' + Ku' = 0 \quad \text{and} \quad v' - Ku' = 0, \tag{3.2}$$

where $\lambda = K$, $\mu = -K$. Since K is a function of u alone, Eqs. (3.2) are exact; the Riemann invariants are

$$r = v + L(u), \qquad s = v - L(u),$$

where

$$dL/du = K.$$

To compute λ_r we write

$$r - s = 2L(u)$$

and differentiate it with respect to r:

$$1 = 2L_u u_r = 2Ku_r.$$

Combining this with

$$\lambda_r = K_r = K_u u_r$$

gives

$$\lambda_r = K_u/2K. \tag{3.3}$$

Differentiate r with respect to x:

$$r_x = v_x + L_u u_x = v_x + Ku_x.$$

Since initially v is zero and $u = y_x$,

$$\max r_x(0) \simeq K(0) \max y(0)_{xx}. \tag{3.4}$$

So, by (2.10), the time beyond which the solution cannot be continued is

$$T_{crit} \simeq 2[K_u(0) \max y_{xx}(0)]^{-1}. \tag{3.5}$$

In Ref. 3 K is taken to be $c(1 + \epsilon u)^{\frac{1}{2}}$ and $y_0(x) = a \sin(\pi x/L)$. Then $K_u(0) = \frac{1}{2}\epsilon c$; so by (3.5),

$$T_{crit} \simeq 4L^2/ca\epsilon\pi^2.$$

The period of vibration of the linearized system is $2L/c$, so the critical number of vibrations is

$$2L/a\epsilon\pi^2. \tag{3.6}$$

This agrees with Eq. (5.21) of Ref. 3.

The above formula is asymptotically valid for large values (3.6). Taking $\epsilon = 1$, this means that the maximum displacement a should be small compared to the length L of the string.

In the calculation in Ref. 4, the values chosen correspond to: $L = 1$, $a = 1$, $c = 1$, $\epsilon = \frac{1}{64}$. Formula (3.6) indicates that breakdown occurs after ~ 13.0 cycles.

[3] N. J. Zabusky, J. Math. Phys. 3, 1028 (1962).
[4] E. Fermi, J. Pasta, and S. Ulam, "Studies of Nonlinear Problems I, Los Alamos Sci. Lab. Rept. LA 1940 (1955).

Boundary Conditions for a Partial-Wave Amplitude*

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A partial-wave amplitude is frequently subject to constraints which specify its values at a given set of points. This happens, for instance, when we insist on its correct threshold behavior. We investigate such constraints in this paper and derive a class of inequalities which are necessary conditions for the existence of such an amplitude.

I. INTRODUCTION

RECENT investigations of partial-wave dispersion relations[1,2] have focused attention on the question of the existence of solutions for these equations satisfying given boundary conditions. Such conditions may specify the asymptotic behavior of the spectral functions and then lead to theorems[1,2] similar to the one proved by Pomeranchuk[3] in a different context. Or they may specify the values of the amplitude at known points in the finite complex plane. This is the case, for example, when an amplitude for orbital angular momentum l is required to have an l-fold zero at threshold. Literature on some aspects of this problem exists[1,2] and the present work may be regarded as an extension of the results contained therein.

For pedagogical reasons, in Sec. II, we begin with a simple situation where the amplitude has two zeros whose positions are subject to some constraints. Certain inequalities are derived involving moments of the spectral function for the unphysical cut and of the inelasticity coefficient and a formalism is developed which expresses these inequalities in a concise form. The distinction between the original dispersion relation and the N/D equation is then utilized to obtain inequalities for bound-state parameters.

In Sec. III, we consider an amplitude which has an arbitrary but finite number of zeros, and prove the associated inequalities. These results can be sharpened if physical information regarding the behavior of the phase shifts over some range of energies can be obtained from experiment. The way to do this is discussed next. As in Sec. II, we can also derive inequalities for bound-state parameters. These are seen to imply some restrictions on the positions of the bound-state poles. Finally, all these results are generalized to boundary conditions which specify the values of the amplitude at some known points. These should prove useful particularly when unstable particles are present in the system.

The material in these two sections refers only to the scattering of a spin-zero by a spin-$\frac{1}{2}$ particle since it presents features not shared by a spin-zero system. The latter is treated briefly in the final section. The scattering of particles of arbitrary spin is not studied in this work, but it appears to involve no serious difficulty.

In the Appendix, the algebraic properties of a certain function are analyzed and used to simplify our previous results somewhat. This is important since the inequalities of Sec. III call for the knowledge of the zeros of a function of several real variables and may not be suitable for numerical work. However, these simplified inequalities do not seem to exhaust the contents of the original ones.

II. SPIN-ZERO-SPIN-½ SCATTERING: AN EXAMPLE

Let $f_{l\pm}$ denote the partial-wave amplitude for orbital angular momentum l and total angular momentum $J = l \pm \frac{1}{2}$. If the center-of-mass energy w is chosen as the complex variable, $f_{l+}(w)$ satisfies the dispersion relation

$$\begin{aligned}\operatorname{Re} f_{l+}(w) &= \operatorname{Re}\left\{\frac{\eta_{l+}(w)\exp(2i\delta_{l+}(w)) - 1}{2ik}\right\} \\ &= \frac{\eta_{l+}(w)\sin 2\delta_{l+}(w)}{2k} = \frac{1}{\pi}\int_U dw'\,\frac{\varphi_{l+}(w')}{w' - w} \\ &+ \frac{P}{\pi}\int_{w_I}^{\infty}\frac{dw'}{2k'}\,\frac{1 - \eta_{l+}(w')}{w' - w} \\ &- \frac{1}{\pi}\int_{-w_I}^{-\infty}\frac{dw'}{2k'}\,\frac{1 - \eta_{(l+1)-}(-w')}{w' - w} \\ &+ \frac{P}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'}\left[\frac{\eta_{l+}(w')\sin^2\delta_{l+}(w')}{w' - w}\right. \\ &\left. - \frac{\eta_{(l+1)-}(w')\sin^2\delta_{(l+1)-}(w')}{w' + w}\right], \quad w \geq w_t, \quad \text{(II.1)}\end{aligned}$$

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[1] G. Frye and R. L. Warnock, Phys. Rev. **130**, 478 (1963).
[2] A. P. Balachandran and F. N. von Hippel (to be published).
[3] I. Ia. Pomeranchuk, Zh. Experim. i Teor. Fiz. **34**, 725 (1958) [Engl. transl.: Soviet Phys. — JETP **7**, 499 (1958)].

where $\eta_{l\pm}(w)$ and $\delta_{l\pm}(w)$ are the transmission coefficients and real parts of the phase shifts for $f_{l\pm}(w)$, w_t, and w_I are the scattering and inelastic thresholds, $\varphi_{l+}(w)$ is the spectral function for the unphysical cut U, and k is the center-of-mass momentum. The choice of the amplitude here (and in Sec. III) is dictated by the desire to avoid all kinematical singularities and is well known in the literature. (Cf. Ref. 1.) The function $\varphi_{l+}(w)$ will contain δ functions if there are poles in (II.1). We are required to solve for $\delta_{l+}(w)$ and $\delta_{(l+1)-}(w)$ when $\varphi_{l+}(w)$, $\eta_{l+}(w)$, and $\eta_{(l+1)-}(w)$ are given and will therefore, as far as possible, state our results entirely in terms of these known functions. In (II.1), we have assumed the absence of any contribution from the circle at infinity. In addition, in this work, we will also assume that $\varphi_{l+}(w)$, the η's, the sin δ's, and their analog for the spin-zero system do not oscillate infinitely as $w \to \infty$. These two assumptions seem to be intimately related and have not been proved hitherto.

It is convenient to combine the first three integrals and write them as

$$I_1 = \frac{P}{\pi}\int_V dw' \frac{\psi_{l+}(w')}{w' - w}, \qquad w \geq w_t, \tag{II.2}$$

where V now runs over all the three cuts and $\psi_{l+}(w)$ takes on appropriate values in the different ranges. If

$$I_2 = 1/\pi \int_V dw' \psi_{l+}(w') \tag{II.3}$$

exists, the following sum rule is true[1,2]:

$$I_2 + \frac{1}{\pi}\int_{w_t}^{\infty} \frac{dw'}{k'} [\eta_{l+}(w') \sin^2 \delta_{l+}(w') + \eta_{(l+1)-}(w') \sin^2 \delta_{(l+1)-}(w')] = 0. \tag{II.4}$$

For, if it were not true, the coefficient of $1/w$ on the left-hand side of (II.1) will not vanish as $w \to \infty$ along the unitarity cut, that is, $\eta_{l+}(\infty) \neq 0$ and $\delta_{l+}(\infty) \neq \frac{1}{2}(n\pi)$ for any integer n. But, then, $\eta_{l+}(\infty) \sin^2 \delta_{l+}(\infty) \neq 0$ and the last integral will behave like ln w/w for large w. Since the left-hand side is $O(1/w)$ for large w, this is a contradiction and proves (II.4).

Now suppose that $f_{l+}(w)$ is required to have zeros at two points z_1 and z_2 which do not lie in either of the intervals $w_t < z_i < \infty$ and $-\infty < z_i < -w_t$. The z_i may of course be threshold zeros. If z_1 is complex, the real analyticity of $f_{l+}(w)$ implies that $z_2 = z_1^*$. By hypothesis, the function

$$g^1_{l+}(w) = f_{l+}(w)/[(w - z_1)(w - z_2)] \tag{II.5}$$

may have no poles at z_1 and z_2 and therefore,

$$\frac{\eta_{l+}(w) \sin 2\delta_{l+}(w)}{2k \prod_{i=1}^{2} (w - z_i)} = \frac{P}{\pi}\int_V dw' \frac{\psi_{l+}(w')}{(w' - w)\prod_{i=1}^{2}(w' - z_i)} + \frac{P}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'}\left[\frac{\eta_{l+}(w') \sin^2 \delta_{l+}(w')}{(w' - w)\prod_{i=1}^{2}(w' - z_i)} - \frac{\eta_{(l+1)-}(w') \sin^2 \delta_{(l+1)-}(w')}{(w' + w)\prod_{i=1}^{2}(w' + z_i)}\right], \quad w \geq w_t. \tag{II.6}$$

It is easily seen that the first integral exists even when z_i falls on U. Let us now introduce a notation, which will prove particularly useful later on, through the definition

$$h^i_n(2) = \frac{1}{\pi}\int_V dw' \frac{\psi_{l+}(w')}{\prod_{i=1}^{2}(w' - z_i)} w'^i \times \prod_{j=2-n+i+1}^{2}(w' - w_j), \qquad n \leq 2, \tag{II.7}$$

where the product in the numerator is to be set equal to 1 if $2 - n + i + 1 > 2$ and the w_j are complex variables in a domain to be specified later. The integrals $h^i_2(2)$ are assumed to exist, which is true if I_2 does. (This restriction will be removed at the end of Sec. III.) The left-hand side of (II.6) is $O(1/w^3)$ for large positive w, and so

$$h^0_0(2) + \frac{1}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'}\left[\frac{\eta_{l+}(w') \sin^2 \delta_{l+}(w')}{\prod_{i=1}^{2}(w' - z_i)} + \frac{\eta_{(l+1)-}(w') \sin^2 \delta_{(l+1)-}(w')}{\prod_{i=1}^{2}(w' + z_i)}\right] \equiv h^0_0(2) + j^0_+ + j^0_- = 0,$$

$$h^1_1(2) + \frac{1}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'} w'\left[\frac{\eta_{l+}(w') \sin^2 \delta_{l+}(w')}{\prod_{i=1}^{2}(w' - z_i)} - \frac{\eta_{(l+1)-}(w') \sin^2 \delta_{(l+1)-}(w')}{\prod_{i=1}^{2}(w' + z_i)}\right] \equiv h^1_1(2) + j^1_+ - j^1_- = 0,$$

$$h^2_2(2) + \frac{1}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'} w'^2\left[\frac{\eta_{l+}(w') \sin^2 \delta_{l+}(w')}{\prod_{i=1}^{2}(w' - z_i)} + \frac{\eta_{(l+1)-}(w') \sin^2 \delta_{(l+1)-}(w')}{\prod_{i=1}^{2}(w' + z_i)}\right] \equiv h^2_2(2) + j^2_+ + j^2_- = 0. \tag{II.8}$$

The last equation is the analog of (II.4). These sum rules immediately lead to inequalities for the known functions $h_i^l(2)$. Thus,

$$h_0^0(2) < 0, \qquad h_2^2(2) < 0. \tag{II.9}$$

The equalities $h_0^0(2) = 0$, $h_2^2(2) = 0$ are possible if and only if there is no scattering and can therefore be ignored. Also, since

$$h_0^0(2) = -(j_+^0 + j_-^0)$$
$$> -\frac{1}{w_i^2}(j_+^2 + j_-^2) = \frac{1}{w_i^2} h_2^2(2), \tag{II.10}$$

we have

$$h_2^2(2) - w_i^2 h_0^0(2) < 0. \tag{II.11}$$

In deriving (II.9) and (II.10), we have used the positive-definiteness of the integrands of $j_\pm^{0,2}$. There is one further inequality which is implied by (II.8). The integral

$$\frac{1}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'}(w' - \lambda)^2 \frac{\eta_{l+}(w')\sin^2\delta_{l+}(w')}{\prod_{i=1}^{2}(w' - z_i)} \tag{II.12}$$

is positive for any real λ. So too is the corresponding integral for $(l+1)-$. That is,

$$\lambda^2 j_\pm^0 - 2\lambda j_\pm^1 + j_\pm^2 > 0 \tag{II.13}$$

for any real λ. Therefore,

$$(j_\pm^1)^2 < j_\pm^0 j_\pm^2. \tag{II.14}$$

It follows that

$$[h_1^1(2)]^2 = (j_+^1 - j_-^1)^2 < (j_+^1)^2 + (j_-^1)^2 + j_+^0 j_-^2 + j_+^2 j_-^0$$
$$< j_+^0 j_+^2 + j_-^0 j_-^2 + j_+^0 j_-^2 + j_+^2 j_-^0 = h_0^0(2)h_2^2(2),$$

i.e.,

$$[h_1^1(2)]^2 < h_0^0(2)h_2^2(2). \tag{II.15}$$

It has been observed previously[1,2] that, if the analytic continuation of I_1 plus its appropriate imaginary part has zeros at z_1 and z_2, (II.1) has no solution with these zeros. This is a special case of our results, for then,

$$\frac{I_1}{\prod_{i=1}^{2}(w - z_i)} = \frac{P}{\pi}\int_V dw' \frac{\psi_{l+}(w')}{(w' - w)\prod_{i=1}^{2}(w' - z_i)}. \tag{II.16}$$

Since $I_1/\prod_{i=1}^{2}(w - z_i)$ is $o(1/w^2)$ for large w, (II.16) tells us that $h_0^0(2) = h_1^1(2) = 0$. This is inconsistent with (II.9) and (II.15), and proves the assertion.

These inequalities are by no means equivalent to the set that can be written down by successively assuming $f_{l+}(w)$ to have a zero first at z_1 and then at z_2. For instance, if $z_1 = z_2$, this will merely give an equation for $f_{l+}(w)$ to have a simple zero at z_1, while the preceding set corresponds to its having a double zero at that point.

Let us derive these results in a different way. Construct the function

$$g_{l+}^2(w) = f_{l+}(w)\prod_{i=1}^{2}\frac{(w - w_i)}{(w - z_i)}, \tag{II.17}$$

where the w_i are complex variables. This gives, instead of (II.4),

$$h_2^0(2) + \frac{1}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'}\left[\eta_{l+}(w')\sin^2\delta_{l+}(w')\prod_{i=1}^{2}\frac{(w' - w_i)}{(w' - z_i)}\right.$$
$$\left. + \eta_{(l+1)-}(w')\sin^2\delta_{(l+1)-}(w')\prod_{i=1}^{2}\frac{(w' + w_i)}{(w' + z_i)}\right] = 0. \tag{II.18}$$

It is readily verified that Eqs. (II.8) and (II.18) imply each other. Eq. (II.18) shows that

$$h_2^0(2) < 0, \tag{II.19}$$

if either (a) $w_1 = w_2$ and takes any real value or

(b) $-w_t \le w_i \le w_t$, $i = 1, 2$.

Since

$$h_2^0(2) = w_1 w_2 h_0^0(2) - (w_1 + w_2)h_1^1(2) + h_2^2(2), \tag{II.20}$$

(a) gives

$$w_1^2 h_0^0(2) - 2w_1 h_1^1(2) + h_2^2(2) < 0, \tag{II.21}$$

for any real w_1. Therefore,

$$[h_1^1(2)]^2 < h_0^0(2)h_2^2(2),$$
$$h_0^0(2) < 0, \qquad h_2^2(2) < 0. \tag{II.22}$$

To reduce (b), observe that, for fixed w_2, $h_2^0(2)$ is a linear function of w_1 and will be negative for $-w_t \le w_1 \le w_t$ if it is negative at the end points $w_1 = \pm w_t$. That is,

$$(\pm w_t)w_2 h_0^0(2) - (\pm w_t + w_2)h_1^1(2)$$
$$+ h_2^2(2) < 0. \tag{II.23}$$

This is in turn a linear function of w_2 and so should be negative for $w_2 = \pm w_t$. Only the sign combination $w_1 = -w_2$ gives a result different from (II.21) and this reads

$$-w_t^2 h_0^0(2) + h_2^2(2) < 0. \tag{II.24}$$

Equations (II.22) and (II.24) are identical with the previous set and are the necessary and sufficient conditions for (II.19) to be true. These are also necessary conditions for the existence of solutions of (II.1) with zeros at z_1 and z_2. The simplicity and generality of the formalism which leads to (II.19) will turn out to be very useful in Sec. III where a complete reduction of the analog of this equation into its component inequalities does not seem feasible.

Equation (II.18) also tells us that $h_2^0(2) < 0$

when $w_2 = w_1^*$, and that it assumes any value. This is not a new equation though, and is implied by (II.21) as a simple calculation shows.

We have remarked that (II.19) is a necessary condition if (II.1) is to have solutions with zeros at z_1 and z_2. However, even if (II.19) is not true, it may very well be that the N/D decomposition possesses solutions with these zeros, since these are not always solutions of (II.1). Suppose now that the N/D function exists and is not a solution of (II.1), either because (II.19) is not satisfied or for some other reason. The function D must then have zeros which give rise to poles in N/D not contained in (II.1). Therefore, if these poles are m in number and are at the points b_i and are all simple,

$$\operatorname{Re} N/D = \frac{\eta_{l+}(w)\sin 2\,\delta'_{l+}(w)}{2k} = I_1 + \sum_{i=1}^{m}\frac{\lambda_i}{w-b_i} + \frac{P}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'}\left[\frac{\eta_{l+}(w')\sin^2\delta'_{l+}(w')}{w'-w} - \frac{\eta_{(l+1)-}(w')\sin^2\delta'_{(l+1)-}(w')}{w'+w}\right], \quad w \geq w_t, \quad \text{(II.25)}$$

where the λ_i's are the residues at the poles, and the prime on δ'_{l+} and $\delta'_{(l+1)-}$ distinguishes these phase shifts from the ones in (II.1). Eq. (II.19) is now replaced by

$$h_2^0(2) - \sum_{i=1}^{m}\lambda_i\prod_{j=1}^{2}\frac{(b_i-w_j)}{(b_i-z_j)} < 0. \quad \text{(II.26)}$$

These poles may be called bound states provided only that the b_i's are not complex and the residues have the proper signs. Eq. (II.26) is thus an inequality for bound state parameters in terms of the known function $h_2^0(2)$.

III. SPIN-ZERO-SPIN-½ SCATTERING: GENERAL

The amplitude $f_{l+}(w)$ is required to have zeros at the n points $z_1, z_2, \cdots, z_n$. In the first instance, let us suppose that none of these lies in the intervals $w_t < z_i < \infty$ and $-\infty < z_i < -w_t$. They are allowed to be threshold zeros. If there are complex zeros, they always occur in conjugate pairs. As in Sec. II, we define the functions

$$g_{l+}^2(w) = f_{l+}(w)\prod_{j=1}^{n}\frac{(w-w_j)}{(w-z_j)}, \quad \text{(III.1)}$$

and

$$h_n^i(m) = \frac{1}{\pi}\int_V dw'\psi_{l+}(w')\times\frac{w'^i\prod_{j=m-n+i+1}^{m}(w'-w_j)}{\prod_{j=1}^{m}(w'-z_j)}, \quad n \leq m, \quad \text{(III.2)}$$

where the product in the numerator is to be set equal to 1 if $m - n + i + 1 > m$ and $h_n^i(n)$ is assumed to exist. This leads to the sum rule

$$h_n^0(n) + \frac{1}{\pi}\int_{w_t}^{\infty}\frac{dw'}{k'}\left[\eta_{l+}(w')\sin^2\delta_{l+}(w')\prod_{i=1}^{n}\frac{(w'-w_i)}{(w'-z_i)} + \eta_{(l+1)-}(w')\sin^2\delta_{(l+1)-}(w')\prod_{i=1}^{n}\frac{(w'+w_i)}{(w'+z_i)}\right] = 0. \quad \text{(III.3)}$$

For any real a and b with $a \leq b$, we will say that $\{w_i\}$ is contained in $D(a, b)$ and write $\{w_i\} \in D(a, b)$ if some pairs of w_i are equal and assume any real value and the rest satisfy the inequaltity $a \leq w_i \leq b$. Similarly, $\{z_i\} \in E(a, b)$ if the z_i fall in neither of the *open* intervals $-\infty < z_i < a$ and $b < z_i < \infty$.

Eq. (III.3) is now seen to imply the following theorem:

Theorem 1. Let Eq. (II.1) be required to have a solution with zeros at $z_1, z_2, \cdots, z_n$ where $\{z_i\} \in E(-w_t, w_t)$. Then, a necessary condition for the existence of such a function is that

$$h_n^0(n) < 0 \quad \text{(III.4)}$$

when $\{w_i\} \in D(-w_t, w_t)$.

With a slight modification, this theorem can also be used in situations where, for instance, the function vanishes like a square root at some point.[1]

If some of these zeros lie on the unitarity cuts, let z_r denote the one among these with the largest positive value and z_l the one with the smallest negative value. Further, let $|z_{r,l}| \geq w_t$. If we rewrite (III.3) in the form

$$h_n^0(n) + \frac{1}{\pi}\left[\int_{w_t}^{z_r} + \int_{z_r}^{\infty}\right]\frac{dw'}{k'}\eta_{l+}(w')\times\sin^2\delta_{l+}(w')\prod_{i=1}^{n}\frac{(w'-w_i)}{(w'-z_i)} + \frac{1}{\pi}\left[\int_{w_t}^{|z_l|} + \int_{|z_l|}^{\infty}\right]\frac{dw'}{k'}\eta_{(l+1)-}(w')\times\sin^2\delta_{(l+1)-}(w')\prod_{i=1}^{n}\frac{(w'+w_i)}{(w'+z_i)} = 0, \quad \text{(III.5)}$$

Lemma 1 is seen to follow:

Lemma 1. Let some of the zeros of $f_{l+}(w)$ lie on the unitarity cuts and let z_r denote the one which occurs farthest to the right on the right-hand unitarity cut and z_l the one which occurs farthest to the left on the left-hand unitarity cut. Then a necessary condition for the existence of such a function is that

$$h_n^0(n) + \frac{1}{\pi}\int_{w_t}^{z_r}\frac{dw'}{k'}\eta_{l+}(w')\sin^2\delta_{l+}(w')\prod_{i=1}^{n}\frac{(w'-w_i)}{(w'-z_i)}$$

$$+\frac{1}{\pi}\int_{w_t}^{|z_l|}\frac{dw'}{k'}\,\eta_{(l+1)-}(w')$$
$$\times\sin^2\delta_{(l+1)-}(w')\prod_{i=1}^{n}\frac{(w'+w_i)}{(w'+z_i)}<0, \qquad \text{(III.6)}$$

when $\{w_i\}\in D(z_l, z_r)$. If z_r does not exist, the second integral in (III.6) is to be removed and the condition $\{w_i\}\in D(z_l, z_r)$ is to be replaced by $\{w_i\}\in D(z_l, w_t)$. A similar change is to be made if z_l does not exist.

Equation (III.6) is much weaker than (III.4) since it involves the phase shifts $\delta_{l+}(w)$ and $\delta_{(l+1)-}(w)$ which are not known *a priori*. For threshold zeros, $z_i = \pm w_t$ and (III.4) and (III.6) give identical results as they should.

In physical situations, the inequality (III.4) is not the best possible one. Often, fairly detailed information regarding the behavior of the phase shifts δ_{l+} and $\delta_{(l+1)-}$ for some ranges of energies $w_{i+}-\Delta_{i+}$ to $w_{i+}+\Delta_{i+}$ $(i=1, 2, \cdots, p)$ and $w_{i-}-\Delta_{i-}$ to $w_{i-}+\Delta_{i-}$ $(i=1, 2, \cdots, q)$ can be obtained from experiment. If such is the case, (III.3) implies

$$h_n^0(n)+\frac{1}{\pi}\sum_{i=1}^{p}\int_{w_{i+}-\Delta_{i+}}^{w_{i+}+\Delta_{i+}}\frac{dw'}{k'}\,\eta_{l+}(w')$$
$$\times\sin^2\delta_{l+}(w')\prod_{j=1}^{n}\frac{(w'-w_j)}{(w'-z_j)}$$
$$+\frac{1}{\pi}\sum_{i=1}^{q}\int_{w_{i-}-\Delta_{i-}}^{w_{i-}+\Delta_{i-}}\frac{dw'}{k'}\,\eta_{(l+1)-}(w')$$
$$\times\sin^2\delta_{(l+1)-}(w')\prod_{j=1}^{n}\frac{(w'+w_j)}{(w'+z_j)}$$
$$\equiv h_n^0(n)+\sum_{i=1}^{p}J_i+\sum_{i=1}^{q}K_i<0, \qquad \text{(III.7)}$$

where some pairs of w_j lie in the intervals $w_{l+}-\Delta_{l+}\le w_j\le w_{i+}+\Delta_{l+}$ and $-(w_{i-}+\Delta_{l-})\le w_j\le -(w_{i-}-\Delta_{l-})$ and the rest of the $\{w_j\}\in D(-w_t, w_t)$. This leads to Lemma 2.

Lemma 2. If the integrals J_i and K_i are known to have the minimum values min J_i and min K_i when some pairs of w_j lie in the intervals $w_{l+}-\Delta_{i+}\le w_j\le w_{i+}+\Delta_{i+}$ and $-(w_{l-}+\Delta_{l-})\le w_j\le -(w_{l-}-\Delta_{l-})$ and the rest of the $\{w_j\}\in D(-w_t, w_t)$, and (II.1) is to have a solution with zeros at $\{z_j\}\in E(-w_t, w_t)$, it is necessary that

$$h_n^0(n)+\sum_{i=1}^{p}\min J_i+\sum_{i=1}^{q}\min K_i<0, \qquad \text{(III.8)}$$

when $\{w_j\}$ lie in these intervals.

If any of the lower limits of J_i ot K_i coincides with w_t, (III.8) can be improved by modifying the ranges of w_j as in Lemma 1.

Equation (III.8) corresponds to the existence of a particular type of solution for (II.1) while (III.4) corresponds to its having some solution. Lemma 2 should therefore prove more useful in practice since it contains more physics.

To get inequalities for bound-state parameters, we proceed as in Sec. II. The result is the next lemma.

Lemma 3. Suppose that $\{z_j\}\in E(-w_t, w_t)$, and suppose further that an N/D solution with these zeros exists and has m poles which are not implied by (II.1). Let these poles be simple and be at the points b_i with residues λ_i. Then

$$h_n^0(n)-\sum_{i=1}^{m}\lambda_i\prod_{j=1}^{n}\frac{(b_i-w_j)}{(b_i-z_j)}<0, \qquad \text{(III.9)}$$

when $\{w_j\}\in D(-w_t, w_t)$.

Let us rewrite (III.9) in the form

$$h_n^0(n)-\sum_{i=1}^{m-1}\lambda_i\prod_{j=1}^{n}\frac{(b_i-w_j)}{(b_i-z_j)}$$
$$-\lambda_m\prod_{j=1}^{n}\frac{(b_m-w_j)}{(b_m-z_j)}<0. \qquad \text{(III.10)}$$

These equations are true regardless of whether the poles are bound states or ghosts. If they are, in fact, bound states, we have the further inequality $-w_t<b_i<w_t$. If

$$h_n^0(n)-\sum_{i=1}^{m-1}\lambda_i\prod_{j=1}^{n}\frac{(b_i-w_j)}{(b_i-z_j)}\ge 0 \qquad \text{(III.11)}$$

as one of the w_j's, say w_k, is varied between two points in the interval $-w_t\le w_k\le w_t$ and the rest of the w_j's are held fixed,

$$-\lambda_m\prod_{j=1}^{n}\frac{(b_m-w_j)}{(b_m-z_j)}<0 \qquad \text{(III.12)}$$

in the same domain of the variables. Hence, b_m cannot lie in this range of w_k, for if it did, the factor (b_m-w_k) will change sign as w_k crosses b_m and (III.12) will be contradicted. For $m>1$, (III.11) involves bound-state parameters while initially, we are given only $h_n^0(n)$. The most interesting result therefore emerges when $m=1$ which we state as a lemma.

Lemma 4. Let $\{z_j\}\in E(-w_t, w_t)$. Then, if there is one bound state, and

$$h_n^0(n)\ge 0 \qquad \text{(III.13)}$$

for some range of one of the w_j's in the gap between the unitarity cuts when the remaining w_j's are held fixed in $D(-w_t, w_t)$, the bound state does not lie in this range.

A corollary is that, if $h_n^0(n)\ge 0$ as one of w_j's varies between $-w_t$ and $+w_t$ and the remaining

w_i's are held fixed in $D(-w_t, w_t)$, there are at least two poles in the N/D solution not contained in (II.1).

We can now consider a related boundary condition where the values of the function are specified at some set of points z_j $(j = 1, 2, \cdots, n)$. Let $f_{l+}(z_j) = a_j$. As before, construct the function

$$g^2_{l+}(w) = f_{l+}(w) \prod_{j=1}^{n} \frac{(w - w_j)}{(w - z_j)}. \qquad \text{(III.14)}$$

This gives

$$h^0_n(n) - \sum_{i=1}^{n} a_i \frac{\prod_{j=1}^{n} (z_i - w_j)}{\prod_{j\neq i}^{n} (z_i - z_j)} + \frac{1}{\pi}\int_{w_t}^{\infty} \frac{dw'}{k'} \times \Big[\eta_{l+}(w') \sin^2 \delta_{l+}(w') \prod_{j=1}^{n} \frac{(w' - w_j)}{(w' - z_j)} + \eta_{(l+1)-}(w') \sin^2 \delta_{(l+1)-}(w') \prod_{j=1}^{n} \frac{(w' + w_j)}{(w' + z_j)}\Big] = 0, \qquad \text{(III.15)}$$

and implies Theorem 2.

Theorem 2. Let $f_{l+}(w)$ be required to assume the values a_j at the points z_j $(j = 1, 2, \cdots, n)$ where $\{z_j\} \in E(-w_t, w_t)$. Then, if such a function is to exist, it is necessary that

$$h^0_n(n) - \sum_{i=1}^{n} a_i \frac{\prod_{j=1}^{n} (z_i - w_j)}{\prod_{j\neq i}^{n} (z_i - z_j)} < 0 \qquad \text{(III.16)}$$

when $\{w_j\} \in D(-w_t, w_t)$.

Equation (III.16) should prove useful if there are unstable particles present in the system which are identified with poles on some unphysical sheet. As an example, consider the continuation of $f_{l+}(w)$ through the elastic unitarity cut (assuming that it exists). This continuation is given by

$$f^{II}_{l+}(w) = f_{l+}(w)/[1 + 2ikf_{l+}(w)]. \qquad \text{(III.17)}$$

Therefore, if there is a pole on this sheet at $w = z_j$,

$$f_{l+}(z_j) = -1/2ik_j, \qquad \text{(III.18)}$$

where $k_j = k(z_j)$. In practice, z_j can be fixed by requiring a resonance of specified mass and width at least when the width is small. Equation (III.18) then determines one of the a_j. Further, $f_{l+}(z^*_j) = a^*_j$. When these values are inserted into (III.16), if the inequality is violated, we may conclude that (II.1) has no solution which is such that $f_{l+}(z_j) = a_j$.

If the integral I_2 in (II.3) diverges, let

$$I_1 \sim -\frac{1}{w}\chi_{l+}(w) \qquad \text{(III.19)}$$

for large positive w. Then, it is known[1,2] that

$$\chi_{l+}(w) \sim -\frac{1}{\pi}\int_{w_t}^{w} \frac{dw'}{k'} [\eta_{l+}(w') \sin^2 \delta_{l+}(w') + \eta_{(l+1)-}(w') \sin^2 \delta_{(l+1)-}(w')], \qquad \text{(III.20)}$$

for large positive w. Therefore[4],

$$\chi_{l+}(w) < 0, \qquad |\chi_{l+}(w)| \leq \frac{4}{\pi} \ln w, \qquad \text{(III.21)}$$

for all sufficiently large positive w. Further,

$$h^0_{n-2}(n) < 0. \qquad \text{(III.22)}$$

These results are summarized in the next theorem.

Theorem 3. If (III.19) is true, where $|\chi_{l+}(w)| \to \infty$ as $w \to \infty$, then (II.1) has a solution with zeros at $\{z_j\} \in E(-w_t, w_t)$ only if

$$\chi_{l+}(w) < 0, \qquad |\chi_{l+}(w)| \leq \frac{4}{\pi} \ln w,$$

for all sufficiently large positive w, and

$$h^0_{n-2}(n) < 0, \qquad \text{(III.23)}$$

when $\{w_j\} \in D(-w_t, w_t)$.

The statement $|\chi_{l+}(w)| \leq (4/\pi) \ln w$ can in fact be strengthened and Ref. 2 should be consulted for a detailed discussion of this point.

Theorems 2 and 3 can be easily extended to cover the situations implied in Lemmas 1–4.

IV. SPIN-ZERO-SPIN-ZERO SCATTERING: GENERAL

In the previous sections, we were obliged to work in the w plane due to the presence of kinematical singularities if $s = w^2$ is chosen as the complex variable. There is, however, no such difficulty for a spinless system. Let

$$f_l(s) = [s^{\frac{1}{2}}/k][\eta_l(s)e^{2i\delta_l(s)} - 1]/2i \qquad \text{(IV.1)}$$

be the partial-wave amplitude for angular momentum l. It satisfies the dispersion relation

$$\frac{s^{\frac{1}{2}}}{2k}\eta_l(s) \sin 2\delta_l(s) = f_l(s_0) + \frac{s - s_0}{\pi} P\int_V ds' \frac{\psi_l(s')}{(s' - s_0)(s' - s)} + \frac{s - s_0}{\pi} P\int_{s_t}^{\infty} ds' \frac{s'^{\frac{1}{2}}}{k'} \frac{\eta_l(s') \sin 2\delta_l(s')}{(s' - s_0)(s' - s)}, \quad s \geq s_t, \qquad \text{(IV.2)}$$

where $s_t = w^2_t$. The subtraction in (IV.2) may or may not be necessary according as whether the integral

$$I_1 = \frac{P}{\pi}\int_V ds' \frac{\psi_l(s')}{s' - s} \qquad \text{(IV.3)}$$

diverges or converges.[2] In particular, for s waves, its existence may imply that there are no arbitrary

[4] G. F. Chew and S. Mandelstam, Nuovo Cimento **19**, 752 (1961).

parameters in the system, as has been suggested by Chew and Frautschi.[5]

We may now define the integrals

$$h_n^i(m) = \frac{1}{\pi}\int_\nu ds' \frac{\psi_l(s')}{\prod_{j=1}^{m}(s'-z_j)} s'^i \times \prod_{j=m-n+i+1}^{m}(s'-s_j), \qquad n \leq m-1, \qquad \text{(IV.4)}$$

and the domains $D(a, b)$ and $E(a, b)$ for $\{s_i\}$ and $\{z_i\}$ as in Sec. III. This leads to Theorem 4.

Theorem 4. Let $f_l(s)$ be required to have zeros at the points z_j $(j = 1, 2, \cdots, n)$, none of which lies in the interval $s_t < z_j < \infty$, that is, $\{z_j\} \in E(-\infty, s_t)$. Two cases are possible.

(a) The integral $h_{n-1}^0(n)$ exists. Then, it is necessary that

$$h_{n-1}^0(n) < 0 \qquad \text{(IV.5)}$$

when $\{s_i\} \in D(-\infty, s_t)$.

(b) The integral $h_{n-1}^0(n)$ does not exist. Let

$$\frac{P}{\pi}\int_\nu ds' \frac{\psi_l(s')}{s'(s'-s)} \sim -\frac{1}{s}\chi_l(s) \qquad \text{(IV.6)}$$

as $s \to \infty$. Then, it is necessary that

$$\chi_l(s) < 0, \qquad |\chi_l(s)| \leq \frac{2}{\pi}\ln s$$

for all sufficiently large positive s, and

$$h_{n-2}^0(n) < 0 \qquad \text{(IV.7)}$$

when $\{s_i\} \in D(-\infty, s_t)$.

Unlike the w_i, the variables s_i are not bounded from below since (IV.2) has no analog of the last integral in (II.1). This results, for instance, in the demand that h_{n-p}^i be negative for every $p \geq 1$ and $i \leq n-p$ while, previously, it was required to be negative only for every even p.

It is clear that in this case too, we can duplicate every result of Sec. III by making a few suitable changes.

Incidentally, all the results of this paper can also be used in potential scattering after a few trivial alterations.

Since the completion of this paper, it has been realized that the questions treated in this paper can be studied in terms of certain reduced moment problems.[6] This observation will be developed further in a paper under completion.

[5] G. F. Chew and S. C. Frautschi, Phys. Rev. Letters 7, 394 (1961); 8, 41 (1962).

[6] J. A. Shohat and J. D. Tamarkin, *The Problem of Moments* (American Mathematical Society, New York, 1943).

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APPENDIX

We wish to study the functions $h_n^i(m)$ and try to deduce a number of simpler equations from (III.4) and (IV.5). The other inequalities can be reduced similarly. Let us first prove the following identity for the $h_n^i(m)$ of (III.2):

$$h_n^i(m) = \sum_{k=0}^{p}(-1)^k c(p, k) h_{n-k}^{i+p-k}(m). \qquad \text{(A1)}$$

The symbol $c(p, k)$ denotes the sum over all combinations of the p variables $w_{m-n+i+1}$, $w_{m-n+i+2}$, $\cdots$, $w_{m-n+i+p}$ taken k at a time, and $c(p, 0)$ is defined to be equal to one. The proof is by induction. For $p = 0$, (A1) is a triviality. Since

$$h_{n-k}^{i+p-k}(m) = h_{n-k}^{i+p+1-k}(m) - w_{m-n+i+p+1}h_{n-k-1}^{i+p-k}(m), \qquad \text{(A2)}$$

we have

$$\begin{aligned} h_n^i(m) &= h_n^{i+p+1}(m) - c(p+1, 1)h_{n-1}^{i+p}(m) \\ &\quad + \sum_{k=2}^{p}(-1)^k c(p, k) h_{n-k}^{i+p+1-k}(m) \\ &\quad + \sum_{k=1}^{p}(-1)^{k+1} c(p, k) w_{m-n+i+p+1} h_{n-k-1}^{i+p-k}(m) \\ &= h_n^{i+p+1}(m) - c(p+1, 1)h_{n-1}^{i+p}(m) \\ &\quad + \sum_{k=2}^{p}(-1)^k c(p, k) h_{n-k}^{i+p+1-k}(m) \\ &\quad + \sum_{k=2}^{p+1}(-1)^k c(p, k-1) w_{m-n+i+p+1} h_{n-k}^{i+p+1-k}(m) \\ &= \sum_{k=0}^{p+1}(-1)^k c(p+1, k) h_{n-k}^{i+p+1-k}(m), \end{aligned} \qquad \text{(A3)}$$

because of the identity

$$c(p, k) + w_{m-n+i+p+1}c(p, k-1) = c(p+1, k). \qquad \text{(A4)}$$

Equation (A3) completes the induction.

We may note two more useful identities. Thus,

$$h_n^i(m) = \sum_{k=0}^{2p}\alpha_{2p-k}^{2p} w_{m-n+i+1}^{2p-k} h_{n+k-2p}^{i+k}(m), \qquad \text{(A5a)}$$

where

$$\alpha_{2p-k}^{2p} = (-1)^k \frac{(2p)!}{k!\,(2p-k)!}, \qquad \text{(A5b)}$$

if

$$w_{m-n+i+1} = w_{m-n+i+2} = \cdots = w_{m-n+i+2p}.$$

Further,

$$h_n^i(m) = \sum_{k=0}^{p} \beta_{p-k}^p w_{m-n+i+1}^{2p-2k} h_{n-2p+2k}^{i+2k}(m), \qquad \text{(A6a)}$$

where

$$\beta_{p-k}^p = (-1)^{p-k} \frac{p!}{k!\,(p-k)!}, \qquad \text{(A6b)}$$

if

$$w_{m-n+i+1} = -w_{m-n+i+2}$$
$$= +w_{m-n+i+3} = \cdots = -w_{m-n+i+2p}.$$

Equations (A5) and (A6) can be proved either by induction or by binomial expansion. For instance, for (A6a), induction leads to a difference equation for β_{p-k}^p:

$$\beta_{p+1-k}^{p+1} + \beta_{p-k}^p - \beta_{p+1-k}^p = 0,$$

with the boundary conditions

$$\beta_p^p = (-1)^p, \qquad \beta_0^p = 1, \qquad \text{(A7)}$$

for which (A6b) is the solution.

It may be verified that the following inequalities are necessary and sufficient for (III.4) to be true:

$$[h_{n-1}^1(n)]^2 < h_{n-2}^0(n) h_n^2(n),$$
$$h_{n-2}^0(n) < 0, \qquad h_n^2(n) < 0, \qquad \text{(A8)}$$
$$h_n^2(n) - w_t^2 h_{n-2}^0(n) < 0.$$

Further reduction with such completeness appears difficult since it requires the location of zeros of polynomials of increasingly high order. We may, however, note the conditions implied by (A8) when $|w_i| \leq w_t$. These are obtained by setting each of the $w_i = \pm w_t$. Let any member of this resultant class of functions be denoted by $j_n^i(m)$. The latter can be computed by using (A1). Equation (A8) therefore leads to the following inequalities for the corresponding members of the class:

$$[j_{n-1-2p}^1(n-2q)]^2 < j_{n-2-2p}^0(n-2q) j_{n-2p}^2(n-2q),$$
$$j_{n-2-2p}^0(n-2q) < 0, \quad j_{n-2q}^2(n-2q) < 0, \qquad \text{(A9)}$$
$$j_{n-2p}^2(n-2q) - w_t^2 j_{n-2-2p}^0(n-2q) < 0,$$

where $q = 0, 2, 4, \cdots$ and $p = q, q+1, \cdots$, integer $\{\frac{1}{2}(n-2), \frac{1}{2}(n-3)\}$. When q is increased by two, every possible choice of two pairs of complex zeros conjugate to each other are to be removed in turn. This rule may require a word of explanation. We have remarked in Sec. II that the inequality $h_n^0(n) < 0$ when $w_{i+1} = w_i^*$ is already implied by the corresponding inequality gotten by setting $w_{i+1} = w_i$ and letting them be real. We can therefore derive $h_{n-2q}^0(n-2q) < 0$ for any q from $h_n^0(n) < 0$ by substituting the values of the complex zeros for the appropriate w_i. But (A9) with $q = 0$ is necessary and sufficient only for that part of (III.4) where one pair of variables are equal and the rest are constrained by $|w_i| \leq w_t$. Thus, when $q = 0$, (A9) enables us to remove one pair of zeros from (III.4), but not two pairs. We should therefore include a separate equation for $q = 2$. The situation then repeats itself and we have to include an equation for $q = 4$ too, and so on. There is no point in associating q with a real zero, however, as such equations follow from (III.4) when one or more of the w_i coincide with these real points and hence are implicit in (A9). For a similar reason, we have not written the equations $j_{n-2p}^2(n-2q) < 0$ for $p \geq q+1$ in (A9) as these are consequences of $j_{n-2-2p}^0(n-2q) < 0$.

Let us investigate (IV.5). The identities (A1), (A5), and (A6) are still true if the w_i are replaced by s_i. Instead of (A8), we find

$$[h_{n-2}^1(n)]^2 < h_{n-3}^0(n) h_{n-1}^2(n),$$
$$h_{n-3}^0(n) < 0, \qquad \text{(A10)}$$
$$h_{n-1}^2(n) < 0,$$
$$h_{n-2}^1(n) - s_t h_{n-3}^0(n) < 0.$$

The following identities can now be verified:

$$h_n^i(m) \xrightarrow[s_{m-n+i+1} \to -\infty]{} |s_{m-n+i+1}|\, h_{n-1}^i(m), \qquad \text{(A11)}$$

$$k_n^i(m) = h_n^i(m)\,|_{s_{m-n+i+1} = s_{m-n+i+2} = \cdots = s_m = s_t}$$
$$= \sum_{p=0}^{n-i} (-1)^p \frac{(n-i)!}{p!\,(n-i-p)!} s_t^p h_{n-p}^{n-p}(m).$$

The last is a consequence of (A1). The analog of (A9) are therefore

$$[k_{n-2-p}^1(n-2q)]^2 < k_{n-3-p}^0(n-2q) k_{n-1-p}^2(n-2q),$$
$$k_{n-3-p}^0(n-2q) < 0, \qquad \text{(A12)}$$
$$k_{n-2q-1}^2(n-2q) < 0,$$
$$k_{n-2-p}^1(n-2q) - s_t k_{n-3-p}^0(n-2q) < 0,$$

where $q = 0, 2, \cdots$ and $p = 2q, 2q+1, \cdots, n-3$. As in (A9), q is associated with the complex zeros.

Study of Exactly Soluble One-Dimensional N-Body Problems

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In this paper it is shown that several cases of one-dimensional N-body problems are exactly soluble. The first case describes the motion of three one-dimensional particles of arbitrary mass which interact with one another via infinite-strength, repulsive delta-function potentials. It is found in this case that the stationary-state solution of the scattering of the three particles is analogous to an electromagnetic diffraction problem which has already been solved. The solution to this analogous electromagnetic problem is interpreted in terms of particles. Next it is shown that the problem of three particles of equal mass interacting with each other via finite- but equal-strength delta-function potentials is exactly soluble. This example exhibits rearrangement and bound-state effects, but no inelastic processes occur. Finally it is shown that the problem of N particles of equal mass all interacting with one another via finite- but equal-strength delta functions is exactly soluble. Again no inelastic processes occur, but various types of rearrangements and an N-particle bound state do occur. These rearrangements and the N-particle bound state are illustrated by means of a series of sample calculations.

I. INTRODUCTION

SINCE the advent of quantum theory, physicists have relied on exactly soluble problems to describe some of the strange effects which have quantum mechanical origin. The way in which the potential enters the Schrödinger wave equation makes this equation soluble only for a very limited class of potentials, and with the exception of the Coulomb potential and the harmonic-oscillator potential, the exactly soluble problems are not particularly good imitations of the interactions which exist in the physical world. On the other hand, these exactly soluble problems illustrate a broad range of effects which are present in the physical world, and therefore at least allow us a qualitative description of the processes which can occur, and perhaps an insight into perturbation and approximation methods which can be used in more physical problems.

One would hope that exact solutions of N-body problems would be of help in producing similar insights into qualitative effects and possible approximation methods for problems of this type. There are, however, additional mathematical difficulties introduced by the presence of more than two particles which have made the exact solution of an N-body problem a more elusive goal.[1,2] These mathematical difficulties are related to the broad range of physical effects which are possible due to the presence of more than two particles.

Let us discuss the kinds of effects which may occur in N-body problems. We know that the many-particle wavefunction will contain all of the information about two-particle interactions because we may isolate two particles by putting the other particles so far away that their influence on the remaining two is negligible. Under these circumstances we will recover the two-particle wavefunction. More complicated effects arise when the N particles are close together in space and time.

Our task is to discuss those effects which arise from the proximity of the N particles, so let us focus our attention on the simplest problem which contains these effects, the three-body problem. Even here we expect a large number of physical effects. We expect finite probabilities for any two particles with an attractive potential between them to be bound in the final state, even though all of the particles are free in the initial state. Also, there will be finite probabilities for the particles to be scattered from a free state to another free state with a different distribution of energy among the particles. If a free particle is incident on a bound state we would expect that this free particle could ionize, excite, or perhaps replace a bound particle. In general we would expect finite matrix elements between any initial and final state which have the same energy.

In view of the many effects which exist in problems of this type it is not surprising that exact solutions or even reliable approximation methods are difficult to find. In order to construct exactly soluble problems we are going to be forced to make many simplifying assumptions. We are going to deal with a three-body problem where all of the particles move in only one dimension and interact with one

[1] E. Lieb and H. Koppe, Phys. Rev. **116**, 367 (1959).
[2] R. Jost, Commun. Math. Helv. **28**, 173 (1954).

another through delta-function potentials. We will later argue that this does not *a priori* restrict the number of physical effects which can occur, except for the fact that two particles which interact through an attractive delta-function potential have only a single bound state, and therefore an incident third particle cannot excite to another bound state, but only to the continuum.

II. FORMULATION OF THE PROBLEM

We consider the Hamiltonian

$$H = -\frac{\hbar^2}{2}\left(\frac{1}{M_1}\frac{d^2}{dx_1^2} + \frac{1}{M_2}\frac{d^2}{dx_2^2} + \frac{1}{M_3}\frac{d^2}{dx_3^2}\right) + A\,\delta(x_1 - x_2) + B\,\delta(x_2 - x_3) + C\,\delta(x_1 - x_3),$$

which arises when three particles of mass M_1, M_2, M_3 at positions x_1, x_2, x_3 interact with one another via delta-function potentials with strengths A, B, C which depend on coordinate differences between particles.

If we make the change of variables

$$z = (M_1 + M_2 + M_3)^{-\frac{1}{2}}(M_1x_1 + M_2x_2 + M_3x_3),$$

$$y = \frac{[M_3(M_1 + M_2)]^{\frac{1}{2}}}{(M_1 + M_2 + M_3)^{\frac{1}{2}}}\left(\frac{M_1x_1 + M_2x_2}{M_1 + M_2} - x_3\right),$$

$$x = (M_1M_2)^{\frac{1}{2}}/(M_1 + M_2)^{\frac{1}{2}}(x_1 - x_2),$$

the resulting Hamiltonian will be

$$H = -\frac{\hbar^2}{2}\left(\frac{d^2}{dz^2} + \frac{d^2}{dy^2} + \frac{d^2}{dx^2}\right) + A\,\delta\left(\frac{1}{\mu_{12}}x\right) + B\,\delta\left(\frac{1}{\mu_{23}}[x\cos\alpha + y\sin\alpha]\right) + C\,\delta\left(\frac{1}{\mu_{13}}[x\cos\beta - y\sin\beta]\right),$$

$$\frac{1}{\mu_{ij}} = \left[\frac{1}{M_i} + \frac{1}{M_j}\right]^{\frac{1}{2}},$$

$$\tan\alpha = [(M_1 + M_2 + M_3)M_2/M_1M_3]^{\frac{1}{2}},$$

$$\tan\beta = [(M_1 + M_2 + M_3)M_1/M_2M_3]^{\frac{1}{2}}.$$

Transformations of this type are discussed in the Appendix. Formulas are derived which are valid for N particles and not restricted to one dimension.

If we remove the center-of-mass motion of all three particles and eliminate the time from Schrödinger's equation, the stationary-state equation for the internal motion of the three particles will be

$$\left[-\frac{\hbar^2}{2}\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2}\right) + A\,\delta\left(\frac{1}{\mu_{12}}x\right) + B\,\delta\left(\frac{1}{\mu_{23}}[x\cos\alpha + y\sin\alpha]\right) + C\,\delta\left(\frac{1}{\mu_{13}}[x\cos\beta - y\sin\beta]\right) - E\right]\psi = 0.$$

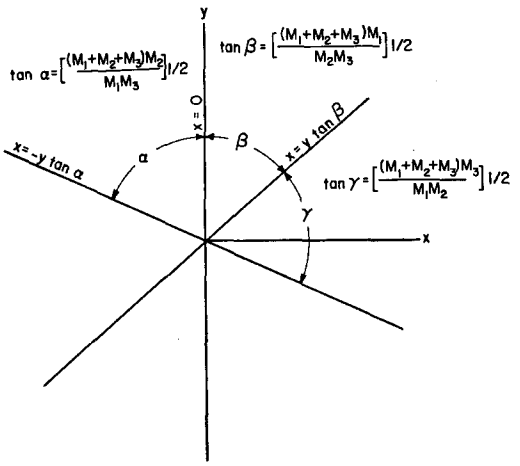

FIG. 1. Potential diagram for three particles interacting in one dimension.

This differential equation may be interpreted as describing the motion of a single particle in a two-dimensional space. Interpreting the differential equation this way may seem awkward since it tends to obscure the true nature of the physical problem, but we will find that the interpretation in terms of particles is not difficult once we have the solution to this mathematically equivalent problem.

The potential in which the single two-dimensional particle moves is zero everywhere except on the lines $x = 0$, $x = y\tan\beta$, $x = -y\tan\alpha$, as shown in Fig. 1. We see that we must solve $(\nabla^2+k^2)\psi=0$ everywhere except on the boundaries provided by the "line" delta functions. It is well known that the boundary condition on such a delta-function line is that there is a discontinuity in the normal derivative of the wavefunction which is equal to the strength of the delta function times the value of the wavefunction on the boundary.

Even this problem is an extremely difficult one mathematically and only limited progress has been made toward its solution. In Sec. IV we will solve a special case of this problem where the masses of the particles and the strengths of the delta functions are chosen in a particular way.

Another special case of interest has already been solved for us. If we take the strength of the delta-function interactions to be infinite, then the wavefunction must approach zero on the delta-function boundaries. This problem is analogous to the diffraction of electromagnetic waves from wedges and corners made of conducting materials, and is soluble for arbitrary angles between the delta-function lines and hence for arbitrary masses of the interacting

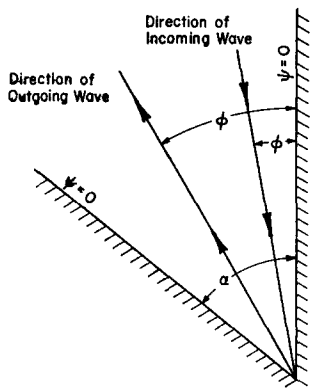

FIG. 2. Coordinate system for the electromagnetic diffraction problem.

particles. We propose to make a quantum mechanical interpretation of the solution to this analogous electromagnetic problem.

III. INFINITE-STRENGTH DELTA FUNCTIONS

A. Discussion of the Solution

The analysis of the infinite-delta-function problem is simplified by the fact that the wavefunction is confined to one of the wedges of Fig. 1. We interpret this as meaning that the particles stay in a particular order in the one dimension. The particles cannot transmit through one another because they cannot penetrate the infinite-strength delta-function wall.

Most readers will recall that certain wedge problems may easily be solved by the method of images, which is equivalent to tracing rays through a wedge until the wave vector for the ray is pointed in such a direction that it will not hit one of the sides of the wedge again. For a wedge of arbitrary angular opening, there will be two such rays emerging from the wedge corresponding to the bifurcation of the incident wave by the two sides of the wedge. If, however, the angular opening of the wedge is π/n, the reflected rays will emerge in parallel with one another and fill all of the space within the wedge. In this case the entire solution to the problem requires only the sum of the incident plus the reflected waves.

For a wedge of arbitrary angular opening, the outgoing waves will emerge in different directions and either overlap or not fill all of the space within the wedge, and thus something must be added to the solution to fit the continuity conditions along the so-called "boundaries of geometric optics" which are the terminators of the regions filled by the outgoing waves.

Diffraction problems of this type have received extensive treatment in the literature beginning with Sommerfeld's paper in 1896.[3] The interested reader can trace the literature from Oberhettinger[4] (our principal source), who has given a particularly convenient treatment for quantum mechanical interpretation.

The solution, as we have argued that it should, consists of all of the reflections in the various regions of space plus a diffraction term which fits the continuity conditions along the boundaries of geometric optics. For the scattering solution we are interested only in the far-field part of this diffraction term. For a discussion of the general boundary conditions and form of the solution of problems of this type, see Ref. [5]. We write the far-field solution as

$$\psi = \psi_{\text{incident}} + \text{two-body reflections} + f(\varphi, \varphi', \alpha)(e^{ikr}/r^{\frac{1}{2}}) + O(r^{-\frac{3}{2}}),$$

where φ and φ' are, respectively, the angles of the incoming and outgoing k vectors, and α is the angular opening of the wedge. The coordinate system is shown in Fig. 2.

Oberhettinger has provided an expansion from which we may calculate f,

$$f(\varphi, \varphi'; \alpha) = \frac{\lambda^{\frac{1}{2}}}{4}\frac{\sin(\pi^2/\alpha)}{\alpha} \times \left[\frac{\sin\frac{\pi\varphi}{\alpha}\sin\frac{\pi\varphi'}{\alpha}}{\left(\sin\frac{\pi\varphi}{\alpha}\sin\frac{\pi\varphi'}{\alpha}\right)^2 - \left(\cos\frac{\pi\varphi}{\alpha}\cos\frac{\pi\varphi'}{\alpha} - \cos\frac{\pi^2}{\alpha}\right)^2}\right].$$

Notice that $f(\varphi, \varphi'; \pi/n) = 0$, so that, as asserted earlier, there is no diffraction when the wedge is of angular opening π/n. The singularity of f along the boundaries of geometric optics, where $\pi \pm (\varphi \pm \varphi') = 2n\alpha$, is required to fit continuity conditions.

Before going further let us analyze a particular example to practice interpreting this solution in terms of particles.

B. Analysis of a Particular Example

As an example we will take the interaction between two particles of equal mass and a third particle of infinite mass. The two light particles interact with each other, but we will assume that only one of the light particles interacts with the massive particle. All interactions are infinite-strength, repulsive delta functions.

The potential diagram for this problem is shown in Fig. 3. We must solve $(\nabla^2 + k^2)\psi = 0$ with $\psi = 0$ on the lines $x = 0$ and $x = y$. The interpretation of the solution of this problem is simplified

[3] A. Sommerfeld, Math. Ann. 47, 317 (1896).

[4] F. Oberhettinger, J. Res. Natl. Bur. Std. 61, 343 (1958).

[5] E. Gerjuoy, Phys. Rev. 109, 1806 (1958).

by the fact that the x coordinate of the potential diagram is the position of the x particle relative to the massive particle (the x particle is the one which interacts with the massive particle), and the y coordinate is the coordinate of the y particle relative to the massive particle.

If the incoming wave is in Region I no three-body reactions occur since Region I is a wedge of π/n. The total solution in this region is a succession of the two-body problems. The experimental arrangement corresponding to Region I would have the y particle starting to the left of the x particle as shown in Fig. 3.

In Region II the situation is more interesting because the angular opening is $\frac{3}{4}\pi$. The experimental arrangement which corresponds to this region has the x particle starting to the left of the y particle, again as shown in Fig. 3.

We will assume that the incoming beam is "collimated" in the sense that the x and y particles in the incoming beam are adjusted so as to be at the origin at about the same time. This introduces a correlated distribution in the incoming state, that is the probability of finding an x particle per unit length depends upon where the y particle is. The collimation is necessary because otherwise the probability per unit volume to find the x particle at x_0 and the y particle at y_0 would depend on interference terms between the incident wave, the two-particle reflected waves and the true three-body waves. By introducing a collimation we have allowed the possibility of positioning the detector outside the beam and the two-particle reflections where the true three-particle effects are directly observable without interference.

As is usual in problems of this type, the probability per second to be scattered into some "solid" angle is proportional to the incident flux. This flux is neither the x-particle flux nor the y-particle flux, but the magnitude of the vector flux in the two-dimensional space. We will assume that the incident beam is normalized such that

$$\psi_{\text{incident}} = (\rho_x\rho_y)^{\frac{1}{2}}e^{ik_x x}e^{ik_y y},$$

where ρ_x and ρ_y are, respectively, the number of x particles per unit length and the number of y particles per unit length. Under these circumstances the magnitude of the flux[6] is $\rho_x\rho_y(v_x^2 + v_y^2)^{\frac{1}{2}}$ and

[6] It can be verified that this quantity is the scale factor for the reaction rate by calculating the reaction rate from the "golden rule" or by analyzing what happens to each Fourier component of a situation where a packet of x particles is incident from the left and a packet of y particles is incident from the right.

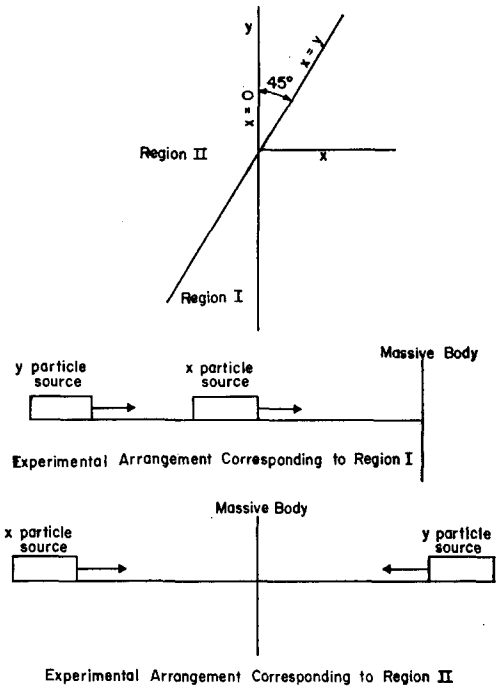

FIG. 3. Potential diagram and corresponding experimental arrangements for the particular example.

the reaction rate is

$$w = \rho_x\rho_y(v_x^2 + v_y^2)^{\frac{1}{2}}\ |f(\varphi)|^2$$

per second per unit solid angle.

A possible experiment would be to place an x-particle momentum detector to the left of the massive particle and measure the outgoing momentum distribution of x particles. This distribution would have two high peaks corresponding to the geometrical reflections of the incoming beam, but it would also have x particles of every possible momentum from zero up to the maximum possible consistent with the conservation of energy. The height of the peaks of the distribution would be proportional to the total number of the incoming particles, whereas the distributed portion of the spectrum would be proportional to the beam flux.

A second type of experiment would be to count coincidences of particle x situated between x_0 and $x_0 + \Delta x_0$ and particle y situated between y_0 and $y_0 + \Delta y_0$. The coincidence rate for this experiment is computed from the reaction rate given above where $\tan\varphi' = x_0/y_0$. For fixed $\Delta x_0\ \Delta y_0$, the coincidence rate would decrease as

$$(x_0^2 + y_0^2)^{-\frac{1}{2}}.$$

C. Summary of the Infinite-Delta-Function Results

The goals of analyzing the infinite-strength delta-function problem were limited. Of the three-body

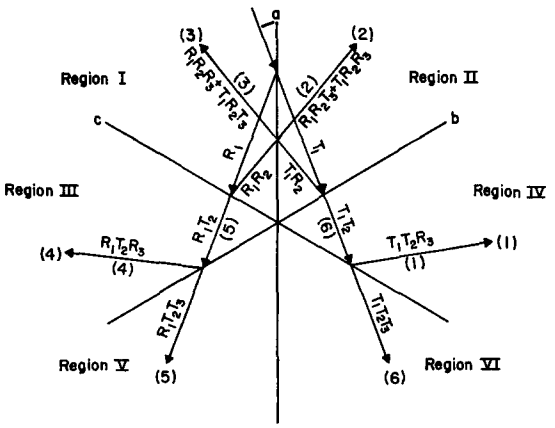

FIG. 4. Ray diagram which applies when the incoming (6) hits potential (a) first.

physical effects outlined in the Indrotuction the only one we expected to see was the redistribution of energy among the three particles, and this we have seen in our particular example. We could not have expected to see any of the other effects, because by using infinite-repulsive delta-functions for all of the interactions we have guaranteed that there will be no bound states to be ionized or rearranged.

We have, however, learned a good deal about the structure of solutions of problems of this type, and we could at least make a guess as to the form the solutions might take if the delta-function walls were transmissive. We would guess that the wave-function would consist of all of the transmitted and reflected waves in the various regions of space, plus diffracted waves which fit the continuity conditions along the boundaries of geometric optics. In spite of these insights no one has yet been able to construct a general solution to the problem where the interpotential angles are arbitrary.

Suppose we could construct a problem which bears the same relations to the finite-strength delta-function case as does the π/n wedge to the infinite-delta-function case, that is a problem in which there is no diffraction. If such a problem exists, all of the angles between the potential walls must be π/n because the transmission from wedge to wedge would assure that there would be some problability to get into a diffracting (non π/n) wedge. Since the three interpotential angles of Fig. 1 must add up to 180° there are only three possibilities for mass ratios where all angles are π/n. These possibilities are:

(1) The masses of two like particles are infinitesimal compared with that of a third particle. The interpotential angles in this case are 45°, 45°, and 90°.

(2) Particle 1 is of infinite mass compared to particle 2 which in turn is three times the mass of particle 3 (90°, 60°, 30°).

(3) All three particles have equal mass (all angles are 60°).

We have examined all three cases and it turns out that the first two possibilities will always diffract if the strengths of all of the potentials involved are finite, but as we will now proceed to show, the third possibility will not diffract if the strengths of all the potentials are the same.

IV. EXPLICIT SOLUTION TO A PROBLEM WITH FINITE-STRENGTH DELTA-FUNCTION POTENTIALS

A. Free-Particle Solution

The Hamiltonian for the internal motion of three-one dimensional particles of equal mass interacting with one another by equal-strength delta-function potentials is

$$H = -\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2}\right) - g\delta(x) - g\delta\left(\frac{1}{2}x + \frac{\sqrt{3}}{2}y\right) - g\delta\left(\frac{1}{2}x - \frac{\sqrt{3}}{2}y\right).$$

We have chosen units so that $\hbar = M = 1$. If c is the "true" strength of the delta-function potentials, the equivalent strength is

$$-g = \sqrt{2}\,c.$$

The potential diagram for this problem is three-line delta functions intersecting at 60° angles. The method of solution will be to trace rays through this complex of delta functions and verify that there are no boundaries of geometric optics and hence no diffraction.

We again wish to take literally the mathematical equivalence of this Hamiltonian to a single particle in a two-dimensional space, and return to the interpretation of one-dimensional particles after we have solved the problem.

The potential diagram and the rays which result are shown in Figs. 4 and 5. Any sequence of reflections of the incident ray result in one of six rays as shown in Fig. 6. As is indicated in Fig. 6, there are three possible angles of incidence for these rays to strike a potential. These angles are φ, $60° + \varphi$, and $60° - \varphi$.

The rays transmit or reflect with an amplitude which is dependent only on the component of momentum perpendicular to the potential surface, that is, the sine of the angle of incidence. As is usual in problems of this type we do not have to

consider path-length effects because two nearby pieces of the phase front travel the same distance between incoming and outgoing wave.

For a delta-function potential of strength g the transmission coefficient may easily be shown to be[7]

$$T = \frac{2ik/g}{2ik/g + 1} = \frac{S}{S + 1}, \qquad S = \frac{2ik}{g}.$$

Similarly, the reflection coefficient is

$$R = \frac{-1}{2ik/g + 1}\frac{-1}{S + 1},$$

where k is the component of the wave vector perpendicular to the delta-function surface.

We denote the six possible plane waves ψ_1 through ψ_6. Their momentum vectors are shown in Fig. 6. For convenience we have labeled the potentials a, b, and c and numbered the Regions I through VI.

In Fig. 4 we consider the incoming wave to be of Type 6 in Region I. The incoming wave may strike potential a first. If it does so it has an amplitude T_1 to be transmitted into Region II and an amplitude R_1 to be reflected into a Type-5 wave and stay in Region I. If the plane wave is transmitted through potential a, it will then hit potential b and again be transmitted or reflected, and so on. Notice that each ray interacts only three times, once at each angle of incidence, before becoming an outgoing ray. This is a consequence of equal-massed particles. Figure 5 illustrates the sequence of reflections we would obtain if the incoming Type-6 plane wave in Region I struck potential b first.

By following rays through the potential complex

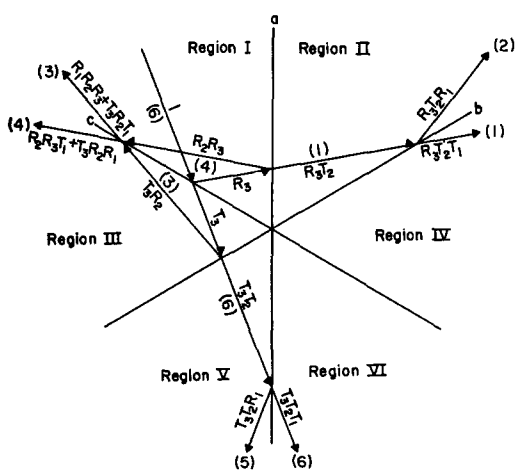

FIG. 5. Ray diagram which applies when the incoming (6) hits potential (c) first.

[7] P. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, p. 1644.

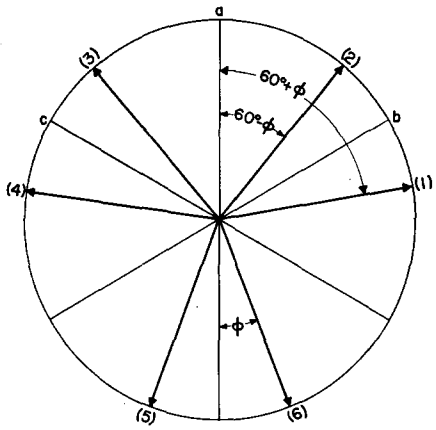

FIG. 6. Representation of the six plane waves which may be generated by reflections in the potential complex.

it is possible to evaluate the amplitude for each type of wave (i.e., Types 1 through 6) to be present in each region. As we have seen in the case of the infinite-strength delta functions, the incoming wave is bifurcated depending on which potential wall it hits first. As we saw in the infinite-delta-function case, the two halves of the plane wave must reunite to form a complete plane wave or diffraction will result. In this problem the two halves of the plane wave must be parallel and fill all of space and be equal in magnitude and phase.

It would seem at first that this problem would contain diffraction because the outgoing 2 in Region II is made up of the sum of two amplitudes from the potential a side and only one amplitude from the b side. From the a side we have

$$T_3R_2R_1 + R_3R_2T_1 = (s_3 + s_1)/(s_1 + 1)(s_2 + 1)(s_3 + 1),$$

but

$$s_2 - s_3 = (2ik/g)[\sin(60° + \varphi) - \sin(60° - \varphi)] = (2ik/g)\sin\varphi = s_1.$$

Thus

$$s_1 + s_3 = s_2$$

$$T_3R_2R_1 + R_3R_2T_1 = s_2/(s_3 + 1)(s_2 + 1)(s_1 + 1) = R_1T_2R_3,$$

which is exactly equal to the contribution from the b side; thus there is no diffraction. A similar situation occurs in Region III and the same relationship between s's again shows that there is no diffraction. In all of the other wedges it is clear that the two halves have the same magnitude and phase because the amplitudes of the two halves are made up of

TABLE I. Amplitude of plane waves in the various regions for the free wave solution.

Wave type	Region I	Region II	Region III
6	1	T_1	T_3
5	R_1		R_1T_2
4	R_2R_3		$T_3R_2R_1 + R_3R_2T_1 = R_1T_2R_3$
3	$R_1R_2R_3 + T_3R_2T_1$	T_1R_2	T_3R_2
2	R_1R_2	$T_1R_2R_3 + R_1R_2T_3 = R_3T_2R_1$	
1	R_3	R_3T_2	
Wave type	**Region IV**	**Region V**	**Region VI**
6	T_1T_2	T_3T_2	$T_1T_2T_3$
5		$T_3T_2R_1$	
4			
3			
2			
1	$T_1T_2R_3$		

the product of three complex numbers which are the same for both halves.

Since there is no diffraction, the solution to the problem may be specified by giving the amplitude for each of the six plane waves in each of the six regions. These amplitudes are given in Table I.

B. Interpretation of the Solution in Terms of Particles

Let us now interpret our solution in terms of particles. If we have the three particles oriented along a line, say in the order 1 2 3 from left to right, and we are interested in the scattering of these three particles off one another, we see first that particle 1 must be traveling to the right faster than particle 2, which in turn must be traveling to the right faster than particle 3. This is because we are interested in a scattering problem and the initial state of a scattering problem must be such that if the state is projected backwards in time there are no collisions. If particle 1 were traveling slower than particle 2 and we projected this state backwards in time, there would be a collision between 1 and 2 at some time in the past. This "no collision in the past" condition is the condition that the incoming plane wave be aimed into a wedge in such a way that the tail of the k vector not intersect any of the delta-function walls.

In the potential diagram we recall that the incoming plane wave was bifurcated by the two walls bounding the Region-I wedge. In terms of particles this means that there are two possible first interactions among the three particles, viz., particle 1 may hit particle 2 or particle 2 may hit particle 3.

When two particles of equal mass collide in one dimension, the amplitude to reflect is the amplitude that the particles retain their original order along the one-dimensional line and the amplitude to transmit is the amplitude that they exchange positions along the line. Each of the six wedges of the potential diagram represent a given order of the particles along the line. If Region I is the order 1 2 3 from left to right, then Region II must be the order 2 1 3 because to get from Region I to Region II, particle 1 must transmit through particle 2 since a is the potential between particles 1 and 2.

In two-body collisions between particles of equal mass no new velocities are generated. That is to say that the particles in the incoming state have the same velocities as the particles in the outgoing state, although the particles may switch velocities during the collision.

What we have demonstrated in our problem is that there are no new velocities generated even though there are three particles present. If we make any small change in our problem, such as letting the strength of one of the delta functions change or one of the masses be slightly different from the other two, the character of the solution will change radically due to the presence of diffraction, and there will be an infinity of new velocities brought into the problem.

We now see that we have calculated the scattering, or S matrix for this problem, which is simply a 6×6 matrix, the elements of which tell how each of the six possible initial permutations of the particles on a line couple to each of the final six permutations of the particles. To specify this 6×6 matrix entirely, it is sufficient to write down how one permutation, say 1 2 3, propagates into the six possible outgoing permutations. This is shown in Table II. The remaining elements of the 6×6 matrix may be derived by a relabeling of the particles in the initial state.

TABLE II. Elements of the S matrix.

Wavefunction	Amplitude	Region
$\exp i(k_1x_1 + k_2x_2 + k_3x_3)$	1 (Incoming Wave)	Region I: $x_1 < x_2 < x_3$
$\exp i(k_3x_1 + k_2x_2 + k_1x_3)$	$\dfrac{-1 - s_1s_3}{(s_1+1)(s_2+1)(s_3+1)}$	Region I: $x_1 < x_2 < x_3$
$\exp i(k_2x_1 + k_3x_2 + k_1x_3)$	$\dfrac{s_2}{(s_1+1)(s_2+1)(s_3+1)}$	Region II: $x_2 < x_1 < x_3$
$\exp i(k_3x_1 + k_1x_2 + k_2x_3)$	$\dfrac{s_2}{(s_1+1)(s_2+1)(s_3+1)}$	Region III: $x_1 < x_3 < x_2$
$\exp i(k_1x_1 + k_3x_2 + k_2x_3)$	$\dfrac{-s_1s_2}{(s_1+1)(s_2+1)(s_3+1)}$	Region IV: $x_2 < x_3 < x_1$
$\exp i(k_2x_1 + k_1x_2 + k_3x_3)$	$\dfrac{-s_2s_3}{(s_1+1)(s_2+1)(s_3+1)}$	Region V: $x_3 < x_1 < x_2$
$\exp i(k_1x_1 + k_2x_2 + k_3x_3)$	$\dfrac{s_1s_2s_3}{(s_1+1)(s_2+1)(s_3+1)}$	Region VI: $x_3 < x_2 < x_1$

C. Rearranged Solutions

Although we have seen that there is no diffraction in the free wave solution there is still the possibility that a particle which is bound in the initial state may be free in the final state.

Suppose we choose particles 1 and 2 to be bound in the initial state. The boundary conditions at infinity requires that there be no incoming waves in particles 1 and 2. The only way this can happen is to make both T_1 and R_1 infinite by choosing $s_1 = -1$ so that the ratio of the amplitudes of the incoming to the outgoing waves in particles 1 and 2 is zero. In the limit as s_1 approaches -1, the ratio of T_1 to R_1 is unity.

Let us evaluate the entries in Table I in this limit, that is, we set $T_1 = R_1 = 1$ and any product of amplitudes which does not contain T_1 or R_1 is set equal to zero. This result is given in Table III. The amplitudes given in Table III may be verified to constitute a solution.

In order to interpret the entries in Table III we return to Fig. 4. The incoming 6 in Region I now is at an imaginary angle of incidence with respect to potential a. Its amplitudes to either transmit or reflect are infinite and equal. This transmission and reflection together represent an incoming wave, bound in potential a. This incoming wave is a decaying exponential in both the positive and negative x direction and a propagating exponential in the y direction.

The outgoing 2 in Region II makes the same imaginary angle to potential b as does the 5 in Region I to potential a. This outgoing 2 together with the outgoing 1 in Region IV form a bound-state wavefunction in the direction perpendicular to b which is propagating in the direction parallel to b. Notice that all of the intermediate states, such as the two in Region I tend to zero exponentially at infinity in the region in which they exist.

There are three outgoing waves, a bound state in potential b propagating up to the right parallel to potential b, a bound state in potential c propagating up to the left parallel to c, and a bound state in potential a propagating down parallel to potential a.

The interpretation in terms of particles may be made without difficulty since we know that potential b, for example, is the potential between particles 1 and 3 and if the outgoing wave is bound in potential b, particles 1 and 3 must be bound together

TABLE III. Amplitudes of waves in various regions for the rearranged solution.

Wave Type	Region I	Region II	Region III
6		1	
5	1		T_2
4			$R_2T_3 + R_3R_2$
3	$R_2R_3 + R_2T_3$	R_2	
2	R_2	$R_2R_3 + R_2T_3$	
1			

Wave Type	Region IV	Region V	Region VI
6	T_2		T_3T_2
5		T_3T_2	
4			
3			
2			
1	T_2R_3		

and particle 2 free. This would represent a rearrangement of our initial state which had particles 1 and 2 bound and particle 3 free.

We follow this line of reasoning and conclude that the amplitude to leave the vertex bound in potential a is the amplitude for no rearrangement to occur. This amplitude is given from Table III,

$$T_3T_2 = \left(\frac{s_3}{s_3+1}\right)\left(\frac{s_2}{s_2+1}\right) = \frac{s_3-1}{s_3+1}.$$

The amplitude to go up to the right along potential b and the amplitude to go up to the left along potential c are interpreted as the amplitudes for the particles 1 and 2, respectively, to have been replaced by the incoming particle 3. They are

$$T_2R_3 = R_2R_3 + R_2T_3 = -s_2/(s_3+1)(s_2+1),$$

since $s_1 = -1$;

$$\tfrac{1}{4}[2i(k_y^2 - \tfrac{1}{4}g^2)^{\frac{1}{2}}]\sin\varphi = -1,$$

$$\sin\varphi = \frac{+ig}{2(k_y^2 - \tfrac{1}{4}g^2)^{\frac{1}{2}}},$$

$$s_2 = \frac{2ik\sin(60^\circ+\varphi)}{g} = \frac{\sqrt{3}\,ik_y}{g} - \frac{1}{2},$$

$$s_3 = \frac{2ik\sin(60^\circ-\varphi)}{g} = \frac{\sqrt{3}\,ik_y}{g} + \frac{1}{2}.$$

The corresponding probabilities are:

Probability that 3 replaces 1 = Probability that 3 replaces 2,

$$\left(\frac{3ky^2}{g^2} + \frac{9}{4}\right)^{-1}.$$

$$\text{Probability of no rearrangement} = \frac{(3k_y^2/g^2 + \frac{1}{4})}{(3k_y^2/g^2 + \frac{9}{4})}.$$

Note the following results of this rearrangement solution:

(1) There is no ionization, that is there is no amplitude for the final state of the system to be three free particles. This is intimately connected with the lack of diffraction in the free wave solutions.

(2) There is no reflection. If some particle is incident from the left in the initial state, some particle will be moving to the right in the final state with the same velocity as the initially incident particle.

(3) Even if the incident particle is moving toward the bound pair with an infinitesimal velocity, it has a probability of $\frac{1}{9}$ to transmit through the bound pair.

D. The Bound State of Three Particles

In addition to the free wave and rearranged solutions there is one totally bound state of the three particles. The condition for this state is that there be no incoming waves in any of the particles. This is achieved by imposing the further condition that $s_3 = -1$ on the rearranged solution. All of the outgoing waves then have equal amplitude. Their k vectors are pure imaginary and are pointed along the bisectors of the angles of the six wedges. Apart from the normalization factor, this wavefunction may be written as

$$\psi = n\exp\{-\sqrt{2}\,g[|x_1-x_2| + |x_2-x_3| + |x_1-x_3|]\},$$

where x_1, x_2, x_3 are the positions of the three particles along the one-dimensional line. This wavefunction is totally symmetric to the interchange of any pair of particles and its energy is $E = -\frac{1}{2}g^2$.

All of the properties of the outgoing wavefunction for the rearranged state and the bound state may be deduced directly from the S matrix by simply considering the behavior of the S matrix at the values of k for which it has a pole when it is analytically continued to complex or imaginary k. The discussion in this section was carried out in terms of the wavefunction for purposes of clarity, henceforth we shall discuss rearrangements and bound states from the analytically continued S matrix.[8]

V. N-PARTICLE SOLUTION

In this section we will show that the corresponding N-particle problem is exactly soluble, that is, the problem of an arbitrary number of particles of equal mass all interacting with one another via equal-strength delta-function potentials.

The Hamiltonian is

$$H = -\frac{\hbar^2}{2M}\sum_{i=1}^{N}\frac{d^2}{dx_i^2} + C\sum_{i>j=1}^{N}\sum\delta(x_i - x_j).$$

We will continue to use the units

$$\hbar = M = 1, \qquad \sqrt{2}\,C = -g.$$

[8] We should note here that there is a universal peculiarity bred into this problem which is retained in all of the problems we shall discuss subsequently. This peculiarity is that there are no bound-state solutions where any two particles are moving with zero relative velocity. From an inspection of the S matrix it would appear that the condition $s_1 = -1$, $s_3 = 0$, $s_2 = -1$ is also a state which has no incoming waves. If one applies this condition and looks at the wavefunction, one finds that it does not satisfy the boundary conditions on the delta-function surfaces. One can construct a wavefunction which does satisfy the boundary conditions on the delta-function surfaces by a careful limiting process, but this wavefunction increases exponentially at infinity in certain domains.

It is apparently quite impossible to continue to think of the N-particle problem as an equivalent one-particle problem in a multidimensional space, for the dimensionality of this equivalent space is $N - 1$. An alternative point of view exists, however, in which the difficulty of increasing dimensionality may be avoided.

Suppose we consider the space–time plot of a two-particle problem. The particles enter at some momentum which dictates the slope of the line in space–time. When the two particles collide they either transmit or reflect, but since no new velocities are generated, the space–time plot looks as shown in Fig. 7. If particle 1 started on the left and particle 2 on the right, then the transmission coefficient is the amplitude for particle 1 to come out on the right and particle 2 to come out on the left. The reflection coefficient is the amplitude for particle 1 to come out on the left and particle 2 to come out on the right.

We should remark here that there is no intention of changing our formulation of the many-particle problem from the stationary-state type to that of space–time. We intend only to argue that by interpreting the space–time plots we may derive all of the information which would be available in a ray tracing argument such as we used in Sec. IV.

Now let us consider the three-particle problem. There are two possible topologically different three-particle space–time diagrams which are again shown in Fig. 7. These two diagrams correspond exactly to the bifurcation of the incoming plane wave with which we dealt in the previous section. If the particles are ordered 1 2 3 from left to right, then the diagram on the left is the diagram which occurs when particle 1 strikes particle 2 first and the diagram on the right is the diagram which occurs when particle 2 strikes particle 3 first. It is now obvious that there is one collision at each of the three possible relative velocities and that there are exactly three collisions between incoming and outgoing waves. As a matter of fact even the "miraculous" property that $s_1 + s_3 = s_2$ is now evident because

$$s_1 = \sqrt{2}\, i(k_1 - k_2)/g,$$

$$s_3 = \sqrt{2}\, i(k_2 - k_3)/g;$$

thus

$$s_1 + s_3 = \sqrt{2}\, i(k_1 - k_3)/g = s_2.$$

What we have shown in the previous section is that, as far as the outgoing waves are concerned, it does not matter which of the two possible diagrams is used, for both give exactly the same result.

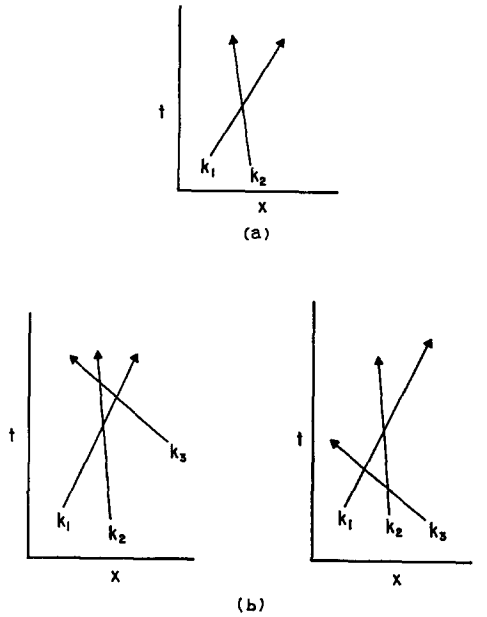

FIG. 7. Space–time plots for (a) two- and (b) three-particle problems.

If we were to change one of the particle masses or one of the delta-function strengths, the two diagrams would not give the same result and diffraction would occur.

In order to calculate the amplitude of the outgoing waves, let us invent two operators T_{ij}^{ll+1} and R_{ij}^{ll+1} which are to operate on some permutation of particles along the line. The indices $ll + 1$ label the position of an adjacent pair of particles which are interacting, and i and j label the k vectors with which the particles are interacting. The operator T interchanges the particle in the lth slot and the particle in the $l + 1$ slot with the amplitude t_{ij} where

$$t_{ij} = \frac{\sqrt{2}\, i(k_i - k_j)/g}{\sqrt{2}\, i(k_i - k_j)/g + 1} = \frac{s_{ij}}{s_{ij} + 1}.$$

The operator R leaves the same particles in the l and $l + 1$ slot, with the amplitude r_{ij} where

$$r_{ij} = -1/(s_{ij} + 1).$$

We denote the order of the particles by (1 3 2) meaning that particle 1 is in the first slot (that is, it is to the left of all of the other particles), particle 3 is in the second slot, and particle 2 is in the last slot. Thus, for example

$$T_{12}^{12}(132) = [s_{12}/(s_{12} + 1)](312),$$

$$R_{12}^{12}(132) = [-1/(s_{12} + 1)](132).$$

We use the three-particle diagrams of Fig. 7

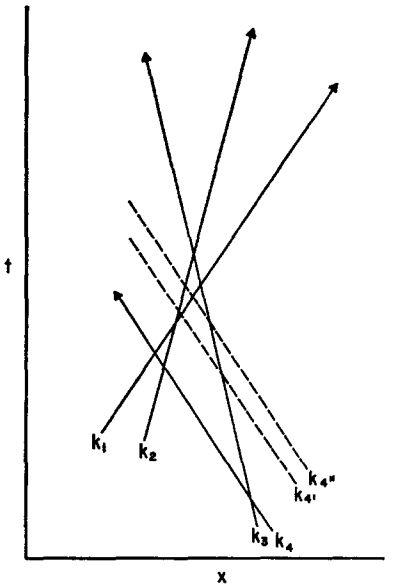

FIG. 8. Four-particle space-time plot.

to tell us in what order these operators work. For example the three-particle diagram on the left in Fig. 7 implies the order

$$(T_{23}^{12} + R_{23}^{12})(T_{13}^{23} + R_{13}^{23})(T_{12}^{12} + R_{12}^{12}),$$

which operates on some linear combination of the initial permutations of the three particles.

The three-particle diagram on the right in Fig. 7 implies the order

$$(T_{12}^{23} + R_{12}^{23})(T_{13}^{12} + R_{13}^{12})(T_{23}^{23} + R_{23}^{23}).$$

It is easily verified that these operators on any permutation of the particles give exactly the same result.

If we go on to four particles it will require fourteen diagrams to fill all space, and there will be six operator products going from incoming to outgoing states. We will now show that the outgoing waves are the same from each of the possible diagrams.

In order to do this let us start with a typical four-particle diagram such as the one shown in Fig. 8. This diagram implies the sequence of six operators

$$O_{24}^{23}\, O_{13}^{34}\, O_{12}^{23}\, O_{14}^{12}\, O_{24}^{23}\, O_{34}^{34},$$

where

$$O_{ij}^{ll+1} = T_{ij}^{ll+1} + R_{ij}^{ll+1}.$$

Suppose we now imagine moving the bottom line, that is, the k_4 line, up the page. We generate a new sequence when this line passes the collision between k_1 and k_2 indicated by the dotted line in Fig. 8. This second sequence of collisions gives exactly the same result as the first because all we have done is change the order of operators and the diagram in exactly the way we changed them in the three-body problem. If we continue to move the k_4 line up the page, another new sequence will be generated when the k_4 line reaches the position indicated by the second dotted line. This sequence involves an interchange of the operators O_{12}^{12} and O_{34}^{34} which commute because they have no slot in common. Thus this diagram gives exactly the same result as do the first two.

A continuation of this argument will show that every possible diagram contributes exactly the same outgoing waves. The argument does not depend on the number of particles, for all that is ever required is to move lines across intersections or to move intersections past commuting intersections. In order to show there is no diffraction, one must show that the amplitudes for every intermediate state which may be reached by more than one route are equal. The argument for these states proceeds in exactly the same way, and requires no more than the operators discussed above.

VI. N-PARTICLE CALCULATIONS

A. The Three-Particle Problem

We are now in a position to calculate amplitudes for various N-particle processes with relative ease. We could now draw some convenient sequence diagram with N k lines, write the appropriate operator sequence, and generate the S matrix by the operator rules of the preceding section. We know that we may pick any sequence whatever to generate the S matrix, for all sequences yield the same result. If it is desired to study scatterings in which particles are bound to one another we simply take ratios of elements of the S matrix where the elements are evaluated at the poles which correspond to the desired bound state.

In order to make the method more clear, let us redo the three-particle problem by the methods of Sec. V.

Let us evaluate the three-particle S matrix by using the space–time sequence diagram on the left in Fig. 7. We will assume that the incoming wave has the particles in the order (123) from left to right. Now

$$\begin{aligned} S(123) &= (T_{23}^{12} + R_{23}^{12})(T_{13}^{23} + R_{13}^{23})(T_{12}^{12} + R_{12}^{12})(123) \\ &= (T_{23}^{12} + R_{23}^{12})(T_{13}^{23} + R_{13}^{23})[t_{12}(213) + r_{12}(123)] \\ &= (T_{23}^{12} + R_{23}^{12})[t_{13}t_{12}(231) + r_{13}t_{12}(213) \end{aligned}$$

$$+ t_{13}r_{12}(132) + r_{13}r_{12}(123)]$$
$$= (t_{23}r_{13}t_{12} + r_{12}r_{13}r_{12})(123)$$
$$+ (r_{23}r_{13}t_{12} + t_{23}r_{13}r_{12})(213) + (r_{23}t_{13}r_{12})(132)$$
$$+ r_{23}t_{13}t_{12}(213) + t_{23}t_{13}r_{12}(312) + t_{23}t_{13}t_{12}(321),$$

if we let

$$s_{12} = s_1, \qquad s_{23} = s_3, \qquad s_{13} = s_2.$$

The elements above are exactly the same as the elements of the S matrix as given in Table II.

Of course, the other sequence diagram of Fig. 7 gives the same result. As we have seen previously, all of the scattering amplitudes for all possible processes as well as the bound-state energies may be calculated from analytic continuation of the S matrix.

The evaluation of S matrices for more particles is a straightforward but tedious process. We will consider here some processes whose amplitudes may be calculated without calculating the entire S matrix.

B. Four-Particle Processes

Suppose we consider the scattering of a pair of bound particles incident on a second bound pair of particles. We will denote the incoming state as

$$|(12)(34)\rangle$$

where the (12) indicates that particles one and two are bound and the order inside the "ket" indicates the order along the one dimension from left to right.

Let us first calculate the amplitude for the bound aggregates to pass through one another, that is, for the outgoing state to be

$$\langle(34)(12)|.$$

We know that the wavefunction is symmetric to the interchange of particles 1 and 2, for the single bound-state wavefunction of two particles bound by a delta-function potential is symmetric. If one of the particles has momentum k_1 and the other has momentum k_2 we know that

$$\sqrt{2}\, i(k_1 - k_2)/g = -1,$$

for this is the condition that the two particles be bound. Similarly the condition

$$\sqrt{2}\, i(k_3 - k_4)/g = -1$$

is the condition that particles 3 and 4 be bound. Let

$$\sqrt{2}\, i(k_2 - k_3)/g = s.$$

If the bound aggregate (12) is to pass through (34), clearly both particles 1 and 2 must transmit through particles 3 and 4. The amplitude for particle 2 to transmit through particle 3 is

$$\langle 32 \mid 23\rangle = \frac{\sqrt{2}\, i(k_2 - k_3)/g}{\sqrt{2}\, i(k_2 - k_3)/g + 1} = \frac{s}{s+1}.$$

The amplitude for 2 to transmit through 4 is

$$\langle 42 \mid 24\rangle = (s-1)/s.$$

Similarly,

$$\langle 31 \mid 13\rangle = (s-1)/s,$$
$$\langle 41 \mid 14\rangle = (s-2)/(s-1).$$

The amplitude for all four of these events is the product of their respective amplitudes and is the amplitude for the aggregate (12) to pass through the aggregate (34). Thus,

$$\langle(34)(12) \mid (12)(34)\rangle = (s-1)(s-2)/s(s+1).$$

Let us write this amplitude in terms of the energy in the center-of-mass system. By use of the formula in the Appendix which relates the energy to the s variables we can write

$$-4E_{tot}/g^2 = [s-1]^2 + 1.$$

The factor $+1$ on the right-hand side is just the binding energy of the two pairs of particles, and in this problem it is more convenient to represent the solution in terms of the kinetic energy of incidence of the bound aggregates in their center of mass; thus if we remove the binding energy term

$$-4E/g^2 = [s-1]^2,$$
$$s = 1 + 2iE^{\frac{1}{2}}/g.$$

The amplitude for transmission is then

$$\langle(34)(12) \mid (12)(34)\rangle = \frac{(2iE^{\frac{1}{2}}/g)(2iE^{\frac{1}{2}}/g - 1)}{(2iE^{\frac{1}{2}}/g + 1)(2 + 2iE^{\frac{1}{2}}/g)},$$

and the probability of transmission is

$$|\langle(34)(12) \mid (12)(34)\rangle|^2 = \frac{E/g^2}{E/g^2 + 1}.$$

So the probability for the (12) aggregate to pass through the (34) aggregate is zero at zero energy and monotonically increasing to unity at infinite energy.

We have several other possibilities for outgoing states. It is possible for one of the particles of the bound aggregate (12) to switch places with one of the bound particles of the aggregate (34). One way this could happen is for the first interaction to be a reflection and for the last three interactions to be

transmissions. Thus we have the amplitude

$$\langle(13)(24) \mid (12)(34)\rangle = (s-1)(s-2)/s^2(s+1),$$

which yields the probability

$$|\langle(13)(24) \mid (12)(34)\rangle|^2 = \frac{4E/g^2}{(4E/g^2+1)(4E/g^2+4)}.$$

This probability is zero both at zero and at infinite energy. It is a "resonance" probability having a maximum at $E = \frac{1}{2}g^2$ where the probability of the production of the $\langle(13)(24) \mid$ state is $\frac{1}{3}$.

There is no easy way to calculate the amplitude for the reflection of the (12) aggragate off the (34) aggregate; one must return to the sequence diagrams and analyze the S matrix at the appropriate poles. We will simply state the result

$$\langle(12)(34) \mid (12)(34)\rangle = 2(s-2)/s^2(s+1),$$

$$|\langle(12)(34) \mid (12)(34)\rangle|^2 = \frac{4}{(4E/g^2+1)(4E/g^2+4)}.$$

C. The Many-Particle Bound State

From the four-particle amplitudes worked out above, we can see that there is a four-particle bound state. Every element of the S matrix is proportional to $1/[s(s+1)]$; thus if we let $s = -1$ there are only outgoing waves, and we will have a bound state. It would also appear that $s = 0$ would give a bound state, but as we have seen in the three-particle case there are no solutions where two particles have zero relative velocity.

The condition for the four-particle bound state is

$$\frac{\sqrt{2}\,i(k_1-k_2)}{g} = \frac{\sqrt{2}\,i(k_2-k_3)}{g} = \frac{\sqrt{2}\,i(k_3-k_4)}{g} = -1.$$

One may show using the many-particle S matrix that the condition for an N-particle bound state is

$$\sqrt{2}\,i(k_j - k_{j+1})/g = -1 = s_j$$

for all j.

Using this condition we may evaluate the energy of the N-particle bound state using the formula derived in the Appendix which relates $k_i - k_{i+1}$ to the internal energy,

$$E = \frac{g^2}{4}\sum_{n=1}^{N-1}\frac{1}{n(n+1)}\left[\sum_{l=1}^{n} l s_l\right]^2 = -\tfrac{1}{48}(g^2)N(N^2-1).$$

There is no saturation; the energy decreases as N^3. The wavefunction is symmetric to the interchange of any pair of particles and the average density of particles in the vicinity of the center of mass is of the order of Ng.

D. Scattering of One-Particle by $N-1$ Bound Particles

As a final example of an N-body calculation let us consider the scattering of one free particle by $N-1$ bound particles. By the usual method the relation between s and kinetic energy in the center of mass is found to be

$$s = \frac{2iN^{\frac{1}{2}}E^{\frac{1}{2}}}{g(N-1)^{\frac{1}{2}}} + \frac{N-2}{2} = \frac{\sqrt{2}\,i(k_1-k_2)}{g}.$$

The amplitude for the incident particle to pass through the bound aggregate of $N-1$ particles is the product of its amplitude to pass through each particle individually, and is

$$\langle(2\cdots N)(1) \mid (1)(2\cdots N)\rangle = \left(\frac{s}{s+1}\right)\left(\frac{s-1}{s}\right)\left(\frac{s-2}{s-1}\right)\cdots\frac{[s-(N-2)]}{s-(N-3)}$$

$$= \frac{s-(N-2)}{s+1} = \frac{2i(NE)^{\frac{1}{2}}/g(N-1)^{\frac{1}{2}} - \frac{1}{2}(N-2)}{2i(NE)^{\frac{1}{2}}/g(N-1)^{\frac{1}{2}} + \frac{1}{2}N}.$$

The amplitude for the incident particle to replace one of the bound particles is the same for all bound particles, and is

$$\langle(13\cdots N)(2) \mid (1)(2\cdots N)\rangle = \langle(124\cdots N)(3) \mid (1)(2\cdots N)\rangle = \left(\frac{-1}{s+1}\right)\left(\frac{s-1}{s}\right)\cdots\frac{s-(N-2)}{s-(N-3)}$$

$$= \left[\frac{-1}{\dfrac{2i(NE)^{\frac{1}{2}}}{g(N-1)^{\frac{1}{2}}} + \frac{1}{2}N}\right]\left[\frac{\dfrac{2i(NE)^{\frac{1}{2}}}{g(N-1)^{\frac{1}{2}}} - \frac{1}{2}(N-2)}{\dfrac{2i(NE)^{\frac{1}{2}}}{g(N-1)} + \frac{1}{2}(N-2)}\right].$$

We noted previously that one of the peculiar things about the three-particle solution was that the amplitude for the incident particle to transmit through the bound aggregate was nonzero even at zero energy. Here we see that this transmission amplitude is always nonzero for one particle incident on $N-1$ particles, and in fact the amplitude to transmit approaches 1 for infinite N. Thus in the limit of large N nothing happens to the incident particle; it simply passes through this extremely dense bound aggregate as though it were not there.

VII. SUMMARY

In the Introduction we stated that one of our objectives in studying exactly soluble N-body prob-

lems was the illustration of physical effects. We have succeeded in this objective to some degree, for we have seen a number of the possible effects outlined in the Introduction. In the infinite-strength delta-function case we have seen particles redistribute their energy among the particles in a way which cannot be understood by a sequence of the two-body interactions. For infinite-strength delta functions we have illustrated the possibility of rearrangement of particles and the existence of N-particle bound states.

On the other hand we have not been able to illustrate any inelastic processes which involve disassociation or recombination of particles out of or into bound states. We have, however, learned to associate these processes with some generalization of diffraction processes in a multidimensional space. This multidimensional diffraction must be dealt with in any successful approximation method so at least in this sense we have provided some insight into the approximation methods which might be used in more physical problems. Moreover, we now have an exactly soluble problem involving a rearrangement of particles which can be used to check the existing approximation methods, and perhaps lead to a better understanding of the lack of convergence which seems to be implicit in problems of this type.[9]

Finally one must wonder about the statistical mechanics of a one-dimensional system of particles of equal mass which interact through equal-strength delta-function potentials. If the particles were bosons or distinguishable particles and the potentials attractive, the problem would make no sense, for the system would collapse into the N-particle bound state independent of temperature. The case of repulsive bosons has recently been worked out by Lieb[10] who, independent of this work, constructed the totally symmetric wavefunction for an arbitrary number of particles of equal mass interacting via finite-strength, repulsive delta-function potentials. The situation with attractive or repulsive fermions remains open and should prove to be an interesting area of further research.

ACKNOWLEDGMENTS

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APPENDIX. DISCUSSION OF COORDINATE SYSTEMS FOR N-BODY PROBLEMS

Consider an N-body Hamiltonian of the form

$$H = -\frac{\hbar^2}{2}\sum_{i=1}^{N}\frac{1}{M_i}\frac{\partial^2}{\partial x_i^2} + \sum_{j>i}^{N}\sum v_{ij}(x_i - x_j).$$

We will take the x_i to be one-dimensional variables, but the results we derive will be independent of dimensionality and may be extended to more dimensions by simply substituting the vector quantities ∇_i^2 for $\partial^2/\partial x_i^2$ and $\mathbf{x}_i$ for x_i.

We wish to make a change of variables which will allow us to separate out the center of mass of the entire system. In addition we will find that a more unified view of N-body problems is attained if we pick a "rationalized" coordinate system so that the second derivative terms in the new variables all have the same coefficient. The following has been shown to be such a coordinate system[11,12]:

$$z_1 = \frac{(M_1M_2)^{\frac{1}{2}}}{(M_1 + M_2)^{\frac{1}{2}}}(x_1 - x_2),$$

$$z_2 = \frac{M_3^{\frac{1}{2}}(M_1 + M_2)^{\frac{1}{2}}}{(M_1 + M_2 + M_3)^{\frac{1}{2}}}\left(\frac{M_1x_1 + M_2x_2}{M_1 + M_2} - x_3\right),$$

$$z_n = \frac{M_{n+1}^{\frac{1}{2}}\left(\sum_{i=1}^{n} M_i\right)^{\frac{1}{2}}}{\left(\sum_{i=1}^{n+1} M_i\right)^{\frac{1}{2}}}\left[\frac{\sum_{i=1}^{n} M_ix_i}{\sum_{i=1}^{n} M_i} - x_{n+1}\right], \quad n < N,$$

$$z_N = \sum_{i=1}^{N} M_ix_i \Big/ \left(\sum_{i=1}^{N} M_i\right)^{\frac{1}{2}}.$$

Pick the first new coordinate to be the relative coordinate between any two particles multiplied by the square root of the reduced mass of those two particles. Pick the second new coordinate to be the coordinate of a third particle relative to the center of mass of the first two multiplied by the square root of the reduced mass of particle three and the sum of the masses of the first two, etc. The last coordinate is the center of mass of the whole system multiplied by the square root of the sum of the masses.

We can verify that this transformation has the property that the coefficients of the new second-derivative terms are equal by observing that the transformation between z and x can be written as an orthogonal matrix times a diagonal matrix, where

[9] R. Aaron, R. D. Amado, and B. W. Lee, Phys. Rev. 121, 319 (1961).

[10] E. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).

[11] D. W. Jepsen and J. O. Hirschfelder, Proc. Natl. Acad. Sci. U. S. 45, 249 (1959).

[12] J. O. Hirschfelder and J. S. Dahler, Proc. Natl. Acad. Sci. U. S. 42, 363 (1956).

the elements of the diagonal matrix are the square roots of the masses of the particles. That is,

$$z = UM^{\frac{1}{2}}x,$$

where

$$M^{\frac{1}{2}} = M_i^{\frac{1}{2}}\delta_{ij},$$

and

$$U_{ni} = (M_{n+1}^{\frac{1}{2}})(M_i^{\frac{1}{2}})\Big/\Big(\sum_{j=1}^{n+1} M_j\Big)^{\frac{1}{2}}\Big(\sum_{j=1}^{n} M_j\Big)^{\frac{1}{2}}, \quad N > n \geq i,$$

$$U_{nn+1} = -\Big[\Big(\sum_{j=1}^{n} M_j\Big)^{\frac{1}{2}}\Big/\Big(\sum_{j=1}^{n+1} M_j\Big)^{\frac{1}{2}}, \qquad N > n,$$

$$U_{Ni} = M_i^{\frac{1}{2}}\Big/\Big(\sum_{j=1}^{N} M_j\Big)^{\frac{1}{2}},$$

$$U_{ni} = 0, \qquad i > n + 1.$$

The operator $\partial/\partial x$ transforms by the rule

$$\partial/\partial x = (M^{\frac{1}{2}}U')\,\partial/\partial z.$$

Thus the quadratic form

$$\Big(\frac{\partial}{\partial x}\Big)'(M)^{-1}\frac{\partial}{\partial x} = \sum_{i=1}^{N}\frac{1}{M_i}\frac{\partial^2}{\partial x_i^2}$$

$$= \Big(\frac{\partial}{\partial z}\Big)'UM^{\frac{1}{2}}(M)^{-1}M^{\frac{1}{2}}U'\frac{\partial}{\partial z} = \sum_{i=1}^{N}\frac{\partial^2}{\partial z_i^2}.$$

To find the arguments of the potentials we invert the transformation between x and z for form $x_i - x_j$. The result is

$$x_i - x_j = \Big(\frac{M_i + M_j}{M_iM_j}\Big)^{\frac{1}{2}} \times \Bigg[\sum_{n=i}^{j-2}\frac{(M_iM_j)^{\frac{1}{2}}}{(M_i + M_j)^{\frac{1}{2}}}\frac{M_{n+1}^{\frac{1}{2}}}{\Big(\sum_{l=1}^{n} M_l\Big)^{\frac{1}{2}}\Big(\sum_{l=1}^{n+1} M_l\Big)^{\frac{1}{2}}}z_n + \frac{\Big(\sum_{l=1}^{j} M_l\Big)^{\frac{1}{2}}M_j^{\frac{1}{2}}}{(M_i + M_j)^{\frac{1}{2}}\Big(\sum_{l=1}^{j-1} M_l\Big)^{\frac{1}{2}}}z_{j-1}$$

$$- \frac{M_i^{\frac{1}{2}}\Big(\sum_{l=1}^{i-1} M_l\Big)^{\frac{1}{2}}}{(M_i + M_j)^{\frac{1}{2}}\Big(\sum_{l=1}^{i} M_l\Big)^{\frac{1}{2}}}z_{i-1}\Bigg].$$

The factor of the square root of the reduced mass is introduced so that the sum of the squares of the coefficients of the z's add up to unity. These coefficients may be looked at as the "direction cosines" of the potential in the multidimensional space.

Another result which we shall find useful is the transformation law between momenta in the two systems. This transformation is

$$\partial/\partial z = [U(M^{\frac{1}{2}})^{-1}]\,\partial/\partial x,$$

$$P_z = U(M^{\frac{1}{2}})^{-1}P_x,$$

which leads to

$$P_{z_n} = \frac{M_{n+1}^{\frac{1}{2}}}{\Big(\sum_{i=1}^{n+1} M_i\Big)^{\frac{1}{2}}\Big(\sum_{n=1}^{n} M_i\Big)^{\frac{1}{2}}}\sum_{i=1}^{n}(P_{x_i} - P_{x_{n+1}}), \qquad n < N.$$

The total energy of internal motion is

$$E = \frac{\hbar^2}{2}\sum_{n=1}^{N-1} P_{z_n}^2.$$

We shall need to calculate this energy for the case when all of the masses are equal. For convenience we set $h = 1$ and $M = 1$. This leads to

$$E = \frac{1}{2}\sum_{n=1}^{N-1}\Bigg[\frac{1}{n^{\frac{1}{2}}(n+1)^{\frac{1}{2}}}\sum_{i=1}^{n}(P_{x_i} - P_{x_{n+1}})\Bigg]^2,$$

which can be written

$$E = \frac{1}{2}\sum_{n=1}^{N-1}\frac{1}{n(n+1)}\Bigg[\sum_{i=1}^{n} ik_i\Bigg]^2,$$

where

$$k_i = P_{x_i} - P_{x_{i+1}}.$$

Application of Nonlocal Field Operators to a System of Hard-Sphere Bose Gas*†

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Some relationships of the nonlocal field operators developed by Siegert *et al.* and the usual free-field operators are obtained. The interaction Hamiltonian derived with the help of these relationships is compared with the pseudopotential recently obtained by Liu and Wong. A study of the fluid dynamical equations at extreme low temperature has been made.

1. INTRODUCTION

RECENTLY Aizu, Dell'Antonio, and Siegert[1,2] have developed a new algebra for bosons interacting as hard spheres. The field operators of their new algebra do not have usual commutation rules. In this paper we have developed some relationships between their nonlocal and the usual field operators. These relationships were then used to obtain the pseudopotential of the many-particle system. It is found that the present method gives the same form of pseudopotential derived by Liu and Wong recently, except for the presence of a projection operator. The purpose of the projection operator is to eliminate those solutions where the Liu and Wong pseudopotential alone does not replace the hard-sphere interaction. These particular solutions were shown clearly in the two-body problem by Liu and Wong[3] [Eq. (27)]. If we expand the projection operator in a free-field-operator representation, we will obtain terms of the nature that can be called three-body and higher-body pseudopotentials. We must however keep in mind that there are many ways in which we can expand the projection operator. Therefore, the form of the higher-body pseudopotentials are actually not unique, and hence not meaningful to be considered separately.

In Sec. 2 we derive some algebraic relationships between A–D–S field operators and the usual field operators. The derivation of the generalized many-body pseudopotential form the main part of Sec. 3. A comparison of the Liu and Wong pseudopotential and the present many-body pseudopotential is also given. In Sec. 4 we rederive the equation of motion of a free-field operator, previously obtained by A–D–S with a slight difference, the difference being that A–D–S consider the equation of motion of a nonlocal field operator, whereas we consider the equation of motion of a usual free-field operator. In the last section, Sec. 5, we study the dynamical equations of a superfluid at extreme low temperature. It is found that instead of purely a continuity equation we have an extra term similar in form to the Boltzmann equation. This is reasonable because the collision of the particles will give rise to a change of the occupation number of the degenerate state of the system. The superfluid equation obtained with the present pseudopotential is also a modification of the London[4] equation. We have a frictional-force term from the surface interaction between spheres. The importance of the presence of these extra terms obviously depend on the density of the system. It is clear that such terms will not arise if we use the Lee, Huang, and Yang[5] pseudopotential. A study of the solutions of these hydrodynamical equations using the L–H–Y pseudopotential has already been done by Wu.[6] In this paper we do not repeat his work.

2. ALGEBRA FOR THE NONLOCAL FIELD OPERATORS

In this section we repeat some algebraic identities which are in A–D–S for the sake of completeness and convenience, since most of these identities will be used in the later sections.

In order to solve a many-particle system with impenetrable spherical core, diameter a, we have essentially to solve the many-particle Schrödinger equation with the interparticle boundary conditions

$$\Phi_N(\mathbf{x}_1, \cdots, \mathbf{x}_N; \nu_N) = 0; \qquad |\mathbf{x}_i - \mathbf{x}_j| \leq a$$

and

$$\lim_{|\mathbf{x}_i - \mathbf{x}_j| \to a} \Phi_N(\mathbf{x}_1, \cdots, \mathbf{x}_N; \nu_N) \to 0,$$

for any pair of position vectors $\mathbf{x}_i$, $\mathbf{x}_j$ and energy

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† Part of this work was submitted as a Ph. D. dissertation at Northwestern University.

[1] A. J. F. Siegert, Phys. Rev. **116**, 1057 (1959).

[2] K. Aizu, G. Dell'Antonio, and A. J. F. Siegert (private communication), herein referred to as A–D–S.

[3] L. Liu and K. W. Wong, Phys. Rev. **132**, 1349 (1963).

[4] F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II, pp. 129–130.

[5] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957), herein referred to as L–H–Y.

[6] T. T. Wu, J. Math. Phys. **2**, 105 (1961).

$E(\nu_N)$. Siegert[1] has shown that we can define a nonlocal field operator in Fock's representation by its matrix element:

$$\langle \nu_{N-1} | \psi(\mathbf{x}) | \nu_N \rangle = N^{\frac{1}{2}} \int \prod_{i=1}^{N-1} d^3x_i \Phi^*_{N-1}(q_{N-1}; \nu_{N-1}) \times \Phi_N(q_{N-1}\mathbf{x}; \nu_N), \quad (2.1)$$

where

$$q_{N-1} \equiv \mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_{N-1}.$$

It is clear that the nonlocal operators span a closed linear subspace H_R, where all configuration coordinates $|\mathbf{x}_i - \mathbf{x}_j| > a$ of the Hilbert space H. There exists a linear mapping $H \to H$ such that the nonlocal field operators can be defined in terms of the standard free-field operators $\psi_0(\mathbf{x})$, $\psi^*_0(\mathbf{x})$ as follows:

$$\begin{aligned} \psi(\mathbf{x}) &\equiv P(\mathbf{x})\psi_0(\mathbf{x}), \\ \psi^*(\mathbf{x}) &\equiv \psi^*_0(\mathbf{x})P(\mathbf{x}), \end{aligned} \quad (2.2)$$

where $P(\mathbf{x})$ is a projection operator

$$P(\mathbf{x}) \equiv \sum_{N=0}^{\infty} \int \prod_{i}^{N} d^3x_i C(\mathbf{x}q_N) P_N(q_N), \quad (2.3)$$

and $C(\mathbf{x}q_N)$ is a step function,

$$\begin{aligned} C(\mathbf{x}q_N) &\equiv C(\mathbf{x}\mathbf{x}_1) \cdots C(\mathbf{x}\mathbf{x}_N) C(\mathbf{x}_1\mathbf{x}_2) \cdots \\ &\quad \times C(\mathbf{x}_1\mathbf{x}_N) \cdots C(\mathbf{x}_{N-1}\mathbf{x}_N), \\ C(\mathbf{x}_i\mathbf{x}_j) &= \begin{cases} 1 & |\mathbf{x}_i - \mathbf{x}_j| > a, \\ 0 & \text{otherwise}, \end{cases} \\ C(0) &= C(\mathbf{x}) = 1, \end{aligned} \quad (2.4)$$

$$P_N(q_N) \equiv (N!)^{-1} \prod_{i=1}^{N} \psi^*_0(\mathbf{x}_i) |0\rangle\langle 0| \prod_{i=1}^{N} \psi_0(\mathbf{x}_i). \quad (2.5)$$

For later convenience we shall rewrite $P(\mathbf{x})$ in the following form:

$$P(\mathbf{x}) \equiv P + \Lambda(\mathbf{x}), \quad (2.6)$$

where

$$P \equiv \sum_{N=0}^{\infty} \int \prod_{i}^{N} d^3x_i C(q_N) P_N(q_N), \quad (2.7)$$

and

$$\Lambda(\mathbf{x}) \equiv \sum_{l=1}^{M} \frac{(-)^l}{l!} \int \cdots \int_{S_{\mathbf{x}}} \prod_{i=1}^{l} \psi^*(\mathbf{x}_i) \times \prod_{i=1}^{l} \psi(\mathbf{x}_i)\, d^3x_i, \quad (2.8)$$

where M is the maximum number of particles of diameter $a + \epsilon$ ($\epsilon > 0 \to 0$) one can pack into a sphere of diameter $3a$, and $S_{\mathbf{x}}$ is the volume bounded by the surface $|\mathbf{x} - \mathbf{x}_i| = \lim_{\epsilon \to 0} a + \epsilon$. Equation (2.6) has already been proven in A–D–S. However, we shall give in our opinion a much more straightforward proof in Appendix A. It is now straightforward to show the following algebraic identities:

$$\begin{aligned} &PP(\mathbf{x}) = P(\mathbf{x}); \qquad P\Lambda(\mathbf{x}) = \Lambda(\mathbf{x}), \\ &\Lambda^n(\mathbf{x}) = (-)^{n+1}\Lambda(\mathbf{x}), \qquad n \geq 1, \\ &[P(\mathbf{x}), P(\mathbf{x}')] = [\Lambda(\mathbf{x}), \Lambda(\mathbf{x}')] = 0, \\ &\psi_0(\mathbf{y})P(\mathbf{x}) = C(\mathbf{x}\mathbf{y})P(\mathbf{x})P(\mathbf{y})\psi_0(\mathbf{y}), \\ &P(\mathbf{x})\psi^*_0(\mathbf{y}) = C(\mathbf{x}\mathbf{y})\psi^*_0(\mathbf{y})P(\mathbf{y})P(\mathbf{x}), \end{aligned} \quad (2.9)$$

and commutation rules

$$\begin{aligned} &[\psi(\mathbf{x}), \psi(\mathbf{x}')] = [\psi^*(\mathbf{x}), \psi^*(\mathbf{x}')] = 0, \\ &\psi(\mathbf{x})\psi(\mathbf{x}') = 0 \quad \text{for} \quad |\mathbf{x} - \mathbf{x}'| \leq a, \\ &\psi(\mathbf{x})\psi^*(\mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')P(\mathbf{x}) \quad \text{for} \quad |\mathbf{x} - \mathbf{x}'| < a. \end{aligned} \quad (2.10)$$

For other properties of these nonlocal field operators, we refer the reader to A–D–S.

3. THE MANY-BODY PSEUDOPOTENTIAL

From the definition of the nonlocal field operators given by Eq. (2.1), and using the unit $\hbar = 1, 2m = 1$, we can simply write the many-body Hamiltonian with periodic boundary conditions as follows:

$$H = -\int d^3x \psi^*(\mathbf{x}) \nabla^2 \psi(\mathbf{x}). \quad (3.1)$$

Using the algebraic identities (2.2), (2.6), and (2.8), we obtain

$$\begin{aligned} H = &-\int d^3x \psi^*_0(\mathbf{x}) \nabla^2 P(\mathbf{x}) \psi_0(\mathbf{x}) \\ &+ \int d^3x' \oint^{\mathbf{x}'} d\sigma_{\mathbf{x}} \psi^*_0(\mathbf{x}) \psi^*_0(\mathbf{x}') \\ &\times \frac{\mathbf{x} - \mathbf{x}'}{a^2} \cdot \nabla |\mathbf{x} - \mathbf{x}'| P(\mathbf{x}')P(\mathbf{x})\psi_0(\mathbf{x}')\psi_0(\mathbf{x}). \end{aligned} \quad (3.2)$$

The proof of Eq. (3.2) is given in Appendix B.

Since

$$\begin{aligned} &\int d^3x' \oint^{\mathbf{x}'} d\sigma_{\mathbf{x}} f(\mathbf{x} - \mathbf{x}') \frac{\mathbf{x} - \mathbf{x}'}{a} \cdot (\nabla - \nabla') g(\mathbf{x} - \mathbf{x}') \\ &= \lim_{\epsilon \to 0} 2 \int d^3x\, d^3x' f(\mathbf{x} - \mathbf{x}')\, \delta(|\mathbf{x} - \mathbf{x}'| - a) \\ &\quad \times \left[\frac{\partial}{\partial |\mathbf{x} - \mathbf{x}'|} g(\mathbf{x} - \mathbf{x}') \right]_{|\mathbf{x} - \mathbf{x}'| = a + \epsilon}, \end{aligned} \quad (3.3)$$

where ϵ is *positive*, we can rewrite H as

$$H = -\int d^3x \psi_0^*(\mathbf{x})\nabla^2 P(\mathbf{x})\psi_0(\mathbf{x}) + \lim_{\epsilon\to 0}\frac{1}{a}\int d^3x\, d^3x' \psi_0^*(\mathbf{x})\psi_0^*(\mathbf{x}')\,\delta(r-a) \times \left[\frac{\partial}{\partial r} rP(\mathbf{x})P(\mathbf{x}')\psi_0(\mathbf{x}')\psi_0(\mathbf{x})\right]_{r=a+\epsilon}, \quad (3.4)$$

with $r \equiv |\mathbf{x} - \mathbf{x}'|$ and $\partial/\partial r$ defined with $\mathbf{x} + \mathbf{x}'$ fixed. This many-body Hamiltonian is very much similar in form to the Hamiltonian given by Liu and Wong[3] (Eq. 3.2). The main difference between the two forms is the presence of the projection operator $P(\mathbf{x})$ in (3.4). Actually, Liu and Wong have already mentioned in their work that their form of the pseudopotential does not replace the hard-core interaction for all scattering energy of the system.

It is clear that in order to replace the hard-core interaction we need, in addition to the Liu and Wong pseudopotential, a projection operator which will force the wavefunction to vanish inside the core. We can expand the projection operator in some specific representation; however, it has been shown clearly by Liu and Wong that the projection operator actually only affects a discrete set of scattering energy. Hence, a poor choice of expansion of $P(\mathbf{x})$ will not only not improve the quantitative calculation of a many-body system, but may actually make the problem meaningless. We might be able to choose a projection operator in momentum representation which will give the exact solution for a two-body problem, but such a projection operator cannot be extended to the many-body system. It may seem to be possible to obtain complicated many-body pseudopotentials by expanding $P(\mathbf{x})$ in some specific representation. However, as we have said before, the form of $P(\mathbf{x})$ is not unique and it acts only on a discrete set of solutions superimposed on a continuum. Any pseudopotential obtained this way has no physical meaning and is not unique.

4. THE NONEQUILIBRIUM BOSE GAS

In order to study the motion of a single hard-core Bose particle put into a system of hard-core Bose gas at equilibrium and nearly completely degenerated into the zero-momentum single-particle state, we shall have to define the time-dependent nonlocal field operator also by its matrix elements, and assume a time-dependent state function $\varphi(\mathbf{x}t)$ for the single particle:

$$\langle \nu_{N-1}\,|\psi(\mathbf{x}t)|\,\nu_N\rangle = N^{\frac{1}{2}}\int \prod_{j=1}^{N-1} d^3x_j \Phi_{N-1}^*(q_{N-1};\nu_{N-1}t) \times \Phi_N(q_{N-1}\mathbf{x};\nu_N t). \quad (4.1)$$

where $\Phi_N(q_N;\nu_N t)$ is the symmetrized time-dependent many-particle wavefunction satisfying hard-core boundary conditions.

It is easy to show that the algebraic relationships derived in Sec. 2 are also valid in the time-dependent case. Hence, it is straightforward to show that the Hamiltonian can be written in the following form:

$$H = -\int d^3x \psi_0^*(\mathbf{x}t)\nabla^2 P(\mathbf{x}t)\psi_0(\mathbf{x}t) + \lim_{\epsilon\to 0}\frac{1}{a}\int d^3x\, d^3x' \psi_0^*(\mathbf{x}t)\psi_0^*(\mathbf{x}'t)\,\delta(r-a) \times \left[\frac{\partial}{\partial r} rP(\mathbf{x}'t)P(\mathbf{x}t)\psi_0(\mathbf{x}'t)\psi_0(\mathbf{x}t)\right]_{r=a+\epsilon}. \quad (4.2)$$

The equation of motion of the field operator $\psi_0(\mathbf{x}t)$ is therefore

$$i\frac{\partial}{\partial t}\psi_0(\mathbf{x}t) = -\nabla^2 P(\mathbf{x}t)\psi_0(\mathbf{x}t) + \lim_{\epsilon\to 0}\frac{2}{a}\int d^3x' \psi_0^*(\mathbf{x}'t)\,\delta(r-a) \times \left[\frac{\partial}{\partial r} rP(\mathbf{x}'t)P(\mathbf{x}t)\psi_0(\mathbf{x}'t)\psi_0(\mathbf{x}t)\right]_{r=a+\epsilon} - \int d^3x' \psi_0^*(\mathbf{x}'t)\nabla'^2 P(\mathbf{x}'t)\psi_0(\mathbf{x}'t) \times (P(\mathbf{x}t)-1)\psi_0(\mathbf{x}t) + \lim_{\epsilon\to 0}\frac{1}{a}\int d^3x'\, d^3x'' \times \psi_0^*(\mathbf{x}'t)\psi_0^*(\mathbf{x}''t)\,\delta(r'-a) \times \left[\frac{\partial}{\partial r'} r'P(\mathbf{x}''t)P(\mathbf{x}'t)\psi_0(\mathbf{x}''t)\psi_0(\mathbf{x}'t)\right]_{r'=a+\epsilon} \times (P(\mathbf{x}t)-1)\psi_0(\mathbf{x}t), \quad (4.3)$$

where

$$r' \equiv |\mathbf{x}' - \mathbf{x}''|.$$

The equation of motion of a physical field operator given in A–D–S differs from the equation of motion of a usual free-field operator given by the above equation in the presence of the term

$$-\int d^3x' \psi_0^*(\mathbf{x}'t)\nabla'^2 P(\mathbf{x}'t)\psi_0(\mathbf{x}'t)(P(\mathbf{x}t)-1)\psi_0(\mathbf{x}t) + \lim_{\epsilon\to 0}\frac{1}{a}\int d^3x'\, d^3x'' \psi_0^*(\mathbf{x}'t)\psi_0^*(\mathbf{x}''t)\,\delta(r'-a) \times \left[\frac{\partial}{\partial r'} r'P(\mathbf{x}''t)P(\mathbf{x}'t)\psi_0(\mathbf{x}''t)\psi_0(\mathbf{x}'t)\right]_{r'=a+\epsilon} \times (P(\mathbf{x}t)-1)\psi_0(\mathbf{x}t). \quad (4.4)$$

It is quite clear that this term will be important only when we have a densely packed system, where

we have to take into account instantaneous many-particle scattering processes. For our present purpose, we shall consider a dilute Bose gas and replace $P(\mathbf{x}t)$ by unity, which is equivalent to using the Liu and Wong pseudopotential. The equation of motion (4.3) reduces to

$$i\frac{\partial}{\partial t}\psi_0(\mathbf{x}t) = -\nabla^2\psi_0(\mathbf{x}t) + \lim_{\epsilon\to 0}\frac{2}{a}\int d^3x'\psi_0^*(\mathbf{x}'t)\,\delta(r-a) \times\left[\frac{\partial}{\partial r}r\psi_0(\mathbf{x}'t)\psi_0(\mathbf{x}t)\right]_{r=a+\epsilon}. \tag{4.5}$$

Let us consider the case where the degeneracy into the single-particle state is nearly complete. The parts of ψ_0^* and ψ_0 corresponding to this one state may be singled out:

$$\begin{aligned}\psi_0^*(\mathbf{x}t) &= \psi_0^{*0}(\mathbf{x}t) + \psi_0^{*'}(\mathbf{x}t),\\ \psi_0(\mathbf{x}t) &= \psi_0^0(\mathbf{x}t) + \psi_0'(\mathbf{x}t),\end{aligned} \tag{4.6}$$

where

$$\begin{aligned}\psi_0^{*0}(\mathbf{x}t) &= \Omega^{-\frac{1}{2}}a_0^*(t)\varphi^*(\mathbf{x}t),\\ \psi_0^0(\mathbf{x}t) &= \Omega^{-\frac{1}{2}}a_0(t)\varphi(\mathbf{x}t),\end{aligned} \tag{4.7}$$

and Ω is the volume of the box, $\varphi(\mathbf{x}t)$ is the single-particle wavefunction, such that $a_0^*(t)$ and $a_0(t)$ are defined as follows:

$$\begin{aligned}a_0^*(t) &= \Omega^{-\frac{1}{2}}\int d^3x\psi_0^*(\mathbf{x}t)\varphi(\mathbf{x}t),\\ a_0(t) &= \Omega^{-\frac{1}{2}}\int d^3x\psi_0(\mathbf{x}t)\varphi^*(\mathbf{x}t).\end{aligned} \tag{4.8}$$

In the present approximation, we shall restrict ourselves to consider only the degenerate single-particle state. The equation of motion of this state is therefore

$$i\frac{\partial}{\partial t}a_0(t)\varphi(\mathbf{x}t) \cong -a_0(t)\nabla^2\varphi(\mathbf{x}t) + \lim_{\epsilon\to 0}\rho_0(t)a_0(t)\frac{2}{a}\int d^3x'\varphi^*(\mathbf{x}'t)\,\delta(r-a) \times\left[\frac{\partial}{\partial r}r\varphi(\mathbf{x}'t)\varphi(\mathbf{x}t)\right]_{r=a+\epsilon}, \tag{4.9}$$

where

$$\begin{aligned}\rho_0(t) &= N_0(t)/\Omega,\\ N_0(t) &= a_0^*(t)a_0(t).\end{aligned} \tag{4.10}$$

Equation (4.9) can be rewritten as

$$ia_0(t)\frac{\partial}{\partial t}\varphi(\mathbf{x}t) \cong -i\varphi(\mathbf{x}t)\frac{\partial}{\partial t}a_0(t) - a_0(t)\nabla^2\varphi(\mathbf{x}t) + \lim_{\epsilon\to 0}\rho_0(t)a_0(t)\frac{2}{a}\int d^3x'\varphi^*(\mathbf{x}'t) \times\delta(r-a)\left[\frac{\partial}{\partial r}r\varphi(\mathbf{x}'t)\varphi(\mathbf{x}t)\right]_{r=a+\epsilon}. \tag{4.11}$$

Even in the present approximation, we observed that the equation of motion of the single-particle wavefunction is a nonlinear integro-differential equation, whereas the same equation obtained by using the L–H–Y pseudopotential is much simpler. Wu[6] has obtained this equation using the L–H–Y pseudopotential. Making use of the Hamiltonian given by (4.2) we obtain

$$i[\partial a_0(t)/\partial t] = \bar{\mathfrak{I}}(t)a_0(t) + 4\pi a\mathfrak{I}(t)\rho_0(t)a_0(t), \tag{4.12}$$

where

$$\bar{\mathfrak{I}}(t) = \Omega^{-1}\int d^3x\,|\nabla\varphi(\mathbf{x}t)|^2, \tag{4.13}$$

and

$$\mathfrak{I}(t) = \lim_{\epsilon\to 0}\Omega^{-1}\frac{1}{2\pi a^2}\int d^3x\,d^3x'\varphi^*(\mathbf{x}t)\varphi^*(\mathbf{x}'t) \times\delta(r-a)\left[\frac{\partial}{\partial r}r\varphi(\mathbf{x}'t)\varphi(\mathbf{x}t)\right]_{r=a+\epsilon}. \tag{4.14}$$

The equation of motion for the single-particle wavefunction $\varphi(\mathbf{x}t)$ can now be written in a form similar to Wu's:

$$i\frac{\partial\varphi(\mathbf{x}t)}{\partial t} = [-\nabla^2 - 4\pi a\rho_0(t)\mathfrak{I}(t) - \bar{\mathfrak{I}}(t)]\varphi(\mathbf{x}t) + \lim_{\epsilon\to 0}\frac{2}{a}\rho_0(t)\int d^3x'\varphi^*(\mathbf{x}'t)\,\delta(r-a) \times\left[\frac{\partial}{\partial r}r\varphi(\mathbf{x}'t)\varphi(\mathbf{x}t)\right]_{r=a+\epsilon}. \tag{4.15}$$

The present equation differs from Wu's mainly in that we have an integro-differential, equation whereas he has a differential equation. We shall show in the next section that this difference gives some extra terms which have physical meaning.

5. DYNAMICAL EQUATIONS OF A SUPERFLUID

The dynamical properties of a dilute hard-core Bose gas at extremely low temperature are contained in Eq. (4.15).

Let us rewrite $\varphi(\mathbf{x}t)$ in a form that will be more convenient:

$$\varphi(\mathbf{x}t) = A(\mathbf{x}t)e^{i\theta(\mathbf{x}t)}, \tag{5.1}$$

where $A(\mathbf{x}t)$ and $\theta(\mathbf{x}t)$ are real functions.

The velocity of a particle is usually defined as

$$\mathbf{v}(\mathbf{x}t) = i(\varphi\nabla\varphi^* - \varphi^*\nabla\varphi)/\varphi^*\varphi = 2\nabla\theta(\mathbf{x}t). \tag{5.2}$$

From this definition of $\mathbf{v}$ it follows that the fluid is irrotational.

The number density of the fluid is given by

$$\rho(\mathbf{x}t) = \rho_0(t)A^2(\mathbf{x}t). \tag{5.3}$$

Considering the imaginary and real parts of Eq. (4.15), we have

$$(\partial/\partial t)A(\mathbf{x}t) = -(\nabla^2\theta)A - 2(\nabla\theta)\cdot(\nabla A) + \operatorname{Im}\mathfrak{L}, \tag{5.4}$$

and

$$-\left(\frac{\partial}{\partial t}\,\theta(\mathbf{x}t)\right)A(\mathbf{x}t) = -\nabla^2 A - 4\pi a\rho_0(t)\mathfrak{z}(t)A + (\nabla\theta)^2 A - \bar{\mathfrak{z}}(t)A + \operatorname{Re}\mathfrak{L}, \tag{5.5}$$

where

$$\mathfrak{L}(\mathbf{x}t) = \lim_{\epsilon\to 0}\frac{2}{a}\,\rho_0(t)\int d^3x' A(\mathbf{x}'t)\,\delta(r-a) \times \{A(\mathbf{x}'t)A(\mathbf{x}t) + aA(\mathbf{x}t)\partial' A(\mathbf{x}'t) + aA(\mathbf{x}'t)\partial A(\mathbf{x}t) + iaA(\mathbf{x}'t)A(\mathbf{x}t)[\partial\theta(\mathbf{x}t) + \partial'\theta(\mathbf{x}'t)]\}_{r=a+\epsilon}. \tag{5.6}$$

The prime indicates the variable $\mathbf{x}'$.

It is now straightforward to show that from Eq. (5.4) we obtain

$$\frac{\partial\rho(\mathbf{x}t)}{\partial t} = A^2(\mathbf{x}t)\,\frac{\partial\rho_0(t)}{\partial t} - \nabla\cdot\rho(\mathbf{x}t)\mathbf{v}(\mathbf{x}t) + 2\rho_0(t)A(\mathbf{x}t)\operatorname{Im}\mathfrak{L}(\mathbf{x}t). \tag{5.7}$$

Equation (5.7) gives the well known Equation of Continuity, except for an extra term

$$A^2(\mathbf{x}t)[\partial\rho_0(t)/\partial t] + 2\rho_0(t)A(\mathbf{x}t)\operatorname{Im}\mathfrak{L}(\mathbf{x}t),$$

where

$$2\rho_0(t)A(\mathbf{x}t)\operatorname{Im}\mathfrak{L}(\mathbf{x}t) = \lim_{\epsilon\to 0}\int d^3x'\rho^{\frac{1}{2}}(\mathbf{x}t)\rho^{\frac{1}{2}}(\mathbf{x}'t)\,\delta(r-a) \times\left\{\rho^{\frac{1}{2}}(\mathbf{x}t)\rho^{\frac{1}{2}}(\mathbf{x}'t)\,\frac{\mathbf{x}'-\mathbf{x}}{a}\cdot[\mathbf{v}(\mathbf{x}'t)-\mathbf{v}(\mathbf{x}t)]\right\}_{r=a+\epsilon}. \tag{5.8}$$

Equation (5.7) is of physical interest. Since we are only considering the motion of a single-particle density in the degenerate state, it is clear that we would have sink and source due to particles in the excited states. Therefore, instead of the equation of continuity, we have a collision term (5.8) and a term due to the change of the occupation number of the degenerate state. This equation is actually very similar to the classical Boltzmann's equation.

From Eq. (5.5) we obtain the usual hydrodynamic equation for a superfluid,

$$\rho(\mathbf{x}t)\,\frac{\partial\mathbf{v}(\mathbf{x}t)}{\partial t} = 2\rho(\mathbf{x}t)\nabla[\rho^{-\frac{1}{2}}(\mathbf{x}t)\nabla^2\rho^{\frac{1}{2}}(\mathbf{x}t)] - \rho(\mathbf{x}t)[\mathbf{v}(\mathbf{x}t)\cdot\nabla]\mathbf{v}(\mathbf{x}t) - 2\rho(\mathbf{x}t)\nabla A^{-1}(\mathbf{x}t)\operatorname{Re}\mathfrak{L}(\mathbf{x}t), \tag{5.9}$$

where

$$2\rho(\mathbf{x}t)\nabla A^{-1}(\mathbf{x}t)\operatorname{Re}\mathfrak{L}(\mathbf{x}t) = [4\rho(\mathbf{x}t)/a]\nabla \times\lim_{\epsilon\to 0}\int d^3x'\rho^{-\frac{1}{2}}(\mathbf{x}t)\rho^{\frac{1}{2}}(\mathbf{x}'t)\,\delta(r-a) \times[\rho^{\frac{1}{2}}(\mathbf{x}'t)\rho^{\frac{1}{2}}(\mathbf{x}t) + a\rho^{\frac{1}{2}}(\mathbf{x}t)\,\partial'\rho^{\frac{1}{2}}(\mathbf{x}'t) + a\rho^{\frac{1}{2}}(\mathbf{x}'t)\,\partial\rho^{\frac{1}{2}}(\mathbf{x}t)]_{r=a+\epsilon}. \tag{5.10}$$

We define the static pressure as:

$$\nabla P = \frac{2\rho(\mathbf{x}t)}{a}\,\nabla\lim_{\epsilon\to 0}\int d^3x'\rho^{-\frac{1}{2}}(\mathbf{x}t) \times\rho^{\frac{1}{2}}(\mathbf{x}'t)\,\delta(r-a)[\rho^{\frac{1}{2}}(\mathbf{x}'t)\rho^{\frac{1}{2}}(\mathbf{x}t)]_{r=a+\epsilon}. \tag{5.11}$$

The static pressure is approximately $4\pi a\rho^2(\mathbf{x}t)$ when a is small.

Let D/Dt be the Lagrangian derivative. Equation (5.9) can be rewritten in a more familiar form,

$$\tfrac{1}{2}\rho(\mathbf{x}t)[D\mathbf{v}(\mathbf{x}t)/Dt] = -\nabla P + \rho\nabla(\rho^{-\frac{1}{2}}\nabla^2\rho^{\frac{1}{2}}) + \mathbf{I}, \tag{5.12}$$

where

$$\mathbf{I}(\mathbf{x}t) = -\lim_{\epsilon\to 0}4\rho(\mathbf{x}t)\nabla\int d^3x'\rho^{-\frac{1}{2}}(\mathbf{x}t)\rho^{\frac{1}{2}}(\mathbf{x}'t)\,\delta(r-a) \times[\rho^{\frac{1}{2}}(\mathbf{x}t)\,\partial'\rho^{\frac{1}{2}}(\mathbf{x}'t) + \rho^{\frac{1}{2}}(\mathbf{x}'t)\,\partial\rho^{\frac{1}{2}}(\mathbf{x}t)]_{r=a+\epsilon}. \tag{5.13}$$

$\mathbf{I}$ is an extra term to the usual London[4] superfluid equation. Actually $\mathbf{I}$ is a frictional-force term similar to the Maxwell stress tensor on a conductor. The importance of the presence of these extra terms is negligible for a very dilute system, but might be of importance in the case of liquid helium II.

APPENDIX A

To prove that $P(\mathbf{x})$ can be written in the form given by Eq. (2.6), we recall the definition of $P(\mathbf{x})$, Eq. (2.3),

$$P(\mathbf{x}) \equiv \sum_{N=0}^{\infty}\int\prod_{i}^{N}d^3x_i C(\mathbf{x}q_N)P_N(q_N). \tag{A1}$$

The step function $C(\mathbf{x}q_N)$ can be written as

$$C(\mathbf{x}q_N) \equiv \prod_{i=1}^{N}[1 - \Delta(\mathbf{x}\mathbf{x}_i)]C(q_N), \tag{A2}$$

where $\Delta(\mathbf{x}\mathbf{x}_i)$ is a step function defined as follows:

$$\Delta(\mathbf{x}\mathbf{x}_i) = \begin{cases} 0 & \text{for } |\mathbf{x} - \mathbf{x}_i| > a, \\ 1 & \text{otherwise.} \end{cases} \tag{A3}$$

Hence, $P(\mathbf{x})$ can be written as follows:

$$P(\mathbf{x}) \equiv P + \Lambda(\mathbf{x}), \tag{A4}$$

where P is defined by Eq. (2.7).

The operator $\Lambda(\mathbf{x})$ can be simplified easily,

$$\begin{aligned}
\Lambda(\mathbf{x}) &= \sum_{N=0}^{\infty} \int \prod_{i}^{N} d^3x_i C(q_N) P_N(q_N) \\
&\times \left[\sum_{l=1}^{N} \frac{(-)^l N!}{l!\,(N-l)!} \prod_{i=1}^{l} \Delta(\mathbf{x}\mathbf{x}_i) \right] \\
&= \sum_{N=1}^{\infty} \sum_{l=1}^{N} \frac{(-)^l}{l!} \int \prod_{j=1}^{l} d^3x_j \prod_{i=1}^{l} \Delta(\mathbf{x}\mathbf{x}_i) \int \prod_{k=1}^{N-l} d^3x'_k \\
&\times \left[C(q_l q'_{N-l}) \prod_{m=1}^{l} \psi_0^*(\mathbf{x}_m) P_{N-l}(q'_{N-l}) \prod_{n=1}^{l} \psi_0(\mathbf{x}_n) \right] \\
&= \sum_{l=1}^{M} \frac{(-)^l}{l!} \int \cdots \int_{S_\mathbf{x}} \prod_{j=1}^{l} d^3x_j \left[\sum_{N=0}^{\infty} \int \prod_{i=1}^{N} d^3x'_i \right. \\
&\left. \times C(q_l q'_N) \prod_{k=1}^{l} \psi_0^*(\mathbf{x}_k) P_N(q'_N) \prod_{m=1}^{l} \psi_0(\mathbf{x}_m) \right],
\end{aligned} \tag{A5}$$

where M is the maximum integer such that $\prod_{i=1}^{M} \Delta(\mathbf{x}\mathbf{x}_i) C(q_M) \not\equiv 0$ and $S_\mathbf{x}$ is the volume bounded by the surface $|\mathbf{x} - \mathbf{x}_i| = \lim_{\epsilon \to 0} a + \epsilon$, $\epsilon > 0$.

APPENDIX B

We recall Eq. (3.2). We have

$$\begin{aligned}
H &= -\int d^3x \psi_0^*(\mathbf{x}) \nabla^2 P(\mathbf{x}) \psi_0(\mathbf{x}) \\
&+ \int d^3x' \oint^{\mathbf{x}'} d\sigma_\mathbf{x} \psi_0^*(\mathbf{x}) \psi_0^*(\mathbf{x}') \frac{\mathbf{x} - \mathbf{x}'}{a} \cdot \nabla \psi(\mathbf{x}') \psi(\mathbf{x}) \\
&+ \sum_{l=2}^{M} \frac{(-)^l}{l!} \int d^3x \int_{S_\mathbf{x}} \psi_0^*(\mathbf{x}) \prod_{j=1}^{l} \psi^*(\mathbf{x}_j) \nabla^2 \\
&\times \prod_{k=1}^{l} \psi(\mathbf{x}_k) \psi(\mathbf{x})\, d^3x_k.
\end{aligned} \tag{B1}$$

The term

$$\sum_{l=2}^{M} \frac{(-)^l}{l!} \int d^3x \int_{S_\mathbf{x}} \psi_0^*(\mathbf{x}) \times \prod_{i=1}^{l} \psi^*(\mathbf{x}_i) \nabla^2 \prod_{j=1}^{l} \psi(\mathbf{x}_j) \psi(\mathbf{x})\, d^3x_i$$

vanishes, since

$$\begin{aligned}
&\sum_{l=2}^{M} \frac{(-)^l}{l!} \int d^3x \int_{S_\mathbf{x}} \psi_0^*(\mathbf{x}) \\
&\times \prod_{i=1}^{l} \psi^*(\mathbf{x}_i) \nabla^2 \prod_{j=1}^{l} \psi(\mathbf{x}_j) \psi(\mathbf{x})\, d^3x_i \\
&= \sum_{l=2}^{M} \frac{(-)^l}{(l-1)!} \int d^3x_1 \oint^{\mathbf{x}_1} d\sigma_\mathbf{x} \int_{S_\mathbf{x}} \psi_0^*(\mathbf{x}) \psi^*(\mathbf{x}_1) \\
&\times \prod_{i=2}^{l} \psi^*(\mathbf{x}_i) \frac{\mathbf{x} - \mathbf{x}_i}{a} \cdot \nabla \prod_{j=2}^{l} \psi(\mathbf{x}_j) \psi(\mathbf{x}_1) \psi(\mathbf{x})\, d^3x_i \\
&- \sum_{l=2}^{M} \frac{(-)^l}{(l-1)!} \int_{|\mathbf{x}-\mathbf{x}_1| \le a} d^3x\, d^3x_1 \Big(\nabla \psi_0^*(\mathbf{x}) \psi^*(\mathbf{x}_1) \\
&\times \int_{S_\mathbf{x}} \prod_{i=2}^{l} \psi^*(\mathbf{x}_i) \prod_{j=2}^{l} \psi(\mathbf{x}_j)\, d^3x_j \Big) \cdot \nabla \psi(\mathbf{x}_1) \psi(\mathbf{x})
\end{aligned} \tag{B2}$$

$$= 0.$$

The surface integral term vanishes because we have the condition $\psi(\mathbf{x}_j)\psi(\mathbf{x}) = 0$ for $|\mathbf{x}_j - \mathbf{x}| \le a$, where $j \neq 1$. The volume integral terms vanish because $\nabla\psi(\mathbf{x}_1)\psi(\mathbf{x})$ vanishes everywhere inside the volume $|\mathbf{x}_1 - \mathbf{x}| \le a$ except on the surface $|\mathbf{x}_1 - \mathbf{x}| = a$ where it is assumed to be bounded.

Therefore, the interaction term can be written simply as

$$\int d^3x' \oint^{\mathbf{x}'} d\sigma_\mathbf{x} \psi_0^*(\mathbf{x}) \psi_0^*(\mathbf{x}') \frac{\mathbf{x} - \mathbf{x}'}{a} \cdot \nabla \psi(\mathbf{x}') \psi(\mathbf{x}). \tag{B3}$$

However, since

$$\lim_{|\mathbf{x}-\mathbf{x}'| \to a} \langle \nu_{N-2} |\psi(\mathbf{x}')\psi(\mathbf{x})| \nu_N \rangle \to 0, \tag{B4}$$

we can multiply Eq. (B3) by a test function $f(r)$ in the following manner:

$$\int d^3x' \oint^{\mathbf{x}'} d\sigma_\mathbf{x} \psi_0^*(\mathbf{x}) \psi_0^*(\mathbf{x}') \frac{\mathbf{x} - \mathbf{x}'}{a f(a)} \cdot \nabla f(r) \times \psi(\mathbf{x}') \psi(\mathbf{x}). \tag{B5}$$

In particular, the function $f(r)$ is chosen to be r. In order to fix the function $f(r)$ we have made use of the method of Liu and Wong in treating the two-body problem.

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Analytic Solution of the Percus–Yevick Equation*

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The properties of the Percus–Yevick approximate integral equation for the pair distribution function in classical statistical mechanics are examined for the class of pair potentials consisting of a hard core plus a short-range tail. For one-dimensional systems, some elementary theorems of complex variable applied to the Laplace-transformed equations enable one to express the direct correlation function in a very simple form, one which becomes explicit and trivial in the absence of a short-range tail. In the presence of the tail, the direct correlation function satisfies a (coupled) integral equation over a finite domain. The impossibility of a phase transition in one dimension is strongly indicated. Analysis of the case of three dimensions proceeds similarly, but is complicated by the appearance of essential parameters other than the density and compressibility. The character of the direct correlation function is qualitatively unchanged. Principal differences in three dimensions are that a phase transition is no longer prohibited, and the pair distribution function cannot be reasonably expressed as a sum of nth-neighbor contributions.

I. INTRODUCTION

SEVERAL approximate integral equations have been proposed for the pair distribution function in classical statistical mechanics. On the basis of numerical comparisons[1] made so far, the Percus–Yevick (PY) equation[2] is the most successful of these. Furthermore the PY equation has been solved exactly for hard spheres,[3,4] representing the first nontrivial system solved for any of these integral equations. In the solution for hard spheres a factorization of the PY equation occurred, which in the original method of solution appeared as a lucky accident. This suggested a more detailed study of the PY equation, exploiting the fact that it is a quadratic integral equation.

The method we have used consists of the application of some elementary theory of the functions of a complex variable to the Laplace-transformed PY equation. We consider the case of hard spheres with a potential tail which becomes identically zero beyond a distance a which is less than the hard sphere diameter R. The potential tail is assumed to be finite or have only integrable singularities, but is otherwise arbitrary. For this system we find a factorization of the PY equation, which may be used to eliminate the pair distribution function, leaving an equation for the direct correlation function alone. In the case of zero tail the solution for hard spheres is obtained in a simple fashion. For the case of nonzero tail the equation for the direct correlation function $C(x)$ is expressed in a form believed suitable for numerical computation. The method used clearly shows the similarity as well as some important differences between the one-dimensional and the three-dimensional case. In the following we carry out both cases explicitly. Since the one-dimensional problem can be solved exactly, any information on the solution of the PY equation in one dimension serves as a welcome check on the adequacy of the PY approximation.

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[1] A. A. Broyles, J. Chem. Phys. **33**, 456 (1960); **34**, 359 (1961); **34**, 1068 (1961); **35**, 493 (1961). A. A. Broyles, S. U. Chung, and H. L. Sahlin, J. Chem. Phys. **37**, 2462 (1962).

[2] J. K. Percus and G. J. Yevick, Phys. Rev. **110**, 1 (1958).

[3] M. S. Wertheim, Phys. Rev. Letters **10**, 321 (1963).

[4] E. Thiele, J. Chem. Phys. **38**, 1959 (1963).

II. ONE DIMENSION

A. Analytic Character of the Integral Equation

In one dimension, the PY equation for a system of particles interacting pairwise with a potential $V(x)$ can be written[2]

$$\tau(x) = 1 - \rho \int_{-\infty}^{\infty} \tau(x')f(x')\,dx' + \rho \int_{-\infty}^{\infty} \tau(x')f(x')\tau(x - x')\,\mathrm{e}(x - x')\,dx', \qquad (1)$$

where $\mathrm{e}(x) \equiv \exp[-\beta V(x)]$, $f(x) = \mathrm{e}(x) - 1$, ρ is the density, and $\beta = (kT)^{-1}$. The pair distribution function $g(x)$ and the direct correlation function $C(x)$ of Ornstein and Zernike[5] are in the PY approximation related to $\tau(x)$ by

$$g(x) = \tau(x)\mathrm{e}(x), \qquad C(x) = \tau(x)f(x).$$

In our case $V(x) = V_{\mathrm{H}} + V_{\mathrm{T}}$, where the hard-

[5] L. S. Ornstein and F. Zernike, Proc. Acad. Sci. Amsterdam **17**, 793 (1914).

rod potential V_H is given by

$$V_H = 0 \quad (|x| > l), \qquad V_H = \infty \quad (|x| < l),$$

and the tail potential V_T satisfies $V_T = 0$ for $|x| > l + a$.

We take the one-side Laplace transform (LT) of (1) for a potential of this form and obtain

$$F(s) + G(s) = (1 + \rho K)/s - \rho[F(s) + F(-s)]G(s) - \rho Y(s) + \rho Y(-s), \qquad (2)$$

where

$$F(s) \equiv -\int_0^{l+a} C(x) \exp(-sx)\, dx,$$

$$G(s) \equiv \int_l^{\infty} g(x) \exp(-sx)\, dx,$$

$$Y(s) \equiv \int_0^{a} y(x) \exp(-sx)\, dx,$$

$$y(x) \equiv -\int_{l+x}^{l+a} C(x')g(x - x')\, dx' \quad (0 < x < a),$$

$$y(x) \equiv 0 \quad (x < 0 \text{ and } x > a),$$

$$K \equiv -2\int_0^{l+a} C(x')\, dx'.$$

Solving for $G(s)$, and letting $1 + \rho K \equiv Q^2$, this becomes

$$G(s) = \frac{Q^2 s^{-1} - F(s) - \rho Y(s) + \rho Y(-s)}{1 + \rho F(s) + \rho F(-s)}. \qquad (3)$$

We assume that $C(x)$ and $g(x)$ are everywhere finite. Therefore $F(s)$ and $Y(s)$, being LT's over a finite interval, are entire functions of s. $G(s)$ is an LT over an infinite interval and is therefore regular in the right half-plane (RHP). In the left-half plane (LHP) $G(s)$ is defined by analytic continuation of the function $G(s)$ in the RHP.

From (3) it follows that

$$G(-s) = \frac{-Q^2 s^{-1} - F(-s) - \rho Y(-s) + \rho Y(s)}{1 + \rho F(-s) + \rho F(s)} \qquad (4)$$

and that the quantity

$$G(s)[Q^2 s^{-1} + F(-s) - \rho Y(s) + \rho Y(-s)]$$

is an even function of s. According to (3), $G(s)$ has a simple pole with principal part s^{-1} at $s=0$. Therefore the quantity $s^2G(s)[Q^2s^{-1}+F(-s)-\rho Y(s)+\rho Y(-s)]$ is regular at the origin and in the RHP, since both factors are regular in the RHP. Since it is also an even function of s, it is also regular in the LHP, and hence it is an entire function of s. Noting that the growth rates of $F(s)$ and $Y(s)$ as we go to infinity in the LHP are $O[s^{-1} \exp(-l - a)s]$ and $O[s^{-1} \exp(-as)]$, respectively, we find by (3) that $G(s)$ goes to $-\rho^{-1}$ as we go to infinity in the LHP, and that the growth rate of $s^2G(s)[Q^2s^{-1} + F(-s) - \rho Y(s) + \rho Y(-s)]$ is $O[s \exp(-as)]$.

Now consider the function

$$H(s) = s^2G(s)[Q^2s^{-1} + F(-s) - \rho Y(s) + \rho Y(-s)] - s^2[Y(s) + Y(-s)].$$

Clearly it is also an even entire function of s. Furthermore, by (3) H is given by

$$H(s) = s^2[1 + \rho F(s) + \rho F(-s)]^{-1}\{Q^4s^{-2} + Q^2s^{-1} \times [F(-s) - F(s) - 2\rho Y(s) + 2\rho Y(-s)] - F(s)F(-s) - 2\rho F(s)Y(-s) - 2\rho F(-s)Y(s) - Y(s) - Y(-s) + \rho^2[Y(s) - Y(-s)]^2\}. \qquad (5)$$

In the LHP, the term with the largest growth rate is $F(s)$ which is $O[s^{-1} \exp(-l - a)s]$. Using $F(-s) = -\tau(0)s^{-1} + O(s^2)$, $Y(-s) = -y(0)s^{-1} + O(s^{-2})$, and $\tau(0) = Q^2 - 2\rho y(0)$ from (1) as we go to infinity in the LHP, we find $H(s) = O(1)$ as we go to infinity along any radius in the LHP. Since $H(s)$ is even, $H(s) = O(1)$ holds also in the RHP. But by Liouville's theorem a bounded entire function is a constant. We evaluate the constant by taking $H(0)$ in (5) and find $H = Q^2$. Therefore

$$G(s)[Q^2/s + F(-s) - \rho Y(s) + \rho Y(-s)] = Q^2/s^2 + Y(s) + Y(-s). \qquad (6)$$

At this point we note that this factorization holds only for a nearest-neighbor-type tail. For $a > l$ the dominant term in the numerator of (5) is $Y^2(s)$, which is $O[s^{-2} \exp(-2as)]$ as we go to infinity in the LHP, and $H(s)$ is $O[s^{-1} \exp(-a + l)s]$ rather than $O(1)$.

Combining (6) with (2), we obtain

$$F(s) + G(s) = Q^2\left(\frac{1}{s} - \frac{\rho}{s^2}\right) - 2\rho Y(s) + \rho^2 Y(-s)G(s) - \rho^2 Y(s)G(s) - \rho F(s)G(s) + \frac{\rho Q^2 G(s)}{s}. \qquad (7)$$

Let us transform (7) back to coordinate space. For hard rods with no tail, $Y = 0$. Moreover $G(s)$, $\rho F(s)G(s)$ and $\rho Q^2 s^{-1}G(s)$ are LT's of functions which are zero for $x < l$. Hence we obtain for $x < l$:

$$-C(x) = Q^2(1 - \rho x), \qquad (8)$$

and, since by (2)

$$\tau(0) = 1 + 2\rho\int_0^l \tau(x)\, dx, \quad Q^2 = 1 - \rho Q^2(2l + \rho l^2),$$

and

$$Q^2 = (1 - \rho l)^{-2}. \tag{9}$$

In this fashion the PY equation is solved for hard rods in an extremely simple way.

B. Elimination of $g(x)$ and Reduction to Finite-Range Equations

Now consider the case of nonzero tail. The right-hand side of (7) contains four types of terms. The term $Q^2(s^{-1} - \rho s^{-2})$ is the LT of $Q^2(1 - \rho x)$, the term $-2\rho Y(s)$ is the LT of $-2\rho y(x)$, which is nonzero only for $0 < x < a$. The term $-\rho^2 Y(-s)G(s)$ is the LT of a function which is zero for $x < l - a$. All the remaining terms are LT's of functions which are zero for $x < l$.

For future convenience we now define

$$-C(x) = -C_0(x) - 2\rho y(x) + p(x - l) + q(x - l),$$

where $-C_0(x) = Q^2(1 - \rho x)$ for $(0 < x < l)$ and $-C_0(x) = 0$ for $x > l$; $p(x) = 0$ for $x < -a$ and $x > 0$; $q(x) = 0$ for $x < 0$ and $x > a$. According to (7), p is given by

$$p(x - l) = \rho^2 \int_{-a}^{x-l} y(-x')g(x - x')\,dx'. \tag{10}$$

We omit the equation for $q(x - l)$, since it still involves $g(x)$ for $x > l + a$ in the inverse LT of the term $\rho^2 Y(-s)G(s)$.

In order to eliminate $g(x)$ for $x > l + a$, and obtain an equation for $C(x)$ alone, it is necessary to return to Eqs. (2) and (6). We define

$$X(s) = [F(s) + 2\rho Y(s) - Q^2 s^{-1} + \rho Q^2 s^{-2}],$$
$$Z(s) = Q^2 s^{-2} + Y(s) + Y(-s).$$

Equations (2) and (6) combined now become

$$[X(s) - \rho Z(s)][X(-s) - \rho Z(s)]$$
$$= -Z(s)[1 + \rho X(s) + \rho X(-s) - 2\rho^2 Z(s)] \tag{11}$$

or

$$X(s)X(-s) = -Z(s) + \rho^2 Z^2(s). \tag{12}$$

Now let

$$X(s) = e^{-sl}\mu(s)\nu(s), \tag{13}$$
$$Z(s) = -\mu(s)\mu(-s). \tag{14}$$

The result is

$$\nu(s)\nu(-s) = \rho^2\mu(s)\mu(-s) + 1 \tag{15}$$

and

$$G(s) = \frac{-\mu(s)}{e^{sl}\nu(-s) + \rho\mu(s)}. \tag{16}$$

The functions $s^2X(s)$ and $s^2Z(s)$ are entire and can therefore be written as canonical Weierstrass products. In the factorization $X(s) = \mu(s)\nu(s)\exp(-sl)$, all the roots of $X(s)$ which are also roots of $Z(s)$ appear in $\mu(s)$, while the common roots of $X(s)$ and $\rho Z(s) - 1$ appear in $\nu(s)$.

So far, $\mu(s)$ and $\nu(s)$ are determined only up to an exponential factor, since simultaneously multiplying $\mu(s)$ by $\exp\phi(s)$ and $\nu(s)$ by $\exp[-\phi(s)]$—with $\phi(s)$ an odd function of s—has no effect on any of the preceding equations. The factor can certainly be chosen to be an entire function. Then $\mu(s)$ and $\nu(s)$ are regular except for a simple pole at $s = 0$. The poles $\rho Q^2 s^{-2}$ in $X(s)$ and $Q^2 s^{-2}$ in $Z(s)$ imply poles Qs^{-1} in $\mu(s)$ and $\rho Q s^{-1}$ in $\nu(s)$. We define

$$\mu(s) = Q/s + M(s), \quad \nu(s) = \rho Q/s - 1 + N(s), \tag{17}$$

where $M(s)$ and $N(s)$ are entire functions. The explicit terms taken out of $\mu(s)$ and $\nu(s)$ are just the hard-rod values of $\mu(s)$ and $\nu(s)$, with the actual Q replacing the hard-rod value of Q.

Substituting (17) into (13), (14), (15), and (16), we obtain

$$M(s)N(s) + \frac{Q}{s}[N(s) + \rho M(s)] - M(s)$$
$$= \frac{Q}{s}[1 - Q(1 - \rho l)] + P(s) + \Pi(s), \tag{18}$$

where

$$P(s) = \int_{-a}^{0} p(x)\exp(-sx)\,dx$$

and

$$\Pi(s) = \int_{0}^{a} q(x)\exp(-sx)\,dx,$$

$$N(s)N(-s) + \frac{\rho Q}{s}[N(-s) - N(s)] - N(-s) - N(s)$$
$$= \rho^2\left\{M(s)M(-s) + \frac{Q}{s}[M(-s) - M(s)]\right\}$$
$$= -\rho^2[Y(s) + Y(-s)], \tag{19}$$

and

$$G(s)\{e^{sl}[-\rho Q/s - 1 + N(-s)]$$
$$+ \rho[Q/s + M(s)]\} = -Q/s - M(s). \tag{20}$$

The right-hand side of (18) is the LT of a function which has the constant value $Q[1 - Q(1 - \rho l)]$ for $x > a$. The inverse LT of the left-hand side of (18) will certainly be of this form if $M(s)$ and $N(s)$ are the LT's of functions $m(x)$ and $n(x)$, one of which is identically zero except in the interval

$0 < x < a$, while the other vanishes identically outside the interval $-a < x < 0$. Similarly the right-hand side of (19) is the LT of a function which is zero for $x > a$, and the left-hand side of (19) will automatically have this behavior if $m(x)$ and $n(x)$ are confined to $-a < x < 0$ and $0 < x < a$.

The correct choice between these two alternatives can be made by testing the consistency of each choice with the two relations between $g(x)$, $q(x)$, $p(x)$, and $y(x)$ already obtained, namely the definition of $y(x) = \int_{x+l}^{a+l} q(x')g(x' - x)\,dx'$ and (10). The correct choice turns out to be $m(x)$ confined to $0 < x < a$, $n(x)$ confined to $-a < x < 0$.

Taking the inverse LT of (18) we obtain

$$p(-x) = Q\int_x^a n(-x')\,dx' + \int_x^a m(x' - x)n(-x')\,dx', \tag{21}$$

$$q(x) = -m(x) - \rho Q\int_x^a m(x')\,dx' + \int_x^a m(x')n(x - x')\,dx', \tag{22}$$

$$1 - Q(1 - \rho l) = \rho\int_0^a m(x')\,dx' + \int_0^a n(-x')\,dx'. \tag{23}$$

The inverse LT of (19) yields

$$\int_x^a n(-x')n(x - x')\,dx' + \rho Q\int_x^a n(-x')\,dx' - n(-x) = \rho^2\left[\int_x^a m(x')m(x' - x)\,dx' + Q\int_x^a m(x')\,dx'\right] = -\rho^2 y(x), \tag{24}$$

and from (20) we obtain, defining $\gamma(x) = g(x + l)$, for the interval $0 < x < a$

$$-\gamma(x) - \rho Q\int_0^x \gamma(x')\,dx' + \int_0^x \gamma(x')n(x' - x)\,dx' = -Q - m(x). \tag{25}$$

Equations (22), (24), and (25) form a closed set of three coupled quadratic integral equations for the quantities $m(x)$, $n(x)$ and $q(x)$—$\gamma(x)$ being related to $q(x)$ by $-\gamma(x)f_T(x + l) = q(x)e_T(x + l)$—with the auxiliary equation (23) relating the value of the parameter Q to $m(x)$ and $n(x)$. Thus the pair distribution function has been eliminated completely, and the interval of integration in the equation for the direct correlation function has been reduced to the range of the tail potential alone. It is a characteristic feature of this reduced form that the square root of the compressibility appears as a parameter, whereas the compressibility itself appears in the original PY equation.

C. Further Considerations

It is still necessary to demonstrate the consistency of (21) through (25) with the definition of y,

$$y(x) = \int_x^a q(x')\gamma(x' - x)\,dx', \tag{26}$$

and (10), which may be rewritten as

$$p(-x) = -\rho^2\int_x^a y(x')\gamma(x' - x)\,dx'. \tag{27}$$

Writing (22) as an equation for $q(x')$, multiplying by $\gamma(x' - x)$ and integrating from x to a, then using (25) to eliminate $\gamma(x)$, we obtain precisely $y(x)$ in terms of $m(x)$ as given by (24). Similarly we may use (24) in the form which gives $y(x')$ as a function of $n(x')$. Multiplying by $\gamma(x' - x)$, integrating from x to a, and using (25) to eliminate $\gamma(x)$, we obtain exactly (21). Had we assumed $m(x)$ confined to $-a < x < 0$ and $n(x)$ confined to $0 < x < a$, then we would have found a contradiction at this point.

One may further verify that, defining a function $\xi(x) = Q\theta(x, l) - \rho^{-1}n(-x) - m(x - l)$, where $\theta(x, l)$ is the step function which is 1 for $0 < x < l$, and zero otherwise, the direct correlation function is given

$$-C(x) = \xi(-x) + \xi(x) + \rho\int_{-\infty}^{\infty} \xi(x')\xi(x' - x)\,dx'. \tag{28}$$

Finally we consider some important consequences of Eq. (15). We may expand both sides of (15) in a Laurent series and equate coefficients for each power of s. In the case $Q = 0$, the leading equation is

$$[N(0) - 1]^2 = \rho^2 M^2(0) + 1. \tag{29}$$

But (24) becomes, for the case $Q = 0$,

$$N(0) - 1 = \rho M(0). \tag{30}$$

The two equations are obvioulsy inconsistent for finite values of $M(0)$ and $N(0)$. Therefore Q can

never attain the value zero for finite $M(0)$ and $N(0)$. It follows that there can be neither a straight line segment in the P–V curve, nor a van der Waals loop. We conclude that the system does not exhibit a first-order phase transition. This seems to be a strong point in favor of the PY equation, since the exact treatment of this system also shows that no phase transition can occur, as first shown by Gürsey.[6]

There remains some question whether Q can become zero through $m(x)$ and $n(x)$ increasing without limit as ρ approaches some density ρ_0. By (15) this would imply that $m(x)$ approaches $n(-x)$ and $g(x)$ approaches $\delta(x-l)$ for $1 \leq x < 2$. We also have $q(x)f(x+l) = -e(x+l)g(x+l)$. On the other hand, $q(x)$ is related to $m(x)$ and $n(x)$ via (22). To make the two relations for $q(x)$ consistent, enormous cancellation of large quantities on the right-hand side of (22) would be required, and it seems unlikely that this is possible.

Next we show how to write $g(x)$ as a sum of nth nearest neighbor distribution functions.

In taking the inverse LT of (16), we can expand the denominator in powers of $\rho\mu(s)/\exp(sl)\nu(-s)$ if the inequality $\rho\,|\mu(s)| < |\nu(-s)\exp sl|$ is satisfied on the contour. The path of integration consists of the y axis from $-i\infty$ to $-i\epsilon$, a small semicircle of radius ϵ in the RHP, and the y axis from $i\epsilon$ to $i\infty$. On the y axis (15) is equivalent to

$$|\nu(iy)|^2 = \rho^2\,|\mu(iy)|^2 + 1 \tag{31}$$

and the inequality is obviously satisfied. Letting $s = \epsilon \exp i\theta$ on the small semicircle, we have

$$\begin{aligned} |s\nu(-s)e^{sl}|^2 &= \rho^2Q^2 \\ &\quad + 2\rho Q[1 - N(0) + Q\rho l]\epsilon\cos\theta + O(\epsilon^2), \\ \rho^2\,|\mu(s)|^2 &= \rho^2Q^2 + 2\rho^2QM(0)\epsilon\cos\theta + O(\epsilon^2), \end{aligned} \tag{32}$$

and, using (23),

$$|s\nu(-s)e^{sl}|^2 - \rho^2\,|\mu(s)|^2 = 2\rho Q\epsilon\cos\theta + O(\epsilon^2). \tag{33}$$

Since $Q > 0$, and $\cos\theta > 0$, the inequality is satisfied on the small semicircle also. Therefore we can expand $G(s) = \sum_{n=1}^{\infty} G_n(s)$, where $G_n(s) = [\mu(s)/\nu(-s)\exp sl]^n$.

Because of the factor $\exp sl$, the inequality is also satisfied on a large semicircle in the RHP. Thus we have a closed contour on which $|\nu(-s)\exp sl| > |\mu(s)|$. Our original hypothesis that $G(s)$ has no pole in the RHP implies that $\nu(-s)\exp sl + \rho\mu(s)$ has no zero in the RHP, since in (16) a zero of the denominator cannot be canceled by a zero of $\mu(s)$, $\mu(s)$ and $\nu(-s)$ by (15) having no common zero. It follows that we can apply Rouché's theorem, and we find that $\nu(-s)$ has no root in the RHP.

In calculating

$$g_n(x) = \frac{1}{2\pi}\int_{-i\infty}^{i\infty} G_n(s)e^{sx}\,dx \tag{34}$$

we close in the RHP for $x < nl$, obtaining zero. For $x > nl$ we close the contour in the LHP, obtaining contributions from the residues of the poles at the zeros of $\nu(-s)$ in the LHP. We also have the relation

$$\int_0^{\infty} g_n(x)\,dx = G_n(0) = \rho^{-1}, \tag{35}$$

which tells us that each $g_n(x)$ is normalized to exactly one particle. It is therefore natural to interpret $g_n(x)$ as the nth nearest neighbor distribution function.

III. THREE DIMENSIONS

A. Preliminary Reduction

In the following we omit mathematical details whenever the argument closely parallels the one-dimensional case, concentrating instead on the important differences between the two cases.

In three dimensions the PY equation can be written[2]:

$$\begin{aligned} \tau(\mathbf{r}) &= 1 - \rho\int \tau(\mathbf{r})f(\mathbf{r})\,d\mathbf{r} \\ &\quad + \rho\int \tau(\mathbf{r}')f(\mathbf{r}')\tau(\mathbf{r}-\mathbf{r}')\,e(\mathbf{r}-\mathbf{r}')\,d\mathbf{r}'. \end{aligned} \tag{36}$$

We assume a spherically symmetric solution, and introduce the coordinates $r' = |\mathbf{r}'|$, $|\mathbf{r}-\mathbf{r}'|$, and a trivial polar angle ϕ. We make the equations dimensionless by defining $x = (r/R)$, $\eta = (\pi R^3\rho/6)$, $a' = (a/R)$, where R is hard-sphere radius, $R + a$ the distance beyond which $V_T(r) = 0$, and take the one side LT of the equation satisfied by $\sigma(x) \equiv x\tau(x)$. Defining

$$\begin{aligned} F(t) &\equiv -\int_0^{1+a'} xC(x)\exp(-tx)\,dx, \\ G(t) &\equiv \int_1^{\infty} xg(x)\exp(-tx)\,dx, \\ K &\equiv -F'(0) = -\int_0^{a'} x^2C(x)\,dx, \\ Y(t) &\equiv \int_0^{a'} y(x)\exp(-tx)\,dx, \\ y(x) &\equiv -\int_{1+x}^{1+a'} x'C(x')(x-x')g(x-x')\,dx', \end{aligned} \tag{37}$$

[6] F. Gürsey, Proc. Cambridge Phil. Soc. 46, 182 (1950).

and noting that $1 + 24\eta K$ is the inverse compressibility $\beta(\partial p/\partial\rho)_\beta$, we obtain

$$t[F(t) + G(t)] = (1 + 24\eta K)/t + 12\eta \times \{[F(t) - F(-t)]G(t) - Y(t) + Y(-t)\}. \quad (33)$$

Solving for $G(t)$, this becomes

$$G(t) = \frac{(1 + 24\eta K)/t^2 - F(t) + (12\eta/t)[Y(-t) - Y(t)]}{1 + (12\eta/t)[F(-t) - F(t)]}. \quad (39)$$

Arguing as in the one-dimensional case, $F(t)$ and $Y(t)$ are entire functions, and $G(t)$ is regular in the RHP and has a double pole at $t = 0$. Furthermore,

$$G(-t) = \frac{(1 + 24\eta K)/t^2 - F(-t) + (12\eta/t)[Y(-t) - Y(t)]}{1 + (12\eta/t)[F(-t) - F(t)]} \quad (40)$$

and hence the function

$$t^4G(t)\{(1 + 24\eta K)t^{-2} - F(-t) + 12\eta t^{-1}[Y(-t) - Y(t)]\}$$

is an even entire function of t. We define

$$H(t) = t^4G(t)\{(1 + 24\eta K)t^{-2} - F(-t) + 12\eta t^{-1}[Y(-t) - Y(t)]\} + Y(t) + Y(-t).$$

By (39), $H(t)$ is given by

$$H(t) = t^4\{1 + 24\eta t^{-1}[F(-t) - F(t)]\}^{-1} \times \{(1 + 24\eta K)^2t^{-4} + (1 + 24\eta K)t^{-2} \times [-F(t) - F(-t) + 24\eta t^{-1}Y(-t) - 24\eta t^{-1}Y(t)] + F(t)F(-t) - 24\eta t^{-1}F(t)Y(-t) + 24\eta t^{-1}F(-t)Y(t) + (12\eta t^{-1})^2[Y(t) - Y(-t)]^2\}. \quad (41)$$

Examining the growth rates at large t in a fashion completely analogous to the one-dimensional case we find $H(t) = O(t^2)$ at large t. Therefore, by a well known extension of Liouville's theorem, $H(t)$ is a quadratic polynomial $H(t) = \lambda_1 + \lambda_2t^2$.

Here the first important difference between one and three dimensions appears. In the original PY equation there appears one parameter, the value of which is given as an integral of the unknown function appearing in the integral equation, namely the inverse compressibility. In one dimension the factored equation also contains just one parameter, which is the square root of the inverse compressibility. In three dimensions, however, two parameters appear in the factored equation. As will be shown later, one of them is again the square root of the inverse compressibility.

Evaluating the constants by expanding $H(t)$ in powers of t in (41), we find

$$\lambda_1 = (1 + 24\eta K),$$
$$\lambda_2 = -2F(0) + 4\eta F'''(0) - 48Y'(0), \quad (42)$$

and

$$G(t)\left\{\frac{1 + 24\eta K}{t^2} - F(-t) + \frac{12\eta}{t}[Y(-t) - Y(t)]\right\} = \frac{\lambda_1}{t^4} + \frac{\lambda_2}{t^2} - Y(t) - Y(-t). \quad (43)$$

Combining (43) and (33) one obtains

$$tF(t) = \frac{\lambda_1}{t} + \frac{12\eta\lambda_2}{t^2} + \frac{12\eta\lambda_1}{t^4} - 24\eta Y(t) - \frac{(12\eta)^2Y(-t)G(t)}{t} + \frac{(12\eta)^2Y(t)G(t)}{t} + 12\eta F(t)G(t) - \frac{12\eta\lambda_1G(t)}{t^2} - tG(t). \quad (44)$$

We first solve the case of zero tail. Then

$$G(t)[12\eta F(t) - 12\lambda_1t^{-2} - t]$$

is the LT of a function which is zero for $x < 1$. For $x < 1$ we obtain

$$-C(x) = \lambda_1 + 6\eta\lambda_2x + \tfrac{1}{2}\eta\lambda_1x^3. \quad (45)$$

Combining (45) with the relations (42), we obtain two simultaneous linear equations for λ_1 and λ_2:

$$\lambda_1 = 1 + 24\eta(\tfrac{1}{3}\lambda_1 + \tfrac{3}{2}\eta\lambda_2 + \tfrac{1}{12}\eta\lambda_1),$$
$$\lambda_2 = -2(\tfrac{1}{2}\lambda_1 + 2\eta\lambda_2 + \tfrac{1}{10}\eta\lambda_1) - 4\eta(\tfrac{1}{5}\lambda_1 + \eta\lambda_2 + \tfrac{1}{16}\eta\lambda_1), \quad (46)$$

the solution of which is

$$\lambda_1 = (1 + 2\eta)^2/(1 - \eta)^4, \quad \lambda_2 = -(1 + \tfrac{1}{2}\eta)^2/(1 - \eta)^4. \quad (47)$$

From λ_1 we obtain the equation of state

$$\beta P\rho^{-1} = (1 + \eta + \eta^2)/(1 - \eta)^3. \quad (48)$$

The factorization method is a much simpler and physically more transparent way of solving the PY equation for hard spheres than the method originally used.[3,4]

B. Finite-Range Equations

Returning to (44) for the case of a nonvanishing tail, we see that $-[xC(x)]'$ can be written

$$-[xC(x)]' = -[xC_0(x)]' - 24\eta y(x) + p(x-1) - q(x-1), \quad (49)$$

where $-[xC_0(x)]' = \lambda_1 + 2\eta\lambda_2 + 2\eta\lambda_1 x^3$ for $0 < x < 1$, and $-[xC_0(x)]' = 0$ for $x > 1$, $y(x)$ is confined to the interval $0<x<a'$, $p(x)$ to $-a'<x<0$, and $q(x)$ to $0 < x < a'$.

Defining

$$X(t) = F(t) - \lambda_1 t^{-2} - 12\eta\lambda_2 t^{-3} - 12\eta\lambda_1 t^{-5} + 24\eta t^{-1} Y(t),$$

$$Z(t) = \lambda_1 t^{-4} + \lambda_2 t^{-2} - Y(t) - Y(-t),$$

we obtain from (39) and (43)

$$\left[X(t) + \frac{12\eta}{t} Z(t)\right]\left[X(-t) - \frac{12\eta}{t} Z(t)\right] = Z(t)\left[1 - \frac{12\eta}{t} X(t) + \frac{12\eta}{t} X(-t) - \frac{2(12\eta)^2}{t^2} Z(t)\right], \quad (50)$$

or

$$X(t)X(-t) = Z(t) - \frac{(12\eta)^2}{t^2} Z^2. \quad (51)$$

Letting $X(t) = e^{-t}\mu(t)\nu(t)$, and $Z(t) = \mu(t)\mu(-t)$, then

$$\nu(t)\nu(-t) = 1 - (12\eta/t)^2\mu(t)\mu(-t) \quad (52)$$

and

$$G(t) = \frac{-\mu(t)}{e^t\nu(-t) - (12\eta/t)\mu(t)}. \quad (53)$$

The singularities of $X(t)$ and $Z(t)$ tell us immediately that the leading powers in the Laurent series are t^{-2} for $\mu(t)$ and t^{-3} for $\nu(t)$. We let

$$\mu(t) = A_2 t^{-2} + A_1 t^{-1} + M(t),$$

$$\nu(t) = B_3 t^{-3} + B_2 t^{-2} + B_1 t^{-1} + 1 + N(t), \quad (54)$$

where $M(t)$ and $N(t)$ are entire functions. We now compare the two equations for $G(t)$, (39) and (53). By (39) $G(t)$ is given in the neighborhood of $t = 0$ by $G(t) = t^{-2} + O(1)$. In (39) the numerator yields $-\mu(t) = -A_2 t^{-2} - A_1 t^{-1} + O(1)$, hence consistency with (53) requires that near zero the denominator satisfy $e^t\nu(-t) - 12\eta t^{-1}\mu(t) = -A_2 - A_1 t + O(t^2)$. Equating the principal part of $e^t\nu(-t) - 12\eta t^{-1}\mu(t)$ to zero yields

$$B_3 = -12\eta A_2, \qquad B_2 = 12\eta(A_1 - A_2),$$
$$B_1 = 12\eta[A_1 - \tfrac{1}{2}A_2 - M(0)].$$

The equations for the coefficients of t^1 and t^0 yield, after expressing the B's in terms of A_2 and A_1:

$$(1 + 2\eta)A_2 - 6\eta A_1 = -1 - N(0) - 12\eta M(0) + 12\eta M'(0),$$

$$\tfrac{3}{2}\eta A_2 + (1 - 4\eta)A_1 = -1 - N(0) + N'(0) - 6\eta M(0) - 12\eta M''(0). \quad (55)$$

Having obtained the parameters A_2 and A_1 in terms of the functions $M(t)$ and $N(t)$, we obtain λ_1 and λ_2 in terms of A_1 and A_2 by equating coefficients in the Laurent series of $\mu(t)\nu(t)e^{-t} = X(t)$. The coefficients of t^{-5} and t^{-3} tell us that

$$A_2^2 = \lambda_1, \qquad A_1^2 - 2A_2 M(0) = -\lambda_2. \quad (56)$$

By an argument closely paralleling the one-dimensional case, $N(t)$ is the LT of a function $n(x)$ confined to $-a' < x < 0$ and $M(t)$ is the LT of $m(x)$ which is confined to $0<x<a'$. We note that $t^{-1}[M(t)-M(0)]$ is also the LT of a function confined to $0 < x < a'$ and equal to $\hat{m}(x) = \int_x^a m(x')\,dx'$ in that interval. Hence $e^{-t}\nu(t) + 12\eta t^{-1}\mu(-t)$ is the LT of $n(1 + x) + \hat{m}(-x) + \delta(x-1) + 12\eta[M(0) - A_1 x + \frac{1}{2}A_2 x^2]\theta(x, 1)$. By (50), expressed in terms of μ and ν, we have

$$1 + \frac{12\eta}{t}[F(-t) - F(t)] = \left[e^{-t}\nu(t) + \frac{12\eta}{t}\mu(-t)\right] \times \left[e^t\nu(-t) - \frac{12\eta}{t}\mu(t)\right]. \quad (57)$$

Recalling the definition of $F(t)$, the inverse LT of (57) can be written

$$\int_{-\infty}^{x} x'C(x')\,dx' = \xi(x) + \xi(-x) + 12\eta\int_{-\infty}^{\infty}\xi(x')\xi(x' - x)\,dx', \quad (58)$$

where

$$\xi(x) = (12\eta)^{-1}n(-x) + \hat{m}(x - 1) + [M(0) - A_1(1 - x) + \tfrac{1}{2}A_2(1 - x)^2]\theta(x, 1).$$

Defining $\gamma(x - 1) = xg(x)$ for $0 < x < a'$, we now write down the three coupled integral equations for $m(x)$, $n(x)$, and $\hat{q}(x)$, where $\hat{q}(x) = \int_0^x q(x')\,dx'$. From $\mu(t)\nu(t)e^{-t} = X(t)$ we obtain for the interval $0<x<a$

$$\hat{q}(x) = m(x) + \int_x^{a'} m(x')n(x - x')\,dx' - 12\eta\int_x^{a'} m(x')[A_1 - \tfrac{1}{2}A_2 - M(0) + (A_1 - A_2)(x - x') - \tfrac{1}{2}A_2(x - x')^2]\,\hat{q}x'. \quad (59)$$

From (52) for $0 < x < a'$ we obtain

$$n(-x) + \int_x^{a'} n(-x')n(x - x')\,dx' - 12\eta \int_x^{a'} n(-x')[A_1 - \tfrac{1}{2}A_2 - M(0) + (A_1 - A_2)(x - x') - \tfrac{1}{2}A_2(x - x')^2]\,dx' = 144\eta^2\Big[\int_x^{a'} \hat{m}(x')\hat{m}(x' - x)\,dx' + \int_x^{a'} \hat{m}(x') \times [M(0) - A_1(x - x') + \tfrac{1}{2}A_2(x - x')^2]\,dx'\Big]. \tag{60}$$

From (53) for $0 < x < a'$ we obtain

$$\gamma(x) + \int_0^x \gamma(x - x')\{n(-x') + 12\eta[\tfrac{1}{2}A_2x'^2 + (A_1 - A_2)x' - A_1 + \tfrac{1}{2}A_2 + M(0)]\}\,dx' = -[\tfrac{1}{2}A_2x + A_1 + m(x)]. \tag{61}$$

Here $\gamma(x)$ and $\hat{q}(x)$ are related by $-\gamma(x)f(1 + x) = \hat{q}(x)e(1 + x)$.

The equations corresponding to (59) and (60) for $x > a'$ just duplicate (55).

We note at this point that vanishing of the inverse compressibility does not lead to a contradiction analogous to the one encountered in one dimension. This does not prove that the PY equation in three dimensions can show a phase transition, or even that a solution for zero inverse compressibility does in fact exist, but at least this possibility is not excluded in the same obvious way that occurred in one dimension.

C. Structure of the Radial Distribution Function

Finally we consider the question of zeros of $\nu(-t)$ in the RHP, and the expansion of $g(x)$ obtained by expanding the denominator of (53) in powers of $\mu(t)/\nu(-t)\exp t$.

We consider first the case of positive compressibility. Taking the same contour considered for the one-dimensional case, we find that the inequality $|12\eta t^{-1}\mu(t)| < |\nu(-t)|$ is satisfied on the y axis and on the large semicircle, but not on the small semicircle. We compute the variation of the argument of $\nu(t)$ around the contour in two steps.

By our original hypothesis, $D(t) = \nu(-t)e^t - 12\eta t^{-1}\mu(t)$ has no zero in the RHP. Hence the variations of the argument $\phi(D)$ of $D(t)$ around the contour considered here is zero. Near $t=0$, $D(t) = -A + O(t)$. This means that the change of $\phi(D)$ on the small semicircle is zero, and by subtraction, the change of $\phi(D)$ going from $-i\epsilon$ to $i\epsilon$ counterclockwise is also zero. On this part of the contour $|12\eta t^{-1}\mu(t)| < |\nu(-t)|$, so that $|\phi(D) - \phi[\nu(-t)]| < \frac{1}{2}\pi$ everywhere, and it suffices to calculate $\phi(D) - \phi[\nu(-t)]$ at the end points to obtain the total change of $\phi[\nu(-t)]$. At $y = \epsilon$, $D(t) = -A_2 + O(\epsilon)$, $\nu(-t) = -12\eta A_2 i\epsilon^{-3} + O(\epsilon^{-2})$; at $y = -\epsilon$, $D(t) = -A_2 + O(\epsilon)$, $\nu(-t) = 12\eta A_2 i\epsilon^{-3} + O(\epsilon^{-2})$. Hence $\phi[\nu(-t)]$ changes by $-\pi$ on this part of the contour. The point $t = 0$ is a triple pole of $\nu(-t)$, and therefore $\phi[\nu(-t)]$ increases by 3π on the small semicircle. Thus the total change in $\phi[\nu(-t)]$ around the contour is 2π, and $\nu(-t)$ has exactly one root in the RHP. In the only solved case,[3,4] hard spheres with no tail, $\nu(-t)$ has two complex-conjugate roots in the LHP and one real root in the RHP.

For zero inverse compressibility, $D(t) = -A_1t + O(t^2)$ and $\nu(-t) = 12\eta A_1t^{-2}$ near $t = 0$. $\phi(D)$ increases by π going from $y = -\epsilon$ to $y = \epsilon$ counterclockwise. At $y = \epsilon$, $D(t) = -A_1i\epsilon + O(\epsilon^2)$; $\nu(-t) = -A_1\epsilon^{-2}$; at $y = -\epsilon$, $D(t) = A_1i\epsilon + O(\epsilon^2)$, $\nu(-t) = -A_1\epsilon^{-2} + O(\epsilon^{-1})$. Hence $\phi[\nu(-t)]$ increases by 0 on this part of the contour. On the small semicircle $\phi[\nu(-t)]$ increases by 2π, since $t = 0$ is a double pole. Thus the total variation of $\phi[\nu(-t)]$ around the contour is 2π. Therefore a solution with zero inverse compressibility also has one root of $\nu(-t)$ in the RHP.

In order to expand $G(t)$ in powers of $\mu(t)/\nu(-t)$ exp t, it is necessary to find a contour on which $|12\eta t^{-1}\mu(t)| < |\nu(-t)e^t|$ is satisfied. From our proof that $\nu(-t)$ has one root in the RHP it follows that there can be no such contour passing from $-i\infty$ to $i\infty$ to the left of the positive root of $\nu(-t)$, since the existence of such a contour would imply that $D(t)$ also has one root in the RHP. On the other hand it is clear that on a sufficiently large semicircle $|t| = P$ in the RHP $|12\eta t^{-1}\mu(t)| < |\nu(-t)|$ is satisfied. If one replaces the segment of the y axis between $y = -P$ and $y = P$ by $|t| = P$, one can expand on the contour. Then $g(x) = \sum_{n=1}^{\infty} g_n(x)$ and

$$xg_n(x) = \frac{1}{12\eta}\sum_i R_i\left\{e^{t(x-n)}\left[\frac{\mu(t)}{12\eta t\nu(-t)}\right]^n\right\} \quad (x > n),$$
$$xg_n(x) = 0 \quad (x < n), \tag{62}$$

where the R_i are the residues of the quantity in braces at the roots of $\nu(-t)$. Since there is always one root in the RHP, each $g_n(x)$ includes a term of exponentially increasing character. Therefore the $g_n(x)$ are never normalizable and never represent nth nearest-neighbor distributions.

In addition to being suitable for numerical computation, the coupled equations are suitable

for obtaining two expansions: a virial expansion in powers of the density, and a perturbation expansion in powers of $f_T(x)$. In the latter case the advantage of eliminating $g(x)$ is particularly striking; while even the first order is difficult to obtain from the original PY equation, the coupled equations in every order of $f_T(x)$ lead to simple linear integral equations which can be solved explicitly by reduction to integrals involving $f_T(x)$ and known functions.

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The Influence of Initial Correlations on the Approach to Equilibrium*

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The irreversible behavior of a particle under the influence of fixed scattering centers is investigated in the weak coupling limit. An ensemble is introduced which statistically describes the scattering centers as well as the particle. This allows the treatment of correlations between the particle and the scattering centers. A new diagrammatic method is used to investigate high-order terms in the perturbation theory. This method yields quite explicit information about the way in which the influence of initial correlations will disappear. In particular, it is quite clear that as one goes to higher order in the perturbation theory one must wait longer times for the influence of initial correlations to disappear. For completeness, the Boltzmann equation is derived and solved to lowest order in the interaction strength.

I. INTRODUCTION

IN the past few years, Van Hove[1] and Prigogine[2] and their coworkers have developed methods of analysis which have improved our understanding of the irreversible behavior of complex systems. These are essentially methods for doing secular perturbation theory (i.e., perturbation theory which is valid for times long compared to the characteristic interaction times of the system). In particular, in Prigogine's method, one uses the perturbation theory to find the time dependence of the lower-order reduced distribution functions. This involves the investigation of the time dependence of various diagrams and summations over infinite sets of these diagrams to obtain kinetic equations for the reduced distribution functions. The theory is somewhat cumbersome in that one works with time and spatial Fourier transforms of the distribution functions rather than the functions themselves. We want to introduce here a method which is closely related to that of Prigogine but which avoids the use of the transforms. This method has the advantage that the time dependence of the diagrams and the existence of various time scales in the kinetic equations become very explicit. It has the disadvantage that it seems applicable only to particles with short-range interactions.

Probably the most important result of this treatment is contained in Eq. (24) and the subsequent discussion, which shows, to each order in perturbation theory, how the influence of correlations in the initial distribution function becomes weaker as time progresses.

The system we want to treat consists of N particles which do not interact with each other but which do interact with N fixed scattering centers. This problem reduces to a single-particle problem, which is dynamically simpler than the interacting gas, but exhibits most of the important points in approach to equilibrium problems.

Previous treatments of this problem have not allowed for correlations between the particle and the scattering centers.

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[1] L. Van Hove, Physica **21**, 517 (1955); **23**, 441 (1957); **25**, 268 (1959).
[2] I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Interscience Publishers, Inc., New York, 1962).

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II. EXPANSION OF THE DISTRIBUTION FUNCTION

Our system will be described by the distribution function

$$f_{2N}(\mathbf{x}_1, \mathbf{p}_1 \cdots \mathbf{x}_N, \mathbf{p}_N, \mathbf{r}_1 \cdots \mathbf{r}_N, t),$$

where $\mathbf{x}_i$, $\mathbf{p}_i$ are the position and momentum of the ith particle, $\mathbf{r}_i$ is the position of the ith scattering center, and t is the time. f_{2N} is an ensemble probability distribution for both the particles and the scattering centers and as such is normalized to 1,

$$\int f_{2N}(\mathbf{x}_1, \mathbf{p}_1 \cdots \mathbf{r}_N, t)\, d\mathbf{x}_1\, d\mathbf{p}_1 \cdots d\mathbf{r}_N = 1.$$

Its time dependence is given by the Liouville equation which we write as

$$i\,\partial f_{2N}/\partial t = L_{2N} f_{2N}, \tag{1}$$

where L_{2N} is the operator

$$L_{2N} = -\frac{i}{m}\sum_{i=1}^{N} \mathbf{p}_i \cdot \frac{\partial}{\partial \mathbf{x}_i} + i \sum_{i,l=1}^{N} \frac{\partial V(\mathbf{x}_i - \mathbf{r}_l)}{\partial \mathbf{x}_i} \cdot \frac{\partial}{\partial \mathbf{p}_i}. \tag{2}$$

$V(\mathbf{x}_i - \mathbf{r}_l)$ is the interaction potential energy between the jth particle and the lth scattering center.

The distribution function for one particle and all of the scattering centers is given by

$$f(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_N, t) = \int f_{2N}(\mathbf{x}, \mathbf{p}, \mathbf{x}_2, \mathbf{p}_2 \cdots \mathbf{x}_N, \mathbf{p}_N, \times \mathbf{r}_1 \cdots \mathbf{r}_N, t)\, d\mathbf{x}_2\, d\mathbf{p}_2 \cdots d\mathbf{x}_N\, d\mathbf{p}_N. \tag{3}$$

Since the particles do not interact with each other, one can integrate (1) over the positions and momenta of all but one particle to obtain

$$i\,\partial f/\partial t = Lf, \tag{4}$$

where L is given by

$$L = -\frac{i}{m}\mathbf{p}\cdot\frac{\partial}{\partial \mathbf{x}} + i\sum_{l=1}^{N} \frac{\partial V(\mathbf{x} - \mathbf{r}_l)}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{p}}. \tag{5}$$

The function f is normalized to one also. We have assumed that the function f_{2N} is chosen symmetric in the variables $\mathbf{x}_1$, $\mathbf{p}_1 \cdots \mathbf{x}_N$, $\mathbf{p}_N$. We shall later make the same assumption about the variables $\mathbf{r}_1 \cdots \mathbf{r}_N$. Since the particles are identical and the scattering centers are identical these are reasonable assumptions.

As usual we eventually want to take the limit as the number of scattering centers N and the volume Ω become infinite with the ratio N/Ω finite. In this limit, f has no physical meaning, and one should work instead with reduced distribution functions or correlation functions. We define the reduced distribution functions by

$$f_s(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_s, t) = N^{s+1} \int f(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_N, t)\, d\mathbf{r}_{s+1} \cdots d\mathbf{r}_N, \quad 0 \le s \le N. \tag{6}$$

It is an assumption that the f_s exist in the limit of large N and Ω. We have used a definition of the reduced distribution functions which differs from the normal one in the factor before the integral. f_s is ordinarily given by

$$f_s = N(N!)/(N-s)! \int f\, d\mathbf{r}_{s+1} \cdots d\mathbf{r}_N;$$

however in the limit of large N, for any s, the two definitions converge to each other. The reason for this choice of f_s will be seen shortly. We now introduce a functional transformation to a new set of functions.

$$\begin{aligned}
f_0(\mathbf{x}, \mathbf{p}, t) &= U(\mathbf{x}, \mathbf{p}, t),\\
f_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, t) &= N/\Omega U(\mathbf{x}, \mathbf{p}, t) + U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, t),\\
f_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, \mathbf{r}_2, t) &= N^2/\Omega^2 U(\mathbf{x}, \mathbf{p}, t)\\
&\quad \times N/\Omega U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, t) + N/\Omega U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_2, t)\\
&\quad + U_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, \mathbf{r}_2, t)\\
&\;\;\vdots\\
f_N(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_N, t) &= (N/\Omega)^N U(\mathbf{x}, \mathbf{p}, t)\\
&\quad + (N/\Omega)^{N-1} \textstyle\sum_i U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, t)\\
&\quad + (N/\Omega)^{N-2} \textstyle\sum_{i \ne j} U_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, \mathbf{r}_j, t)\\
&\quad + \cdots U_N(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_N, t).
\end{aligned} \tag{7}$$

From these equations one obtains the inverse equations

$$\begin{aligned}
U(\mathbf{x}, \mathbf{p}, t) &= f_0(\mathbf{x}, \mathbf{p}, t),\\
U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, t) &= f_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, t) - N/\Omega f_0(\mathbf{x}, \mathbf{p}, t),\\
U_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, \mathbf{r}_2, t) &= f_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, \mathbf{r}_2, t)\\
&\quad - N/\Omega f_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_1, t) - N/\Omega f_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_2, t)\\
&\quad + (N/\Omega)^2 f_0(\mathbf{x}, \mathbf{p}, t)\\
&\;\;\vdots
\end{aligned} \tag{8}$$

Now from Eqs. (7) and (8) one can show that the U_s have the property that

$$\int U_s(x, p, r_1 \cdots r_s, t)\, dr_k = 0, \quad s \ge 1, \quad 1 \le k \le s. \tag{9}$$

This property will be useful later and is the reason for our particular definition of the f_s. Combining Eqs. (6) and (7), one obtains the desired expansion for f, which we shall write as

$$\Omega^N N f(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_N, t) = U(\mathbf{x}, \mathbf{p}, t) + \Omega/N \sum_i U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, t) + (\Omega/N)^2 \sum_{i \neq j} U_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, \mathbf{r}_j, t) + \cdots . \quad (10)$$

This expansion corresponds to that of Prigogine's except that we work directly with f rather than its Fourier transform. We shall now assume that the distribution of scattering centers is homogeneous and that there are no correlations between scattering centers. In this case the functions introduced in Eq. (7) are, in the limit of large N, particle-scattering center correlation functions. If one wants to include correlations between scattering centers one must introduce scattering center–scattering center correlation functions. This can be done without difficulty but the expansion for f becomes somewhat more complicated.

III. TIME EVOLUTION OF THE SYSTEM

We now turn to the central problem, that of finding the time dependence of the U_s. In particular, we examine the time dependence of $U(\mathbf{x}, \mathbf{p}, t)$. To do this we use a method developed by Zwanzig.[3]

Suppose one has a vector $x(t)$ in a Hilbert space which satisfies

$$i\, \partial x(t)/\partial t = Lx(t),$$

where L is a time-independent linear operator. Then if P is any linear operator one can show that

$$i\, \partial Px(t)/\partial t = PLPx(t) - i \int_0^t PLG(s)(1 - P) \times LPx(t - s)\, ds + PLG(t)(1 - P)x(0), \quad (11a)$$

$$(1 - P)x(t) = -i \int_0^t G(s)(1 - P)LPx(t - s)\, ds + G(t)(1 - P)x(0), \quad (11b)$$

where G is the operator

$$G(t) = e^{-it(1-P)L}. \quad (11c)$$

In our application we choose $x(t) = \Omega^N N f(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_N, t)$ and $P = 1/\Omega^N \int d\mathbf{r}_1 \cdots d\mathbf{r}_N$. We take L as given by Eq. (5) and split it into two parts:

$$L = L_0 + \delta L, \quad (12a)$$

$$L_0 = -i/m\mathbf{p}\cdot\partial/\partial\mathbf{x}, \quad (12b)$$

$$\delta L = i \sum_i \frac{\partial V(\mathbf{x} - \mathbf{r}_i)}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{p}}. \quad (12c)$$

With these choices it is easy to show that

$$P^2 = P, \qquad (1 - P)^2 = (1 - P), \quad (13a)$$

$$PL_0 = L_0 P, \quad (13b)$$

$$P\delta LP = 0, \quad (13c)$$

$$PL_0P = L_0P. \quad (13d)$$

Using these properties and the expansion (10) for f, one obtains from (11a)

$$i\, \partial U(\mathbf{x}, \mathbf{p}, t)/\partial t = L_0 U(\mathbf{x}, \mathbf{p}, t) - i \int_0^t P\delta LG(s)\delta LU(\mathbf{x}, \mathbf{p}, t - s)\, ds + P\delta LG(t)[\Omega/N \sum_i U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, 0) + (\Omega/N)^2 \sum_{i \neq j} U_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, \mathbf{r}_j, 0) + \cdots]. \quad (14)$$

This gives us an equation for $U(\mathbf{x}, \mathbf{p}, t)$ which depends on the value of U_s, $s \geq 1$ at $t = 0$, i.e., on the initial correlations. The central question is now what kind of correlations can one have at $t = 0$ and still obtain solutions of (14) for $U(\mathbf{x}, \mathbf{p}, t)$ which approach equilibrium, and furthermore how long must one wait to get near this equilibrium.

The correlations at $t = 0$ we shall assume to be of finite range, that is, we assume a length R such that

$$U_s(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_s, 0) = 0 \quad (15)$$

if $|\mathbf{x} - \mathbf{r}_k| > R$ for any $k \leq s$ and all $s \geq 1$. We have assumed here that the correlation range R is independent of s.

With this assumption we want to investigate the solutions of (14). These solutions depend on the operator $G(t)$ whose structure is so complex that one must use some kind of a perturbation expansion for it. One can in this problem assume the density of scattering centers is low and expand $G(t)$ in powers of this density or one can assume weak interactions between the scattering centers and the particle. The latter choice is the simpler so we shall take an expansion of $G(t)$ in powers of the potential term δL.

We assume that

$$G(t) = \sum_{n=0}^{\infty} G^n(t), \quad (16)$$

where $G^n(t)$ is of order $(\delta L)^n$. In Appendix I we show by the usual methods that

[3] R. Zwanzig, *Lectures in Theoretical Physics*, Boulder, Colorado, 1960 (Interscience Publishers, Inc., New York, 1961), Vol. III.

$$G^n(t) = (-1)^n \int_0^t \int_0^{t_1} \cdots \int_0^{t_{n-1}} \sum_{i_1} \cdots$$
$$\times \sum_{i_n} (1 - P) \frac{\partial V(\mathbf{x} - \mathbf{v}[t - t_1] - \mathbf{r}_{i_1})}{\partial \mathbf{x}}$$
$$\times \partial_1 (1 - P) \frac{\partial V(\mathbf{x} - \mathbf{v}[t - t_2] - \mathbf{r}_{i_2})}{\partial \mathbf{x}}$$
$$\times \partial_2 \cdots (1 - P) \frac{\partial V(\mathbf{x} - \mathbf{v}[t - t_n] - \mathbf{r}_{i_n})}{\partial \mathbf{x}}$$
$$\times \partial_n \{e^{-iL_0(t-t_n)} P + e^{-iL_0 t}(1 - P)\}, \qquad (17)$$

where

$$\partial_i = [\partial/\partial \mathbf{p} + (t - t_i)/m \partial/\partial \mathbf{x}], \qquad \mathbf{v} = \mathbf{p}/m.$$

In particular, $G^0(t) = P + e^{-iL_0 t}(1 - P)$.

In Eq. (14) we shall replace $G(t)$ by $G^0(t)$. The first term to consider is $P\delta L G^0(s)\delta L U(\mathbf{x}, \mathbf{p}, t - s)$. From Appendix II we see that this term can be written as

$$P\delta L G^0(s)\delta L U(\mathbf{x}, \mathbf{p}, t - s)$$
$$= -\sum_{i_0} \sum_{i_1} P \frac{\partial V(\mathbf{x} - \mathbf{r}_{i_0})}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{p}}$$
$$\times \frac{\partial V(\mathbf{x} - \mathbf{v}s - \mathbf{r}_{i_1})}{\partial \mathbf{x}} \cdot \left(\frac{\partial}{\partial \mathbf{p}} + \frac{s}{m} \frac{\partial}{\partial \mathbf{x}}\right)$$
$$\times u(\mathbf{x} - \mathbf{v}s, \mathbf{p}, t - s). \qquad (18)$$

All of the terms in this double sum vanish except those for which $i_0 = i_1$. To see this, change the derivatives with respect to $\mathbf{x}$ to derivatives with respect to $\mathbf{r}_{i_0}$ and $\mathbf{r}_{i_1}$ and remember that P integrates over all the $\mathbf{r}$ variables. Therefore,

$$P\delta L G^0(s)\delta L U(\mathbf{x}, \mathbf{p}, t - s)$$
$$= -\sum_i P \frac{\partial V(\mathbf{x} - \mathbf{r}_i)}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{p}}$$
$$\times \frac{\partial V(\mathbf{x} - \mathbf{v}s - \mathbf{r}_i)}{\partial \mathbf{x}} \cdot \left(\frac{\partial}{\partial \mathbf{p}} + \frac{s}{m} \frac{\partial}{\partial \mathbf{x}}\right)$$
$$\times U(\mathbf{x} - \mathbf{v}s, \mathbf{p}, t - s). \qquad (19)$$

Now if we assume that $V(\mathbf{x}) = 0$ for $|\mathbf{x}| > a$, we must have both $|\mathbf{x} - \mathbf{r}_i| < a$ and $|\mathbf{x} - \mathbf{v}s - \mathbf{r}_i| < a$ if (19) is not to vanish. But this means

$$P\delta L G^0(s)\delta L U(\mathbf{x}, \mathbf{p}, t - s) = 0$$
$$\text{for} \quad s > 2a/v. \qquad (20)$$

This term vanishes then for times longer than a collision time $t_c = 2a/v$. In Appendix II, by means of a diagrammatic method we generalize this result to all orders in δL and prove

$$P\delta L G^n(s)\delta L u(\mathbf{x}, \mathbf{p}, t - s) = 0$$
$$\text{for} \quad s > (n/2 + 1)t_c. \qquad (21)$$

Now let us consider the lowest-order contributions from the correlation terms in (14). Using the definition of $G^0(t)$ and Eq. (9) we can write

$$P\delta L G^0(t)[\Omega/N \sum_i U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, 0)$$
$$\times (\Omega/N)^2 \sum_{i \neq j} U_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, \mathbf{r}_j, 0) + \cdots]$$
$$= iP \sum_{i_0} \frac{\partial V(\mathbf{x} - \mathbf{r}_{i_0})}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{p}} [\Omega/N \sum_i$$
$$\times U_1(\mathbf{x} - \mathbf{v}t, \mathbf{p}, \mathbf{r}_i, 0) + (\Omega/N)^2 \sum_{i \neq j}$$
$$\times U_2(\mathbf{x} - \mathbf{v}t, \mathbf{p}, \mathbf{r}_i, \mathbf{r}_j, 0) + \cdots]. \qquad (22)$$

Consider the U_1 term. We must have $i_0 = i$ in the double sum or this term vanishes because of the $\partial V(\mathbf{x} - \mathbf{r}_{i_0})/\partial \mathbf{x} = -\partial V(\mathbf{x} - \mathbf{r}_{i_0})/\partial \mathbf{r}_{i_0}$ factor. Similarly in the U_2 term we must put either $i_0 = i$ or $i_0 = j$. Suppose $i_0 = i$. Then $j \neq i = i_0$ and this term vanishes anyhow because of the integration of U_2 over $\mathbf{r}_j$ [see Eq. (9)]. The same is true for all the U_i, $i > 1$. So

$$P\delta L G^0(t)[\Omega/N \sum_i U_1(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, 0) + (\Omega/N)^2$$
$$\times \sum_{i \neq j} U_2(\mathbf{x}, \mathbf{p}, \mathbf{r}_i, \mathbf{r}_j, 0) + \cdots] = \Omega/NP$$
$$\times \sum_i \frac{\partial V(\mathbf{x} - \mathbf{r}_i)}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{p}} U_1(\mathbf{x} - \mathbf{v}t, \mathbf{p}, \mathbf{r}_i, 0). \qquad (23)$$

For this term to be nonzero we must have $|\mathbf{x} - \mathbf{r}_i| < a$ and from (15) also $|\mathbf{x} - \mathbf{v}t - \mathbf{r}_i| < R$. This means (23) vanishes unless $t < (R + a)/v$. We define $t_R = R/v$ as the correlation time. Then (23) vanishes for $t > \frac{1}{2}t_c + t_R$. In Appendix III we find to all orders that

$$P\delta L G^n(t) U_l(0) = 0 \quad \text{for all} \quad t \quad \text{if} \quad l > n + 1; \qquad (24)$$

for $t > [\frac{1}{2}(n - l) + \frac{3}{2}]t_c + t_R$ if $l \leq n + 1$. Equation (24) gives a rather exact description of how the influence of the initial correlations disappears from Eq. (14). In the first place, the initial correlations of higher order contribute only in high order in the perturbation theory and therefore could hopefully be neglected in a really weakly coupled system unless these correlations were extremely strong. In the second place, any correlations which must be considered vanish to any order in the perturbation theory after a well defined time which increases as the order of perturbation theory increases. The time one must wait in order to neglect the initial correlations is now well defined in the sense that its dependence on the range of forces, range of initial correlations, strength of initial correlations, and order of perturbation theory is known. If we assume that we have waited long enough to neglect the correlations, Eq. (14) becomes a self-contained

equation for $U(\mathbf{x}, \mathbf{p}, t)$, in particular,

$$i\partial U(\mathbf{x}, \mathbf{p}, t)/\partial t = L_0 U(\mathbf{x}, \mathbf{p}, t) - i\int_0^t P\delta L G(s)\, \delta L U(\mathbf{x}, \mathbf{p}, t-s)\, ds. \quad (25)$$

One would now like to show that the solutions of (25) show approach to equilibrium behavior. Time-convoluted equations of this form are by now familiar in nonequilibrium statistical mechanics and they are usually treated by reducing them to a Boltzmann-type equation, whose solutions are known (see Ref. 2). Most of these methods seem unsatisfactory in that the reduction takes place only in the limit of long times, and the length of time required is unclear. For completeness we shall include a simple reduction of (25) to a Boltzmann equation, to lowest order in the perturbation theory. We hope in a later paper to be able to treat the time-convoluted equation. The simplest reduction is obtained by the following argument. Replace $G(s)$ by $G^0(s)$ in (25). From (20), $P\delta L G^0(s)\delta L$ is zero for $s > 2a/v = 2ma/p$. For large p this is a very short time. If $U(\mathbf{x}, \mathbf{p}, t)$ does not vary much over this time interval, the $G^0(s)$ acts like a δ function and we can set $s = 0$ in the $U(\mathbf{x}, \mathbf{p}, t-s)$ term. From Eq. (19) we see that U must also be a slowly varying function of $\mathbf{x}$, over a distance a, to permit this treatment. If $t > t_c$ we can set $t = \infty$ in the upper limit of the integral since $G^0(s) = 0$ for $t > t_c$.

Using this approximation we show in Appendix IV that (25) can be written in component form as

$$\partial U(\mathbf{x}, \mathbf{p}, t)/\partial t = -1/mp_i\, \partial/\partial x_i U(\mathbf{x}, \mathbf{p}, t) - mN/\Omega\left(\int_0^\infty g'(\alpha)/\alpha\, d\alpha\right)\partial/\partial p_i \times (\delta_{ij}/p - p_i p_j/p^3)\, \partial/\partial p_j U(\mathbf{x}, \mathbf{p}, t), \quad (26)$$

where

$$g(\alpha) = \int V(\mathbf{y})V(\mathbf{y} - \boldsymbol{\alpha})\, d\mathbf{y}. \quad (27)$$

If we assume that V is a decreasing function of y (repulsive forces), then $g(\alpha)$ is a decreasing function of α, so

$$\int_0^\infty g'(\alpha)/\alpha\, d\alpha < 0. \quad (28)$$

Equation (26) is the Boltzmann equation for this problem, in the weak coupling limit. The first term on the right is the streaming term, the second is the collision term. That the solutions of this equation show approach to equilibrium can be proven by the well known H-function method.

In the homogeneous case, where $\partial/\partial x_i U(\mathbf{x}, \mathbf{p}, t) = 0$, we can write explicit solutions. We expand $U(\mathbf{p}, t)$ in spherical harmonics,

$$U(\mathbf{p}, t) = \sum_{l,m} C_{lm}(p, t) Y_l^m(\theta, \varphi). \quad (29)$$

Putting this expansion into Eq. (27) and using Eq. (IV.7) and the orthonormality of $Y_l^m(\theta, \varphi)$ we have

$$\partial C_{lm}(p, t)/\partial t = mN/\Omega \times \left(\int_0^\infty g'(\alpha)/\alpha\, d\alpha\right) l(l+1)/p^3 C_{lm}(p, t), \quad (30)$$

which has solutions

$$C_{lm}(p, t) = A_{lm}(p) e^{\lambda(l,p)t}, \quad (31)$$

where

$$\lambda(l, p) = mN/\Omega\left(\int_0^\infty g'(\alpha)/\alpha\, d\alpha\right) l(l+1)/p^3. \quad (32)$$

Note that $\lambda(p, l) \leq 0$ by virtue of (28). After a long time all terms but the $l = 0$ term disappear and we are left with the spherically symmetric equilibrium distribution.

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I would like to thank Professor Max Dresden for many hours of stimulating discussion on this subject.

APPENDIX I

We want to derive the expansion given by Eq. (17) for the operator $G(t) = e^{-i(1-P)Lt}$. Using the normal field-theoretic techniques one can write

$$G(t) = \sum_{n=0}^\infty G^n(t),$$

where

$$G^n(t) = (-i)^n \int_0^t e^{-i(1-P)L_0(t-t_1)}(1-P)\, \delta L \times \int_0^{t_1} e^{-i(1-P)L_0(t_1-t_2)}(1-P)\, \delta L \cdots \times \int_0^{t_{n-1}} e^{-i(1-P)L_0(t_{n-1}-t_n)}(1-P)\, \delta L \times e^{-i(1-P)L_0 t_n}\, dt_1 \cdots dt_n. \quad (I.1)$$

In particular, $G^0(t) = e^{-i(1-P)L_0 t}$.

If one expands $e^{-i(1-P)L_0 t}$ in a power series and remembers that $PL_0 = L_0 P$, one can show that

$$e^{-i(1-P)L_0 t} = P + e^{-iL_0 t}(1-P). \quad (I.2)$$

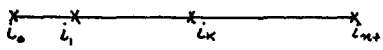

FIG. 1. Representation of general nth-order term.

Substituting this into (I.1) and using $P(1-P)=0$, one obtains

$$G^n(t) = (-i)^n \int_0^t e^{-iL_0(t-t_1)}(1-P)\,\delta L \times \int_0^{t_1} e^{-iL_0(t_1-t_2)} \cdots (1-P)\,\delta L \times \int_0^{t_{n-1}} e^{-iL_0(t_{n-1}-t_n)}(1-P)\,\delta L \times \{P + e^{-iL_0t_n}(1-P)\}\,dt_1 \cdots dt_n. \quad (I.3)$$

Now we need the following identities:

$$e^{-iL_0t}h(\mathbf{x}) = \exp(-\mathbf{p}t/m\cdot\partial/\partial\mathbf{x})h(\mathbf{x}) = h(\mathbf{x}-\mathbf{p}t/m)e^{-iL_0t}. \quad (I.4)$$

This is just the well known definition of a displacement operator,

$$e^{-iL_0t}\,\partial/\partial\mathbf{p} = (\partial/\partial\mathbf{p} + t/m\,\partial/\partial\mathbf{x})e^{-iL_0t}. \quad (I.5)$$

Equation (I.5) can be obtained by letting both sides act on an arbitrary function of $\mathbf{x}$ and $\mathbf{p}$ and using (I.4). Using (I.4) and (I.5), one has

$$e^{-iL_0t}\delta L = ie^{-iL_0t}\sum_l \frac{\partial V(\mathbf{x}-\mathbf{r}_l)}{\partial\mathbf{x}}\cdot\frac{\partial}{\partial\mathbf{p}} = i\sum_l \frac{\partial V(\mathbf{x}-\mathbf{r}_l-\mathbf{p}/mt)}{\partial\mathbf{x}}\cdot\left(\frac{\partial}{\partial\mathbf{p}} + \frac{t}{m}\frac{\partial}{\partial\mathbf{x}}\right)e^{-iL_0t}. \quad (I.6)$$

Putting (I.6) in (I.3) we can move all of the exponential operators to the extreme right to obtain

$$G^n(t) = (-1)^n \int_0^t \cdots \int_0^{t_{n-1}} \sum_{i_1}\cdots \times \sum_{i_n}(1-P)\frac{\partial V(\mathbf{x}-\mathbf{r}_{i_1}-\mathbf{v}[t-t_1])}{\partial\mathbf{x}} \times \partial_1(1-P)\cdots(1-P)\frac{\partial V(\mathbf{x}-\mathbf{r}_{i_n}-\mathbf{v}[t-t_n])}{\partial\mathbf{x}} \times \partial_n\{e^{-iL_0(t-t_n)}P + e^{-iL_0t}(1-P)\}\,dt_1\cdots dt_n, \quad (I.7)$$

where $\mathbf{v} = \mathbf{p}/m$ and $\partial_i = (\partial/\partial\mathbf{p} + (t-t_i)/m\partial/\partial\mathbf{x})\cdot$ It should be noted that the operators ∂_i in (I.7) act on everything to their right.

APPENDIX II

We want to develop a graphical method for investigating the time dependence of terms of the form $P\delta LG^n(s)\delta LU(\mathbf{x}, \mathbf{p}, t-s)$ and

$$P\delta LG^n(t)U_l(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_l, 0).$$

Let us look at $P\delta LG^n(s)\delta LU(t-s)$ first. From Eq. (17) we have

$$P\delta LG^n(s)\delta LU(\mathbf{x}, \mathbf{p}, t-s) = (-1)^n \int_0^t \int_0^{t_1} \cdots \times \int_0^{t_{n-1}} \sum_{i_0}\cdots\sum_{i_{n+1}} P\frac{\partial V(\mathbf{x}-\mathbf{r}_{i_0})}{\partial\mathbf{x}}\cdot\frac{\partial}{\partial\mathbf{p}} \times (1-P)\frac{\partial V(\mathbf{x}-\mathbf{r}_{i_1}-\mathbf{v}[s-t_1])}{\partial\mathbf{x}}\cdot\partial_1\cdots \times \frac{\partial V(\mathbf{x}-\mathbf{r}_{i_n}-\mathbf{v}[s-t_n])}{\partial\mathbf{x}}\cdot\partial_n(1-P) \times \frac{\partial V(\mathbf{x}-\mathbf{r}_{i_{n+1}}-\mathbf{v}s)}{\partial\mathbf{x}}\cdot\left(\frac{\partial}{\partial\mathbf{p}} + \frac{s}{m}\frac{\partial}{\partial\mathbf{x}}\right) \times U(\mathbf{x}-\mathbf{v}s, \mathbf{p}, t-s)\,dt_1\cdots dt_n. \quad (II.1)$$

The general nth-order term will be represented by a line with $n+2$ marks on it. With each mark is associated a summation variable i_k, and a factor $\{\partial V(\mathbf{x}-\mathbf{r}_{i_k}-\mathbf{v}[s-t_k])/\partial\mathbf{x}\}\cdot\partial_k$, except for the first and last marks i_0, i_{n+1} for which the factors are

$$\frac{\partial V(\mathbf{x}-\mathbf{r}_{i_0})}{\partial\mathbf{x}}\cdot\frac{\partial}{\partial\mathbf{p}}$$

and

$$\frac{\partial V(\mathbf{x}-\mathbf{r}_{i_{n+1}}-\mathbf{v}s)}{\partial\mathbf{x}}\cdot\left(\frac{\partial}{\partial\mathbf{p}} + \frac{s}{m}\frac{\partial}{\partial\mathbf{x}}\right),$$

respectively (see Fig. 1).

In the expression (I.1), $n+2$ summations appear. Let us consider terms of this sum which have the property that the i_k index is different from all other indices. Now $P = \prod_{l=1}^N P_l = \prod_{l=1}^N 1/\Omega \int d\mathbf{r}_l$. For terms of the above type the P_{i_k} operates only on a term of the form $\{\partial V(\mathbf{x}-\mathbf{r}_{i_k}-\mathbf{v}[s-t_k])/\partial\mathbf{x}\}$, and this gives zero if we change the $\mathbf{x}$ derivative to a $\mathbf{r}_{i_k}$ derivative and use the fact that V has finite range. The net result is that only those terms of (I.1) are nonzero which have every index the same as *at least* one other index. To indicate graphically when two indices are the same, we shall connect them by a loop [see Figs. 2(a) and 2(b)]. We have shown then that only those diagrams contribute in which every mark has at least one loop attached. If one can get from the first mark to the last mark by means of connecting loops only, then the diagram is said to be linked [Fig. 2(a)]; otherwise it is unlinked [Fig. 2(b)]. We now prove:

Theorem. The terms in (I.1) corresponding to unlinked diagrams are identically zero.

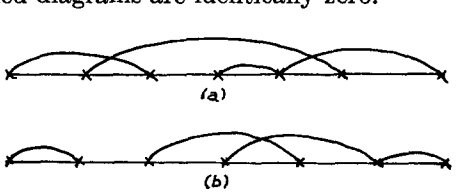

FIG. 2. 5th-order diagram: (a) linked, (b) unlinked.

Proof: Suppose that the diagram is unlinked between the i_k and i_{k+1} index (or mark). Then none of the variables $\mathbf{r}_{i_1} \cdots \mathbf{r}_{i_k}$ are the same as any of the variables $\mathbf{r}_{i_{k+1}} \cdots \mathbf{r}_{i_{n+1}}$ in (I.1).

Then the $(1 - P)$ that stands before the i_{k+1} term can be replaced by $1 - P_{i_{k+1}}P_{i_{k+2}} \cdots P_{i_{n+1}}$. We can also take the P that stands before the first mark and separate off a factor $P_{i_{k+1}} \cdots P_{i_{n+1}}$ which we can bring over to the i_{k+1} term so that we have standing before the i_{k+1} term a factor

$$(P_{i_{k+1}}P_{i_{k+2}} \cdots P_{i_{n+1}})(1 - P_{i_{k+1}}P_{i_{k+2}} \cdots P_{i_{n+1}}) = 0.$$

Hence the terms in the sum corresponding to unlinked diagrams are zero.

Now the index of a linked diagram is defined to be the number of loops that one must traverse to get from the first mark to the last. The final result that we want is:

Theorem. The contribution of a linked diagram of index l vanishes for $s > lt_0$.

Proof: To illustrate the method of this proof let us take a fourth-order linked diagram of index two. [See Fig. 3.] From (I.1) we see that with each mark except the first there is associated a time variable. From the limits on the integrations we know that $s > t_1 > t_2 > t_3 > t_4$. Now from the fact that the third and first mark are connected, we see that the expression (I.1) vanishes unless both $|\mathbf{x}-\mathbf{r}_{i_0}| < a$ and $|\mathbf{x} - \mathbf{r}_{i_0} - \mathbf{v}[s - t_2]| < a$, or unless $v\ |s-t_2| < a$ or $|s - t_2| < 2a/v = t_0$. Similarly the fact that the second and last marks are connected implies that (I.1) vanishes unless $|\mathbf{x} - \mathbf{r}_{i_1} - \mathbf{v}(s - t_1)| < a$ and $|\mathbf{x} - \mathbf{r}_{i_1} - \mathbf{v}s| < a$, or unless $vt_1 < 2a$ or $t_1 < t_0$. Then (I.1) vanishes unless $s < t_2 + t_0 < t_1 + t_0 < 2t_0$. This proves the theorem for this particular diagram.

It should be clear that the same type argument applies to any linked diagram. One can also see quite easily by example that this type of result is not available for unlinked diagrams, so it is fortunate that they give zero contribution to (I.1).

Now to complete the proof of (29a) all one need notice is that the index of any nth-order diagram is less than or equal to $\frac{1}{2}(n + 2)$.

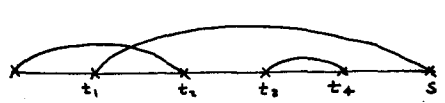

FIG. 3. 4th-order linked diagram of index 2.

APPENDIX III

In this appendix we shall consider the time

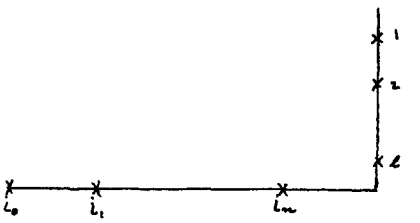

FIG. 4. General diagram for correlations.

dependence of terms of the form

$$P\delta LG^n(t)U_l(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_l, 0)$$

by methods similar to those of Appendix II.

From Eq. (17) we have

$$P\delta LG^n(t)U_l(\mathbf{x}, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_l, 0) = (-1)^n \int_0^t \cdots$$

$$\times \int_0^{t_n} \sum_{i_0} \cdots \sum_{i_n} P \frac{\partial V(\mathbf{x} - \mathbf{r}_{i_0})}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{p}} (1 - P)$$

$$\times \frac{\partial V(\mathbf{x} - \mathbf{r}_{i_1} - \mathbf{v}[t - t_1])}{\partial \mathbf{x}} \cdot \partial_1 \cdots (1 - P)$$

$$\times \frac{\partial V(\mathbf{x} - \mathbf{r}_{i_n} - \mathbf{v}[t - t_n])}{\partial \mathbf{x}} \cdot \partial_n$$

$$\times U_l(\mathbf{x} - \mathbf{v}t, \mathbf{p}, \mathbf{r}_1 \cdots \mathbf{r}_l, 0)\, dt_1 \cdots dt_n. \qquad \text{(III.1)}$$

We represent the general term by a horizontal line with $n + 1$ marks and a vertical line with l marks (Fig. 4). By virtue of Eq. (9) and the same arguments as in Appendix II, we see that the only terms in the sum which are nonzero are those for which each mark is connected to at least one other. We may connect horizontal to horizontal marks or horizontal to vertical marks, but not vertical to vertical marks since in Eq. (10) no two indices are ever the same. This means that any diagram for which $l > n + 1$ vanishes identically since there is no way to connect all the vertical marks to different horizontal marks.

Again as in Appendix II one proves that only linked diagrams are nonzero. The index of a linked diagram is again defined to be the minimum number of loops one must traverse to get from the first horizontal mark to the vertical line. Let us consider in particular a diagram of fifth-order and index three (Fig. 5).

From the structure of this diagram and the arguments in Appendix II we see that its contribu-

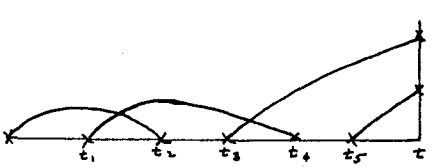

FIG. 5. 5th-order diagram of index 3.

tion will vanish unless

(a) $|t - t_2| < t_c$, since the first and third marks are connected;

(b) $|t_4 - t_1| < t_c$, since the second and fifth marks are connected;

(c) $t_3 < t_c + t_R$, since the fourth mark is connected to the vertical line.

We have then

$$t < t_c + t_2 < t_c + t_1 < 2t_c + t_4 < 2t_c + t_3 < 3t_c + t_R.$$

One can generalize this to show that the contribution of any diagram of index k vanishes for $t > kt_c + t_R$. One can see that for a given n and l all diagrams have index less than or equal to $\frac{1}{2}(n + 1 - l) + 1$. Then for a given n and l all contributions vanish for $t > [\frac{1}{2}(n - l) + \frac{3}{2}]t_c + t_R$.

APPENDIX IV

We want to find the explicit form of the expression

$$\int_0^\infty P\delta LG^0(s)\delta LU(\mathbf{x}, \mathbf{p}, t - s)\, ds = -\int_0^\infty \sum_i 1/\Omega \int_{r_i} \frac{\partial V(\mathbf{x} - \mathbf{r}_i)}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{p}} \times \frac{\partial V(\mathbf{x} - \mathbf{vs} - \mathbf{r}_i)}{\partial \mathbf{x}} \cdot \left(\frac{\partial}{\partial \mathbf{p}} + \frac{s}{m}\frac{\partial}{\partial \mathbf{x}}\right) d\mathbf{r}_i \times U(\mathbf{x} - \mathbf{vs}, \mathbf{p}, t - s)\, ds.$$

[See Eq. (19).]

Since the value of the integral over $\mathbf{r}_i$ is independent of j we may remove the sum. We also change the variable of integration from $\mathbf{r}_i$ to $y = \mathbf{x} - \mathbf{r}_i$ to obtain

$$\int_0^\infty P\delta LG^0(s)\delta LU(\mathbf{x}, \mathbf{p}, t - s)\, ds = -N/\Omega \times \int_0^\infty \int_y \frac{\partial V(\mathbf{y})}{\partial \mathbf{y}} \cdot \frac{\partial}{\partial \mathbf{p}} \frac{\partial V(\mathbf{y} - \mathbf{vs})}{\partial \mathbf{y}} \cdot \left(\frac{\partial}{\partial \mathbf{p}} + \frac{s}{m}\frac{\partial}{\partial \mathbf{x}}\right) \times U(\mathbf{x} - \mathbf{vs}, \mathbf{p}, t)\, d\mathbf{y}\, ds.$$

Since $[\partial V(\mathbf{y})/\partial \mathbf{y}][\partial V(\mathbf{y} - \mathbf{vs})/\partial \mathbf{y}] = 0$ when $vs > 2a$, the appropriate approximation is to set $s = 0$ except in the $V(\mathbf{y} - \mathbf{vs})$ term to obtain

$$\int_0^\infty P\delta LG^0(s)\delta LU(\mathbf{x}, \mathbf{p}, t - s)\, ds = -N/\Omega \times \int_0^\infty \int_y \frac{\partial V(\mathbf{y})}{\partial \mathbf{y}} \cdot \frac{\partial}{\partial \mathbf{p}} \frac{\partial V(\mathbf{y} - \mathbf{vs})}{\partial \mathbf{y}} \cdot \frac{\partial}{\partial \mathbf{p}}\, d\mathbf{y}\, ds \times U(\mathbf{x}, \mathbf{p}, t). \quad \text{(IV.1)}$$

To make this approximation we have assumed that $U(\mathbf{x}, \mathbf{p}, t)$ is a slowly varying function of $\mathbf{x}$ over the distance a and slowly varying in t over times of the order $t_c = 2a/v$. Using component notation and integrating by parts on $\mathbf{y}$, (IV.1) can be written as

$$\int_0^\infty P\delta LG^0(s)\delta LU(\mathbf{x}, \mathbf{p}, t - s)\, ds = N/\Omega\, \partial/\partial p_i \times \int_0^\infty \int_y V(\mathbf{y})\, \partial/\partial y_i\, \partial/\partial y_i \times V(\mathbf{y} - \mathbf{vs})\, d\mathbf{y}\, ds\, \partial/\partial p_i U(\mathbf{x}, \mathbf{p}, t). \quad \text{(IV.2)}$$

Remembering that $\mathbf{v} = \mathbf{p}/m$ we can now change the y_i derivatives to p_i derivatives to obtain

$$\int_0^\infty P\delta LG^0(s)\delta LU(\mathbf{x}, \mathbf{p}, t - s)\, ds = N/\Omega\, \partial/\partial p_i \times \left[\partial/\partial p_i\, \partial/\partial p_i \int_0^\infty \int_y m^2/s^2 V(\mathbf{y}) \times V(\mathbf{y} - \mathbf{ps}/m)\, d\mathbf{y}\, ds\right](\partial/\partial p_i)U(\mathbf{x}, \mathbf{p}, t). \quad \text{(IV.3)}$$

We now assume that V has spherical symmetry so that the integral over $\mathbf{y}$ can depend only on the magnitude of $\mathbf{ps}/m$. We set

$$g(ps/m) = \int V(\mathbf{y})V(\mathbf{y} - \mathbf{ps}/m)\, d\mathbf{y}. \quad \text{(IV.4)}$$

Note that if V vanishes for $|\mathbf{y}| > a$, then g vanishes for $ps/m > 2a$ or $s > t_c$. Because of the spherical symmetry, g has zero derivative at the origin, that is, $g'(0) = 0$. We note that

$$\partial g(ps/m)/\partial p_i = s/mg'(ps/m)p_i/p,$$

and

$$\partial^2 g(ps/m)/\partial p_i\, \partial p_i = s^2/m^2 g''(ps/m)p_i p_i/p^2 + s/mg'(ps/m)(\delta_{ii}/p - p_i p_i/p^3).$$

This yields

$$\int_0^\infty P\delta LG^0(s)\delta LU(\mathbf{x}, \mathbf{p}, t - s)\, ds = N/\Omega\, \partial/\partial p_i \times \int_0^\infty [g''(ps/m)p_i p_i/p^2 + m/sg'(ps/m) \times (\delta_{ii}/p - p_i p_i/p^3)\, \partial/\partial p_i]\, dsU(\mathbf{x}, \mathbf{p}, t). \quad \text{(IV.5)}$$

When we integrate over s from 0 to ∞, the g'' term vanishes since $g'(0) = g'(\infty) = 0$. In the g' term we change the variable of integration to $\alpha = ps/m$ so that the integral is independent of p and obtain

$$\int_0^\infty P\delta LG^0(s)\ \delta L\, ds = mN/\Omega \int_0^\infty g'(\alpha)/\alpha\, d\alpha \times \partial/\partial p_i(\delta_{ii}/p - p_i p_i/p^3)\, \partial/\partial p_i\ . \quad \text{(IV.6)}$$

It is useful to note that in spherical coordinates

$$\partial/\partial p_i(\delta_{ii}/p - p_i p_i/p^3)\, \partial/\partial p_i = 1/p^3[1/\sin\theta\, \partial/\partial\theta \times (\sin\theta\, \partial/\partial\theta) + 1/\sin^2\theta\, \partial^2/\partial\varphi^2].$$

The eigenvectors of this operator are the spherical harmonics $Y_l^m(\theta, \varphi)$ and its eigenvalues are $-l(l + 1)$.

Multiple Scattering in the Diffusion Approximation*

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The passage of classical particles through a grainy scattering medium can be described by a linearized Boltzmann equation. A discussion is given of the physical conditions which justify the use of the Fokker–Planck diffusion approximation to this equation. Some limiting properties of the solutions of the diffusion equation are first discussed for the initial-value problem in an infinite medium characterized by a diffusion length D. For a total path length $\ell \ll D$ convenient formulas are given for the distribution of scattering angles θ and, for given θ, the first few moments of the final position vector are computed. These results are taken as a basis for approximate treatment of steady-state boundary-value problems. The case of a particle beam incident on a thin plane parallel slab of thickness $d \ll D$ is considered. Approximate formulas are given for the angular distribution of the transmitted beam and for the (very small) fraction of the beam which emerges from the entrance face. Errors are assessed, and the behavior for grazing angles of incidence or exit is discussed in a conjectural way.

I. THE DIFFUSION APPROXIMATION

IN the analysis of problems involving the passage of particles through a grainy scattering medium, one is sometimes justified in adopting the Fokker–Planck diffusion approximation to the linear Boltzmann equation.[1] It is our main purpose here to discuss some limiting properties of the solutions of the resulting diffusion equation, in order to bring out what may be useful approximation schemes for situations in which the geometric dimensions of the scattering medium are small compared to the diffusion length. In this first section, however, we are concerned with establishing the nature of the physical conditions that warrant the transition to a diffusion equation description of multiple scattering.

The general problem under discussion has to do with the motion of classical point particles in a medium filled with fixed spherical scattering centers, randomly located on a fine-grained scale.[2] The coarse-grained number density of scattering centers, n, we take to be uniform over the medium and constant in time. In the collision of a particle with a scattering center, it is only the orientation, not the magnitude, of the velocity vector $\mathbf{v}$ that undergoes change. Let $\sigma_{\mathbf{v},\mathbf{v}'}$ be the differential cross section for scattering from the direction of $\mathbf{v}$ to the direction of $\mathbf{v}'$; and let $f(\mathbf{x}, \mathbf{v}, \ell)\, d^3x\, d\Omega$ be the the probability (in an ensemble sense) that, at time $t = \ell/v$, the particle is located in a spatial volume element d^3x centered about $\mathbf{x}$, with velocity vector lying in an element of solid angle $d\Omega$ centered about the direction of $\mathbf{v}$. We suppose that the distribution function f satisfies the Boltzmann equation

$$\frac{\partial f(\mathbf{x}, \mathbf{v}, \ell)}{\partial \ell} + \frac{\mathbf{v}}{v}\cdot\nabla f(\mathbf{x}, \mathbf{v}, \ell) = n \int d\Omega'\, \sigma_{\mathbf{v},\mathbf{v}'}\{f(\mathbf{x}, \mathbf{v}', \ell) - f(\mathbf{x}, \mathbf{v}, \ell)\}. \quad (1)$$

Suppose now that we are dealing with a scattering function $\sigma_{\mathbf{v},\mathbf{v}'} \equiv \sigma(\psi)$, $\psi = \cos^{-1}(\mathbf{v}\cdot\mathbf{v}'/v^2)$, which is strongly peaked at very small scattering angles ψ. In this circumstance we are tempted to approximate the collision integral above by expanding $f(\mathbf{x}, \mathbf{v}', \ell)$ in a Taylor series about $\mathbf{v}' = \mathbf{v}$, retaining only the lowest nonvanishing terms. This leads to the diffusion equation of interest. Denote by θ and φ the polar and azimuthal angles which describe the orientation of the vector $\mathbf{v}$ with respect to fixed axes; and let $\cos\theta \equiv \mu$. We then find

$$\frac{\partial f}{\partial \ell} + \frac{\mathbf{v}}{v}\cdot\nabla f = \frac{1}{D}\left\{\frac{\partial}{\partial \mu}(1-\mu^2)\frac{\partial f}{\partial \mu} + \frac{1}{1-\mu^2}\frac{\partial^2 f}{\partial \varphi^2}\right\}, \quad (2)$$

where the diffusion length D is given by

$$1/D = \frac{2\pi n}{4}\int_0^\pi \psi^2 \sigma(\psi) \sin\psi\, d\psi. \quad (3)$$

Before proceeding to our study of the mathe-

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[1] For a general review, see S. Chandrasekhar, Rev. Mod. Phys. 15, 1 (1943).

[2] There is a vast literature on this problem of multiple scattering without energy loss which goes beyond the diffusion approximation. See, for example, S. Goudsmit and J. L. Saunderson, Phys. Rev. 57, 24 (1939); Phys. Rev. 58, 36 (1940); C. Grosjean, Physica 19, 29 (1953); E. P. Wigner, Phys. Rev. 94, 17 (1954).

matical properties of the solutions of the diffusion equation, let us first consider what errors are involved in this transition from the Boltzmann equation to a diffusion equation. It is of course not easy to assess the errors in general terms, since they must depend not only on the nature of the scattering law $\sigma(\psi)$ but also on the boundary and initial conditions and on the region in phase space and time for which the assessment is to be made. A crude discussion, however, can be given along the following lines, for a representative problem of motion in an infinite medium.

Consider a situation in which a particle is moving along the z axis at the initial time. We ask for the distribution in orientation of the velocity vector at some later time (or at some path length $\ell = vt$), irrespective of the spatial position of the particle. Hence we regard f as a function of θ and ℓ, where θ is the polar angle, and normalize according to $\int f(\theta, \ell)\, d\Omega = 1$. Throughout the rest of the discussion we shall be concerned only with path lengths ℓ small compared to the diffusion length D. For $\ell \ll D$ we expect that f will be peaked at small angles θ; and, in the small angle approximation, the diffusion equation is solved by

$$f_{diff}(\theta, \ell) = \frac{1}{\pi \overline{\theta^2}} \exp\left[-\theta^2/\overline{\theta^2}\right], \tag{4}$$

where

$$\overline{\theta^2} = 4l/D \ll 1. \tag{5}$$

We now attempt to assess how seriously this departs from the true solution f of the Boltzmann equation, employing a kind of iteration test for the purpose. Let us insert the approximation (4) into the true Boltzmann collision integral. In the small angle approximation this gives

$$\frac{\partial f(\theta, \ell)}{\partial \ell} = \frac{n}{\pi \overline{\theta^2}} \exp\left[-\theta^2/\overline{\theta^2}\right] \int_0^{2\pi} d\alpha \int_0^{\pi} d\psi$$

$$\times \sin\psi\sigma(\psi)\{\exp\left[-(\psi^2 - 2\theta\psi\cos\alpha)/\overline{\theta^2}\right] - 1\}. \tag{6}$$

In the diffusion equation approximation to the collision integral, on the other hand, the expression in curly brackets above is expanded to lowest order in ψ^2; thus

$$\frac{\partial f_{diff}}{\partial l} = \frac{n}{\pi \overline{\theta^2}} \exp\left[-\frac{\theta^2}{\overline{\theta^2}}\right] \frac{2\pi}{\overline{\theta^2}} \left(1 - \frac{\theta^2}{\overline{\theta^2}}\right) \int_0^{\pi} d\psi$$

$$\times \sin\psi\sigma(\psi)\psi^2. \tag{7}$$

The diffusion approximation is justified, for given θ and ℓ, insofar as (7) adequately approximates (6).

It is clear that the diffusion equation can be meaningful only if the scattering function $\sigma(\psi)$ falls off sufficiently rapidly with increasing ψ. For the present discussion let us in fact restrict our considerations to functions which everywhere fall off monotonically with increasing ψ and which have the property that there exists some critical angle $\psi_0 \ll 1$ such that

$$\int_{\psi_0}^{\pi} d\psi\, \psi^2 \sin\psi\sigma(\psi) \ll \int_0^{\psi_0} d\psi\, \psi^2 \sin\psi\sigma(\psi). \tag{8}$$

For example, the scattering function

$$\sigma(\psi) = a^2/(\psi_0^2 + \psi^2)^n \tag{9}$$

has the indicated properties, provided $\psi_0 \ll 1$ and $n > 2$.

On comparing Eqs. (6) and (9) we see immediately that one necessary condition for validity of the diffusion approximation is

$$\overline{\theta^2} = 4l/D \gg \psi_0^2; \tag{10}$$

i.e., in no case can we take the diffusion equation seriously for times ℓ/v which are too short. This is reasonable on physical grounds. After the first mean collision time interval, the true distribution should already be filled out to angles up to a value of order ψ_0. Hence, not until enough time has elapsed so that $(\overline{\theta^2})^{\frac{1}{2}}$ exceeds ψ_0 can we accept any assertions which follow from the diffusion equation, since the latter presupposes that many scatterings have occurred in any time interval of interest. Throughout the remaining discussion we shall assume that the condition (10) is satisfied.

It is also clear that the expansion to terms linear in ψ^2 in the curly bracket term of (6) must surely go wrong unless

$$\theta \ll \overline{\theta^2}/\psi_0, \tag{11}$$

i.e., (11) is a necessary, though not a sufficient condition for adequacy of the diffusion equation solution. This too can be seen on physical grounds. A typical collision involves a scattering through angle of order ψ_0. In a sequence of N collisions, with random changes in azimuthal angle, the mean net turning angle $(\overline{\theta^2})^{\frac{1}{2}}$ is given by $N^{\frac{1}{2}}\psi_0$. On the other hand, the improbable sequence of N such collisions in which the velocity vector remains essentially in a fixed plane yields a net angular deflection $\theta \approx N\psi_0$. We may be sure that such a coherent chain of scatterings is not properly accounted for in the diffusion approximation, hence we expect the diffusion equation solution to go wrong when $\theta > N\psi_0 \approx \overline{\theta^2}/\psi_0$ as in Eq. (11).

We have said that Eq. (11) represents a *necessary*

condition for validity of the diffusion approximation. On the other hand, a *sufficient* condition is simply

$$\theta^2 < \overline{\theta^2}, \tag{12}$$

as one expects on physical grounds and can verify by inspection of Eq. (6). To improve this estimate of sufficiency, we can employ the following considerations. We ask for the contribution to $f(\theta, \ell)$, for $\theta^2 \gg \overline{\theta^2} \equiv \bar{\theta}^2$, which comes from a single large angle scattering having taken place during the path-length interval ℓ. Since the bulk of the probability distribution is confined to angles up to a value of order $\bar{\theta} \ll \theta$, such a scattering must involve an angular change which is essentially equal to θ itself. This single scattering contribution is therefore given by

$$f_s(\theta, \ell) \approx 2\pi n \ell \sigma(\theta), \qquad \theta \gg \bar{\theta}. \tag{13}$$

Notice, from (5) and (13), that

$$f_s/\overline{\theta^2} = (2\pi n/4) D\sigma(\theta); \tag{14}$$

and from (3), that

$$1/D \gtrsim (2\pi n/4)\psi_0^4 \sigma(\psi_0). \tag{15}$$

We first show that the total probability $P(\theta, \ell)$ for single scattering through angles of order θ or larger is small compared to unity: since $\psi_0 \ll \bar{\theta} \ll \theta \ll \pi$, and since $\theta^4\sigma(\theta)$ is a monotonically decreasing function, we have

$$P(\theta, l) = \frac{\pi n}{2} \overline{\theta^2}\, D \int_\theta^\pi \sigma(\theta') \sin\theta'\, d\theta'$$

$$\sim n\overline{\theta^2}\, D\theta^2\sigma(\theta) \lesssim \frac{\overline{\theta^2}}{\overline{\theta^2}} \frac{\theta^4\sigma(\theta)}{\psi_0^4\sigma(\psi_0)} \ll 1. \tag{16}$$

Since this probability is small we can certainly neglect multiple large angle scattering for all $\theta \gg \bar{\theta}$. However, single large angle scattering can be neglected only when $f_s(\theta, \ell) \ll f_{diff}(\theta, \ell)$. The diffusion equation is then adequate provided θ satisfies (11) and is also less than a critical angle θ_c determined by $f_{diff}(\theta_c, \ell) \approx f_s(\theta_c, \ell)$. Thus,

$$\frac{1}{\pi\overline{\theta^2}} \exp\left[-\theta_c^2/\overline{\theta^2}\right] \approx 2\pi n \ell \sigma(\theta_c), \tag{17}$$

or, from (5) and (15):

$$\exp\left[-\theta_c^2/\overline{\theta^2}\right] \approx \pi(\overline{\theta^2}/\psi_0^2)^2(\psi_0^2/\theta_c^2)^4. \tag{18}$$

These results can also be understood from a direct comparison of (6) and (7). For $\theta \gg \bar{\theta}$ the expression in curly brackets in (6), regarded as a function of ψ, has a sharp bump of height $\approx \exp[\theta^2/\overline{\theta^2}]$ and width $\approx \bar{\theta}$, centered at $\psi = \theta$. In the integral on the right-hand side of (6) this bump makes a contribution which is just of order $f_s(\theta, \ell)/\ell$; i.e., it is just the contribution of a single large angle scattering. Indeed, if the condition (11) is met, the right side of (6) is essentially the sum of two terms:

$$\partial f/\partial \ell \approx \partial f_{diff}/\partial \ell + f_s/\ell. \tag{19}$$

We can now summarize our findings in the following manner: (1) The transition from the Boltzmann to the diffusion equation can at best make sense only if the scattering function $\sigma(\psi)$ falls off sufficiently rapidly with increasing ψ—faster than ψ^{-4}—beyond some small angle ψ_0. (2) Even then, any solution of the diffusion equation must be thought of as representing a smoothing of the true distribution function over path-length intervals large compared to $\ell_0 = \frac{1}{4}D\psi_0$ [see Eq. (10)]. Where the distribution function has already come to be rather smoothly varying in phase space, this delicacy is no longer important; but if, as in the example we have analyzed, the initial f is sharply peaked in phase space, the diffusion solution cannot be believed until an interval of time ℓ_0/v has elapsed. In any case, if $\sigma(\psi)$ is slowly varying in the interval $0 < \psi < \psi_0$, changes in the distribution function over an interval $\Delta\ell < \ell_0$ can always be obtained from a straight *single* scattering analysis. (3) If at some initial time the distribution function is essentially confined to a narrow region in phase space, its subsequent development within a larger domain of phase space, over an interval $\ell_0 \ll \ell \ll D$, is adequately approximated by regarding f as a direct sum of the diffusion equation solution f_{diff} and a contribution f_s coming from single, large angle scatterings:

$$f \approx f_{diff} + f_s, \tag{20}$$

where we understand by this that f_s is to be included only for angles large compared to the mean angle for f_{diff}. In the sample problem analyzed above, the domain of validity of (20) corresponds to $0 < \theta \ll \overline{\theta^2}/\psi_0$ [see Eq. (11)], the f_s term being appended only for $\theta \gg \bar{\theta}$ and becoming important only beyond some critical angle θ_c determined by setting $f_{diff} \approx f_s$ and taking the root, if any, which lies well above $\bar{\theta}$. Finally, we must emphasize again that a proper assessment of the errors involved in any approximation scheme for treating multiple scattering must depend on the details of the problem at hand. The above discussion was intended only to provide a very rough idea of the circumstances which permit a treatment of the Boltzmann problem

based on the diffusion equation approximation, as supplemented perhaps by consideration of single, large angle scattering effects.

We have fixed our attention here on the diffusion approximation for classical point particles moving in a scattering medium. Two other problems of interest are the passage of Schrödinger waves through a medium filled with randomly placed quantum mechanical scattering potentials, and the passage of electromagnetic waves through a medium with fluctuating refractive index.[3] The exact equations for these problems are of course entirely different from the Boltzmann equation (1). Nevertheless, under certain restrictive conditions the motion of wave packets in these problems can also be described approximately by the diffusion equation (2). The errors which are introduced in this approximation for situations involving wave packets are of course entirely different than for classical particle problems. We shall however not pursue any further the physical basis of the diffusion equation. We instead turn to the mathematical properties of the equation, using for descriptive purposes the language of classical point particles.

In the remaining sections we shall be concerned with multiple scattering effects for problems of the following sort, assuming without further apology that the diffusion approximation is always relevant. Suppose that a beam of particles impinges on a scattering medium, the geometrical conditions being such that most of the particles emerge from the medium in times short compared to the diffusion time D/v. (For example, it may be that some characteristic dimension of the medium is small compared to the diffusion length.) In such circumstances the net scattering angle will be small for most beam particles. But we will be interested in estimating the probability of occurrence for those rare events in which the net scattering angle is large. Multiple small angle scattering plays two distinct roles here. For one thing it may compete with single large angle scattering contributions to the events in question. For another, even where single large angle scattering effects dominate, their quantitative contribution can be appreciably influenced by a possible loss of beam intensity within the medium, this effect coming about from leakage through the walls produced by multiple small angle scattering phenomena.

These multiple scattering effects clearly depend sensitively on geometrical details; but there is little hope of obtaining closed solutions of the diffusion equation with general boundary conditions. Our procedure then is to first analyze the time-dependent diffusion problem for an infinite medium, in order to extract insights which can suggest approximation schemes for the time-independent problem with boundary conditions.

[3] See, L. Chernov, *Wave Propagation in a Random Medium* (McGraw-Hill Book Company, Inc., New York, 1960).

II. THE INFINITE MEDIUM DIFFUSION PROBLEM

Suppose that at the initial time a particle is located at the spatial origin $\mathbf{x} = 0$ with velocity vector $\mathbf{v}$ directed along the positive z axis. The development in time ℓ/v of the phase-space distribution function $f(\mathbf{x}, \theta, \varphi, \ell)$ is governed by the diffusion equation (2); and for convenience we scale out the diffusion length D by measuring all distances in units of D. A full solution to this initial value problem does not seem to be attainable in closed form, and we resort instead to studying the dependence on orientation of the velocity vector of the low spatial moments of f, in particular for times which are small compared to the diffusion time, i.e., for $\ell \ll 1$.

Consider first the zeroth spatial moment

$$f_0(\theta, l) = \int f(\mathbf{x}, \theta, \varphi, \ell)\, d^3x, \tag{21}$$

which describes the distribution in velocity vector orientation, irrespective of spatial position. For this moment the diffusion equation reduces to

$$\frac{\partial}{\partial \mu}(1 - \mu^2)\frac{\partial f_0}{\partial \mu} = \frac{\partial f_0}{\partial l}, \qquad \mu = \cos\theta, \tag{22}$$

and the solution consistent with the given initial condition is

$$f_0 = \frac{1}{4\pi}\sum_{n=0}^{\infty}(2n + 1)P_n(\theta)e^{-n(n+1)\ell}, \tag{23}$$

where $P_n(\theta)$ is the Legendre function of nth order.

For $\ell \gg 1$ this series converges rapidly, and hence is already in useful form. For $\ell \ll 1$ we seek another, more rapidly convergent representation. This can be arrived at in the following manner. For $\theta < \pi$ the Legendre function can be written as

$$P_n(\theta) = \frac{\sqrt{2}}{\pi}\int_{\theta}^{\pi} d\alpha\, \frac{\sin[(n + \frac{1}{2})\alpha]}{(\cos\theta - \cos\alpha)^{\frac{1}{2}}}, \tag{24}$$

so that

$$4\pi f_0 = \frac{1}{\sqrt{2}\,\pi}\int_{\theta}^{\pi} d\alpha\, \frac{\Sigma(\alpha)}{(\cos\theta - \cos\alpha)^{\frac{1}{2}}},$$

$$\Sigma(\alpha) = \sum_{n=-\infty}^{\infty}(2n + 1)\sin[(n + \tfrac{1}{2})\alpha]e^{-n(n+1)\ell}.$$

We now use the Poisson sum formula[4] to cast $\Sigma(\alpha)$ into the form

$$\Sigma(\alpha) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dx\, e^{-2\pi i m x}(2x+1) \times \sin[(x+\tfrac{1}{2})\alpha] e^{-x(x+1)\ell}$$

$$= -2\frac{\partial}{\partial\alpha}\sum_m (-1)^m \int_{-\infty}^{\infty} dx\, e^{-2\pi i m x} \times \cos\alpha x e^{-\ell x^2} e^{\ell/4}.$$

For ℓ sufficiently small, only the $m = 0$ term need be retained in the above expression and we find

$$4\pi f_0 \underset{\ell\to 0}{\to} \frac{1}{\sqrt{2\pi}}\frac{1}{\ell^{\frac{1}{2}}}\int_\theta^\pi d\alpha \frac{\alpha e^{-\alpha^2/4\ell}}{(\cos\theta - \cos\alpha)^{\frac{1}{2}}}.$$

Evaluating this in the limit $\ell\to 0$ (but for arbitrary θ) we obtain finally

$$f_0 \underset{\ell\to 0}{\to} \frac{1}{4\pi\ell}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}} e^{-\theta^2/4\ell}. \tag{25}$$

For small θ this agrees with the solution, Eq. (4), anticipated earlier.

We next turn to the higher moments of the distribution in the z coordinate of spatial position, regarded as functions of velocity vector orientation:

$$f_{(n;z)}(\theta, l) = \int z^n f(\mathbf{x}, \theta, \varphi, \ell)\, d^3x. \tag{26}$$

These moments are clearly independent of azimuth φ. Multiplying the diffusion Eq. (2) by z^n, integrating over all space, averaging over azimuth of velocity vector orientation, we find

$$\frac{\partial f_{(n;z)}}{\partial l} - \frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial f_{(n;z)}}{\partial\mu} = \mu n f_{(n-1;z)}. \tag{27}$$

This is to be solved subject to the initial condition $f_{(n;z)} = 0$ at $\ell = 0$, provided $n > 0$. It is evident on inspection that the solution for $f_{(n;z)}$, in terms of $f_{(n-1;z)}$, is given by

$$f_{(n;z)}(\theta, \ell) = \frac{n}{4\pi}\int_0^\ell d\ell' \sum_m (2m+1)P_m(\theta)e^{-m(m+1)(\ell-\ell')} \times \int d\Omega' P_m(\theta')\cos\theta' f_{(n-1;z)}(\theta', \ell'). \tag{28}$$

Since the zeroth moment f_0 is already known, all of the higher moments can be obtained in succession.

In particular, on using Eq. (23) for f_0, we find for $f_{(1;z)}$ the expression

$$f_{(1;z)} = \frac{1}{8\pi}\sum_{m=0}^{\infty} P_m(\theta)\{e^{-m(m-1)\ell} - e^{-(m+1)(m+2)\ell}\}. \tag{29}$$

As with Eq. (23), this expression is already in convenient form for large ℓ. For small ℓ we seek a more rapidly converging representation. Using the Poisson sum formula as before we find for the limit $\ell\to 0$ the result

$$f_{(1;z)} \underset{\ell\to 0}{\to} \ell\left(\frac{\sin\theta}{\theta}\right) f_0(\theta, \ell).$$

Now

$$\bar{z}(\theta, l) = f_{(1;z)}(\theta, \ell)/f_0(\theta, \ell) \tag{30}$$

is the expectation value of the z displacement at "time" ℓ for particles whose velocity vector makes an angle θ with respect to the z axis; so we have

$$\bar{z}(\theta, \ell) \underset{\ell\to 0}{\to} \ell(\sin\theta/\theta). \tag{31}$$

This same result can be obtained in another way, as follows. Substituting $f_{(1;z)} = \bar{z}f_0$ into Eq. (27) for $n = 1$ and using the corresponding equation (22) satisfied by f_0, we find

$$\frac{\partial\bar{z}}{\partial_l} - \frac{\partial^2\bar{z}}{\partial\theta^2} - \cot\theta\frac{\partial\bar{z}}{\partial\theta} - 2\frac{\partial\ln f_0}{\partial\theta}\frac{\partial\bar{z}}{\partial\theta} = \cos\theta \tag{32}$$

where, in the limit $\ell\to 0$, we have

$$\frac{\partial}{\partial\theta}\ln f_0 \to -\theta/2\ell. \tag{33}$$

To lowest order, $\bar{z}$ must be linear in ℓ; and to this order we obtain

$$\bar{z} + \theta\,\partial\bar{z}/\partial\theta = \ell\cos\theta.$$

The solution, finite at $\theta = 0$, is just that given by (31).

In order to estimate the dispersion about the mean given by Eq. (31), we turn next to a computation of the second moment $f_{(2;z)}(\theta, \ell)$. The expression which emerges directly from a substitution of (29) into (28) is not in convenient form to display the behavior of this function in the limit as $\ell\to 0$. In order to study this limiting structure, we work directly with the differential equation (27), writing

$$f_{(2;z)}(\theta, \ell) = [\bar{z}^2(\theta, \ell) + h(\theta, \ell)]f_0(\theta, \ell). \tag{34}$$

We substitute this into (27) for $n = 2$, exploit the same equation for $n = 1$ as well as Eq. (22), and find

$$-2\left(\frac{\partial\bar{z}}{\partial\theta}\right)^2 + \left[\frac{\partial h}{\partial l} - \frac{\partial^2 h}{\partial\theta^2} - \cot\theta\frac{\partial h}{\partial\theta}\right] - 2\frac{\partial h}{\partial\theta}\frac{\partial}{\partial\theta}\ln f_0 = 0. \tag{35}$$

[4] See P. M. Morse and H. Feshback, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. I, p. 466.

From (31) and (32) we now see that

$$h(\theta, \ell) \underset{\ell \to 0}{\to} \ell^3 H(\theta), \tag{36}$$

and in this limit (35) reduces to

$$\theta \frac{dH}{d\theta} + 3H = 2\left[\frac{d}{d\theta}\left(\frac{\sin\theta}{\theta}\right)\right]^2. \tag{37}$$

This has the solution

$$H(\theta) = \frac{1}{\theta^2}\left\{1 + \left(\frac{\sin\theta}{\theta}\right)\cos\theta - 2\left(\frac{\sin\theta}{\theta}\right)^2\right\} \underset{\theta \to 0}{\to} \frac{2}{45}\theta^2. \tag{38}$$

The dispersion about the mean is determined by

$$\overline{(\Delta z)^2} = \overline{z^2} - \bar{z}^2 = \ell^3 H(\theta). \tag{39}$$

We consider next the question of the transverse spread with time of a group of particles all located initially at the origin, with velocity vectors directed along the z axis. Form the moments

$$f_{(n;x)}(\theta, \varphi, \ell) = \int x^n f(\mathbf{x}, \theta, \varphi, \ell)\, d^3x. \tag{40}$$

The diffusion equation then reduces to

$$\frac{\partial f_{(n;x)}}{\partial \ell} - \left\{\frac{\partial}{\partial \mu}(1 - \mu^2)\frac{\partial f_{(n;x)}}{\partial \mu} + \frac{1}{1 - \mu^2}\frac{\partial^2 f_{(n;x)}}{\partial \varphi^2}\right\} = n \sin\theta \cos\varphi f_{(n-1;x)}, \tag{41}$$

which, for $n > 0$, must be solved subject to $f_{(n;x)} = 0$ as $\ell \to 0$. This has the solution

$$f_{(n;x)}(\theta, \varphi, \ell) = n \int_0^\ell d\ell' \sum_{\lambda=0}^{\infty} \sum_{m=-\lambda}^{\lambda} Y_\lambda^m(\theta, \varphi) e^{-\lambda(\lambda+1)(\ell - \ell')} \times \int d\Omega'\, Y_\lambda^{m*}(\theta', \varphi') \sin\theta' \cos\varphi' f_{(n-1;x)}(\theta', \varphi', \ell'), \tag{42}$$

where the Y_λ^m are spherical harmonic functions. To determine the moment functions we proceed exactly as before.

Thus, for the first moment we set $n = 1$ in Eq. (42) and substitute for f_0 on the right side the expression given by Eq. (23). We then find

$$f_{(1;x)}(\theta, \varphi, \ell) = \frac{\cos\varphi}{8\pi}\frac{\partial}{\partial\theta}\sum_{n=1}^{\infty}\frac{1}{n}[P_{n-1}(\theta) - P_n(\theta)] \times \{e^{-n(n-1)\ell} - e^{-n(n+1)\ell}\}. \tag{43}$$

This expression is, of course, not in useful form for small ℓ. To bring out the behavior for this limit, we work directly, as before, with the differential equation (41). We set

$$f_{(1;x)}(\theta, \varphi, \ell) = \bar{x}(\theta, \varphi, \ell) f_0(\theta, \ell), \tag{44}$$

insert this into (41), and, in the resulting equation for $\bar{x}$, retain only the linear term in an expansion in powers of ℓ. The result is given by

$$\bar{x}(\theta, \varphi, \ell) \underset{\ell \to 0}{\to} \ell \cos\varphi\left(\frac{1 - \cos\theta}{\theta}\right). \tag{45}$$

What this signifies is the following. Let $\boldsymbol{\varrho}$ be the projection on the $x - y$ plane of the position vector $\mathbf{x}$; and let $\mathbf{v}_\rho$ be a *unit* vector directed along the projection of $\mathbf{v}$ in the $x - y$ plane. Then the expectation value of $\boldsymbol{\varrho}$ is expressed by

$$\langle \boldsymbol{\varrho} \rangle \underset{\ell \to 0}{\to} \ell\left(\frac{1 - \cos\theta}{\theta}\right)\mathbf{v}_\rho. \tag{46}$$

To estimate the dispersion about the mean we turn to the second moment $f_{(2;x)}(\theta, \varphi, \ell)$. Repeating procedures used above, we write

$$f_{(2;x)}(\theta, \varphi, \ell) = \{\bar{x}^2(\theta, \varphi, \ell) + g(\theta, \varphi, \ell)\} f_0(\theta, \ell), \tag{47}$$

and insert this into (41) for $n = 2$, exploiting the corresponding equations for $n = 1$ and $n = 0$. For small ℓ, g is found to be proportional to ℓ^3; and with

$$g(\theta, \varphi, \ell) \underset{\ell \to 0}{\to} \ell^3\{G_1(\theta)\cos^2\varphi + G_2(\theta)\sin^2\varphi\}, \tag{48}$$

one obtains the results

$$G_1(\theta) = \frac{1}{\theta^2}\left\{1 - \left(\frac{\sin\theta}{\theta}\right)\cos\theta - 2\left(\frac{1 - \cos\theta}{\theta}\right)^2\right\}, \tag{49}$$

$$G_2(\theta) = \frac{2}{\theta^2}\left\{\frac{2\sin\theta}{\theta(1 + \cos\theta)} - 1\right\}. \tag{49'}$$

For small values of θ, one finds $G_1 \approx G_2 \approx \frac{1}{6}$. From (44), (47), and (48) we observe that, for particles whose velocity vectors lie in the x–z plane and make an angle θ with respect to the z axis, the fluctuations about the mean spatial position in the x–y plane are given by

$$\overline{(\Delta x)^2} = \overline{x^2} - \bar{x}^2 = \ell^3 G_1(\theta), \tag{50}$$

$$\overline{(\Delta y)^2} = \overline{y^2} = \ell^3 G_2(\theta). \tag{50'}$$

We have discussed above the distribution moments in x and y for given velocity vector orientation. One can also easily find, directly, or from the above results, the moments of the distribution function averaged over velocity orientations. These are given by

$$\bar{x} = \bar{y} = 0; \qquad \overline{x^2} = \overline{y^2} = \tfrac{2}{3}\ell^3.$$

III. MODEL FOR THE STEADY-STATE FINITE MEDIUM PROBLEM

For most practical purposes, it is not the time-dependent diffusion problem for an infinite medium that is of direct interest, but rather the steady-state problem of a beam impinging on a finite medium. This latter problem, however, poses formidable mathematical difficulties. In fixing attention on the infinite medium case, it was our hope that a good enough physical picture of multiple scattering would emerge so as to permit at least a qualitative analysis of the steady-state problem. In the present work, we are restricting our interest to situations in which the mean path length of a beam particle traversing the medium is small compared to the diffusion length.

Let us then recapitulate some of the results obtained above for the infinite medium problem, in the limit of small path lengths. Recall that all distances are measured in units of the diffusion length D. Suppose that a particle is located initially at the spatial point $\mathbf{x}_0$, with velocity vector $\mathbf{v}_0$. Choosing the z axis to lie along the direction of $\mathbf{v}_0$, we describe the orientation of the velocity vector $\mathbf{v}$ at any later time by the polar angle θ and azimuthal angle φ. For small times $t = \ell/v (\ell \ll 1)$ the distribution in velocity orientation, irrespective of spatial position, is given by

$$f_0(\mathbf{v}, \ell) = \frac{1}{4\pi l}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}} e^{-\theta^2/4\ell}$$

and the mean spatial position, for given orientation of the velocity vector, is determined by

$$\begin{aligned} \bar{x}(\theta, \varphi, \ell) &= x_0 + \ell\cos\varphi\left(\frac{1-\cos\theta}{\theta}\right), \\ \bar{y}(\theta, \varphi, \ell) &= y_0 + \ell\sin\varphi\left(\frac{1-\cos\theta}{\theta}\right), \\ \bar{z}(\theta, \ell) &= z_0 + \ell\left(\frac{\sin\theta}{\theta}\right). \end{aligned} \tag{51}$$

The dispersion about the mean is indicated by Eqs. (39), (50), and (50′).

The results on mean spatial location can be given a simple geometric description (see Fig. 1). For given velocity vector $\mathbf{v}$, the mean position vector $\bar{\mathbf{x}}$ is just the position vector which a particle would have if it had travelled at uniform speed $\mathbf{v}$ on a circular arc of radius $R = \ell/\theta$, starting at the initial time from the point $\mathbf{x}_0$ with velocity $\mathbf{v}_0$ and ending up at "time" ℓ with velocity vector $\mathbf{v}$. We speak of this, in short, as motion along a circular arc.

If we are prepared to neglect dispersion about the mean, the full distribution function in phase space would be written

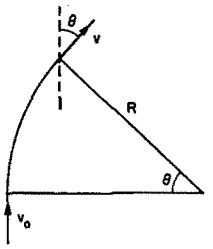

FIG. 1. Illustration of mean motion along a circular arc.

$$f_1(\mathbf{x}, \mathbf{v}; \mathbf{x}_0, \mathbf{v}_0, \ell) = \frac{1}{4\pi\ell}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}} e^{-\theta^2/4\ell} \times \delta(x-\bar{x})\delta(y-\bar{y})\delta(z-\bar{z}). \tag{52}$$

We adopt this approximation in what follows.

Suppose now that we wish to deal with a steady-state situation in which there is a steady source of new particles. Let $\Phi(\mathbf{x}_0\mathbf{v}_0)$ be the source function, which describes the rate at which new particles are created in a unit element of spatial volume centered on $\mathbf{x}_0$ and in a unit element of solid angle centered about the direction of $\mathbf{v}_0$. The steady-state distribution is then given by

$$f_1(\mathbf{x}, \mathbf{v}) = \frac{1}{v}\int_0^\infty d\ell \times \int \Phi(\mathbf{x}_0, \mathbf{v}_0) f_1(\mathbf{x}, \mathbf{v}; \mathbf{x}_0, \mathbf{v}_0, \ell)\, d^3x_0\, d\Omega_0. \tag{53}$$

Of practical interest, we consider the case of a beam of particles impinging on a finite medium. Suppose that the beam travels along the z axis, and that the beam flux F is uniform over a plane normal to the z axis. For this situation, (53) reduces to

$$f_1(\mathbf{x}, \mathbf{v}) = \frac{F}{v}\int_0^\infty d\ell \times \int_\Sigma f_1(\mathbf{x}, \mathbf{v}; \mathbf{x}_0, \mathbf{v}_0, \ell)\, dx_0\, dy_0, \tag{54}$$

where the spatial integration goes over that portion of the surface of the medium which intercepts the beam, with $z_0 = z_0(x_0, y_0)$ evaluated here on the surface. In the approximation envisaged in the present discussion, the boundary conditions are taken into account by our setting $f_1(\mathbf{x}, \mathbf{v}; \mathbf{x}_0\mathbf{v}_0, \ell) = 0$ for any point $(\mathbf{x}, \mathbf{v})$ in phase space which does not connect to the point $(\mathbf{x}_0, \mathbf{v}_0)$ according to our picture, described above, of motion at uniform speed on a circular arc which lies entirely in the medium.

Let us turn immediately to an example, which will serve to illustrate the procedure and also the

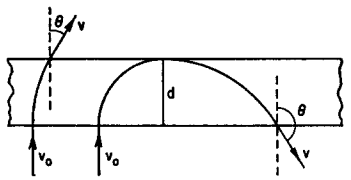

FIG. 2. Mean paths for transmitted and reflected particles.

nature of the errors involved. Suppose that a beam of particles is incident normally on a slab of thickness $d \ll 1$ (recall again that all distances are measured in units of the diffusion length D). Choose the z axis to lie along the beam direction and take the slab to be infinite in the x and y directions (see Fig. 2). The distribution function f depends only on the velocity orientation angle θ and on the spatial coordinate z. From (52) and (54) we find the result

$$f_1(\theta, z) = \frac{1}{4\pi z}\left(\frac{F_0}{v}\right)\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}} e^{-\theta \sin\theta/4z}, \qquad (55)$$

where F_0 is the beam flux.

We may expect that for not too large values of θ, and for spatial positions well away from the boundary surfaces, $0 \ll z \ll d$, this taking over of results for the infinite medium problem is reasonable, since the infinite medium function f has in any case received little contribution here from particles which have passed beyond $z = d$ or below $z = 0$ in their prior history over the short "time" interval $\ell = z\theta/\sin\theta$ and which could therefore know that the boundaries really exist. An appropriate measure of error is provided by the infinite medium estimate for $|\Delta z|$, the root mean square fluctuation about average $\bar{z}(\theta, \ell)$. According to Eq. (39) this is given by

$$|\Delta z| = \ell^{\frac{1}{2}} H^{\frac{1}{2}}(\theta).$$

Now in adopting the approximations which leads to (55), we have in effect taken over the infinite medium results, with the replacement

$$\ell \rightarrow z\theta/\sin\theta. \qquad (56)$$

This ignores boundary effects, which must surely matter for points near to one or another of the boundary surfaces. The uncertainty in the identification (56) is measured by

$$|\Delta\ell| \sim |\Delta z|\,(\theta/\sin\theta) \sim z^{3/2}(\theta/\sin\theta)^{5/2} H^{1/2}(\theta). \qquad (57)$$

In particular, suppose that we are interested in computing the angular distribution of the beam particles which emerge from the upper surface at $z = d$. The flux $F_t(\theta)$ of transmitted particles, i.e., the number of particles crossing a unit area of surface per unit time interval in a unit element of solid angle, is given by

$$F_t(\theta) = v f_1(\theta, d)\cos\theta, \qquad \theta < \tfrac{1}{2}\pi. \qquad (58)$$

The error corresponding to (57) is given by

$$|\Delta F_t/F_t| \sim |(\theta \sin\theta/4d) - 1|\,[dH(\theta)]^{\frac{1}{2}}[\theta/\sin\theta]^{\frac{1}{2}}.$$

In the small angle approximation we have $H(\theta) \sim \theta^2$, hence our estimate for the transmitted flux begins to go wrong for $\theta \gtrsim d^{\frac{1}{2}}$. For small slab thicknesses, $d \ll 1$, this limiting angle greatly exceeds the mean angle $\bar{\theta} = 2d^{\frac{1}{2}}$.

In summary, we suggest that the transmitted flux is adequately represented by

$$F_t(\theta) = \frac{F_0}{4\pi d}\left(\frac{\theta}{\sin\theta}\right)^{\frac{1}{2}} e^{-\theta \sin\theta/4d} C(\theta, d)\cos\theta, \qquad (59)$$

where the correction factor $C(\theta, d)$ is close to unity for angles satisfying

$$\theta < d^{\frac{1}{2}}; \qquad (60)$$

and even beyond this limit we expect that $C(\theta, d)$ varies more slowly with θ than does the exponential factor in Eq. (59).

As for the flux of reflected particles, $F_r(\theta) = v f_1(\theta, z = 0)\cos\theta$, $\theta > \frac{1}{2}\pi$, an estimate based on (55) is totally worthless; this equation gives a vanishing reflected flux. For thin slabs we indeed expect F_r to be small, but at the present level of approximation we are unable to estimate this small quantity. Regarding (55) as a first-order approximation to the true distribution function f, we can now proceed to a second-order correction by appealing to Eq. (53), with the source function $\Phi(\mathbf{x}_0, \mathbf{v}_0)$ set equal to $v f_1(\mathbf{x}, \mathbf{v})$. That is, with

$$f(\mathbf{x}, \mathbf{v}) = f_1(\mathbf{x}, \mathbf{v}) + f_2(\mathbf{x}, \mathbf{v}) + \cdots$$

we write

$$f_2(\mathbf{x}, \mathbf{v}) = \int_0^\infty d\ell \times \int f_1(\mathbf{x}_0, \mathbf{v}_0) f_1(\mathbf{x}, \mathbf{v}; \mathbf{x}_0, \mathbf{v}_0, l)\, d^3x_0\, d\Omega_0. \qquad (61)$$

Recall, however, that $f_1(\mathbf{x}, \mathbf{v}; \mathbf{x}_0, \mathbf{v}_0, \ell)$ is set equal to zero for points $(\mathbf{x}_0, \mathbf{v}_0)$ and $(\mathbf{x}, \mathbf{v})$ which are not connected by motion on a circular arc, in the sense described before. For the rest it is determined by Eq. (52); and $f_1(\mathbf{x}_0, \mathbf{v}_0)$ is as given in (55). Even for the simple problem at hand, the integrations of (61) cannot fully be carried out in closed form. However, we see that f_2 is a product of two first-order distribution functions corresponding to mean motion of a beam particle on a path composed of two circular arcs (see Fig. 2); and the main contributions to f_2 come from those paths for which

the radii are as large as possible, consistent with geometric constraints. The probability associated with a turn through angle θ on an arc of radius R is $R^{-1}e^{-\theta/4R}$; and indeed, a rough analysis of (61) for the particular case of f_2 evaluated at the lower surface $z = 0$ gives

$$f_2(\theta, z = 0) \approx \frac{1}{d}\, e^{-\theta_1/4R_1 - \theta_2/4R_2} \left(\frac{F_0}{v}\right),$$

where

$$\theta_1 = \tfrac{1}{2}\pi, \quad \theta_2 = \theta - \theta_1, \quad R_1 = d, \quad R_2 = d/(1 - \sin\theta).$$

Hence, our estimate for the flux function $F_r(\theta)$ for reflected particles, $F_r = vf(\theta, z=0)\cos\theta = vf_2(\theta, 0)\cos\theta$, is just

$$\frac{F_r(\theta)}{F_0} \approx \frac{\cos\theta}{d}$$

$$\times \exp\{-(1/4d)[\theta(1 - \sin\theta) + \tfrac{1}{2}\pi \sin\theta]\}. \quad (62)$$

We believe this to be "exponentially" correct in its dependence on θ.

As further illustration of a second-order effect, suppose now that the incident beam makes an angle α with respect to the slab, as shown in Fig. 3. We ask for the flux of directly back-scattered particles. There is no first-order contribution here; i.e., no circular arc lying in the medium leads directly to back scattering. In second order, however, the relevant paths are available, composed of two circular arcs. Once again, the main contributions come from paths which involve the largest possible radii. Employing the rough kinds of estimates used before, we find

$$\frac{F_b}{F_0} \approx \frac{\sin^2\alpha}{d}\, e^{-\theta_1/4R_1 - \theta_2/4R_2}$$

with

$$\theta_1 = \pi - \alpha, \qquad \theta_2 = \alpha,$$

$$R_1 = d/(1 + \cos\alpha), \qquad R_2 = d/(1 - \cos\alpha);$$

hence

$$F_b/F_0 \approx (\sin^2\alpha/d)$$

$$\times \exp\{-(1/4d)[\pi(1 + \cos\alpha) - 2\alpha\cos\alpha]\}. \quad (63)$$

It is clear that the approximation scheme being described here for finite medium diffusion problems is at its worst just at the surfaces of the scattering medium for grazing orientations of the velocity vector. At these points in phase space, our technique of following the mean motion of a particle, with neglect of dispersion, amounts to a violent maltreatment of the boundary conditions of the problem.

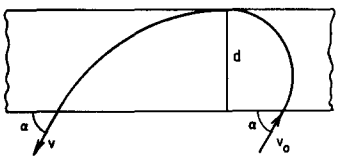

FIG. 3. Mean motion for non-normal back scattering.

The distribution function which we obtain [proportional to $\sin^{-2}\alpha$ times the expression in Eq. (63)] is in general nonvanishing for precisely grazing angles at the boundary surfaces. On the other hand, it is physically clear that the true distribution function must vanish at the boundary surfaces for grazing orientations of the velocity vectors. Similarly, it is physically clear that in the limit of very small grazing angle for the incident beam, the distribution function at all angles appreciably different from the beam angle will become very small. It is possible to show, from the principle that transverse momentum is conserved on the average in collisions on a spherical scattering center, that the distribution function vanishes no more rapidly than linearly in the grazing angle as it approaches zero. We conjecture that Eq. (63) is of the correct order of magnitude if $\alpha^3 \gtrsim d \ll 1$ and that it should be multiplied by a factor of order of magnitude $(\alpha^3/d)^\nu$, where the exponent ν lies between zero and one-third if $\alpha^3 \ll d$. However, we have been unable to prove this conjecture rigorously or to estimate the value of the exponent ν.

As discussed in the Introduction, under certain conditions the Boltzmann function for a finite medium problem can be regarded as a direct sum of two distinct terms. One of them describes contributions from multiple, small angle scatterings; the other, from single, large angle scatterings. For large net scattering angles the latter effect may well dominate. Nevertheless, even here small angle scattering can play an important, if indirect role, in producing a leakage of beam particles through the boundary surfaces of the scattering medium. The general reasoning is clear enough. It will suffice here to illustrate this leakage effect with a simple example.

Suppose that a beam of particles is incident normally on the face of a long cylinder of cross sectional radius R. Once again, we measure all distances in units of the diffusion length; and let us suppose that $R \ll 1$. It is clear that the beam intensity will fall off with increasing penetration distance, owing to the losses induced by multiple small angle scattering effects. In order to estimate an effective penetration distance, we can appeal to Eq. (52). Roughly speaking, at distance z into

the cylinder, the mean transverse displacement of a beam particle will be given by $r \sim z\bar{\theta} \sim z^{\frac{3}{2}}$. We therefore expect the beam intensity to begin falling off exponentially as a function of z for $z \gtrsim R^{\frac{1}{2}}$, i.e., the effective penetration distance is of order $R^{\frac{1}{2}}$.

More precisely, from (52) we find for the Boltzmann function

$$f(r, z) \approx \frac{1}{\pi z^3}\left(\frac{F_0}{v}\right)\int_0^R r_0\, dr_0 \int_0^{2\pi} d\varphi_0 \times \exp\left\{\frac{-r^2 - r_0^2 + 2rr_0\cos\varphi_0}{z^3}\right\},$$

where F_0 is the initial flux. In particular, the intensity on the axis is then given by

$$F(0, z)/F_0 \approx e^{-R^3/z^3},$$

confirming that the exponential fall-off distance is $z_0 \approx R^{\frac{1}{2}}$.

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One-Speed Neutron Transport in Two Adjacent Half-Spaces

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(Received 5 September 1963)

Using Case's method for solving the one-speed transport equation with isotropic scattering, the Milne problem solution, the solution for a constant source in one half-space, and the Green's function solution are obtained for two adjacent half-spaces. These problems have been solved previously by other methods. Here the derivations are greatly simplified by using Case's method.

I. INTRODUCTION

THE one-speed neutron transport equation has been solved in closed form for isotropic scattering in full-space, half-space, and two adjacent half-space media using a number of rather cumbersome techniques.[1-5] Recently Case[6] has developed a new method for treating the one-speed transport equation in which the solution of the general problem is written as a superposition of the singular solutions of the homogeneous equation. Several full- and half-space problems have been solved using this method,[6,7] including certain types of anisotropic scattering.[8,9]

In this work Case's method is applied to three problems for two adjacent half-spaces with isotropic scattering. In Sec. II, we review the normal-mode solutions. In Sec. III, we consider some of the general features of the two-half-space problems. In Secs. IV, V, and VI, we solve the Milne problem, the problem of a uniform isotropic source in one half-space, and the Green's function problem, respectively.

II. THE NORMAL MODES AND THE HALF-SPACE FUNCTIONS

Assuming isotropic scattering, the homogeneous one-speed neutron transport equation for plane symmetry is

$$\mu\frac{\partial\psi(x, \mu)}{\partial x} + \psi(x, \mu) = \frac{c}{2}\int_{-1}^{1}\psi(x, \mu')\, d\mu', \qquad \text{(II.1)}$$

where $\psi(x, \mu)$ is the angular density, x is the distance in units of mean free path, μ is the cosine of the angle between the neutron velocity and the x axis, and c is the average number of neutrons produced per collision. The solutions of Eq. (II.1) as discussed by Case;[6] consist of two discrete modes;

$$\psi_{0\pm}(x, \mu) = \phi_{0\pm}(\mu)e^{\mp x/\nu_0}, \qquad \text{(II.2)}$$

where

$$\phi_{0\pm}(\mu) = \tfrac{1}{2}c[\nu_0/(\nu_0 \mp \mu)], \qquad \text{(II.3)}$$

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[3] S. Chandrasekhar, *Radiative Transfer* (Oxford University Press, London, 1950).
[4] K. M. Case, Rev. Mod. Phys. 29, 651 (1957).
[5] T. Auerbach, Rept. No. BNL 676 (T-225), Brookhaven National Laboratory (1961).
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[7] J. R. Mika, *Asymptotic Reactor Theory in Plane Geometry* (Polish Academy of Sciences, Institute of Nuclear Research, Rept. No. 305/II, Warsaw, 1962).
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and $\pm\nu_0$ are the two zeros of

$$\Lambda(\nu) = 1 - \frac{c\nu}{2}\int_{-1}^{1} d\mu/(\nu - \mu)$$
$$= 1 - c\nu \tanh^{-1}(1/\nu), \qquad \text{(II.4)}$$

and a set of continuum modes

$$\psi_\nu(x, \mu) = \phi_\nu(\mu)e^{-x/\nu}, \qquad \text{(II.5)}$$

where

$$\phi_\nu(\mu) = \tfrac{1}{2}(c)P[\nu/(\nu - \mu)] + \lambda(\nu)\delta(\mu - \nu), \qquad \text{(II.6)}$$

and

$$\lambda(\nu) = 1 - c\nu \tanh^{-1}\nu, \qquad \text{(II.7)}$$

and ν is real and in the interval $-1 \leq \nu \leq 1$. The P in Eq. (II.6) signifies the Cauchy principal value. Notice that $\Lambda(\nu)$ has a cut from -1 to 1 in the complex ν plane. If we define $\Lambda^+(\nu)$ and $\Lambda^-(\nu)$ as the boundary values of $\Lambda(\nu)$ approaching the cut from above and below, respectively, we have

$$\Lambda^\pm(\nu) = \lambda(\nu) \pm \tfrac{1}{2}(i\pi c\nu). \qquad \text{(II.8)}$$

In obtaining the solution to the general half-space problem, Case[6] constructed the following function:

$$X(z) = \frac{1}{1 - z}\exp\left\{\frac{1}{\pi}\int_0^1 \frac{d\mu}{\mu - z}\arg\Lambda^+(\mu)\right\}. \qquad \text{(II.9)}$$

Some of the properties of this function are[6]:

(1) It is analytic in the complex z plane cut from 0 to $+1$.

(2) It is nonvanishing, along with its boundary values, in the entire finite z plane.

(3) It goes as $1/z$ as z approaches infinity.

(4) Its boundary values satisfy the "ratio condition"

$$X^+(\nu)/X^-(\nu) = \Lambda^+(\nu)/\Lambda^-(\nu); \quad 0 < \nu < 1. \qquad \text{(II.10)}$$

(5) It can be shown to satisfy the following identities:

$$X(z) = \int_0^1 \frac{d\mu}{\mu - z}\frac{c\mu}{2}\frac{X^-(\mu)}{\Lambda^-(\mu)}, \qquad \text{(II.11)}$$

$$X(z)X(-z) = \Lambda(z)/[(1 - c)(\nu_0^2 - z^2)], \qquad \text{(II.12)}$$

$$X(0) = 1/[\nu_0(1 - c)^{\frac{1}{2}}], \qquad \text{(II.13)}$$

$$X(z) = \frac{c}{2(1 - c)}\int_{-1}^{0} \frac{\mu\, d\mu}{(\nu_0^2 - \mu^2)X(\mu)(\mu + z)}. \qquad \text{(II.14)}$$

III. THE TWO-HALF-SPACE FUNCTIONS

Two adjacent half-spaces may be characterized by the following convention. Let $x = 0$ denote the interface, and let the subscripts 1 and 2 denote the quantities appropriate to the right- and left-hand half-spaces, respectively. The solutions of the transport equation will then involve $\psi_{1\nu}(x, \mu)$ and $\psi_{10\pm}(x, \mu)$ for $x > 0$; and $\psi_{2\nu}(x, \mu)$ and $\psi_{20\pm}(x, \mu)$ for $x < 0$.

A problem which is encountered in the solution of two-half-space problems is the expansion of a function $\psi'(\mu)$ in terms of the $\phi_{1\nu}(\mu)$ for $0 < \nu < 1$ and $\phi_{2\nu}(\mu)$ for $-1 < \nu < 0$. That is, functions $A_1(\nu)$ and $A_2(\nu)$ are sought such that

$$\psi'(\mu) = \int_{-1}^{0} A_2(\nu)\phi_{2\nu}(\mu)\, d\nu + \int_0^1 A_1(\nu)\phi_{1\nu}(\mu)\, d\nu. \qquad \text{(III.1)}$$

The construction of this expansion has been discussed by Case.[6] We will repeat the relevant parts of Case's discussion here. Let us introduce the following notation:

$$c(\mu) = \begin{cases} c_1, & 0 < \mu < 1, \\ c_2, & -1 < \mu < 0; \end{cases}$$
$$A(\mu) = \begin{cases} A_1(\mu), & 0 < \mu < 1, \\ A_2(\mu), & -1 < \mu < 0; \end{cases}$$
$$\Lambda^\pm(\mu) = \begin{cases} \Lambda_1^\pm(\mu), & 0 < \mu < 1, \\ \Lambda_2^\pm(\mu), & -1 < \mu < 0; \end{cases} \qquad \text{(III.2)}$$
$$\lambda(\mu) = \begin{cases} \lambda_1(\mu), & 0 < \mu < 1, \\ \lambda_2(\mu), & -1 < \mu < 0. \end{cases}$$

With this notation, Eq. (III.1) can be written as follows:

$$\psi'(\mu) = \lambda(\mu)A(\mu) + \tfrac{1}{2}P\int_{-1}^{1} \frac{c(\nu)\nu A(\nu)\, d\nu}{\nu - \mu}. \qquad \text{(III.3)}$$

Now we introduce the function

$$N(z) = \frac{1}{2\pi i}\int_{-1}^{1} \frac{c(\nu)\nu A(\nu)}{2(\nu - z)}\, d\nu. \qquad \text{(III.4)}$$

If $A(\nu)$ is sufficiently well behaved, $N(z)$ has the following properties:

(a) It is analytic in the complex z plane cut from -1 to 1.

(b) It goes to zero at least as fast as $1/z$ at infinity.

(c) It is bounded by $D_\mp/|z \pm 1|^\gamma$, where $D_\mp$ are constants and $\gamma < 1$, as z approaches ∓ 1.

The boundary values of $N(z)$ are

$$N^\pm(\mu) = \frac{1}{2\pi i}P\int_{-1}^{1} \frac{c(\nu)\nu A(\nu)}{2(\nu - \mu)}\, d\nu \pm \frac{1}{2}\frac{c(\mu)\mu A(\mu)}{2}. \qquad \text{(III.5)}$$

Equation (III.3) can be written in terms of $\Lambda(z)$ and $N(z)$ as follows:

$$\frac{\Lambda^+(\mu)}{\Lambda^-(\mu)} N^+(\mu) - N^-(\mu) = \frac{\mu c(\mu)\psi'(\mu)}{2\Lambda^-(\mu)}. \quad \text{(III.6)}$$

The solution of Eq. (III.6) for $N(z)$ is[6]

$$N(z) = \frac{1}{2\pi i\chi(z)} \int_{-1}^{1} \frac{\gamma(\mu)\psi'(\mu)\, d\mu}{\mu - z}, \quad \text{(III.7)}$$

where

$$\chi(z) = X_1(z)X_2(-z), \quad \text{(III.8)}$$

and

$$\gamma(\mu) = \tfrac{1}{2}[\mu c(\mu)][\chi^-(\mu)/\Lambda^-(\mu)]. \quad \text{(III.9)}$$

Since $\chi(z) \sim 1/z^2$ as z approaches infinity, $N(z) \sim 1/z$ at infinity, as required, only if

$$\int_{-1}^{1} \gamma(\mu)\psi'(\mu)\, d\mu = 0,$$

and

$$\int_{-1}^{1} \mu\gamma(\mu)\psi'(\mu)\, d\mu = 0. \quad \text{(III.10)}$$

Hence $A(\mu)$ may be determined from Eqs. (III.5) and (III.7) for any $\psi'(\mu)$ that satisfies Eqs. (III.10).

Also, $\chi(z)$ satisfies a number of useful identities similar to those for the half-space function $X(z)$. The derivations of these identities are entirely analogous to the half-space cases, so we will omit the details and simply state the results.

$$\chi(z) = \int_{-1}^{1} \frac{\gamma(\mu)\, d\mu}{\mu - z}, \quad \text{(III.11)}$$

$$z\chi(z) = \int_{-1}^{1} \frac{\mu\gamma(\mu)\, d\mu}{\mu - z}, \quad \text{(III.12)}$$

$$\chi(z) = \frac{c_2}{2(1 - c_2)} \int_{-1}^{0} \frac{\mu X_1(\mu)\, d\mu}{X_2(\mu)(\nu_{02}^2 - \mu^2)(\mu - z)} + \frac{c_1}{2(1 - c_1)} \int_{0}^{1} \frac{\mu X_2(-\mu)\, d\mu}{X_1(-\mu)(\nu_{01}^2 - \mu^2)(\mu - z)}, \quad \text{(III.13)}$$

$$z\chi(z) = \frac{c_2}{2(1 - c_2)} \int_{-1}^{0} \frac{\mu^2 X_1(\mu)\, d\mu}{X_2(\mu)(\nu_{02}^2 - \mu^2)(\mu - z)} + \frac{c_1}{2(1 - c_1)} \int_{0}^{1} \frac{\mu^2 X_2(-\mu)\, d\mu}{X_1(-\mu)(\nu_{01}^2 - \mu^2)(\mu - z)}. \quad \text{(III.14)}$$

IV. THE MILNE PROBLEM

For the Milne problem, the angular density satisfies the following equation:

$$\mu \frac{\partial\psi(x, \mu)}{\partial x} + \psi(x, \mu) = \frac{c_1}{2} \int_{-1}^{1} \psi(x, \mu')\, d\mu', \quad x > 0,$$

$$= \frac{c_2}{2} \int_{-1}^{1} \psi(x, \mu')\, d\mu', \quad x < 0, \quad \text{(IV.1)}$$

with the following boundary conditions:

(1) $\lim_{x\to\infty} \psi(x, \mu) = \phi_{10-}(\mu)e^{+x/\nu_{01}}$

(i.e., neutrons are assumed to enter the system at plus infinity, and $c_1 < 1$).

(2) $\lim_{x\to-\infty} \psi(x, \mu) = 0$

(i.e., $c_2 < 1$).

(3) $\psi(0^-, \mu) = \psi(0^+, \mu)$

(i.e., the angular density is continuous across the interface).

Boundary conditions (1) and (2) require the following form for the expansion of $\psi(x, \mu)$:

$$\psi(x, \mu) = \phi_{10-}(\mu)e^{x/\nu_{01}} + a_{0+}\phi_{10+}(\mu)e^{-x/\nu_{01}} + \int_{0}^{1} A_1(\nu)\phi_{1\nu}(\mu)e^{-x/\nu}\, d\nu, \quad x > 0;$$

$$= -a_{0-}\phi_{20-}(\mu)e^{x/\nu_{02}} - \int_{-1}^{0} A_2(\nu)\phi_{2\nu}(\mu)e^{-x/\nu}\, d\nu, \quad x < 0. \quad \text{(IV.2)}$$

From boundary condition (3), we have

$$\psi'(\mu) = \int_{-1}^{0} A_2(\nu)\phi_{2\nu}(\mu)\, d\nu + \int_{0}^{1} A_1(\nu)\phi_{1\nu}(\mu)\, d\nu, \quad \text{(IV.3)}$$

where

$$\psi'(\mu) = -\phi_{10-}(\mu) - a_{0+}\phi_{10+}(\mu) - a_{0-}\phi_{20-}(\mu). \quad \text{(IV.4)}$$

From the analysis of Sec. III, the solution of Eq. (IV.3) can be written down immediately,

$$A(\nu) = [2/\nu c(\nu)][N^+(\nu) - N^-(\nu)], \quad \text{(IV.5)}$$

where

$$N(z) = \frac{1}{2\pi i\chi(z)} \int_{-1}^{1} \frac{\gamma(\mu)\psi'(\mu)\, d\mu}{\mu - z}.$$

The coefficients a_{0+} and a_{0-} can be determined from Eqs. (III.10), (III.11), (III.12), and (IV.4),

$$a_{0+} = \frac{\chi(-\nu_{01})}{\chi(\nu_{01})} \frac{(\nu_{02} - \nu_{01})}{(\nu_{02} + \nu_{01})}$$

$$a_{0-} = -\frac{\chi(-\nu_{01})}{\chi(-\nu_{02})} \frac{2c_1\nu_{01}^2}{c_2\nu_{02}(\nu_{02} + \nu_{01})}. \quad \text{(IV.6)}$$

The expression for $N(z)$ can be simplified by using Eqs. (IV.4), (III.11), (III.12), and (IV.6),

$$N(z) = -\frac{1}{2\pi i}[\phi_{10-}(z) + a_{0+}\phi_{10+}(z) + a_{0-}\phi_{20-}(z)] + \frac{1}{2\pi i} \frac{c_1\nu_{01}^2\chi(-\nu_{01})}{(\nu_{01}^2 - z^2)\chi(z)} \frac{\nu_{02} - \nu_{01}}{\nu_{02} + z}. \quad \text{(IV.7)}$$

The expansion coefficient $A(\nu)$ can be determined from Eqs. (IV.5) and (IV.7),

$$\frac{\nu c(\nu)}{2} A(\nu) = \frac{1}{2\pi i} \frac{c_1 \nu_{01}^2 (\nu_{02} - \nu_{01}) \chi(-\nu_{01})}{(\nu_{01}^2 - \nu^2)(\nu_{02} + \nu)} \times \left[\frac{1}{\chi^+(\nu)} - \frac{1}{\chi^-(\nu)} \right].$$

One can show that the following identity holds for the χ-functions:

$$\frac{1}{\chi^+(\nu)} - \frac{1}{\chi^-(\nu)} = \frac{-c_1 \pi i \nu}{\Lambda_1^+(\nu)\Lambda_1^-(\nu)} \frac{X_1(-\nu)}{X_2(-\nu)} (\nu_{01}^2 - \nu^2)(1 - c_1), \quad \nu > 0;$$

$$= \frac{-c_2 \pi i \nu}{\Lambda_2^+(+\nu)\Lambda_2^-(+\nu)} \frac{X_2(\nu)}{X_1(\nu)} (\nu_{02}^2 - \nu^2)(1 - c_2), \quad \nu < 0. \tag{IV.8}$$

Hence,

$$A_1(\nu) = -\frac{c_1(1 - c_1)\nu_{01}^2(\nu_{02} - \nu_{01})\chi(-\nu_{01})X_1(-\nu)}{(\nu_{02} + \nu)\Lambda_1^+(\nu)\Lambda_1^-(\nu)X_2(-\nu)},$$

$$A_2(\nu) = -\frac{c_1(1 - c_2)\nu_{01}^2(\nu_{02} - \nu_{01})\chi(-\nu_{01})(\nu_{02} - \nu)X_2(\nu)}{(\nu_{01}^2 - \nu^2)\Lambda_2^+(-\nu)\Lambda_2^-(-\nu)X_1(\nu)}. \tag{IV.9}$$

The solution of the Milne problem for the angular density is complete since all of the expansion coefficients in Eq. (IV.2) have been determined.

The expression for the angular density at the interface ($x = 0$) can be further simplified. Notice that the angular density at the interface can be written as follows:

$$\psi(0, \mu) = \begin{cases} \phi_{10-}(\mu) + a_{0+}\phi_{10+}(\mu) + f(\mu), & \mu < 0, \\ -a_{0-}\phi_{20-}(\mu) - g(\mu), & \mu > 0, \end{cases} \tag{IV.10}$$

where

$$f(z) = \frac{c_1}{2} \int_0^1 \frac{\nu A_1(\nu)\, d\nu}{\nu - z},$$

$$g(z) = \frac{c_2}{2} \int_{-1}^0 \frac{\nu A_2(\nu)\, d\nu}{\nu - z}.$$

The functions $f(z)$ and $g(z)$ have the following properties:

(1a) $f(z)$ is analytic in the complex z plane cut from 0 to $+1$ and vanishes at infinity.

(1b) $g(z)$ is analytic in the complex z plane cut from -1 to 0 and vanishes at infinity.

(2a) $f(z)$ has a discontinuity across the cut given by

$$f^+(\mu) - f^-(\mu) = \pi i[c_1 \mu A_1(\mu)].$$

(2b) $g(z)$ has a discontinuity across the cut given by:

$$g^+(\mu) - g^-(\mu) = \pi i[c_2 \mu A_2(\mu)].$$

One can construct functions satisfying conditions (1) and (2a), and (1) and (2b), respectively. By Liouville's theorem, these functions are unique. Thus, we can write[10]

$$f(z) = T(z) - \phi_{10-}(z) - a_{0+}\phi_{10+}(z), \qquad g(z) = R(z) - a_{0-}\phi_{20-}(z), \tag{IV.11}$$

where

$$T(z) = \frac{(\nu_{02} - z)c_1\nu_{01}^2 X_2(z)X_1(-\nu_{01})}{(\nu_{01}^2 - z^2)(\nu_{02} + \nu_{01})X_1(z)X_2(-\nu_{01})},$$

and

$$R(z) = -\frac{c_2(1 - c_1)\nu_{01}^2 X_1(-z)X_1(-\nu_{01})}{(1 - c_2)(\nu_{02} + z)(\nu_{02} + \nu_{01})X_2(-z)X_2(-\nu_{01})}.$$

From Eqs. (IV.9) and (IV.10), we can determine the angular density at the interface in terms of X functions,

$$\psi(0, \mu) = \frac{c_1\nu_{01}^2(\nu_{02} - \mu)X_2(\mu)X_1(-\nu_{01})}{(\nu_{01}^2 - \mu^2)(\nu_{02} + \nu_{01})X_1(\mu)X_2(-\nu_{01})}, \quad \mu < 0;$$

$$= \frac{c_2(1 - c_1)\nu_{01}^2 X_1(-\mu)X_1(-\nu_{01})}{(1 - c_2)(\nu_{02} + \mu)(\nu_{02} + \nu_{01})X_2(-\mu)X_2(-\nu_{01})}, \quad \mu > 0. \tag{IV.12}$$

The total density and current at the interface are

$$\rho(0) = \int_{-1}^1 \psi(0, \mu)\, d\mu,$$

$$j(0) = \int_{-1}^1 \mu\psi(0, \mu)\, d\mu.$$

These integrals can be done using Eq. (III.13) and (III.14),

$$\rho(0) = \frac{2\nu_{01}(1 - c_1)^{\frac{1}{2}}X_1(-\nu_{01})}{(\nu_{02} + \nu_{01})(1 - c_2)^{\frac{1}{2}}X_2(-\nu_{01})}, \tag{IV.13}$$

$$j(0) = -\nu_{01}[(1 - c_1)(1 - c_2)]^{\frac{1}{2}}\rho(0). \tag{IV.14}$$

One further quantity of interest is the extrapolated end point z_0, given by

$$0 = e^{-z_0/\nu_{01}} + a_{0+}e^{z_0/\nu_{01}},$$

$$z_0 = \frac{\nu_{01}}{2} \ln \left[\frac{\nu_{01} + \nu_{02}}{\nu_{01} - \nu_{02}} \frac{X_1(\nu_{01})X_2(-\nu_{01})}{X_1(-\nu_{01})X_2(\nu_{01})} \right]. \tag{IV.15}$$

The results of this section and many of the

[10] Note that $T(z)$ and $R(z)$ supply the proper discontinuity and $f(z)$ and $g(z)$ have removable singularities.

results in the following sections can be compared to Davison's[1] results by recognizing the relation between the X function and Davison's h function,

$$h^+(i/\mu) = (1 + \mu)X(-\mu)\nu_0(1 - c)^{\frac{1}{2}}.$$

Similarly, a comparison with Chandrasekhar's[3,5] results can be made by recognizing the relation between the X function and Chandrasekhar's H function,

$$H(\mu) = 1/(\nu_0 + \mu)(1 - c)^{\frac{1}{2}}X(-\mu).$$

V. THE UNIFORM SOURCE

Consider a uniform, isotropic source in the right-hand half-space. The transport equation is

$$\mu \frac{\partial \psi(x, \mu)}{\partial x} + \psi(x, \mu) = \frac{c_1}{2}\int_{-1}^{1} \psi(x, \mu')\, d\mu' + s, \qquad x > 0,$$

$$= \frac{c_2}{2}\int_{-1}^{1} \psi(x, \mu')\, d\mu', \qquad x < 0, \tag{V.1}$$

with the following boundary conditions:

(1) $\lim_{x\to\infty} \psi(x, \mu) = \dfrac{s}{1 - c_1}$ (i.e., $c_1 < 1$),

(2) $\lim_{x\to-\infty} \psi(x, \mu) = 0$ (i.e., $c_2 < 1$),

(3) $\psi(0^+, \mu) = \psi(0^-, \mu)$ (continuity).

The expansion of $\psi(x, \mu)$ in the normal modes, including the restrictions of boundary conditions (1) and (2), is

$$\psi(x, \mu) = \frac{s}{1 - c_1} - a_{0+}\phi_{10+}e^{-x/\nu_{01}} + \int_0^1 A_1(\nu)e^{-x/\nu}\phi_{1\nu}(\mu)\, d\nu, \qquad x > 0;$$

$$= a_{0-}\phi_{20-}(\mu)e^{x/\nu_{02}} - \int_{-1}^{0} A_2(\nu)e^{-x/\nu}\phi_{2\nu}(\mu)\, d\nu, \qquad x < 0. \tag{V.2}$$

Boundary condition (3) then requires that

$$\psi'(\mu) = \int_0^1 A_1(\nu)\phi_{1\nu}(\mu)\, d\nu + \int_{-1}^{0} A_2(\nu)\phi_{2\nu}(\mu)\, d\nu, \tag{V.3}$$

where

$$\psi'(\mu) = a_{0-}\phi_{20-}(\mu) + a_{0+}\phi_{10+}(\mu) - s/(1 - c_1).$$

Again, we can determine the discrete coefficients from Eqs. (III.10), (III.11), and (III.12),

$$a_{0+} = -2s/(1 - c_1)c_1\nu_{01}(\nu_{01} + \nu_{02})\chi(\nu_{01}),$$
$$a_{0-} = -2s/(1 - c_1)c_2\nu_{02}(\nu_{01} + \nu_{02})\chi(-\nu_{02}). \tag{V.4}$$

The expression for $N(z)$,

$$N(z) = \frac{1}{2\pi i\chi(z)}\int_{-1}^{1} \frac{\gamma(\mu)}{\mu - z}\psi'(\mu)\, d\mu,$$

can be evaluated by using Eqs. (III.11), (III.12), and (V.3),

$$N(z) = \frac{1}{2\pi i}\left[a_{0+}\phi_{10+}(z) + a_{0-}\phi_{20-}(z) - \frac{s}{1 - c_1}\right] - \frac{1}{2\pi i\chi(z)}\left[\frac{a_{0+}c_1\nu_{01}\chi(\nu_{01})}{2(\nu_{01} - z)} + \frac{a_{0-}c_2\nu_{02}\chi(-\nu_{02})}{2(\nu_{02} + z)}\right]. \tag{V.5}$$

The continuum expansion coefficient can be computed by using Eq. (III.5),

$$A_1(\nu) = -\frac{s(\nu_{01} + \nu)X_1(-\nu)}{(\nu_{02} + \nu)X_2(-\nu)\Lambda_1^+(\nu)\Lambda_1^-(\nu)},$$
$$A_2(\nu) = \frac{-s(1 - c_2)(\nu_{02} - \nu)X_2(\nu)}{(1 - c_1)(\nu_{01} - \nu)X_1(\nu)\Lambda_2^+(-\nu)\Lambda_2^-(-\nu)}, \tag{V.6}$$

where we have used the explicit expressions for a_{0+} and a_{0-} [Eq. (V.4)], and Eq. (IV.8). Thus the solution of this problem is complete since the expansion coefficients in Eq. (V.2) have been determined.

There is a further simplification in the expression for the angular density at the interface,

$$\psi(0, \mu) = \begin{cases} s/(1 - c_1) - a_{0+}\phi_{10+}(\mu) + f(\mu), & \mu < 0, \\ a_{0-}\phi_{20-}(\mu) - g(\mu), & \mu > 0, \end{cases} \tag{V.7}$$

where

$$f(z) = \frac{c_1}{2}\int_0^1 \frac{\nu A_1(\nu)\, d\nu}{\nu - z},$$

$$g(z) = \frac{c_2}{2}\int_1^0 \frac{\nu A_2(\nu)\, d\nu}{\nu - z}.$$

These functions $f(z)$ and $g(z)$ satisfy conditions (1a), (1b), (2a), and (2b) in Sec. IV, with $A_1(\mu)$ and $A_2(\mu)$ given by Eq. (V.6). Again we can construct unique functions satisfying these conditions,[10]

$$f(z) = T(z) - \frac{sc_1(1 - c_2)}{(c_1 - c_2)(1 - c_1)} + a_{0+}\phi_{10+}(z),$$
$$g(z) = R(z) - sc_2/(c_2 - c_1) + a_{0-}\phi_{20-}(z), \tag{V.8}$$

where

$$T(z) = \frac{sc_1(1 - c_2)(\nu_{02} - z)X_2(z)}{(c_1 - c_2)(1 - c_1)(\nu_{01} - z)X_1(z)},$$

and

$$R(z) = \frac{sc_2(\nu_{01} + z)X_1(-z)}{(c_2 - c_1)(\nu_{02} + z)X_2(-z)}.$$

The angular density at the interface now can be determined by using these results,

$$\psi(0, \mu) = \frac{sc_1(1 - c_2)(\nu_{02} - \mu)X_2(\mu)}{(c_1 - c_2)(1 - c_1)(\nu_{01} - \mu)X_1(\mu)} - \frac{sc_2}{c_1 - c_2}, \quad \mu < 0;$$
$$= \frac{sc_2(\nu_{01} + \mu)X_1(-\mu)}{(c_1 - c_2)(\nu_{02} + \mu)X_2(-\mu)} - \frac{sc_2}{c_1 - c_2}, \quad \mu > 0. \tag{V.9}$$

The total density at the interface,

$$\rho(0) = \int_{-1}^{1} \psi(0, \mu)\, d\mu,$$

can be found using Eqs. (III.13) and (III.14),

$$\rho(0) = \frac{2s}{c_1 - c_2}\left[\frac{(1 - c_2)^{\frac{1}{2}}}{(1 - c_1)^{\frac{1}{2}}} - 1\right]. \tag{V.10}$$

There does not appear to be a corresponding simplification in the expression for the current at the interface, since we do not have an identity similar to Eqs. (III.13) and (III.14) for $z^2\chi(z)$.

VI. THE TWO-HALF-SPACE GREEN'S FUNCTION

Consider a monodirectional plane source in the right-hand half-space. The transport equation becomes

$$\frac{\mu\partial\psi(x, \mu; x_0, \mu_0)}{\partial x} + \psi(x, \mu; x_0, \mu_0) = \frac{c_1}{2}\int_{-1}^{1} \psi(x, \mu'; x_0, \mu_0)\, d\mu' + \frac{\delta(x - x_0)\delta(\mu - \mu_0)}{2\pi}, \quad x > 0,$$
$$= \frac{c_2}{2}\int_{-1}^{1} \psi(x, \mu'; x_0, \mu_0)\, d\mu', \quad x < 0, \tag{VI.1}$$

where

(1) $\lim_{x\to\pm\infty} \psi(x, \mu; x_0, \mu_0) = 0 \quad (c_1, c_2 < 1)$,

(2) $\psi(x_0^+, \mu; x_0, \mu_0) - \psi(x_0^-, \mu; x_0, \mu_0) = \frac{1}{2\pi\mu}\delta(\mu - \mu_0)$,

(3) $\psi(0^+, \mu; x_0, \mu_0) = \psi(0^-, \mu; x_0, \mu_0)$.

A solution which conforms to boundary condition (1) is

$$\psi(x, \mu; x_0, \mu_0) = a_{0+}\phi_{10+}(\mu)e^{-x/\nu_{01}} + \int_0^1 A(\nu)\phi_{1\nu}(\mu)e^{-x/\nu}\, d\nu, \quad x > x_0;$$
$$= -b_{0+}\phi_{10+}(\mu)e^{-x/\nu_{01}} - b_{0-}\phi_{10-}(\mu)e^{x/\nu_{01}} - \int_{-1}^{1} B(\nu)\phi_{1\nu}(\mu)e^{-x/\nu}\, d\nu, \quad 0 < x < x_0;$$
$$= d_{0-}\phi_{20-}(\mu)e^{+x/\nu_{01}} + \int_{-1}^{0} D(\nu)\phi_{2\nu}(\mu)e^{-x/\nu}\, d\nu; \quad x < 0. \tag{VI.2}$$

Applying boundary condition (2) we have

$$(a_{0+} + b_{0+})\phi_{10+}(\mu)e^{-x_0/\nu_{01}} + b_{0-}\phi_{10-}(\mu)e^{x_0/\nu_{01}} + \int_0^1 \{A(\nu) + B(\nu)\}\phi_{1\nu}(\mu)e^{-x_0/\nu}\, d\nu + \int_{-1}^{0} B(\nu)\phi_{1\nu}(\mu)e^{-x_0/\nu}\, d\nu = \frac{1}{2\pi\mu}\delta(\mu - \mu_0). \tag{VI.3}$$

The ϕ's satisfy the following orthogonality relation:

$$\int_{-1}^{+1} \mu\phi_{1\nu}(\mu)\phi_{1\nu'}(\mu)\, d\mu = 0; \quad \nu \neq \nu', \tag{VI.4}$$

where the indices ν and ν' refer to both the discrete and continuum eigenvalues. The normalization is[6]

$$N_{10\pm} = \int_{-1}^{+1} \mu\phi_{10\pm}^2(\mu)\, d\mu = \pm\frac{c_1\nu_{01}^3}{2}\left[\frac{c_1}{\nu_{01}^2 - 1} - \frac{1}{\nu_{01}^2}\right],$$
$$N_1(\nu)\delta(\nu - \nu') = \int_{-1}^{1} \mu\phi_{1\nu}(\mu)\phi_{1\nu'}(\mu)\, d\mu = \nu\Lambda_1^+(\nu)\Lambda_1^-(\nu)\,\delta(\nu - \nu'). \tag{VI.5}$$

Using Eqs. (VI.4) and (VI.5) in Eq. (VI.3), we have

$$a_{0+} + b_{0+} = \frac{1}{2\pi}\frac{\phi_{10+}(\mu_0)e^{x_0/\nu_{01}}}{N_{10+}},$$
$$b_{0-} = \frac{1}{2\pi}\frac{\phi_{10-}(\mu_0)e^{-x_0/\nu_{01}}}{N_{10-}},$$
$$A(\nu) + B(\nu) = \frac{\phi_{1\nu}(\mu_0)e^{x_0/\nu}}{2\pi N_1(\nu)}, \quad \nu > 0,$$
$$B(\nu) = \frac{\phi_{1\nu}(\mu_0)e^{x_0/\nu}}{2\pi N_1(\nu)}, \quad \nu < 0. \tag{VI.6}$$

Applying boundary condition (3) and the identity

$$(c_1/c_2)\phi_{2\nu}(\mu) = \phi_{1\nu}(\mu) + [(c_1 - c_2)/c_2]\delta(\nu - \mu),$$

we have

$$\psi'(\mu) = \int_0^1 B(\nu)\phi_{1\nu}(\mu)\, d\nu + \int_{-1}^{0}\left\{\frac{c_1}{c_2}B(\nu) + D(\nu)\right\}\phi_{2\nu}(\mu)\, d\nu, \tag{VI.7}$$

where

$$\psi'(\mu) = -b_{0+}\phi_{10+}(\mu) - b_{0-}\phi_{10-}(\mu) - d_{0-}\phi_{20-}(\mu) - \frac{c_2 - c_1}{c_2}\frac{\phi_{1\mu}(\mu_0)e^{x_0/\mu}H(-\mu)}{2\pi N_1(\mu)};$$

$$H(x) = \begin{cases} 1, & x > 0; \\ 0, & x < 0. \end{cases}$$

Equation (VI.7) is in the form of Eq. (III.1), and we can use the methods outlined in Sec. III to determine the coefficients

$$\begin{gathered} B(\nu), \quad \nu > 0; \\ b_{0+}, \quad d_{0+}; \\ \frac{c_1}{c_2}B(\nu) + D(\nu), \quad \nu < 0. \end{gathered} \tag{VI.8}$$

Applying Eqs. (III.10, 11, 12) and (VI.6), we have

$$\begin{aligned} b_{0+} &= -2\frac{\nu_{02}\alpha + \beta}{c_1\nu_{01}\chi(\nu_{01})(\nu_{02} + \nu_{01})}, \\ d_{0-} &= 2\frac{\nu_{01}\alpha - \beta}{c_2\nu_{02}\chi(-\nu_{02})(\nu_{02} + \nu_{01})}, \end{aligned} \tag{VI.9}$$

where

$$\alpha(x_0, \mu_0) = -\frac{c_1\nu_{01}}{4\pi}\frac{\phi_{10-}(\mu_0)e^{-x_0/\nu_{01}}\chi(-\nu_{01})}{N_{10-}} + \frac{c_1 - c_2}{4\pi(1 - c_2)}\int_{-1}^{0}\frac{\nu\phi_{1\nu}(\mu_0)e^{x_0/\nu}X_1(\nu)}{N_1(\nu)(\nu_{02}^2 - \nu^2)X_2(\nu)}\,d\nu,$$

$$\beta(x_0, \mu_0) = \frac{c_1\nu_{01}^2}{4\pi}\frac{\phi_{10-}(\mu_0)e^{-x_0/\nu_{01}}\chi(-\nu_{01})}{N_{10-}} + \frac{c_1 - c_2}{4\pi(1 - c_2)}\int_{-1}^{0}\frac{\nu^2\phi_{1\nu}(\mu_0)e^{x_0/\nu}X_1(\nu)}{N_1(\nu)(\nu_{02}^2 - \nu^2)X_2(\nu)}\,d\nu.$$

Applying Eq. (III.4), we have

$$N(z) = -\frac{1}{2\pi i}\{b_{0+}\phi_{10+}(z) + b_{0-}\phi_{10-}(z) + d_{0-}\phi_{20-}(z)\} + \frac{1}{2\pi i\chi(z)}\{b_{0+}\phi_{10+}(z)\chi(\nu_{01}) + b_{0-}\phi_{10-}(z)\chi(-\nu_{01}) + d_{0-}\phi_{20-}(z)\chi(-\nu_{02})\} - \frac{1}{2\pi i\chi(z)}\frac{c_2 - c_1}{4\pi(1 - c_2)} \times \int_{-1}^{0}\frac{\mu\phi_{1\mu}(\mu_0)e^{x_0/\mu}X_1(\mu)}{N_1(\mu)(\mu - z)(\nu_{02}^2 - \mu^2)X_2(\mu)}\,d\mu. \tag{VI.10}$$

Now, using Eqs. (III.5) and (VI.6), we have

$$B(\nu) = -\Big\{b_{0+}\phi_{10+}(\nu)\chi(\nu_{01}) + b_{0-}\phi_{10-}(\nu)\chi(-\nu_{01}) + d_{0-}\phi_{20-}(\nu)\chi(-\nu_{02}) + \frac{c_1 - c_2}{4\pi(1 - c_2)} \times \int_{-1}^{0}\frac{\mu\phi_{1\mu}(\mu_0)e^{x_0/\mu}X_1(\mu)}{N_1(\mu)(\mu - \nu)(\nu_{02}^2 - \mu^2)X_2(\mu)}\,d\mu\Big\} \times \left\{\frac{(\nu_{01}^2 - \nu^2)(1 - c_1)X_1(-\nu)}{\Lambda_1^+(\nu)\Lambda_1^-(\nu)X_2(-\nu)}\right\}, \quad \nu > 0, \tag{VI.11}$$

$$A(\nu) = -B(\nu) + \phi_{1\nu}(\mu_0)e^{x_0/\nu}/2\pi N_1(\nu), \quad \nu > 0.$$

$$D(\nu) = -\frac{c_1}{c_2}\frac{\phi_{1\nu}(\mu_0)}{2\pi N_1(\nu)}e^{x_0/\nu} - \frac{(\nu_{02}^2 - \nu^2)(1 - c_2)X_2(\nu)}{\Lambda_2^+(\nu)\Lambda_2^-(\nu)X_1(\nu)} \times \{b_{0+}\phi_{10+}(\nu)\chi(\nu_{01}) + b_{0-}\phi_{10-}(\nu)\chi(-\nu_{01}) + d_{0-}\phi_{20-}(\nu)\chi(-\nu_{02})\} + \frac{(c_2 - c_1)(\nu_{02}^2 - \nu^2)X_2(\nu)}{4\pi\Lambda_2^+(\nu)\Lambda_2^-(\nu)X_1(\nu)} \times P\int_{-1}^{0}d\mu\,\frac{\mu\phi_{1\mu}(\mu_0)e^{x_0/\mu}X_1(\mu)}{N_1(\mu)(\mu - \nu)(\nu_{02}^2 - \mu^2)X_2(\mu)} - \frac{(c_2 - c_1)\lambda_2(\nu)\phi_{1\nu}(\mu_0)}{2\pi c_2\Lambda_2^+(\nu)\Lambda_2^-(\nu)N_1(\nu)}e^{x_0/\nu}, \quad \nu < 0.$$

Now with Eqs. (VI.6), (VI.9), and (VI.11), the Green's function is completely determined.[11] In this case, there does not appear to be a simplification at the interface corresponding to that found in the previous problems.

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[11] Case has obtained results for the two-half-space Green's function. (See Ref. 4.)

Simple Derivation of the Faxén Solution to the Lamm Equation

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In this paper a Hankel transform technique is used to derive the Faxén solution to the Lamm equation when the sedimentation coefficient is constant and when it varies linearly with concentration.

THE properties of the Lamm equation for the sedimentation of substances in a centrifugal field have been studied by many authors.[1-4] A solution to the Lamm equation which has proved to be of great utility for practical applications is that of Faxén. This solution describes the sedimentation of a substance in an infinite wedge rotating at constant speed around an axis through the vertex of the wedge. There have been several derivations of Faxén's result, many of which are rather complicated in their mathematical details. It is the purpose of this note to provide a derivation of Faxén's solution which is quite simple and to show that the technique can be used to find the Faxén solution for the Lamm equation when the sedimentation coefficient depends linearly on concentration.

The Lamm equation is

$$\frac{\partial c}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD\frac{\partial c}{\partial r} - s\omega^2 r^2 c\right], \tag{1}$$

where ω is the frequency of rotation, assumed constant, s is the sedimentation coefficient, and D is the diffusion constant. The initial condition is usually taken to be $c(r, 0) = 0$ for $r \leq r_0$ and $c(r, 0) = c_0$ for $r > r_0$. We shall, however, assume a general initial condition. Let the dependent and independent variables be subjected to the transformations

$$\psi = \frac{c}{c_0}e^{\tau}, \quad y = 2e^{-\tau/2}\frac{r}{r_0}, \quad \eta = \frac{2D}{s\omega^2 r_0}(1 - e^{-\tau}), \tag{2}$$

where $\tau = 2\omega^2 st$, and c_0 and r_0 are constants introduced to normalize the equations. The substitutions of Eq. (2) convert Eq. (1) into

$$\partial\psi/\partial\eta = \partial^2\psi/\partial y^2 + (1/y)\,\partial\psi/\partial y, \tag{3}$$

as given by Fujita.[3] If one now assumes the separation of variables $\psi(y, \eta) = Y(y)N(\eta)$ to be valid, one finds for $N(\eta)$

$$N(\eta) = \exp(-\lambda^2\eta), \tag{4}$$

and $Y(y)$ satisfies

$$Y''(y) + \frac{1}{y}Y'(y) + \lambda^2 Y(y) = 0 \tag{5}$$

with the solution

$$Y(y) = AY_0(\lambda y) + BJ_0(\lambda y), \tag{6}$$

where $J_0(\lambda y)$ and $Y_0(\lambda y)$ are Bessel functions of the first and second kinds, respectively. The only solution of physical significance is one in which $\psi(y, t)$ remains finite at $y = 0$. Consequently we can set the coefficient of $Y_0(\lambda y)$ equal to zero. Therefore we are led to assume a solution to Eq. (3) of the form

$$\psi(y, \eta) = \int_0^\infty g(\lambda)J_0(\lambda y)e^{-\lambda^2\eta}\,d\lambda, \tag{7}$$

where $g(\lambda)$ is to be found from the initial condition.

The initial condition yields the relation

$$\int_0^\infty g(\lambda)J_0(\lambda y)\,d\lambda = \psi(y, 0). \tag{8}$$

This type of integral equation can be recognized as a form of Hankel transform, and has the inverse

$$g(\lambda) = \lambda\int_0^\infty u\psi(u, 0)J_0(\lambda u)\,du. \tag{9}$$

We therefore have the representation

$$\psi(y, \eta) = \int_0^\infty \lambda J_0(\lambda y)e^{-\lambda^2\eta}\,d\lambda \times \int_0^\infty u\psi(u, 0)J_0(\lambda u)\,du. \tag{10}$$

A change in the order of integration can be justified for functions $\psi(u, 0)$ which are of interest, so that

$$\psi(y, \eta) = \int_0^\infty u\psi(u, 0)\,du \times \int_0^\infty \lambda J_0(\lambda y)J_0(\lambda u)e^{-\lambda^2\eta}\,d\lambda. \tag{11}$$

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[1] O. H. Faxén, Arkiv Math. Astron. Fys. **21B**, 4 (1929).
[2] W. J. Archibald, Phys. Rev. **54**, 371 (1938).
[3] H. Fujita, *Mathematical Theory of Sedimentation Analysis* (Academic Press Inc., New York 1962).
[4] M. Gehatia, E. Katchalski, J. Chem. Phys. **30**, 1334 (1959).

The integral over λ is known,[5]

$$\int_0^\infty \lambda J_0(\lambda y)J_0(\lambda u)e^{-\lambda^2\eta}\,d\lambda$$

$$= \frac{1}{2\eta}\int_0^\infty ue^{-(u^2+y^2)/4\eta}I_0\left(\frac{uy}{2\eta}\right)\psi(u, 0)\,du, \qquad (12)$$

and leads to the representation

$$\psi(y, \eta) = \frac{1}{2\eta}\int_0^\infty ue^{-(u^2+y^2)/4\eta}I_0\left(\frac{uy}{2\eta}\right)\psi(u, 0)\,du, \qquad (13)$$

which is the form given by Faxén,[1] and Gehatia and Katchalski.[4]

In particular, the initial condition

$$\psi(u, 0) = 0 \qquad 0 \le u \le 2,$$
$$= 1 \qquad u > 2,$$

leads to the solution given by Fujita[3]

$$\psi(y, \eta) = \frac{1}{2\eta}\int_2^\infty ue^{-(u^2+y^2)/4\eta}I_0\left(\frac{uy}{2\eta}\right)du. \qquad (14)$$

A similar technique can be used to find an exact solution to Eq. (1) when the sedimentation coefficient is of the form

$$s = s_0(1 - kc). \qquad (15)$$

This problem has been discussed by Fujita,[6] who derived an approximate solution valid only for small values of the parameter $(4Dt)/r_0^2$. In order to reduce Eq. (1) to simpler form we introduce transformations related to those of Fujita,

$$\alpha = kc_0, \qquad \epsilon = 2D/\omega^2 s_0^2 r_0^2, \qquad \tau = 2\omega_0^2 s_0^2 t,$$
$$\theta = \alpha c/c_0, \qquad x = (1/\epsilon)(r/r_0)^2, \qquad (16)$$

where c_0 is a normalizing value of the concentration, and r_0 is a normalizing value of radius. It is easily seen that $\alpha \le 1$ and that $c/c_0 \le 1$ are necessary for the sedimentation coefficient to remain positive. The substitutions of Eq. (16) convert Eq. (1) into

$$\frac{\partial\theta}{\partial\tau} = \frac{\partial}{\partial x}\left\{x\left[\frac{\partial\theta}{\partial x} - \theta(1 - \theta)\right]\right\}, \qquad (17)$$

which must be solved with a given initial condition $\theta(x, 0)$. Noticing that the operator in parentheses in Eq. (17) is a Ricatti operator, we make the further substitutions

$$\theta = \frac{\partial}{\partial x}\ln u, \quad \zeta = 1 - e^{-\tau}, \quad z = 2(xe^{-\tau})^{\frac{1}{2}}, \qquad (18)$$

leading to the result

$$\frac{\partial u}{\partial\zeta} = \frac{\partial^2 u}{\partial z^2} - \frac{1}{z}\frac{\partial u}{\partial z}, \qquad (19)$$

which must be solved with the initial condition

$$u(z, 0) = \exp\tfrac{1}{2}\int_0^z x\theta(x, 0)\,dx. \qquad (20)$$

This type of linearization of a nonlinear differential equation which describes a separation process has been applied in the past to thermal diffusion[7] and to general cascade processes.[8] However, those papers were concerned with a linear rather than a radial geometry.

Again one can separate variables in Eq. (19) and follow the same reasoning as used in the analysis of Eq. (3) to find the general solution

$$u(z, \zeta) = \int_0^\infty zJ_1(\lambda z)e^{-\lambda^2\zeta}g(\lambda)\,d\lambda, \qquad (21)$$

where $g(\lambda)$ is

$$g(\lambda) = \lambda\int_0^\infty J_1(\lambda\sigma)u(\sigma, 0)\,d\sigma. \qquad (22)$$

Hence, integrating over λ in Eq. (21) we find

$$u(z, \zeta) = z\int_0^\infty u(\sigma, 0)\,d\sigma\int_0^\infty \lambda J_1(\lambda\sigma)J_1(\lambda z)e^{-\lambda^2\zeta}\,d\lambda$$

$$= \frac{z}{2\zeta}e^{-z^2/4\zeta}\int_0^\infty e^{-\sigma^2/4\zeta}I_1\left(\frac{z\sigma}{2\zeta}\right)u(\sigma, 0)\,d\sigma. \qquad (23)$$

The final form of the solution for $\theta(x, \zeta)$ is therefore

$$\theta(x, \zeta) = \frac{(1 - \zeta)^{\frac{1}{2}}}{2\zeta x^{\frac{1}{2}}}\frac{P_0(x, \zeta)}{P_1(x, \zeta)} - \left(\frac{1 - \zeta}{\zeta} + \frac{1}{2x}\right), \qquad (24)$$

where

$$P_0(x, \zeta) = \int_0^\infty \sigma u(\sigma, 0)e^{-\sigma^2/4\zeta}I_0\left(\frac{\sigma x^{\frac{1}{2}}(1 - \zeta)^{\frac{1}{2}}}{\zeta}\right)d\sigma,$$
$$P_1(x, \zeta) = \int_0^\infty u(\sigma, 0)e^{-\sigma^2/4\zeta}I_1\left(\frac{\sigma x^{\frac{1}{2}}(1 - \zeta)^{\frac{1}{2}}}{\zeta}\right)d\sigma. \qquad (25)$$

A more complete analysis of the consequences of Eq. (24) will be published elsewhere.

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[5] G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, Cambridge, England.) Second Ed., 1958.

[6] H. Fujita, J. Chem. Phys. **24**, 1084 (1956).

[7] C. D. Majumdar, Phys. Rev. **81**, 844 (1951).

[8] E. W. Montroll and G. F. Newell, J. Appl. Phys. **23**, 184 (1952).

Phase-Space Formulation of the Dynamics of Canonical Variables*

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Statistical reformulation of quantum mechanics in terms of phase-space distribution functions as given by Moyal using Weyl's correspondence rule between classical functions and operators has been extended to various different correspondence rules. The dynamical bracket in the Weyl correspondence (the "Moyal" or the "sine" bracket) is shown to be a Lie bracket. It is further shown that if the theory is restricted to Lie brackets of the form

$$[u(p, q), v(p, q)] = \left\{f\left(\frac{\partial^2}{\partial q_1\,\partial p_2} - \frac{\partial^2}{\partial q_2\,\partial p_1}\right)u(p_1, q_1)v(p_2, q_2)\right\}_{},$$

evaluated for $p_1 = p_2 = p$; $q_1 = q_2 = q$ after differentiation, then the only admissible functional form of f is $f(x) = \beta[(\sin \alpha x)/\alpha]$, where α and β are constants. A law of multiplication which is associative and distributive with respect to addition is also introduced in each case. It gives a correct correspondence between operator multiplication and the multiplication of classical functions. The dynamical brackets obtained in each case are also found to be Lie brackets. Conditions on the phase-space distribution functions to describe pure states are also given.

I. INTRODUCTION

THE possibility of expressing quantum mechanical expectation values as averages over phase-space distribution of noncommuting variables has been discussed by many authors.[1-8] The basic problem one is interested in, is the following:[9]

Given a quantum mechanical state described by the wavefunction $\psi(q)$, one finds the expectation value of any operator $\mathbf{G}(\mathbf{p}, \mathbf{q})$ in the state ψ by the relation[10]

$$\langle \mathbf{G} \rangle = \int \psi^*(q)\mathbf{G}(\mathbf{p}, \mathbf{q})\psi(q)\, dq. \qquad (1.1)$$

We now wish to determine a "phase-space distribution function" $F(p, q)$ of two variables, such that the statistical average of the function $G(p, q)$ with respect to this distribution is identical with the expectation value given by (1.1); i.e.,

$$\overline{G(p, q)} = \iint G(p, q)F(p, q)\, dp\, dq \equiv \langle \mathbf{G}(\mathbf{p}, \mathbf{q}) \rangle. \qquad (1.2)$$

It should be noted that since the operators $\mathbf{p}$ and $\mathbf{q}$ do not commute,[11] the association of $G(p, q)$ with $\mathbf{G}(\mathbf{p}, \mathbf{q})$ may in some cases be ambiguous.

Several rules for the association of a quantum mechanical operator with the corresponding classical function have been proposed.[12] The most commonly used association is that due to Weyl[13] in which a classical function is expressed as a Fourier integral,

$$G(p, q) = \iint \gamma(\tau, \theta)e^{i(\tau p + \theta q)}\, d\tau\, d\theta; \qquad (1.3)$$

the corresponding quantum operator is then defined as that operator which is obtained by replacing p and q on the right-hand side of Eq. (1.3) by the corresponding operators.

$$\mathbf{G}(\mathbf{p}, \mathbf{q}) = \iint \gamma(\tau, \theta)e^{i(\tau \mathbf{p} + \theta \mathbf{q})}\, d\tau\, d\theta. \qquad (1.4)$$

It may be easily shown that in this association the operator corresponding to the function $p^m q^n$ is the coefficient of $[(m + n)!/m!n!]\lambda^m\mu^n$ in the expansion of $(\lambda \mathbf{p} + \mu \mathbf{q})^{m+n}$. Other rules for the association of operators to functions will be given later.

It was shown by Moyal[2] that if Weyl's association between classical functions and quantum mechanical

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[1] E. P. Wigner, Phys. Rev. **40**, 749 (1932).
[2] J. E. Moyal, Proc. Cambridge Phil. Soc. **45**, 99 (1949).
[3] G. A. Baker, Jr., Phys. Rev. **109**, 2198 (1958).
[4] T. F. Jordan and E. C. G. Sudarshan, Rev. Mod. Phys. **33**, 515 (1961).
[5] H. J. Groenewold, Physica **12**, 405 (1946).
[6] T. Takabayasi, Progr. Theoret. Phys. (Kyoto) **11**, 341 (1954).
[7] E. C. G. Sudarshan, *Lectures in Theoretical Physics*, Brandeis University Summer Institute, 1961 (W. A. Benjamin Company, Inc., New York, 1962), Vol. 2, p. 178.
[8] E. C. G. Sudarshan, Phys. Rev. Letters **10**, 277 (1963).
[9] We restrict ourselves to single degree of freedom. Generalization to any finite number of degrees of freedom is however, trivial.
[10] When no limits are specified, all integrals are to be understood as extending from $-\infty$ to $+\infty$.
[11] Their commutator is given by $[\mathbf{q}, \mathbf{p}]_- = i\hbar$. In the present paper, the operators are denoted throughout by boldface letters, and the corresponding classical functions by ordinary (lightface) letters.
[12] J. R. Shewell, Am. J. Phys. **27**, 16 (1959); also see references given in this paper.
[13] H. Weyl, *The Theory of Groups and Quantum Mechanics*, translated from German by H. P. Robertson (Dover Publications, Inc., New York, 1931), p. 274.

operators is used, then the following phase-space distribution function is obtained:

$$F_W(p, q) = \frac{1}{2\pi}\int \psi^*(q - \tfrac{1}{2}\hbar\tau) \times e^{-i\tau p}\psi(q + \tfrac{1}{2}\hbar\tau)\, d\tau. \quad (1.5)$$

This expression is identical with the one first given by Wigner.[1] Moyal has further shown that with this choice of phase-space distribution function, the quantum equation of motion is equivalent to the equation

$$\partial F_W(q, p, t)/\partial t = -[F, H]_W, \quad (1.6)$$

if the state of the system is considered time-dependent and dynamical variables as time-independent (Schrödinger picture). Here H is the Hamiltonian of the system and the bracket $[\ ]_W$ (known as "Moyal" or "sine" bracket) is defined by the formula

$$[A(p, q), B(p, q)]_W = \frac{2}{\hbar}\sin\frac{\hbar}{2}\left\{\frac{\partial^2}{\partial q_1\,\partial p_2} - \frac{\partial^2}{\partial q_2\,\partial p_1}\right\}A(p_1, q_1)B(p_2, q_2)\Big|_{\substack{p_1=p_2=p,\\ q_1=q_2=q}} \quad (1.7)$$

with $p_1 = p_2 = p$ and $q_1 = q_2 = q$ after differentiation as indicated. If, on the other hand, the time dependence is associated with the dynamical variables (Heisenberg picture), then the equation of motion for any variable $G(p, q, t)$ is[14]

$$(d/dt)G(p, q, t) = [G, H]_W. \quad (1.8)$$

It can easily be shown that the operator corresponding to the sine bracket of two arbitrary functions $A(p, q)$ and $B(p, q)$ is nothing but the commutator divided by $i\hbar$, of the operators $\mathbf{A}$ and $\mathbf{B}$ corresponding to the functions A and B. That is,

$$\left.\begin{aligned}&\text{if } \mathbf{A}(\mathbf{p}, \mathbf{q}) \to A(p, q), \mathbf{B}(\mathbf{p}, \mathbf{q}) \to B(p, q),\\ &\text{then } (\mathbf{AB} - \mathbf{BA})/i\hbar \to [A, B]_W.\end{aligned}\right\} \quad (1.9)$$

Further properties of these brackets have been studied by Baker[3] and Jordan and Sudarshan.[4] In particular, Jordan and Sudarshan have shown explicitly that these brackets are Lie brackets. However, their proof contains an error which led them to some incorrect conclusions.[15]

In Appendix A we give a corrected proof that sine brackets do satisfy the conditions of Lie brackets and show also that, if we restrict ourselves to the Lie brackets of the form

$$[u, v] = \left\{f\left(\frac{\partial^2}{\partial q_1\,\partial p_2} - \frac{\partial^2}{\partial q_2\,\partial p_1}\right) \times u(p_1, q_1)v(p_2, q_2)\right\}_{\substack{p_1=p_2=p,\\ q_1=q_2=q}} \quad (1.12)$$

then the only admissible function is

$$f(x) = \beta[(\sin\alpha x)/\alpha], \quad (1.13)$$

where α and β are constants. (We note that Poisson brackets correspond to the case $\alpha = 0$.)

Besides the phase-space formulation based on Weyl's rule of associating operators with classical functions, it is of interest to consider other phase-space distribution functions when different rules of association are used. It is the purpose of this paper to examine systematically these various phase-space formulations.

II. STANDARD ORDERING

We first investigate some consequences of the rule of association in which the operator corresponding to a classical function is obtained by replacing q and p by the corresponding operators $\mathbf{q}$ and $\mathbf{p}$ after q and p have been put in a "standard" order. By standard order is meant here the order in which all powers of $\mathbf{q}$ precede all powers of $\mathbf{p}$. Thus, for example, if

$$G(p, q) = \sum g_{mn}q^m p^n, \quad \text{then } \mathbf{G}(\mathbf{p}, \mathbf{q}) = \sum g_{mn}\mathbf{q}^m\mathbf{p}^n, \quad (2.1)$$

[14] Note the difference of signs on the right-hand side of Eqs. (1.7) and (1.9). This is analogous to a similar situation which holds in connection with quantum equations of motion, expressed in density matrix notation, viz.,

$$i\hbar(\partial\varrho/\partial t) = -[\varrho, \mathbf{H}]_-, \quad (1.6a)$$

$$i\hbar(\partial\mathbf{G}/\partial t) = +[\mathbf{G}, \mathbf{H}]_-, \quad (1.8a)$$

where $[\ ]_-$ denotes the usual commutator.

[15] Thus, for example, according to Jordan and Sudarshan (Ref. 4, p. 524), the bracket defined by

$$[u, v] = \sum_{n=0}^{\infty}\frac{(-1)^n C(n)}{(2n+1)!}\left(\frac{\partial^2}{\partial q_1\,\partial p_2} - \frac{\partial^2}{\partial q_2\,\partial p_1}\right)^{2n+1} \times u(p_1, q_1)v(p_2, q_2)\Big|_{\substack{p_1=p_2=p,\\ q_1=q_2=q}} \quad (1.10)$$

where $C(n)$ are arbitrary (but which ensure the convergence of the series on the right), is a Lie bracket. However, this statement cannot be correct, for if we take, for example,

$$C(n) = \delta_{1n}, \quad u = q^3, \quad v = q^2p^4 \text{ and } w = qp^4,$$

then a straightforward calculation shows that the Jacobi identity

$$[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0 \quad (1.11)$$

is *not* satisfied.

or if

$$G(p, q) = \iint \gamma(\tau, \theta) e^{i(\tau p + \theta q)}\, d\tau\, d\theta,$$

$$\text{then} \quad \mathbf{G}(\mathbf{p}, \mathbf{q}) = \iint \gamma(\tau, \theta) e^{i\theta \mathbf{q}} e^{i\tau \mathbf{p}}\, d\tau\, d\theta. \tag{2.2}$$

A. Distribution Function

With the above correspondence, the characteristic function of the phase-space distribution function $F_S(p, q)$,

$$M_S(\tau, \theta) = \iint F_S(p, q) e^{i(\tau p + \theta q)}\, dp\, dq, \tag{2.3}$$

for a state defined by a wavefunction $\psi(q)$ is given by

$$\begin{aligned} M_S(\tau, \theta) &= \int \psi^*(q) e^{i\theta q} e^{i\tau p} \psi(q)\, dq \\ &= \int \psi^*(q) e^{i\theta q} \psi(q + \hbar\tau)\, dq. \end{aligned} \tag{2.4}$$

From (2.3) and (2.4) we obtain

$$\begin{aligned} F_S(p, q) &= \frac{1}{4\pi^2} \iint d\tau\, d\theta \int dq' \psi^*(q') \\ &\qquad \times \psi(q' + \hbar\tau) e^{-i\tau p} e^{i\theta(q' - q)} \\ &= \frac{1}{2\pi} \int \psi^*(q) e^{-i\tau p} \psi(q + \hbar\tau)\, d\tau. \end{aligned} \tag{2.5}$$

It may be noted that the phase-space distribution function $F_S(p, q)$ given by (2.5) even though being normalizable, is not everywhere real. This was, however, to be expected since the correspondence such as (2.1) or (2.2) does not always associate Hermitian operators with real functions. It may further be noted that if $F_S(p, q)$ is integrated over one of the variables, then the resulting distribution over the remaining variable is *positive-definite*.[16] It also satisfies the constraint

$$\iint dp\, dq F_s(p, q) e^{-i\hbar\partial^2/\partial p \partial q_2} \times A(p, q_1) A^*(p, q_2)\big|_{q_1 = q_2 = q} \geq 0, \tag{2.6}$$

where $A(p, q)$ is any arbitrary function of p and q and $A^*(p, q)$ is its complex conjugate.

$F_S(p, q)$ may also be expressed in the following alternative forms:

$$F_S(p, q) = h^{-\frac{1}{2}} \psi^*(q) \phi(p) e^{ipq/\hbar}, \tag{2.7}$$

$$F_S(p, q) = \frac{1}{2\pi} \int \phi^*(p + \hbar\theta) e^{-i\theta q} \phi(p)\, d\theta, \tag{2.8}$$

where

$$\phi(p) = h^{-\frac{1}{2}} \int \psi(q) e^{-iqp/\hbar}\, dq \tag{2.9}$$

is the wavefunction in momentum space.

If we insert the expansion of the wavefunction ψ in terms of an orthonormal set

$$\psi(q) = \sum_l a_l \psi_l(q) \tag{2.10}$$

in the expression (2.5) for $F_S(p, q)$, we obtain the following expansion for $F_S(p, q)$:

$$F_S(p, q) = \sum_{m,n} \sum a_m^* a_n f_{mn}^S(p, q), \tag{2.11}$$

where the phase-space eigenfunctions $f_{mn}^S(p, q)$ are given by

$$f_{mn}^S(p, q) = \frac{1}{2\pi} \int \psi_m^*(q) e^{-i\tau p} \psi_n(q + \hbar\tau)\, d\tau. \tag{2.12}$$

As in the case of Weyl's association[2] the functions $f_{mn}^S(p, q)$ form a complete orthogonal set, {in the Hilbert space of the phase-space functions $F_S(p, q)$} satisfying the relations

$$\iint f_{mn}^S(p, q) f_{m'n'}^{S*}(p, q)\, dp\, dq = h^{-1}\, \delta_{mm'}\, \delta_{nn'}, \tag{2.13}$$

$$\sum_m \sum_n f_{mn}^S(p, q) f_{mn}^{S*}(p', q') = h^{-1}\, \delta(p - p')\, \delta(q - q'), \tag{2.14}$$

and also the self-orthogonality relations

$$\iint f_{mn}^S(p, q)\, dp\, dq = \delta_{mn}, \tag{2.15}$$

$$\sum_m f_{mm}^S(p, q) = h^{-1}. \tag{2.16}$$

B. Dynamics

To study the dynamics, we must first find a correspondence between the commutator brackets and classical brackets. For this purpose we first determine a "law" for the product of two functions. Let $A(p, q)$ and $B(p, q)$ be two functions given by

$$A(p, q) = \iint \phi_A(k, s) e^{i(kp + sq)}\, dk\, ds, \tag{2.17}$$

and

$$B(p, q) = \iint \phi_B(k, s) e^{i(kp + sq)}\, dk\, ds. \tag{2.18}$$

Then according to the standard ordering law of association, we obtain

$$\begin{aligned} \mathbf{A} \cdot \mathbf{B} = \int \cdots \int dk_1\, dk_2\, ds_1\, ds_2 \phi_A(k_1, s_1) \phi_B(k_2, s_2) \\ \times e^{is_1 \mathbf{q}} e^{ik_1 \mathbf{p}} e^{is_2 \mathbf{q}} e^{ik_2 \mathbf{p}}. \end{aligned} \tag{2.19}$$

[16] The same is true for the case of Wigner distribution given by Eq. (1.6).

Using the well-known identity[17]:

$$e^{\mathbf{L}}e^{\mathbf{M}} = e^{\mathbf{L}+\mathbf{M}+\frac{1}{2}[\mathbf{L},\mathbf{M}]-} = e^{\mathbf{M}}e^{\mathbf{L}}e^{[\mathbf{L},\mathbf{M}]-}, \quad (2.20)$$

where $\mathbf{L}$ and $\mathbf{M}$ are operators commuting with their commutator, Eq. (2.19) can be written as

$$\mathbf{A}\cdot\mathbf{B} = \int \cdots \int dk_1\, dk_2\, ds_1\, ds_2 \phi_A(k_1, s_1)\phi_B(k_2, s_2) \times e^{i\hbar k_1 s_2} e^{i(s_1+s_2)q} e^{i(k_1+k_2)p}.$$

Thus, we see that, if a "law" of multiplication of two functions $A(p, q)$ and $B(p, q)$ be given by

$$A \times B = [e^{-i\hbar(\partial^2/\partial p_1 \partial q_2)} A(p_1, q_1)B(p_2, q_2)]_{\substack{p_1=p_2=p,\\ q_1=q_2=q}} \quad (2.21)$$

then we obtain a correct association of operator multiplication.

The right-hand side of (2.21) may also be written in an integral form[18] (see Appendix B), which shows explicitly the nonlocal nature of the law of multiplication:

$$A(p, q) \times B(p, q) = \frac{1}{h}\iint e^{(-i/\hbar)(\eta-p)(\tau-q)} A(\eta, q)B(p, \tau)\, d\eta\, d\tau. \quad (2.22)$$

It may be easily verified that this law of multiplication is associative (see Appendix C), i.e.,

$$A \times (B \times C) = (A \times B) \times C, \quad (2.23)$$

but is not commutative. The commutator now becomes

$$(1/i\hbar)(\mathbf{AB} - \mathbf{BA}) \to (1/i\hbar)(A \times B - B \times A) = [A, B]_S \equiv (1/i\hbar)\{e^{-i\hbar(\partial^2/\partial p_1 \partial q_2)} - e^{-i\hbar(\partial^2/\partial q_1 \partial p_2)}\} A(p_1, q_1)B(p_2, q_2)\Big|_{\substack{p_1=p_2=p.\\ q_1=q_2=q}} \quad (2.24)$$

It may further be verified explicitly that the bracket defined by (2.24) also satisfies the conditions of a Lie bracket (see Appendix C). This is, of course, not surprising since the ordinary commutator bracket is a Lie bracket. One can further show by a similar analysis, as in Appendix A, that if restriction is made to a Lie bracket of the type

$$[u, v] = \left\{f\left(\frac{\partial^2}{\partial p_1\, \partial q_2}\right) + g\left(\frac{\partial^2}{\partial p_2\, \partial q_1}\right)\right\} u(p_1, q_1)v(p_2, q_2)\Big|_{\substack{p_1=p_2=p,\\ q_1=q_2=q}} \quad (2.25)$$

then the only admissible functional forms are

$$f(x) \equiv -g(x) = (\beta/\alpha)e^{-\alpha x} + \gamma, \quad (2.26)$$

where α, β and γ are constants ($\alpha = 0$ giving the Poisson bracket).

Further it may be noted that in the limit $\hbar \to 0$, Eq. (2.21) or (2.22) reduces to

$$A \times B = A \cdot B, \quad (2.27)$$

where the dot represents ordinary multiplication, and the correspondence (2.24) reduces to the usual Poisson bracket correspondence.

It is now clear that if the time dependence is associated with the dynamical variables, (Heisenberg picture) then the equation of motion for them can be written as

$$\partial A(p, q, t)/\partial t = [A, H]_S. \quad (2.28)$$

If the time dependence is associated with the distribution function rather than with the dynamical variables, then the equation of motion for the distribution function is not given by (1.7) with $[\ ]_W$ replaced by $[\ ]_S$, but instead is given by

$$\frac{\partial F(p, q, t)}{\partial t} = \frac{1}{i\hbar}\{e^{i\hbar(\partial^2/\partial p_2 \partial q_1)} - e^{i\hbar(\partial^2/\partial p_1 \partial q_2)}\} \times e^{i\hbar(\partial^2/\partial q_1 \partial p_1)} H(p_1, q_1)F(p_2, q_2, t)\Big|_{\substack{p_1=p_2=p.\\ q_1=q_2=q}} \quad (2.29)$$

C. Condition for a Pure State

Instead of a pure state described by a wave-function $\psi(q)$, consider now a mixed state described by a density matrix

$$\varrho = \sum_{m,n} \rho_{mn}\psi_m(q)\psi_n^*(q), \quad (2.30)$$

(where ψ_m form a complete orthonormal set). The quantum average or the expectation value of an operator $\mathbf{G}(\mathbf{p}, \mathbf{q})$ is now given by

$$\langle \mathbf{G} \rangle = \mathrm{Tr}\,(\varrho \mathbf{G}) = \sum_{m,n} \rho_{mn} \int \psi_n^*(q)\mathbf{G}\psi_m(q)\, dq. \quad (2.31)$$

The corresponding distribution function is then given by

$$F_S(p, q) = \sum_{m,n} \frac{1}{2\pi} \rho_{mn} \int \psi_n^*(q)e^{-i\tau p}\psi_m(q + \hbar\tau)\, d\tau = \sum_{m,n} \rho_{mn} f_{nm}^S(p, q). \quad (2.32)$$

The necessary and sufficient condition for a state described by the density matrix ϱ (Eq. 2.30) to be pure is given by

$$\varrho^2 = \varrho, \quad (2.33)$$

[17] A. Messiah, *Quantum Mechanics* (North-Holland Publishing Company, Amsterdam, and John Wiley & Sons, Inc., New York, 1961), Vol. I, p. 442.

[18] It is assumed here that the functions A and B and all their derivatives are zero for infinite values of their arguments.

or equivalently, by the condition that the coefficients ρ_{mn} may be expressed in the form

$$\rho_{mn} = \rho_m \rho_n^*. \tag{2.34}$$

We ask for a similar condition on the distribution function $F_S(p, q)$ in order that it may describe a pure state. It is shown below that the required condition is

$$e^{i\hbar(\partial^2/\partial p_1 \partial q_2)} F_S(p_1, q_1) F_S(p_2, q_2)\Big|_{\substack{p_1=p_2=p \\ q_1=q_2=q}} = h^{-1} F_S(p, q). \tag{2.35}$$

In this connection one may also note that the phase-space eigenfunctions (2.12) satisfy the relations

$$e^{i\hbar(\partial^2/\partial p_1 \partial q_2)} f^S_{mn}(p_1, q_1) f^S_{m'n'}(p_2, q_2)\Big|_{\substack{p_1=p_2=p \\ q_1=q_2=q}} = h^{-1} \delta_{nm'} f^S_{mn'}(p, q). \tag{2.36}$$

In order to show that (2.35) is necessary for $F_S(p, q)$ to describe a pure state, we write using (2.32) and (2.34),

$$F_S(p, q) = \sum_{m,n} \rho_m \rho_n^* f^S_{nm}(p, q). \tag{2.37}$$

We then obtain

$$e^{i\hbar(\partial^2/\partial p_1 \partial q_2)} F_S(p_1, q_1) F_S(p_2, q_2)\Big|_{\substack{p_1=p_2=p \\ q_1=q_2=q}} = \sum_{m,n} \sum_{m',n'} \rho_m \rho_n^* \rho_{m'} \rho_{n'}^* h^{-1} \delta_{mn'} f^S_{nm'}(p, q), \tag{2.38}$$

where use has been made of (2.36). Since $F_S(p, q)$ is normalized, we have

$$\sum_m \rho_m \rho_m^* = 1,$$

and (2.38) then gives

$$e^{i\hbar(\partial^2/\partial p_1 \partial q_2)} F_S(p_1, q_1) F_S(p_2, q_2)\Big|_{\substack{p_1=p_2=p \\ q_1=q_2=q}} = h^{-1} F_S(p, q).$$

To show that (2.35) is also sufficient, we write

$$F_S(p, q) = \sum_{m,n} \rho_{mn} f^S_{nm}(p, q). \tag{2.39}$$

Equation (2.35) then gives

$$\sum_{m',n} \sum_m \rho_{mn} \rho_{m'm} f^S_{nm'}(p, q) = \sum_{m,n} \rho_{mn} f^S_{nm}(p, q). \tag{2.40}$$

However, since f^S_{nm} are orthogonal, we obtain

$$\sum_m \rho_{m'm} \rho_{mn} = \rho_{m'n},$$

a relation which is equivalent to (2.33). Hence $F_S(p, q)$ describes a pure state.

We shall now consider corresponding results for cases when the rule of association is not standard ordering. Only the main steps will be indicated, as the analysis is similar to that given in the present section.

III. NORMAL ORDERING

If we introduce two new independent variables[19]

$$a = (q + ip)/(2\hbar)^{\frac{1}{2}}, \qquad a^* = (q - ip)/(2\hbar)^{\frac{1}{2}}, \tag{3.1}$$

then, as is well-known, the corresponding operators $\mathbf{a}$ and $\mathbf{a}^*$ may be interpreted as destruction and creation operators, respectively, satisfying the commutation relation

$$[\mathbf{a}, \mathbf{a}^*]_- = 1. \tag{3.2}$$

In this section we shall discuss the case in which the operator corresponding to a classical function is obtained by replacing a and a^* by the corresponding operators $\mathbf{a}$ and $\mathbf{a}^*$ after they are put in a normal order. By normal order is meant here, the order in which all the creation operators occur on the left of the destruction operators. Thus, if

$$G(p, q) = \sum_{m,n} g_{mn} \left(\frac{q - ip}{(2\hbar)^{\frac{1}{2}}}\right)^m \left(\frac{q + ip}{(2\hbar)^{\frac{1}{2}}}\right)^n,$$

then

$$\mathbf{G}(\mathbf{p}, \mathbf{q}) = \sum_{m,n} g_{mn} \left(\frac{\mathbf{q} - i\mathbf{p}}{(2\hbar)^{\frac{1}{2}}}\right)^m \left(\frac{\mathbf{q} + i\mathbf{p}}{(2\hbar)^{\frac{1}{2}}}\right)^n. \tag{3.3}$$

This association is of particular interest in connection with field-theoretical calculations, where the normal ordered products are usually employed. This formulation, for example, has been found very useful in investigations relating to the connection between the semiclassical and quantum description of optical coherence phenomena.[8,20] It may be noted that this rule associates Hermitian operators with real classical functions. Hence, we expect that the phase-space distribution function will be real though not necessarily positive-definite.

A. Distribution Function

The characteristic function of the distribution function is given by

$$\begin{aligned} M_N(\tau, \theta) &= \iint F_N(p, q) e^{i(\tau p + \theta q)}\, dp\, dq \\ &= \iint F_N(p, q) \exp\left[i\left(\frac{\hbar}{2}\right)^{\frac{1}{2}} a^*(\theta + i\tau)\right] \\ &\quad \times \exp\left[i\left(\frac{\hbar}{2}\right)^{\frac{1}{2}} a(\theta - i\tau)\right] dp\, dq \\ &= \int \psi^*(q) \exp\left[i\left(\frac{\hbar}{2}\right)^{\frac{1}{2}} \mathbf{a}^*(\theta + i\tau)\right] \\ &\quad \times \exp\left[i\left(\frac{\hbar}{2}\right)^{\frac{1}{2}} \mathbf{a}(\theta - i\tau)\right] \psi(q)\, dq. \end{aligned} \tag{3.4}$$

[19] We use the asterisk to denote complex-conjugate quantities for ordinary functions and Hermitian adjoints for operators.

[20] C. L. Mehta and E. Wolf (to be published).

Simplifying Eq. (3.4) and taking the Fourier inverse, we obtain

$$F_N(p, q) = \frac{1}{2\pi} \exp\left[-\tfrac{1}{4}\hbar\left(\frac{\partial^2}{\partial p^2} + \frac{\partial^2}{\partial q^2}\right)\right] \times \int \psi^*(q - \tfrac{1}{2}\hbar\tau)e^{-i\tau p}\psi(q + \tfrac{1}{2}\hbar\tau)\, d\tau. \quad (3.5)$$

It is easily seen that $F_N(p, q)$, given by (3.5), is real as expected. An explicit form for a similar distribution function, obtained from density matrix in Fock representation, has also recently been given by Sudarshan in a different connection.[8]

B. Dynamics

Following the methods given in Sec. IIB, we now find the following law relating to multiplication:

$$A(p, q) \times B(p, q) = \exp\left\{\frac{\hbar}{2}\left(\frac{\partial^2}{\partial q_1\, \partial q_2} + \frac{\partial^2}{\partial p_1\, \partial p_2} + i\frac{\partial^2}{\partial q_1\, \partial p_2} - i\frac{\partial^2}{\partial q_2\, \partial p_1}\right)\right\} \times A(p_1, q_1)B(p_2, q_2)\Big|_{\substack{p_1=p_2=p\cdot \\ q_1=q_2=q}} \quad (3.6)$$

It is easily verified that this law of multiplication is also associative and reduces to an ordinary product in the limit $\hbar \to 0$. The commutator of two functions now takes the form

$$(1/i\hbar)(A \times B - B \times A) = [A, B]_N, \quad (3.7)$$

where the bracket on the right-hand side is defined by

$$[A(p, q), B(p, q)]_N = \exp\left\{\frac{\hbar}{2}\left(\frac{\partial^2}{\partial q_1\, \partial q_2} + \frac{\partial^2}{\partial p_1\, \partial p_2}\right)\right\} \times \frac{2}{\hbar}\sin\frac{\hbar}{2}\left(\frac{\partial^2}{\partial q_1\, \partial p_2} - \frac{\partial^2}{\partial q_2\, \partial p_1}\right) \times A(p_1, q_1)B(p_2, q_2)\Big|_{\substack{p_1=p_2=p\cdot \\ q_1=q_2=q}} \quad (3.8)$$

By analogy with the previous cases, we have the association

$$(1/i\hbar)[\mathbf{A}, \mathbf{B}]_- \to [A, B]_N. \quad (3.9)$$

This correspondence shows that the normal bracket defined by (3.8) is also a Lie Bracket.

The equation of motion, appropriate to the Heisenberg picture now takes the form

$$\partial A(p, q, t)/\partial t = [A, H]_N. \quad (3.10)$$

On the other hand, the corresponding equation of motion for the distribution function (Schrödinger picture) is

$$\frac{\partial F_N}{\partial t} = \frac{2}{\hbar}\exp\left\{-\frac{\hbar}{2}\left(\frac{\partial^2}{\partial q_1\, \partial q_2} + \frac{\partial^2}{\partial p_1\, \partial p_2} + \frac{\partial^2}{\partial p_2^2} + \frac{\partial^2}{\partial q_2^2}\right)\right\}\sin\frac{\hbar}{2}\left(\frac{\partial^2}{\partial q_2\, \partial p_1} - \frac{\partial^2}{\partial q_1\, \partial p_2}\right) \times F_N(p_1, q_1)H(p_2, q_2)\Big|_{\substack{p_1=p_2=p\cdot \\ q_1=q_2=q}} \quad (3.11)$$

C. Condition for a Pure State

Again, following the methods given in Sec. IIC, we obtain the condition which the distribution function $F_N(p, q)$ must satisfy in order that it represents a pure state. This is found to be

$$\exp\left\{-\frac{\hbar}{2}\left(\frac{\partial^2}{\partial q_1\, \partial q_2} + \frac{\partial^2}{\partial p_1\, \partial p_2}\right)\right\} \times \cos\frac{\hbar}{2}\left(\frac{\partial^2}{\partial q_1\, \partial p_2} - \frac{\partial^2}{\partial q_2\, \partial p_1}\right) \times F_N(p_1, q_1)\cdot F_N(p_2, q_2)\Big|_{\substack{p_1=p_2=p \\ q_1=q_2=q}} = h^{-1}F_N(p, q). \quad (3.12)$$

Finally, we note that Eq. (3.6) may also be written in an integral form,

$$A(p, q) \times B(p, q) = \frac{2}{h}\iint e^{(2i/\hbar)\tau\eta} \times A(p - i\tau, q + \tau)B(p + \eta, q - i\eta)\, d\tau\, d\eta. \quad (3.13)$$

Similar integral representations for the bracket (3.8) and the condition for pure state (3.12) may also be readily derived.

IV. RIVIER RULE

From considerations of the correspondence with infinitesimal canonical transformations and infinitesimal unitary transformations, Rivier proposed the following rule of association between classical functions and quantum operators: If the function $G(p, q)$ is written as a Fourier integral

$$G(p, q) = \iint \gamma(\tau, \theta)e^{i(\tau p + \theta q)}\, d\tau\, d\theta, \quad (4.1)$$

then the corresponding operator is given by

$$\mathbf{G(p, q)} = \iint \gamma(\tau, \theta)\tfrac{1}{2}(1 + e^{-i\hbar\tau\theta})e^{i\mathbf{p}\tau}e^{i\mathbf{q}\theta}\, d\tau\, d\theta. \quad (4.2)$$

It may be easily seen that (4.2) may be written as

$$\mathbf{G(p, q)} = \iint \gamma(\tau, \theta)\tfrac{1}{2}(e^{i\mathbf{p}\tau}e^{i\mathbf{q}\theta} + e^{i\mathbf{q}\theta}e^{i\mathbf{p}\tau})\, d\tau\, d\theta, \quad (4.3)$$

which implies that this rule is simply a symmetrized form of the standard ordering rule, i.e., to the

classical function $p^m q^n$ is associated the quantum operator $\frac{1}{2}(\mathbf{p}^m\mathbf{q}^n + \mathbf{q}^n\mathbf{p}^m)$.

It is clear that this rule associates real functions with Hermitian operators, and hence the phase-space distribution in this case must be expected to be real. If we carry out similar calculations as in the previous cases, we obtain the following expression for the distribution function in the case of Rivier association:

$$F_R(p, q) = \frac{1}{4\pi}\int d\tau e^{-i\tau p}\{\psi^*(q)\psi(q + \hbar\tau) + \psi^*(q - \hbar\tau)\psi(q)\}. \quad (4.4)$$

It should be noted that the distribution function $F_R(p, q)$ given by (4.4) is just the real part of $F_S(p, q)$ [cf. Eq. (2.5)].

The product law, dynamical brackets, and the condition for pure state are more complicated and hence are not given here.

V. RELATION BETWEEN VARIOUS PHASE-SPACE DISTRIBUTION FUNCTIONS

In the previous sections we determined expressions for the phase-space distribution functions appropriate to the different rules of association between operators and classical functions, starting from a given quantum mechanical wavefunction (in the case of pure state) or density matrix (in case of mixed state). The inverse of this problem is also of interest. Given a phase-space distribution function and the rule of association, to determine the density matrix (or the wavefunction if the given distribution function describes a pure state). This problem can be solved by first expanding the distribution function in terms of the phase-space eigenfunctions (appropriate to the given rule of association),

$$F(p, q) = \sum_{l,m} a_{lm} f_{lm}(p, q), \quad (5.1)$$

where the coefficients a_{lm} obtained by using orthogonality relations between phase-space eigenfunctions (2.13) are given by

$$a_{lm} = h\iint F(p, q) f^*_{lm}(p, q)\, dp\, dq. \quad (5.2)$$

The density matrix is then simply given by

$$\varrho = \sum a_{lm}\psi_m(q)\psi^*_l(q). \quad (5.3)$$

It is also of interest to examine how the distribution functions appropriate to different rules of association are interrelated. Writing (1.7) in the form [See Eq. (3.10) of the paper by Moyal[2]]

$$F_W(p, q) = h^{-\frac{1}{2}}e^{-\frac{1}{2}i\hbar(\partial^2/\partial p\partial q)}\{\psi^*(q)\phi(p)e^{ipq/\hbar}\}, \quad (5.4)$$

where $\phi(p)$ is given by (2.9), we obtain the following relation between the distribution function corresponding to the case of Weyl's association and that corresponding to the case of standard ordering [cf. Eq. (2.7)]:

$$F_S(p, q) = e^{\frac{1}{2}i\hbar(\partial^2/\partial p\partial q)}F_W(p, q). \quad (5.5)$$

Similarly, one obtains from Eqs. (1.7) and (3.5) the relation

$$F_N(p, q) = \exp\left\{-\frac{\hbar}{4}\left(\frac{\partial^2}{\partial p^2} + \frac{\partial^2}{\partial q^2}\right)\right\}F_W(p, q), \quad (5.6)$$

and from (4.4) and (5.4) the relation

$$F_R(p, q) = \mathrm{Re}\, F_S(p, q) = \cos\left[\tfrac{1}{2}\hbar(\partial^2/\partial p\, \partial q)\right]F_W(p, q), \quad (5.7)$$

where Re denotes the real part.

In particular, the relations (5.5)–(5.7) connect polynomials of a given order in p and q with polynomials of the same order.

It is interesting to note that if a distribution function is bivariate Gaussian in p and q for the Weyl's association, it remains Gaussian for the normal-ordering association also. Thus, for example, if F_W is given by

$$F_W(p, q) = (\Delta^{\frac{1}{2}}/2\pi) \times \exp\{-\tfrac{1}{2}(a_1p^2 + a_2q^2 + 2a_3pq)\}, \quad (5.8)$$

where a_1, a_2, a_3 are constants and $\Delta = a_1a_2 - a_3^2$, then

$$F_N(p, q) = \frac{1}{2\pi}\frac{\Delta}{\Delta'^{\frac{1}{2}}}\exp\left\{-\frac{1}{2}\frac{\Delta}{\Delta'}\left[\left(a_1 - \frac{\hbar}{2}\Delta\right)p^2 + \left(a_2 - \frac{\hbar}{2}\Delta\right)q^2 + 2a_3pq\right]\right\}, \quad (5.9)$$

where

$$\Delta' = \Delta[1 - \tfrac{1}{2}\hbar(a_1 + a_2) + \tfrac{1}{4}\hbar^2\Delta]. \quad (5.10)$$

VI. CONCLUDING REMARKS

We have seen that the nature of the phase-space distribution function and the dynamics depends much on the rule of association of operators with classical functions. The distribution function may not only be negative in some cases, but may even become complex. If, however, the association between the operators and classical functions is such that Hermitian operators correspond to real functions, then the distribution function is real. In most cases, if one integrates over one of the variables, then one obtains a positive-definite quantity. This is not true for the case of normal ordering, discussed in

Sec. III. The fact that one is dealing with quantities which are simultaneously unobservable seems to be reflected in the nonpositivity of the distribution function. From the expressions for these distribution functions, one can, in fact, derive Heisenberg's uncertainty relation and even the Schrödinger equation.[21] Thus, we see that if negative and even complex probability distributions are admitted, and such descriptions are called "semiclassical" as has been suggested elsewhere in the discussion of related problems,[8,20] then such a semiclassical description is completely equivalent to the quantum mechanical description.

Throughout the preceding treatment, only the case of one degree of freedom was considered. However, our whole discussion can readily be extended to the case of finite number of degrees of freedom.

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APPENDIX A. CONDITION UNDER WHICH THE BRACKET DEFINED BY

$$[u(p,q), v(p,q)] = \left\{ f\left(\frac{\partial^2}{\partial q_1\,\partial p_2} - \frac{\partial^2}{\partial q_2\,\partial p_1}\right) \times u(p_1, q_1)v(p_2, q_2)\right\}_{\substack{p_1=p_2=p \\ q_1=q_2=q}}$$

BECOMES A LIE BRACKET

Let us start with the bracket defined by Eq. (1.12) viz:

$$[u(p,q), v(p,q)] = \left\{ f\left(\frac{\partial^2}{\partial q_1\,\partial p_2} - \frac{\partial^2}{\partial q_2\,\partial p_1}\right) \times u(p_1, q_1)v(p_2, q_2)\right\}_{\substack{p_1=p_2=p, \\ q_1=q_2=q}} \tag{A1}$$

and ask for the form of the function f such that this be a Lie bracket, i.e., which satisfies the following three conditions:

(1) Linearity:

$$[u, a_1v + a_2w] = a_1[u, v] + a_2[u, w], \tag{A2}$$

where a_1 and a_2 are constants;

(2) Antisymmetry:

$$[u, v] = -[v, u]; \tag{A3}$$

(3) Jacobi identity:

$$[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0. \tag{A4}$$

The condition (A2) is obviously satisfied by (A1) for arbitrary f. For condition (A3) to be valid, $f(x)$ itself must be antisymmetric, i.e.,

$$f(x) = -f(-x). \tag{A5}$$

To examine Jacobi identity, we write each u, v, w as Fourier transforms:

$$u(p, q) = \iint \phi_u(k_1, s_1)e^{i(k_1p+s_1q)}\,dk_1\,ds_1, \quad \text{etc.} \tag{A6}$$

We then have

$$[u, v] = \int \cdots \int \phi_u(k_1, s_1)\phi_v(k_2, s_2)f(k_1s_2 - k_2s_1) \times e^{i(k_1+k_2)p+i(s_1+s_2)q}\,dk_1\,ds_1\,dk_2\,ds_2,$$

and hence

$$[w, [u, v]] = \int \cdots \int \phi_u\phi_v\phi_w e^{i(k_1+k_2+k_3)p+i(s_1+s_2+s_3)q} \times f(k_1s_2 - k_2s_1)f\{k_3(s_1 + s_2) - s_3(k_1 + k_2)\}\,dk_1\,dk_2\,dk_3\,ds_1\,ds_2\,ds_3. \tag{A7}$$

Since the Jacobi identity has to be satisfied for arbitrary u, v, and w, i.e., for arbitrary ϕ_u, ϕ_v, and ϕ_w, we must have

$$\sum_{\substack{\text{cyclic} \\ \text{permutation}}} f(k_1s_2 - k_2s_1)f(k_3s_1 - s_3k_1 + k_3\,s_2 - s_3k_2) = 0. \tag{A8}$$

Writing symbolically

$$\vec{x} = \vec{k} \times \vec{s} \qquad \text{(i.e., } x_1 = k_2s_3 - k_3s_2, \text{ etc.)}, \tag{A9}$$

we obtain

$$\sum_{\substack{\text{cyclic} \\ \text{permutation}}} f(x_3)f(x_2 - x_1) = 0. \tag{A10}$$

which gives, on using (A5),

$$\sum_{cp} f(x_1 - x_2)f(x_3) = 0. \tag{A11}$$

Now, since $f(x)$ is an odd function, we can write

$$f(x) = \sum_{n=0}^{\infty} C_n x^{2n+1}. \tag{A12}$$

Then

$$f(x_1 - x_2)f(x_3) = \sum_{n,m=0}^{\infty} C_mC_n \sum_{r=0}^{2m+1} \frac{(2m+1)!\,(-1)^r}{r!\,(2m+1-r)!}\,x_1^{2m+1-r}x_2^r x_3^{2n+1}$$

[21] See, for example, Ref. 2, Appendixes 1 and 4.

$$= \sum_{n,m=0}^{\infty} \sum_{r=0}^{m} C_m C_n (2m+1)! \left\{ \frac{x_1^{2m+1-2r} x_2^{2r} x_3^{2n+1}}{(2r)!\,(2m+1-2r)!} - \frac{x_1^{2m-2r} x_2^{2r+1} x_3^{2n+1}}{(2r+1)!\,(2m-2r)!} \right\}. \tag{A13}$$

The order of summation over r and m in (A13) can be interchanged by properly changing the limits and we obtain

$$f(x_1 - x_2) f(x_3) = \sum_{n,r=0}^{\infty} \sum_{m=r}^{\infty} (2m+1)!\, C_m C_n \times \left\{ \frac{x_1^{2m+1-2r} x_2^{2r} x_3^{2n+1}}{(2r)!\,(2m+1-2r)!} - \frac{x_1^{2m-2r} x_2^{2r+1} x_3^{2n+1}}{(2r+1)!\,(2m-2r)!} \right\}. \tag{A14}$$

By substituting $m - r = M$, Eq. (A14) can be written as

$$f(x_1 - x_2) f(x_3) = \sum_{n,r,M=0}^{\infty} C_n C_{M+r} (2M+2r+1)! \times \left\{ \frac{x_1^{2M+1} x_2^{2r} x_3^{2n+1}}{(2r)!\,(2M+1)!} - \frac{x_1^{2M} x_2^{2r+1} x_3^{2n+1}}{(2r+1)!\,(2M)!} \right\}. \tag{A15}$$

Thus, we obtain

$$\begin{aligned} \sum_{cp} f(x_1 - x_2) f(x_3) = \sum_{n,m,r=0}^{\infty} C_n C_{m+r} \frac{(2m+2r+1)!}{(2r)!\,(2m+1)!} \\ \times \{ x_2^{2r} (x_1^{2m+1} x_3^{2n+1} - x_1^{2n+1} x_3^{2m+1}) \\ + x_3^{2r} (x_2^{2m+1} x_1^{2n+1} - x_2^{2n+1} x_1^{2m+1}) \\ + x_1^{2r} (x_3^{2m+1} x_2^{2n+1} - x_3^{2n+1} x_2^{2m+1}) \}. \end{aligned} \tag{A16}$$

Since each of the three terms in the curly brackets on the right-hand side of (A16) is of different nature, condition (A11) gives

$$\sum_{n,m,r=0}^{\infty} C_n C_{m+r} \frac{(2m+2r+1)!}{(2r)!\,(2m+1)!} x_2^{2r} \times (x_1^{2m+1} x_3^{2n+1} - x_1^{2n+1} x_3^{2m+1}) = 0,$$

or

$$C_n C_{m+r} \frac{(2m+2r+1)!}{(2m+1)!} = C_m C_{n+r} \frac{(2n+2r+1)!}{(2n+1)!} \tag{A17}$$

for all integral values of n, m, and r. Setting

$$C_n = D_n/(2n+1)!, \tag{A18}$$

we obtain from (A17) the condition

$$D_n D_{m+r} = D_m D_{n+r} \tag{A19}$$

for all n, m, and r. It can be easily seen that the only solution of (A19) is

$$D_n = D_0 a^n, \tag{A20}$$

where a is a constant (which can be equal to zero; then $D_n = D_0 \delta_{n0}$). Using Eqs. (A12), (A18), and (A20), we obtain

$$f(x) = \sum_{n=0}^{\infty} D_0 \frac{a^n}{(2n+1)!} x^{2n+1}. \tag{A21}$$

Putting $a = -\alpha^2$ and $D_0 = \beta$, we obtain the required solution

$$f(x) = \beta[(\sin \alpha x)/\alpha], \tag{A22}$$

given by the Eq. (1.14) of the text. The bracket defined by (A1) now becomes

$$[u, v] = (\beta/\alpha) \sin \alpha \left(\frac{\partial^2}{\partial q_1\, \partial p_2} - \frac{\partial^2}{\partial q_2\, \partial p_1} \right) \times u(p_1, q_1) v(p_2, q_2) \Big|_{\substack{p_1 = p_2 = p \\ q_1 = q_2 = q}}. \tag{A23}$$

One can further verify (by using the Fourier representation) that any of the brackets which satisfy relation (A24), (A25), or (A26) is a Lie bracket,

$$[u, v]_1 = e^{\gamma(\partial^2/\partial q_1 \partial q_2)} [u, v] \Big|_{q_1 = q_2 = q}, \tag{A24}$$

$$[u, v]_2 = e^{\gamma(\partial^2/\partial p_1 \partial p_2)} [u, v] \Big|_{p_1 = p_2 = p}, \tag{A25}$$

$$[u, v]_3 = e^{\gamma(\partial^2/\partial q_1 \partial p_2 + \partial^2/\partial p_1 \partial q_2)} [u, v] \Big|_{\substack{p_1 = p_2 = p \\ q_1 = q_2 = q}}. \tag{A26}$$

Here $[u, v]$ on the right-hand side itself stands for a bracket of the form (A23) or for any of the brackets $[u, v]_1$, $[u, v]_2$, and $[u, v]_3$. Thus, if we substitute (A23) in (A26), and set $\alpha = \gamma = -i\theta$, we obtain the "exponential" brackets

$$[u, v]_3 = \frac{\beta}{\theta} \{ e^{\theta(\partial^2/\partial q_1 \partial p_2)} - e^{\theta(\partial^2/\partial q_2 \partial p_1)} \} \times u(p_1, q_1) v(p_2, q_2) \Big|_{\substack{p_1 = p_2 = p \\ q_1 = q_2 = q}} \tag{A27}$$

defined by (2.24). Similarly from (A23), (A24), and (A25), we obtain

$$[u, v]_4 = \frac{\beta}{\alpha} e^{\gamma(\partial^2/\partial q_1 \partial p_2 + \partial^2/\partial q_2 \partial p_1)} \times \sin \alpha \left(\frac{\partial^2}{\partial q_1\, \partial p_2} - \frac{\partial^2}{\partial q_2\, \partial p_1} \right) u(p_1, q_1) v(p_2, q_2) \Big|_{\substack{p_1 = p_2 = p, \\ q_1 = q_2 = q}}$$

which is the bracket defined in (3.8).

APPENDIX B. PROOF OF THE EQUIVALENCE OF RELATIONS (2.21) AND (2.22)

Starting with the integral form of the multiplication law (2.22)

$$A \times B = \frac{1}{h}\iint e^{-(i/\hbar)(\eta-p)(\tau-q)}A(\eta, q)B(p, \tau)\,d\tau\,d\eta, \quad \text{(B1)}$$

and making a change of variables,[18] we obtain

$$\begin{aligned} A \times B &= \iint e^{-2\pi i x y}A(p + h^{\frac{1}{2}}x, q) \\ &\qquad \times B(p, q + h^{\frac{1}{2}}y)\,dx\,dy \\ &= \sum_{m,n}\iint e^{-2\pi i x y}\frac{h^{n/2}x^n}{n!}\frac{\partial^n A(p, q)}{\partial p^n} \\ &\qquad \times \frac{h^{\frac{1}{2}m}y^m}{m!}\frac{\partial^m B(p, q)}{\partial q^m}\,dx\,dy \\ &= \sum_{m,n}\int \frac{h^{\frac{1}{2}(m+n)}}{m!\,n!}\frac{\partial^n A(p, q)}{\partial p^n} \\ &\quad \times \frac{\partial^m B(p, q)}{\partial q^m}\,y^m\left(\frac{i}{2\pi}\frac{\partial}{\partial y}\right)^n\delta(y)\,dx\,dy \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-i\hbar\frac{\partial^2}{\partial p_1\,\partial q_2}\right)^n \\ &\qquad \times A(p_1, q_1)B(p_2, q_2)\Big|_{\substack{p_1=p_2=p,\\ q_1=q_2=q}} \end{aligned} \quad \text{(B2)}$$

as given by (2.21).

APPENDIX C. PROOF OF THE ASSOCIATIVE LAW OF MULTIPLICATION (EQ. 2.23)

From Eq. (2.22) we obtain

$$B(p, q) \times C(p, q) = \frac{1}{h}\iint e^{-(i/\hbar)(\eta-p)(\tau-q)}B(\eta, q)C(p, \tau)\,d\tau\,d\eta.$$

Hence

$$\begin{aligned} A(p, q) \times (B(p, q) \times C(p, q)) &= \frac{1}{h^2}\int\cdots\int d\tau\,d\tau'\,d\eta\,d\eta' e^{-(i/\hbar)(\eta-p)(\tau-q)}A(\eta, q) \\ &\quad \times e^{-(i/\hbar)(\eta'-p)(\tau'-\tau)}B(\eta', \tau)C(p, \tau'), \end{aligned} \quad \text{(C1)}$$

whereas

$$\begin{aligned} (A(p, q) \times B(p, q)) \times C(p, q) &= \frac{1}{h^2}\int\cdots\int d\tau\,d\tau'\,d\eta\,d\eta' e^{-(i/\hbar)(\eta-p)(\tau-q)} \\ &\quad \times e^{-(i/\hbar)(\eta'-\eta)(\tau'-q)}A(\eta', q)B(\eta, \tau')C(p, \tau). \end{aligned} \quad \text{(C2)}$$

If we interchange primed and unprimed variables on the right-hand side of (C2) we obtain the expression given on the right-hand side of (C1). Hence

$$A \times (B \times C) = (A \times B) \times C. \quad \text{(C3)}$$

We further have

$$A \times (B + C) = A \times B + A \times C. \quad \text{(C4)}$$

If the product law satisfies (C3) and (C4), then the bracket defined by

$$[A, B] = A \times B - B \times A \quad \text{(C5)}$$

is automatically a Lie bracket. This proves explicitly that the bracket $[\ ]_S$ defined by Eq. (2.24) is also a Lie bracket.

The corresponding product law in the case of Weyl's association,

$$A \times B = e^{-\frac{1}{2}i\hbar(\partial^2/\partial p_1\partial q_2 - \partial^2/\partial q_1\partial p_2)} \times A(p_1, q_1)B(p_2, q_2)\Big|_{\substack{p_1=p_2=p,\\ q_1=q_2=q}} \quad \text{(C6)}$$

can also be shown to be associative. This furnishes another proof that sine brackets are Lie brackets.

Norm Invariance of Mass-Zero Equations under the Conformal Group*

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It is known that a suitable collection of solutions of the free-field Maxwell's equations is a Hilbert space with respect to an appropriate norm, and that the inhomogeneous Lorentz group acts on this Hilbert space in a unitary and irreducible manner. It is shown that this representation extends to a unitary representation of the conformal group of Minkowski space. Similar results are obtained for other mass-zero relativistic equations.

1. INTRODUCTION

IT has been known for a long time that Maxwell's equations are invariant not only under the ten-dimensional inhomogeneous Lorentz group but also under the conformal group of Minkowski space.[1] The conformal group is a fifteen-dimensional Lie group which contains the inhomogeneous Lorentz group and whose principal physical interpretations are as follows: (1) it is the largest group of coordinate transformations of Minkowski space which leave invariant the speed of light, and (2) three of the five extra dimensions correspond to transformations to a coordinate system whose origin is moving with uniform proper acceleration.[2]

In recent years the conformal invariance of other mass-zero relativistic wave equations has been established.[3] The principal use made of this extra invariance has been to establish conservation laws for the wave equations.[3,4] Other attempts have been made, however, to make the conformal group play a more fundamental role in theoretical physics, namely the role of a basic symmetry group for the laws of physics, the role now enjoyed by the inhomogeneous Lorentz group. Wigner[5] in 1939 pointed out that Lorentz invariance in quantum theories is synonomous with unitary invariance under the Lorentz group, i.e., he showed that invariance of a quantum system under the Lorentz group implies the existence of a unitary representation (up to a factor) of the Lorentz group on the Hilbert-state space of the quantum system. His argument moreover applies to any symmetry group of the quantum system. In 1948 Bargmann and Wigner[6] established a one-to-one correspondence between certain relativistic wave equations and equivalence classes of irreducible unitary representations (up to a factor) of the inhomogeneous Lorentz group. In this correspondence the Lorentz group acts on a Hilbert space consisting of solutions of the given wave equation. Taking the group representation as the more fundamental of the two sides of this correspondence, Segal[7] showed how one might begin to construct a theory of elementary particles with the conformal group as the basic invariance group. He showed that one could expect the conformal group to lead to a discrete mass spectrum and possibly a fundamental length, while at the same time the conformal group approximates the inhomogeneous Lorentz group for small values of the fundamental length in the same sense that the Lorentz group approximates the Galilean group for large values of the light velocity. In order to carry forward this theory it is necessary to determine the irreducible unitary representations of the conformal group and to determine which ones correspond to which particles. The first point has been investigated by Murai[8] with applications to physics in mind, and also by Graev,[9] apparently incidental to his investigations of representations of real simple Lie groups. One might expect that a unitary representation of the conformal group corresponding to the photon arises from Maxwell's equations in the same way that a unitary representation of the Lorentz group does, i.e., that one could extend the Maxwell representation of the Lorentz group to a unitary representation of the conformal group. No matter what theory the conformal group might be

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[1] H. Bateman, Proc. London Math. Soc. **8**, 223, 469 (1910); E. Cunningham, *ibid.* 77 (1910).

[2] L. Page, Phys. Rev. **49**, 254 (1936); H. T. Engstrom and M. Zorn, *ibid.* 701 (1936), E. L. Hill, *ibid.* **67**, 358 (1945); **72**, 143 (1947); **84**, 1165 (1951).

[3] J. A. McLennan, Nuovo Cimento **3**, 1360 (1956); J. S. Lomont, *ibid.* **22**, 673 (1961).

[4] E. Bessel-Hagen, Math. Ann. **84**, 258 (1921).

[5] E. P. Wigner, Ann. Math. **40**, 149 (1939).

[6] V. Bargmann and E. P. Wigner, Proc. Natl. Acad. Sci. U. S. **34**, 211 (1949).

[7] I. E. Segal, Duke Math. J. **18**, 221 (1951).

[8] Y. Murai, Progr. Theoret. Phys. (Kyoto) **9**, 147 (1953); *ibid.* **11**, 441 (1954).

[9] M. I. Graev, Dokl. Akad. Nauk SSSR **98**, 517 (1954).

utilized in, its relevance to a quantum mechanical theory would be severely limited if this extension were not possible. In this paper we show that this representation of the inhomogeneous Lorentz group does in fact extend to a unitary representation of the conformal group, and that the same is true of the other mass-zero, discrete spin representations of the Lorentz group.

2. THE PHOTON SPACE

We denote by C the double-napped cone in energy–momentum space consisting of those points $k = (k_1, k_2, k_3, k_0)$ which satisfy $k^2 = 0$ and $k \neq 0$. We shall use the metric with signature $+++-$. We denote by C^+ the subset of C for which $k_0 > 0$. If k is the above four-vector, then $\mathbf{k}$ will denote the three-vector (k_1, k_2, k_3). Consider 3-dimensional vector-valued functions $e(k)$, $h(k)$ with complex components defined on C for which $\mathbf{k}\cdot e(k) = 0$ and $h(k) = \mathbf{k}\times e(k)/k_0$ for each k in C. Since $k_0 = |\mathbf{k}|$ on C^+, C^+ can be identified with 3-dimensional space with the origin excluded. This identification is often made and we shall sometimes use it. It is well-known that the volume element $dk_1dk_2dk_3/|k_0|$ on C is Lorentz-invariant. The photon space is the space $\mathfrak{C}$ of pairs of functions $e(k)$, $h(k)$ on C satisfying the above restrictions, and for which

$$||e, h||^2 = \int_C \frac{e(k)\cdot e(k)^\star + h(k)\cdot h(k)^\star}{k_0^2}\frac{dk_1\, dk_2\, dk_3}{|k_0|} < \infty. \quad (1)$$

A star denotes complex conjugate.

Associated with an element of $\mathfrak{C}$ is a solution E, H of Maxwell's equations in free space, defined as follows:

$$E(x) = \int_C e(k)e^{ik\cdot x}\frac{d^3k}{|k_0|}, \qquad H(x) = \int_C h(k)e^{ik\cdot x}\frac{d^3k}{|k_0|}. \quad (2)$$

More precisely, these expressions define differentiable solutions of Maxwell's equations if $e(k)$ and (consequently) $h(k)$ vanish fast enough for large $|k|$. For an arbitrary element of $\mathfrak{C}$ these expressions define generalized functions on space–time which are generalized solutions of Maxwell's equations. We shall elaborate on this point later. For each k, $h(k)$ is determined by $e(k)$, and since $e(k)$ is orthogonal to $\mathbf{k}$, $e(k)$ has two (complex) degrees of freedom which as is well-known corresponds to the existence of two independent states of polarization of a plane wave.

In order to establish the Lorentz invariance of Eq. (1) we consider momentarily the 4-potential. Let $a(k) = [a_1(k), a_2(k), a_3(k), a_0(k)] = [\mathbf{a}(k), a_0(k)]$ be a complex 4-vector function on C satisfying $k\cdot a(k) = 0$ for each k in C. Then the function $e(k) = ik_0\mathbf{a}(k) - i\mathbf{k}a_0(k)$ satisfies $\mathbf{k}\cdot e(k) = 0$. Hence $e(k)$ and the function $h(k) = \mathbf{k}\times e(k)/k_0$ satisfy the correct algebraic condition to be in $\mathfrak{C}$. Furthermore, $0 \leq e(k)\cdot e(k)^\star = k_0^2 a\cdot a^\star$. Thus

$$\int_C \frac{e(k)\cdot e(k)^\star + h(k)\cdot h(k)^\star}{k_0^2}\frac{d^3k}{|k_0|} = 2\int_C a\cdot a^\star\frac{d^3k}{|k_0|}. \quad (3)$$

Hence if a is such that the right-hand side of Eq. (3) is finite, then the pair e, h will be in $\mathfrak{C}$. For every e, h in $\mathfrak{C}$, there is at least one function $a(k)$ related to e, h as above, namely, $a = (\mathbf{a}, 0)$ where $\mathbf{a}(k) = e(k)/k_0$. The right side of Eq. (3), although always nonnegative, is not positive-definite on the considered class of functions $a(k)$. It is zero if and only if $a(k)$ has the form $a(k) = kf(k)$ almost everywhere on C where f is an arbitrary (measurable) complex-valued function on C. It follows that $e = h = 0$ almost everywhere if and only if $a(k)$ has this form.

The 4-potential $A(x)$ defined by

$$A(x) = \int_C a(k)e^{ik\cdot x}\frac{d^3k}{|k_0|}$$

is readily verified to be a 4-potential for the fields defined in Eq. (2). Consequently, an inhomogeneous Lorentz transformation $x \to L(x + b)$, where b is a four-vector and L is a homogeneous Lorentz transformation, acts on the fields E and H by transforming $A(x)$ into $A'(x) = LA(L^{-1}x + b)$. This transformation of A is obtained by transforming $a(k)$ into $e^{ik\cdot b}La(L^{-1}k)$ (utilizing the Lorentz invariance of $d^3k/|k_0|$). Consequently, the natural action of the inhomogeneous Lorentz group on $\mathfrak{C}$ is unitary in view of the invariance of the right side of Eq. (3) under the transformation $a \to a'(k) = e^{ik\cdot b}La(L^{-1}k)$.

We have been somewhat sketchy here since the above facts are known. In order to establish that the conformal group acts in a unitary manner on H, it will be necessary to describe the norm (1) directly in terms of E and H. For this purpose we let $\hat{k} = (\mathbf{k}, -k_0)$. Then from Eq. (2) we have

$$E(\mathbf{x}, 0) = \int_{C^+}\frac{e(k) + e(\hat{k})}{k_0}e^{i\mathbf{k}\cdot\mathbf{x}}\,d^3k,$$

$$H(\mathbf{x}, 0) = \int_{C^+}\frac{h(k) + h(\hat{k})}{k_0}e^{i\mathbf{k}\cdot\mathbf{x}}\,d^3k.$$

Since

$$h(k)\cdot h(\hat{k}) = \frac{\mathbf{k}\times e(k)}{k_0}\cdot\frac{\mathbf{k}\times e(\hat{k})}{-k_0} = -e(k)\cdot e(\hat{k}),$$

the expression in Eq. (1) can be written

$$\int_{C^+} \frac{|e(\hat{k}) + e(k)|^2 + |h(k) + h(\hat{k})|^2}{k_0^2}\frac{d^3k}{k_0}. \tag{4}$$

Let $f(\mathbf{k}) = [e(\mathbf{k}, k_0) + e(\mathbf{k}, -k_0)]/k_0$ where $k_0 = |\mathbf{k}|$. We write henceforth $E(\mathbf{x})$ in place of $E(\mathbf{x}, 0)$. Then

$$E(\mathbf{x}) = \int f(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}\, d^3k, \tag{5}$$

and

$$f(\mathbf{k}) = (2\pi)^{-3}\int E(\mathbf{x})e^{-i\mathbf{k}\cdot\mathbf{x}}\, d^3x.$$

The electric field contribution to (4) is

$$\int |f(\mathbf{k})|^2\frac{d^3k}{|\mathbf{k}|}.$$

We denote by $\mathfrak{C}'$ the dense submanifold of $\mathfrak{C}$ consisting of those pairs e, h which are bounded and for which $E(\mathbf{x})$ and $H(\mathbf{x})$ are bounded functions integrable over all space. Then in view of the equality

$$\int_{|\mathbf{k}|<R} \exp(i\mathbf{k}\cdot\mathbf{z})\,|\mathbf{k}|^{-1}\, d^3k = 4\pi(1 - \cos|\mathbf{z}|R)/|\mathbf{z}|^2,$$

we have for e, h in $\mathfrak{C}'$

$$\int_{E_3}\frac{f(\mathbf{k})\cdot f(\mathbf{k})^*}{|\mathbf{k}|}d^3k = \frac{1}{(2\pi)^6}\int_{E_3}\frac{d^3k}{|\mathbf{k}|}\iint e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}E(\mathbf{x})\cdot E(\mathbf{y})^*\, d^3x\, d^3y$$

$$= \frac{4\pi}{(2\pi)^6}\lim_{R\to\infty}\int_{E_3}\int_{E_3}\frac{E(\mathbf{x})\cdot E(\mathbf{y})^*}{|\mathbf{x}-\mathbf{y}|^2} \times (1 - \cos|\mathbf{x}-\mathbf{y}|R)\, d^3x\, d^3y.$$

Now

$$\lim_{R\to\infty}\int_{E_3}\int_{E_3}\frac{E(\mathbf{x})\cdot E(\mathbf{y})^*}{|\mathbf{x}-\mathbf{y}|^2}\cos|\mathbf{x}-\mathbf{y}|R\, d^3x\, d^3y = \lim_{R\to\infty}\int_{E_3}\int_{E_3}\frac{E(\mathbf{y}+\mathbf{z})\cdot E(\mathbf{y})^*}{|\mathbf{z}|^2}\cos|\mathbf{z}|R\, d^3x\, d^3y.$$

Since $E(\mathbf{y}+\mathbf{z})\cdot E(\mathbf{y})^*/|\mathbf{z}|^2$ is an integrable function of $\mathbf{y}$ and $\mathbf{z}$, the one-dimensional Riemann–Lebesgue lemma applied to the function of $|\mathbf{z}|$, obtained by integrating $E(\mathbf{y}+\mathbf{z})\cdot E(\mathbf{y})^*/|\mathbf{z}|^2$ with respect to $\mathbf{y}$ and the two angular spherical coordinates of $\mathbf{z}$, shows that the last-indicated limit is zero.

A similar argument applied to H shows that for e, h in $\mathfrak{C}'$ the expression (1) can be written

$$||E, H||^2 = \frac{4\pi}{(2\pi)^6} \times\int_{E_3}\int_{E_3}\frac{E(\mathbf{x})\cdot E(\mathbf{y})^* + H(\mathbf{x})\cdot H(\mathbf{y})^*}{|\mathbf{x}-\mathbf{y}|^2}\, d^3x\, d^3y. \tag{6}$$

3. CONFORMAL INVARIANCE OF PHOTON NORM

The conformal group is generated by the inhomogeneous Lorentz group and two other types of transformations, namely, uniform dilations $x\to ax$ $a>0$ and inversion in the unit hyperboloid $x\to x/x^2$. The manner in which the electric and magnetic fields transform is determined by putting these together to form a skew-symmetric tensor in a well-known way. The skew-symmetric tensor is then transformed as a bivector (also known as a two-form) is normally transformed. Under the dilation $x\to ax$ the result is $E\to E'(x) = a^{-2}E(a^{-1}x)$ and $H\to H'(x) = a^{-2}H(a^{-1}x)$. It follows immediately from Eq. (6) that $||E, H||^2 = ||E', H'||^2$ when E, H is in the dense set $\mathfrak{C}'$. Moreover, from Eq. (2) we see that $e\to e'(k) = e(ak)$ and $h\to h'(k) = h(ak)$ for all pairs e, h in $\mathfrak{C}$, and from Eq. (1) it follows that uniform dilations are unitary.

We now turn to the main result of this paper which is to show that $\mathfrak{C}$ is transformed unitarily under the inversion $x\to x/x^2$. The effect of the inversion $Tx = x/x^2$ on E and H can be computed directly by transforming the corresponding 2-form (bivector). The result for the plane $t = 0$ is[10]

$$\begin{cases} E'(\mathbf{x}) = \dfrac{1}{|\mathbf{x}|^4}E(T^{-1}\mathbf{x}) - \dfrac{2\mathbf{x}}{|\mathbf{x}|^6}[\mathbf{x}\cdot E(T^{-1}\mathbf{x})], \\ H'(\mathbf{x}) = -\dfrac{1}{|\mathbf{x}|^4}H(T^{-1}\mathbf{x}) + \dfrac{2\mathbf{x}}{|\mathbf{x}|^6}\mathbf{x}\cdot H(T^{-1}\mathbf{x}). \end{cases} \tag{7}$$

We remark that in the $t = 0$ plane the inversion T is inversion in the unit sphere. Let $\mathfrak{C}_0$ be the dense submanifold of $\mathfrak{C}$ consisting of those pairs e, h in $\mathfrak{C}$ which are zero outside of a bounded set in C and also in a neighborhood of the vertex, and are at least six times continuously differentiable. If e, h is a pair in $\mathfrak{C}_0$ we shall usually refer to the corresponding pair E, H also as being in $\mathfrak{C}_0$. We note that $\mathfrak{C}_0\subset\mathfrak{C}'$. Moreover it is important to note that if E, H is in $\mathfrak{C}_0$, then E', H' given by Eq. (7) is in $\mathfrak{C}'$. In order to see this we observe that $E(\mathbf{x})$ and $H(\mathbf{x})$ go to zero at ∞ at least as fast as $1/r^6$ and are bounded. Consequently, by

[10] E. Cunningham, footnote 1, p. 89.

Eq. (7), E' and H' are bounded (and go to zero at $\mathbf{x} = 0$) and are $O(r^{-4})$ at ∞. Hence E', H' are both integrable over all space. Using Eq. (5) to define a function $f'(\mathbf{k})$ [and similarly $g'(\mathbf{k})$ for H'], and using the fact that $E'(\mathbf{x})$ and $H'(\mathbf{x})$ are known to satisfy Maxwell's equations, it follows that the equations $\mathbf{k}\cdot e'(k) = \mathbf{k}\cdot e'(\hat{k}) = 0, e'(k) + e'(\hat{k}) = k_0 f'(\mathbf{k},)$ and $\mathbf{k}\times[e'(k) - e'(\hat{k})] = k_0^2 g'(\mathbf{k})$ can be solved for e'—and in view of the derivation of Eq. (6), e', h' is in $\mathfrak{H}'$. Consequently inversion carries $\mathfrak{H}_0$ into $\mathfrak{H}'$.

We consider now an element E, H of $\mathfrak{H}_0$. We may use the form of Eq. (6) for the norm of E, H and also to compute the norm of E', H'.

The Jacobian of the inversion $\mathbf{x} \to \mathbf{x}/|\mathbf{x}|^2$ is readily computed to be $1/|\mathbf{x}|^6$. Substituting E' and H' as given by Eq. (7) into the expression of Eq. (6) and making the change of variables $\mathbf{x} \to T\mathbf{x}$, $\mathbf{y} \to T\mathbf{y}$, we obtain

$$\frac{(2\pi)^6}{4\pi}\,||E'H'||^2 = \iint d^3x\, d^3y \left[\frac{\{|\mathbf{x}|^2 E(\mathbf{x}) - 2\mathbf{x}[\mathbf{x}\cdot E(\mathbf{x})]\}\cdot\{|\mathbf{y}|^2 E(\mathbf{y}) - 2\mathbf{y}[\mathbf{y}\cdot E(\mathbf{y})]\}^\star}{|\mathbf{x}|^2\,|\mathbf{y}|^2\left|\frac{\mathbf{x}}{|\mathbf{x}|}\,|\mathbf{y}| - \frac{\mathbf{y}}{|\mathbf{y}|}\,|\mathbf{x}|\right|^2} + \text{similar } H \text{ terms}\right]. \quad (8)$$

Now the triangle spanned by 0, $\mathbf{x}$, and $\mathbf{y}$ is congruent to the triangle spanned by 0, $\mathbf{y}\,|\mathbf{x}|/|\mathbf{y}|$, and $\mathbf{x}|\mathbf{y}|/|\mathbf{x}|$. Hence

$$\left|\frac{\mathbf{x}}{|\mathbf{x}|}\,|\mathbf{y}| - \frac{\mathbf{y}}{|\mathbf{y}|}\,|\mathbf{x}|\right| = |\mathbf{y} - \mathbf{x}|.$$

Substituting this into Eq. (8) and writing $\hat{x}$ for the unit vector in the direction of $\mathbf{x}$ we get

$$\frac{(2\pi)^6}{4\pi}\,||E', H'||^2 = \iint d^3x\, d^3y\, \frac{E(\mathbf{x})\cdot E(\mathbf{y})^\star}{|\mathbf{x} - \mathbf{y}|^2} + B + \text{similar } H \text{ terms},$$

where

$$B = \int d^3x \int d^3y\, \frac{4\hat{x}\cdot\hat{y}[\hat{x}\cdot E(\mathbf{x})][\hat{y}\cdot E(\mathbf{y})]^\star - 2[\hat{y}\cdot E(\mathbf{x})][\hat{y}\cdot E(\mathbf{y})]^\star - 2[\hat{x}\cdot E(\mathbf{y})]^\star[\hat{x}\cdot E(\mathbf{x})]}{|\mathbf{x} - \mathbf{y}|^2}.$$

It suffices to show that $B = 0$. The first term in B doesn't change upon interchanging $\mathbf{x}$ and $\mathbf{y}$, while the third term becomes the conjugate of the second. Hence

$$B = 4\,\mathrm{Re}\int d^3x \int d^3y \times \frac{(\hat{x}\cdot\hat{y})\hat{x}\cdot E(\mathbf{x})\hat{y}\cdot E(\mathbf{y})^\star - \hat{y}\cdot E(\hat{x})\hat{y}\cdot E(\mathbf{y})^\star}{|\hat{x} - \mathbf{y}|^2}$$

$$= 4\,\mathrm{Re}\int d^3y\, \frac{(\hat{y}\cdot E(\mathbf{y}))^\star}{|\mathbf{y}|} \times \int d^3x\, \frac{(\hat{x}\cdot\mathbf{y})\hat{x}\cdot E(\mathbf{x}) - \mathbf{y}\cdot E(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|^2}. \quad (9)$$

Now

$$\int d^3x\, \frac{(\hat{x}\cdot\mathbf{y})\hat{x}\cdot E(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|^2} = \int d^3x\, \frac{(\hat{x}\cdot\mathbf{y} - \mathbf{x})\hat{x}\cdot E(\mathbf{x}) + [x\cdot E(\mathbf{x})]}{|\mathbf{x} - \mathbf{y}|^2} = \int d^3x\, \frac{(\hat{x}\cdot\mathbf{y} - \mathbf{x})\hat{x}\cdot E(\mathbf{x}) + [\mathbf{x} - \mathbf{y}\cdot E(\mathbf{x})] + \mathbf{y}\cdot E(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|^2}.$$

Denote by $S_r(\mathbf{y})$ the sphere of radius r centered at $\mathbf{y}$, by $B_r(\mathbf{y})$ the solid ball, and by n the outward-drawn unit normal. Then

$$\int d^3x\, \frac{(\mathbf{x} - \mathbf{y})\cdot E(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|^2} = \int_0^\infty dr \int_{S_r(\mathbf{y})} \frac{n\cdot E(\mathbf{x})}{r}\, dA = \int_0^\infty \frac{dr}{r} \int_{B_r(\mathbf{y})} \nabla\cdot E(\mathbf{x})\, d^3x = 0.$$

Hence

$$\int d^3x\, \frac{(\hat{x}\cdot\mathbf{y})\hat{x}\cdot E(\mathbf{x}) - \mathbf{y}\cdot E(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|^2} = \int d^3x\, \frac{(\mathbf{x}\cdot\mathbf{y} - \mathbf{x})[\hat{x}\cdot E(\mathbf{x})]}{|\mathbf{x} - \mathbf{y}|^2\,|\mathbf{x}|}. \quad (10)$$

On the other hand,

$$\int d^3x\, \frac{(\mathbf{x}\cdot\mathbf{y} - \mathbf{x})[\hat{x}\cdot E(\mathbf{x})]}{|\mathbf{x} - \mathbf{y}|^2\,|\mathbf{x}|} = \int d^3x\, \frac{(\mathbf{x} - \mathbf{y}\cdot\mathbf{y} - \mathbf{x})[\hat{x}\cdot E(\mathbf{x})]}{|\mathbf{x} - \mathbf{y}|^2\,|\mathbf{x}|} + \frac{(\mathbf{y}\cdot\mathbf{y} - \mathbf{x})[\hat{x}\cdot E(\mathbf{x})]}{|\mathbf{x} - \mathbf{y}|^2\,|\mathbf{x}|} = -\int d^3x\, \frac{\hat{x}\cdot E(\mathbf{x})}{|\mathbf{x}|} + \int d^3x\, \frac{(\mathbf{y}\cdot\mathbf{y} - \mathbf{x})\hat{x}\cdot E(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|^2\,|\mathbf{x}|}.$$

The first term on the right is

$$\int_0^\infty \frac{dr}{r} \int_{S_r(0)} n\cdot E\, dA = \int_0^\infty \frac{dr}{r} \int_{B_r(0)} \nabla\cdot E\, d^3x = 0.$$

Hence

$$\int d^3x \frac{(\mathbf{x}\cdot\mathbf{y})\hat{x}\cdot E(\mathbf{x}) - \mathbf{y}\cdot E(\mathbf{x})}{|\mathbf{x}-\mathbf{y}|^2} = \int d^3x \frac{(\mathbf{y}\cdot\mathbf{y} - \mathbf{x})[\hat{x}\cdot E(\mathbf{x})]}{|\mathbf{x}-\mathbf{y}|^2\,|\mathbf{x}|}. \quad (11)$$

From Eqs. (9) and (11) we get, interchanging $\mathbf{x}$ and $\mathbf{y}$ in the second line,

$$B = 4\,\mathrm{Re}\int d^3y \int d^3x \frac{[\hat{y}\cdot E(\mathbf{y})]^\star[\hat{x}\cdot E(\mathbf{x})](\mathbf{y}\cdot\mathbf{y} - \mathbf{x})}{|\mathbf{x}|\,|\mathbf{y}|\,|\mathbf{x}-\mathbf{y}|^2}$$

$$= 4\,\mathrm{Re}\int d^3x \int d^3y \frac{[\hat{x}\cdot E(\mathbf{x})]^\star[\hat{y}\cdot E(\mathbf{y})](\mathbf{x}\cdot\mathbf{x} - \mathbf{y})}{|\mathbf{y}|\,|\mathbf{x}|\,|\mathbf{x}-\mathbf{y}|^2}$$

$$= 4\,\mathrm{Re}\int d^3x \int d^3y \frac{[\hat{x}\cdot E(\mathbf{x})][\hat{y}\cdot E(\mathbf{y})]^\star(\mathbf{x}\cdot\mathbf{x} - \mathbf{y})}{|\mathbf{y}|\,|\mathbf{x}|\,|\mathbf{x}-\mathbf{y}|^2}.$$

Upon substituting Eq. (10) into Eq. (9), however, we get exactly the negative of this. Hence $B = 0$.

We have shown that inversion is norm-preserving when applied to elements of $\mathfrak{K}_0$. Since $\mathfrak{K}_0$ is dense in $\mathfrak{K}$, it follows that there exists a unique continuous extension U of T from $\mathfrak{K}_0$ to $\mathfrak{K}$ and that this extension preserves the norm. We must show that U actually agrees with T on the elements of $\mathfrak{K}$ outside $\mathfrak{K}_0$ and that $U^2 = I$. However T has not been defined yet on some of the elements outside $\mathfrak{K}_0$ since these are not functions on space–time, but generalized functions. In order to define T on these elements in the natural way appropriate for generalized functions, we let ϕ stand for a test 2-form (bivector), i.e., ϕ is an infinitely differentiable 2-form on Minkowski space with bounded support set. If F is the 2-form constructed from E and H given by Eq. (2) where e, h are in $\mathfrak{K}_0$, we shall imply, say, F is in $\mathfrak{K}_0$. The generalized function corresponding to F is the functional of ϕ given by $\int_{E_4} F(x)\cdot\phi(x)\, d^4x$ where the dot denotes the Lorentz-invariant bilinear form $F_{\mu\nu}(x)\phi^{\mu\nu}(x)$.

Now if TF denotes the transformed solution of Maxwell's equations under inversion T, then (see discussion in Sec. 4) (TF) is given by

$$(TF)(x) = (1/x^4)L_x \wedge L_x F(Tx),$$

where L_x is a Lorentz transformation and $L_x \wedge L_x$ is the linear transformation[11] on bivectors corresponding to L_x.

From Eq. (23) it follows that $L_{Tx} = L_x$. Thus, since absolute value of Jacobian $T = 1/x^8$,

$$\int TF(x)\cdot\phi(x)\, d^4x = \int \frac{1}{x^4} L_x \wedge L_x F(Tx)\cdot\phi(x)\, d^4x$$

$$= \int F(Tx)\cdot L_x \wedge L_x\phi(x)\frac{1}{x^4}\, d^4x$$

$$= \int F(x)\cdot L_x \wedge L_x\phi(Tx)x^4 \frac{d^4x}{x^8}.$$

Thus

$$\int (TF)(x)\cdot\phi(x)\, d^4x = \int F(x)\cdot(T\phi)(x)\, d^4x. \quad (12)$$

We shall use Eq. (12) to define the generalized function TF when F is an arbitrary element of H, and shall show that T then agrees with U. Since $T^2 = I$ it will then follow that $U^2 = I$ and that U is consequently unitary.

In order to see to what extent the right side of Eq. (12) makes sense as a generalized function for an arbitrary element F of H, we observe first that $\int F(x)\cdot\phi(x)\, d^4x$ corresponds formally to

$$\int_{C^+} \int_{E_4} f_{\mu\nu}(k)\hat{\phi}^{\mu\nu}(k)\frac{d^3k}{|k_0|}, \quad (13)$$

where

$$\hat{\phi}^{\mu\nu}(k) = \int_{E_4} e^{ik\cdot x}\phi^{\mu\nu}(x)\, d^4x.$$

The expression in Eq. (13) is of course the definition of $\int F(x)\cdot\phi(x)\, d^4x$ when F is not a function. That this is a continuous linear functional of ϕ follows from the easy-to-establish facts that the components $f_{\mu\nu}(k)$ are in $L^2(C,\ d^3k/|k_0|^3)$ and so are $k_0^2\phi^{\mu\nu}(k)$, while convergence of a sequence $\phi_n^{\mu\nu}(x)$ in the usual sense for test functions implies convergence of $k_0^2\phi_n^{\mu\nu}(k)$ in $L^2(C,\ d^3k/|k_0|^3)$. At the same time we see that $\int F(x)\cdot\phi(x)\, d^4x$ is a continuous function of F in the $\mathfrak{K}$ norm for fixed ϕ.

Now if ϕ is a test form, then $T\phi$ will have its components in $L^2(E_4)$ but not necessarily in $L^1(E_4)$, and this leads to some technical difficulties in interpreting $\int F(x)\cdot(T\phi)(x)\, d^4x$ for arbitrary F in $\mathfrak{K}$. We consider therefore the set $\mathfrak{D}_0$ of test 2-forms ϕ whose support set is disjoint from the light cone $x^2 = 0$. For such a test form ϕ, one readily verifies that $T\phi$ is again in $\mathfrak{D}_0$. One must define $T\phi$ to be zero on the light cone to make $T\phi$ continuous. Thus for an arbitrary F in $\mathfrak{K}$ and ϕ in $\mathfrak{D}_0$ the expression $\int F(x)\cdot T\phi(x)\, d^4x$ makes sense by defining it as in Eq. (13) with ϕ replaced by $T\phi$. What we shall prove is that there exists a unique element F' in $\mathfrak{K}$ such that for all ϕ in $\mathfrak{D}_0$ we have

$$\int F'(x)\cdot\phi(x)\, d^4x = \int F(x)\cdot T\phi(x)\, d^4x. \quad (14)$$

[11] If $L_x = (a_{\mu\nu})$, then $(L_x \wedge L_x F)_{\mu\nu} = a_{\mu\sigma}a_{\nu\tau}F_{\sigma\tau}$.

For the existence let $F' = UF$ and let F_n be a sequence of elements in $\mathfrak{K}_0$ converging in $\mathfrak{K}$ to F. Then UF_n converges to F' in $\mathfrak{K}$. The following steps are justified by the above mentioned continuity in F:

$$\begin{aligned}\int F(x)\cdot T\phi(x)\,d^4x &= \int \lim F_n\cdot T\phi\,d^4x\\ &= \lim \int F_n\cdot T\phi\,d^4x\\ &= \lim \int TF_n\cdot\phi\,d^4x\\ &= \int \lim TF_n\cdot\phi\,d^4x\\ &= \int F'\cdot\phi\,d^4x.\end{aligned}$$

The linear functionals on $\mathfrak{K}$ determined as in Eq. (13) by the Fourier transforms of elements of $\mathfrak{D}_0$ are dense in $\mathfrak{K}$ since the components of forms in $\mathfrak{D}_0$ are dense in $L^1(E_4)$. Consequently F' is unique. Thus

$$\int UF\cdot\phi\,d^4x = \int F\cdot T\phi\,d^4x$$

$$\text{for } \phi \text{ in } \mathfrak{D}_0 \text{ and } F \text{ in } \mathfrak{K}. \qquad (15)$$

In view of Eq. (12) the natural definition of TF for an arbitrary F in $\mathfrak{K}$ is that it is the F' appearing in Eq. (14). With this definition we then have obviously $TF = UF$ for all F in $\mathfrak{K}$. Since

$$\begin{aligned}\int U^2F\cdot\phi\,d^4x &= \int UF\cdot T\phi\,d^4x\\ &= \int F\cdot T^2\phi\,d^4x = \int F\cdot\phi\,d^4x,\end{aligned}$$

we have $U^2 = I$. Hence the range of U is all of $\mathfrak{K}$ and U is unitary.

4. OTHER SPINS

We utilize the description by Bargmann and Wigner[6] of the wavefunctions for particles of mass zero and spin $s = \frac{1}{2}N$, $N = 1, 2, \cdots$ except for change in signature. Thus if S denotes four-dimensional complex spin space with positive-definite inner product $(,)$, we denote by S^+ and S^- the two 2-dimensional eigenspaces of γ_5. We let K_N denote the direct sum of the space of symmetric N tensors over S^+ with the space of symmetric N tensors over S^-. Thus

$$K_N = S^+ \otimes_s \cdots \otimes_s S^+ + S^- \otimes_s \cdots \otimes_s S^-.$$

We denote by γ_0, γ_1, γ_2, γ_3 the Dirac matrices acting on S satisfying $\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2g_{\mu\nu}$. γ_0 is assumed skew-Hermitian and the other three Hermitian. Denote by $P^{(j)}$ the operator

$$P^{(j)} = 1 \otimes \cdots \otimes \gamma^\mu(\partial/\partial x^\mu) \otimes \cdots \otimes 1,$$

where the nonidentity factor is in the jth position. This operator acts on functions on space–time with values in $S \otimes \cdots \otimes S$ (N factors).

The Dirac wavefunctions then for spin s and mass zero are functions ψ on space–time with values in K_N satisfying

$$P^{(j)}\psi(x) = 0, \qquad j = 1, \cdots N. \qquad (16)$$

Actually any one of these N equations imply all the others because of the symmetry of $\psi(x)$.

The Hilbert space $\mathfrak{K}_N$ associated with spin $s = \frac{1}{2}N$ may be described most easily in momentum space. An element in $\mathfrak{K}_N$ is a function $\phi(k)$ defined on the light cone C with values in K_N satisfying

$$k^{(j)}\phi(k) = 0, \qquad j = 1, \cdots, N, \qquad (17)$$

where

$$k^{(j)} = 1 \otimes \cdots \otimes \gamma^\mu k_\mu \otimes \cdots \otimes 1,$$

and the nonidentity factor is in the jth position.

The normalization condition is

$$||\phi||^2 = \int_C (\phi(k), \phi(k))\,\frac{d^3k}{|k_0|^{N+1}} < \infty. \qquad (18)$$

The wavefunction $\psi(x)$ is related to $\phi(k)$ by

$$\psi(x) = \int_C \phi(k)e^{ik\cdot x}\,\frac{d^3k}{|k^0|}. \qquad (19)$$

ψ is a generalized function satisfying Eq. (16). The space $\mathfrak{K}_2$ is the photon space described differently in Sec. 2. The equivalence of the two descriptions proceeds from the fact that there is an isomorphism between K_2 and the bivectors over complex Minkowski space which establishes an equivalence between the natural representations of the homogeneous Lorentz group in these two spaces. The isomorphism also carries the inner product in K_2 into the inner product on bivectors used in (1) and carries the Dirac equations (16) into Maxwell's equations.[12]

The norm (18) expressed in terms of ψ is

$$\begin{aligned}||\psi||^2 &= \frac{4\pi}{(2\pi)^6}\int_0^\infty \frac{du}{u^{N-2}}\\ &\times \iint (\psi(\mathbf{x}), \psi(\mathbf{y}))\,\frac{\sin|\mathbf{y}-\mathbf{x}|\,u}{|\mathbf{y}-\mathbf{x}|}\,d^3x\,d^3y. \qquad (20)\end{aligned}$$

[12] C. C. Chevalley in *The Algebraic Theory of Spinors* (Columbia University Press, New York, 1954), pp. 89–96; E. M. Corson, *Introduction to Tensors, Spinors, and Relativistic Wave Equations* (Hafner Publishing Company, New York, 1953).

To derive this, one uses the fact[13] that Eq. (17) implies that $\phi(\mathbf{k}, k_0)$ is always orthogonal to $\phi(\mathbf{k}, -k_0)$. However, this expression for the norm will not be very useful. In the spin-$\frac{1}{2}$ case, Eqs. (18) and (19), the orthogonality of $\phi(\mathbf{k}, k_0)$ and $\phi(\mathbf{k}, -k_0)$, and the Plancheral formula show that

$$||\psi||^2 = (2\pi)^{-6} \times \int (\psi(\mathbf{x}, 0), \psi(\mathbf{x}, 0))\, d^3x, \qquad s = \tfrac{1}{2}. \tag{21}$$

Under a dilation $x \to ax$, $a > 0$, the spin-s wavefunction ψ transforms into $\psi'(x) = a^{-s-1}\psi(a^{-1}x)$. This is easily verified to be unitary with respect to the norm (18) or (20), and ψ' clearly satisfies (16) when ψ does.

We consider now how ψ transforms under the inversion $Tx = x/x^2$. The general form to be expected is $\psi'(x) = A\psi(T^{-1}x)$, where A is a linear transformation on the space of values of ψ. If ψ were a tensor field instead of a spinor field, A would simply be the differential dT_x at x applied in a standard manner to tensors. The differential dT_x is the linear transformation on Minkowski space given by the Jacobian matrix, or more directly,

$$(dT_x)y = \frac{dT(x + ty)}{dt}\bigg|_{t=0}. \tag{22}$$

In the present case, however, ψ is a spinor field so that A ought to be a spin transformation (depending on x) corresponding to dT_x. However dT_x is not a Lorentz transformation, but rather a scalar multiple of a Lorentz transformation.[14] Specifically, Eq. (22) applied to the inversion T yields

$$(dT_x)y = \frac{y - 2x(y\cdot x)/x^2}{x^2}, \qquad x^2 \neq 0. \tag{23}$$

The numerator is a reflection in the hyperplane Lorentz orthogonal to x, and hence is a Lorentz transformation. We denote it by $-L_x$. Now the spin transformations on S corresponding to L_x are the scalar multiples of $\sum_{\mu=0}^{3} x_\mu\gamma^\mu$. It is to be expected therefore that A should have the form[15]

$$A = C_N(x)x_\mu\gamma^\mu \otimes \cdots \otimes x_\alpha\gamma^\alpha \quad (N \text{ factors}) \tag{24}$$

for spin $s = \frac{1}{2}N$ where $C_N(x)$ is a scalar.

In fact, for the case $N = 2$ (photon), the isomorphism between K_2 and complex bivectors mentioned above can be used to establish that the known transformation [Eq. (7)] of the electromagnetic field under inversion agrees with Eq. (24) if $C_2(x) = x^{-6}$. On this basis then it is reasonable to seek an A of the form (24) with $C_N(x)$ a power of x^2. A more or less straightforward computation shows that there is only one power of x^2 which allows the transformed wavefunction to satisfy the wave equations (16). The result is as follows. Let x stand for $\sum_{\mu=0}^{3} x^\mu\gamma_\mu$ when x operates on a spinor. Then (since $T = T^{-1}$),

$$\psi'(x) = \frac{x \otimes x \otimes \cdots \otimes x}{x^{2N+2}}\, \psi(Tx). \tag{25}$$

It is straightforward to verify that $\psi'(x)$ does indeed satisfy Eq. (16) except that one needs the fact that

$$1 \otimes \cdots \otimes 1 \otimes \gamma^\mu \otimes 1 \otimes \cdots \otimes 1 \otimes \gamma_\mu \otimes 1 \otimes \cdots \otimes 1$$

acting on elements of K_N is zero. In order to prove this, it suffices to prove it for K_2, i.e., to prove that $C = \gamma^\mu \otimes \gamma_\mu$ carries elements of K_2 into zero. For then $\gamma^\mu \otimes \gamma_\mu \otimes 1 \otimes \cdots \otimes 1$ is zero on K_N and this operator goes into the desired one upon permuting the factors in K_N. Now in view of the isomorphism between K_2 and bivectors, the operator C acting on K_2 can be determined by computing how it acts on bivectors. The isomorphism carries C into the operator $v \to \sum_\mu e^\mu v e_\mu$ where e_μ is a basis of Minkowski space corresponding to γ_μ, v is a bivector and the product is Clifford multiplication. Taking $v = x \wedge y$ with x, y 4-vectors, it is simple to compute explicitly that $\sum_\mu e^\mu v e_\mu = 0$. Another proof consists in using the representation

$$\gamma_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix}, \qquad \gamma_0 = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

for the Dirac matrices, where

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \text{etc.}$$

Since $\sum_\mu \gamma^\mu \otimes \gamma_\mu$ is Hermitian it suffices to show that the trace of $(\sum_\mu \gamma^\mu \otimes \gamma_\mu)^2$ with respect to the subspace K_2 is zero. The trace can be computed explicitly using this representation. One has $(\sum_\mu \gamma^\mu \otimes \gamma_\mu)^2 = 4I + \sum_{\mu\neq\nu} \gamma^\mu\gamma^\nu \otimes \gamma_\mu\gamma_\nu$. The trace on K_2 of $\gamma^\mu\gamma^\nu \otimes \gamma_\mu\gamma_\nu$ (no sum) is -2 trace on $S^+ \otimes_s S^+$ of $\sigma_i \otimes \sigma_i = -2$ in all cases. Since K_2 is six-dimensional trace, $C^2 = 0$.

In the spin-$\frac{1}{2}$ case, the unitarity of the transformation $\psi \to \psi'$ given in Eq. (25) is easy to

[13] Setting $u = \phi_1(k)$ and $v = \phi_2(\hat{k})$, we have $k_0(u, v) = (\gamma_0 k_0\gamma^0 u, v) = -(\gamma_0 u, k_0\gamma^0 v) = -(\gamma_0 u, \mathbf{k}\cdot\gamma v) = (\gamma_0\mathbf{k}\cdot\gamma u, v) = -(\gamma_0 k_0\gamma^0 u, v) = -k_0(u, v)$.

[14] This is the case for any conformal transformation since by definition they preserve angles in the Lorentz metric.

[15] Summation convention is in force in this paper.

demonstrate. The Hilbert space is the space of spinor-valued functions satisfying Eq. (16) (generalized solution), and for which the norm (21) is finite. Substituting ψ' into Eq. (21) we get

$$||\psi'||^2 = \frac{1}{(2\pi)^6} \times \int \left(\frac{\mathbf{x}}{|\mathbf{x}|^4}\,\psi\left(0, \frac{\mathbf{x}}{|\mathbf{x}|^2}\right), \frac{\mathbf{x}}{|\mathbf{x}|^4}\,\psi\left(0, \frac{\mathbf{x}}{|\mathbf{x}|^2}\right)\right) d^3x = \frac{1}{(2\pi)^6} \int \frac{1}{|\mathbf{x}|^6}\,(\psi(T\mathbf{x}), \psi(T\mathbf{x}))\, d^3x,$$

where we have used the fact that $\mathbf{x} = \sum_{i=1}^3 x_i\gamma^i$ is Hermitian and $\mathbf{x}^2 = |\mathbf{x}|^2$. Now a transformation of coordinates $\mathbf{x} \to T\mathbf{x} = \mathbf{x}/|\mathbf{x}|^2$ shows $||\psi'||^2 = ||\psi||^2$ since the Jacobian of T in space is $1/|\mathbf{x}|^6$. Thus T is unitary in the spin-$\frac{1}{2}$ case.

The spin-1 case has already been treated in Sec. 3. For higher spins it becomes algebraically very complicated to prove that Eq. (25) defines a unitary transformation. We shall prove instead something weaker, and in fact we shall be somewhat informal in our proofs. Let T_a denote translation by a: $T_a x = x + a$, where a is an arbitrary element in Minkowski space. Let T denote inversion as before. The transformations TT_aT form a four-dimensional subgroup of the conformal group. We shall show that the infinitesimal generators of this subgroup are formally skew-adjoint. Since all the other eleven generators are already known to be (actually) skew-adjoint, we shall have an informal proof of unitarity. Translation acts on ψ by just translating the argument. Thus $(T_a\psi)(x) = \psi(T_a^{-1}x) = \psi(x - a)$. The infinitesimal generator D_a of the one parameter group TT_aT may be computed as follows:

$$\begin{aligned}(TT_{ta}T\psi)(x) &= \frac{x \otimes \cdots \otimes x}{x^{2N+2}}\,(T_{ta}T\psi)(Tx)\\ &= \frac{x \otimes \cdots \otimes x}{x^{2N+2}}\,(T\psi)(T^{-1}_{ta}Tx)\\ &= \frac{x \otimes \cdots \otimes x}{x^{2N+2}}\,(T\psi)\left(\frac{x}{x^2} - ta\right)\\ &= \frac{x \otimes \cdots \otimes x}{x^{2N+2}} \times \frac{(x/x^2 - ta) \otimes \cdots \otimes (x/x^2 - ta)}{(x/x^2 - ta)^{2N+2}} \times \psi\left(\frac{x - tax^2}{1 - 2tax + t^2a^2x^2}\right).\end{aligned}$$

Hence

$$\begin{aligned}(D_a\psi)(x) &\equiv \frac{d}{dt}\,(TT_{ta}T\psi)(x)|_{t=0}\\ &= [-(xa \otimes 1 \otimes \cdots \otimes 1 + \cdots + 1 \otimes \cdots \otimes 1 \otimes xa) + (2N + 2)(a\cdot x) - x^2a\cdot\nabla + 2(a\cdot x)(x\cdot\nabla)]\psi(x). \qquad (26)\end{aligned}$$

Now we Fourier-transform D_a using Eq. (19). It is more convenient to determine its action on $\chi(\mathbf{k}) = (\phi(k) + \phi(\hat{k}))/|k_0|$ where $\hat{k} = (\mathbf{k}, -k_0)$. First we consider the case where a is a space vector $a = (\mathbf{a}, 0)$. Consider formula (26) in the plane $x_0 = 0$. The right side of Eq. (26) then does not involve any multiplication by x_0 or differentiation with respect to x_0. Furthermore, from Eq. (19),

$$\psi(\mathbf{x}) = \int_{E_3} e^{i\mathbf{k}\cdot\mathbf{x}}\chi(\mathbf{k})\, d^3k.$$

Hence, letting

$$\nabla = \frac{1}{i}\sum_{\mu=1}^3 \gamma^\mu \frac{\partial}{\partial k^\mu}, \quad \text{and} \quad \Delta = -\nabla^2,$$

we have

$$\begin{aligned}D_a\psi(\mathbf{x}) = \int_{E_3} e^{i\mathbf{k}\cdot\mathbf{x}}\, d^3k[&(\nabla\mathbf{a} \otimes 1^{N-1} + \cdots\\ &+ 1^{N-1} \otimes \nabla\mathbf{a} - (2N + 2)\mathbf{a}\cdot\nabla\\ &+ i\Delta\mathbf{a}\cdot\mathbf{k} + 2i(\mathbf{a}\cdot\nabla)\nabla\cdot\mathbf{k}]\chi(\mathbf{k}). \qquad (27)\end{aligned}$$

A differentiation operator is to be understood here as differentiating all functions of $\mathbf{k}$ that appear to its right. As usual an operator on spinors involving a vector such as $\mathbf{a}$ means $\sum_{i=1}^3 a_i\gamma^i$, while $\nabla\cdot\mathbf{k}\chi(\mathbf{k}) = i^{-1}\sum_{j=1}^3 \partial(k_j\chi)/\partial k_j$. The integrations by parts used to obtain Eq. (27) are legal if $\chi(\mathbf{k})$ has two continuous derivatives and, say, vanishes outside of a bounded set. We shall assume this and also that χ vanishes in a neighborhood of 0. The functions ϕ for which χ has these properties form a dense set $\mathfrak{M}$ in $\mathfrak{H}_N$ and *we show that D_a is formally antisymmetric on this domain.*

Since[13] $\phi(k)$ and $\phi(\hat{k})$ are orthogonal elements of K_N, the norm of Eq. (18) can be written

$$||\phi||^2 = \int_{E_3} \frac{d^3k}{|\mathbf{k}|^{N-1}}\,(\chi(\mathbf{k}), \chi(\mathbf{k})), \qquad (28)$$

and correspondingly, the inner product is

$$(\phi_1, \phi_2) = \int_{E_3} \frac{d^3k}{|\mathbf{k}|^{N-1}}\,(\chi_1(\mathbf{k}), \chi_2(\mathbf{k})). \qquad (29)$$

We wish to show that $(D_a\phi_1, \phi_2) = -(\phi_1, D_a\phi_2)$, or more explicitly, denoting the operator in square

brackets in Eq. (27) by A, we want

$$\int \frac{d^3k}{|\mathbf{k}|^{N-1}} (A\chi_1(\mathbf{k}), \chi_2(\mathbf{k})) = -\int \frac{d^3k}{|\mathbf{k}|^{N-1}} (\chi_1(\mathbf{k}), A\chi_2(\mathbf{k})).$$

Proving this is largely a matter of integration by parts which is straightforward though lengthy, and we omit most of it. After applying only integration by parts (dropping all boundary terms), we obtain without using the wave equation or the special nature of the space K_N

$$\begin{aligned}\int_{E_s} \frac{d^3k}{|\mathbf{k}|^{N-1}} &(A\chi_1(\mathbf{k}), \chi_2(\mathbf{k})) \\ &= -\int_{E_s} \frac{d^3k}{|\mathbf{k}|^{N-1}} (\chi_1(\mathbf{k}), A\chi_2(\mathbf{k})) \\ &\quad + (N-1)\int_{E_s} (\chi_1(\mathbf{k}), [N\mathbf{a}\cdot\mathbf{k} - (\mathbf{ak} \otimes 1^{N-1} \\ &\quad + \cdots + 1^{N-1} \otimes \mathbf{ak})]\chi_2(\mathbf{k})) \frac{d^3k}{i\,|\mathbf{k}|^{N+1}}, \end{aligned} \tag{30}$$

where 1^{N-1} means $1 \otimes \cdots \otimes 1$ ($N-1$ factors). In order to show that D_a is formally antisymmetric, it is necessary and sufficient to show that the last integral in Eq. (30) is zero.

Since χ_1 and χ_2 are symmetric, the integral can also be written

$$N(N-1) \times \int_{E_s} (\chi_1(\mathbf{k}), [\mathbf{a}\cdot\mathbf{k} - \mathbf{ak} \otimes 1^{N-1}]\chi_2(\mathbf{k})) \frac{d^3k}{i\,|\mathbf{k}|^{N+1}}.$$

For $N = 1$, this is zero. For $N \geq 2$, it will be zero for all χ_1, χ_2 if and only if the integrand is zero, since the wave equations impose only pointwise conditions on the χ's i.e., a multiple of χ by an arbitrary smooth complex-valued function is again a χ. But for $N = 2$ (photon), we have already seen that inversion is unitary. Hence so is TT_aT unitary for this case, and D_a is therefore antisymmetric in case $N = 2$. Thus

$$\{\chi_1(k), [\mathbf{a}\cdot\mathbf{k} - \mathbf{ak} \otimes 1]\chi_2(\mathbf{k})\} = 0$$

when χ_1 and χ_2 come from photon wavefunctions. Now a general spin-s, ($s > 1$) wavefunction ϕ_1 can be written as a sum of products $\phi_1(k) = \sum_i \phi_i'(k) \otimes v_i$, where ϕ_i' is a photon wavefunction and v_i is in K_{N-2}. To see this we need only take the v_i to be an orthonormal basis of K_{N-2}. The representation exists since K_N is contained in $K_2 \otimes K_{N-2}$. The ϕ_i' are photon wavefunctions since $0 = k \otimes 1^{N-1}\phi_1(k) = \sum_i [(k \otimes 1)\phi_i'(k)] \otimes v_i$ and the v_i are linearly independent. Thus if

$$\chi_i(\mathbf{k}) = \sum_i \chi_i^{(i)}(\mathbf{k}) \otimes v_i, \qquad i = 1, 2,$$

then

$$(\chi_1(\mathbf{k}), [\mathbf{a}\cdot\mathbf{k} - \mathbf{ak} \otimes 1^{N-1}]\chi_2(\mathbf{k})) = \sum_i (\chi_i^{(1)}(\mathbf{k}), [\mathbf{a}\cdot\mathbf{k} - \mathbf{ak} \otimes 1]\chi_i^{(2)}(\mathbf{k})) = 0.$$

Hence D_a is symmetric on the domain $\mathfrak{M}$ we have described. In order to show that D_a is antisymmetric on $\mathfrak{M}$ for vectors a other than those with time-component zero, we need only observe that if L is a homogeneous Lorentz transformation and $U(L)$ is the unitary transformation associated with L in the (already known to be) unitary representation of the Lorentz group on $\mathfrak{H}_N$, then $U(L)$ leaves $\mathfrak{M}$ invariant and moreover $U(L)D_aU(L)^{-1} = D_{La}$. The last equation follows from the fact that inversion T commutes with any homogeneous Lorentz transformation, for then

$$LTT_aTL^{-1} = TLT_aL^{-1}T = TT_{La}T.$$

Thus

$$\begin{aligned}U(L)D_aU(L)^{-1}\psi &= (d/dt)U(L)TT_{ta}TU(L)^{-1}\psi|_{t=0} \\ &= (d/dt)TT_{tLa}T\psi|_{t=0} = D_{La}\end{aligned}$$

when ψ is in $\mathfrak{M}$. Hence D_{La} is skew-symmetric when D_a is, and then so is D_{La-a} since this equals $D_{La} - D_a$. Since every 4-vector has the form $La - a$, where a has zero time component and L is an orthochronous homogeneous Lorentz transformation, it follows that D_a is skew-symmetric for all 4-vectors a.

Existence of a New Conservation Law in Electromagnetic Theory

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Ten new extensive quantities that appear to be independent of stress–energy, but that analogously characterize the physical state of an electromagnetic field, are exhibited and are shown to be conserved in vacuum because of Maxwell's equations. These new quantities are shown to be capable of retrograde flow in a circularly polarized plane-wave field.

1. INTRODUCTION

In a general study of time-periodic electromagnetic fields in vacuum, it was noticed that the real vector field $[\frac{1}{2}j\beta(\mathbf{E}^*\times\mathbf{E} + \mathbf{H}^*\times\mathbf{H})]$, which has the mathematical form of a time-averaged quantity, is solenoidal because of Maxwell's equations. This vector field was therefore recognized to be capable of representing the time-averaged flux of a conserved physical quantity. Simple considerations reveal that the more general expression for the instantaneous flux of this conserved quantity in a nonperiodic field is $(\mathbf{E}\times\partial\mathbf{E}/\partial T + \mathbf{H}\times\partial\mathbf{H}/\partial T)$, and that the spatial density of the conserved quantity is identifiable as $[\mathbf{E}\cdot(\text{curl }\mathbf{E}) + \mathbf{H}\cdot(\text{curl }\mathbf{H})]$. In other words, for an arbitrary electromagnetic field in vacuum, Maxwell's equations were found to guarantee the validity of the differential conservation law,

$$\text{div}\left[\mathbf{E}\times\frac{\partial\mathbf{E}}{\partial T} + \mathbf{H}\times\frac{\partial\mathbf{H}}{\partial T}\right] + \frac{\partial}{\partial T}[\mathbf{E}\cdot(\text{curl }\mathbf{E}) + \mathbf{H}\cdot(\text{curl }\mathbf{H})] = 0. \quad (1)$$

Curiosity concerning the significance of this unusual conservation law stimulated a successful attempt to express it in homogeneous tensor notation, and led to the discovery that it involved a tensor of valence three. The tensorial form of Eq. (1) was then found to express nine additional conservation laws, akin to Eq. (1), and of equally unfamiliar form. This unexpected discovery of a complete set of ten new conservation equations is a source of mathematical *embarras de richesses* because of the lack of any ready physical interpretation for the quantities that are found to be conserved. Nevertheless, the existence of an extensive formal superstructure of new conserved quantities in the classical electromagnetic theory of the vacuum may be of some interest; these new conserved quantities augment the known stress–energy quantities of the electromagnetic field, and appear to be mathematically independent of those quantities. The present paper details the basic mathematical facts concerning the new conserved quantities, including the proof of their conservation based upon Maxwell's equations, and deduces a few simple properties of these quantities.

2. NOTATION

A system of inertia is assumed and is referred to orthogonal, rectilinear, real coordinates $(T = ct, x, y, z) \equiv (x^0, x^1, x^2, x^3)$ in which the metric tensor g_{ik} takes the diagonal Minkowskian form of signature -2. Four-dimensional index notation is used, but is augmented by 3-vector notation in those places where the latter may be convenient or more expressive. Tensor indices have the range 0, 1, 2, 3, except if they precede g in the alphabet, where the restricted range 1, 2, 3 applies. An index of the latter type, enclosed in parentheses, indicates the corresponding Cartesian component of any 3-vector expression to which it is attached. The Einstein summation convention is employed for all doubled indices, over the range appropriate to them, and the comma denotes partial differentiation. ϵ^{ijkm} is the completely antisymmetric tensor density for four dimensions, and ϵ_{abc} is the similar permutation symbol for three dimensions ($\epsilon^{0123} = \epsilon_{123} = +1$). The electromagnetic field $(\mathbf{E}, \mathbf{H})$ or (E_a, H_a) is expressed in Gaussian units and is represented in a conventional way by means of an antisymmetric tensor ϕ_{jk} defined by $\phi_{a0} = E_a$ and $\phi_{ab} = \epsilon_{abc}H_c$. Maxwell's equations for vacuum are then expressed concisely as

$$\epsilon^{mnpq}\phi_{np,q} = 0, \quad (2)$$

$$g^{pq}\phi_{np,q} = 0. \quad (3)$$

3. BASIC STATEMENT OF THE CONSERVATION LAW

Consider the tensor Z^{ijk} (of valence 3 and weight

+1) that is defined as follows:

$$Z^{ijk} = [\tfrac{1}{4}g^{ir}g^{kn}\epsilon^{jpmq} + \tfrac{1}{4}g^{jr}g^{kn}\epsilon^{ipmq} + \tfrac{1}{4}g^{ir}g^{jq}\epsilon^{kpmn} + \tfrac{1}{4}g^{jr}g^{iq}\epsilon^{kpmn} - \tfrac{1}{2}g^{nq}g^{im}\epsilon^{jkrp} - \tfrac{1}{2}g^{nq}g^{jm}\epsilon^{ikrp} - \tfrac{1}{2}g^{nq}g^{ip}\epsilon^{jkrm} - \tfrac{1}{2}g^{nq}g^{jp}\epsilon^{ikrm}]\phi_{mn}\phi_{pq,r}. \quad (4)$$

This tensor has the symmetry property

$$Z^{ijk} = Z^{jik}, \quad (5)$$

which can be verified by inspection of Eq. (4), and satisfies the divergence equation

$$Z^{ijk}{}_{,k} = 0, \quad (6)$$

which is a weak identity based upon the Maxwell vacuum equations. Because of the symmetry expressed by Eq. (5), the set (6) contains at most ten independent equations.

The divergence equation (6) can be interpreted as expressing differential conservation laws for ten quantities that may be hypothesized to possess some important physical significance. The tensor components Z^{ij0} are to be interpreted as the spatial densities of the conserved quantities, and the remaining tensor components Z^{ijc} are to be interpreted as the components of the spatial 3-vectors expressing the fluxes of the conserved quantities. The conserved quantities may therefore conveniently be labeled by the first two indices of the descriptive tensor Z^{ijk}.

Thus, with reference to any closed, stationary Gaussian surface S enclosing a vacuum region of space, the extensive quantity Z^{ij} defined by volume integration inside S,

$$Z^{ij} = \int Z^{ij0}\, dx\, dy\, dz, \qquad (=Z^{ji}), \quad (7)$$

expresses the total amount of the (i, j)th conserved quantity that S momentarily contains. The extensive quantity F^{ij} defined by surface integration over S,

$$F^{ij} = \int Z^{ijc}\, dS_c, \qquad (=F^{ji}), \quad (8)$$

correspondingly represents the total rate at which the (i, j)th conserved quantity is momentarily flowing out of the volume bounded by S. The integral form of the conservation law expressed by Eq. (6), in terms of the extensive quantities Z^{ij} and F^{ij} just defined, is

$$dZ^{ij}/dT = -F^{ij}. \quad (9)$$

4. PROOF OF THE CONSERVATION LAW

By differentiating Eq. (4) to form the divergence $Z^{ijk}{}_{,k}$, the following expression is obtained for that divergence:

$$Z^{ijk}{}_{,k} = [\tfrac{1}{4}g^{ir}g^{kn}\epsilon^{jpmq} + \tfrac{1}{4}g^{jr}g^{kn}\epsilon^{ipmq} + \tfrac{1}{4}g^{ir}g^{jq}\epsilon^{kpmn} + \tfrac{1}{4}g^{jr}g^{iq}\epsilon^{kpmn} - \tfrac{1}{2}g^{nq}g^{im}\epsilon^{jkrp} - \tfrac{1}{2}g^{nq}g^{jm}\epsilon^{ikrp} - \tfrac{1}{2}g^{nq}g^{ip}\epsilon^{jkrm} - \tfrac{1}{2}g^{nq}g^{jp}\epsilon^{ikrm}]\phi_{mn}\phi_{pq,rk} + [\tfrac{1}{4}g^{ir}g^{kn}\epsilon^{jpmq} + \tfrac{1}{4}g^{jr}g^{kn}\epsilon^{ipmq} + \tfrac{1}{4}g^{ir}g^{jq}\epsilon^{kpmn} + \tfrac{1}{4}g^{jr}g^{iq}\epsilon^{kpmn} - \tfrac{1}{2}g^{nq}g^{im}\epsilon^{jkrp} - \tfrac{1}{2}g^{nq}g^{jm}\epsilon^{ikrp} - \tfrac{1}{2}g^{nq}g^{ip}\epsilon^{jkrm} - \tfrac{1}{2}g^{nq}g^{jp}\epsilon^{ikrm}]\phi_{mn,k}\phi_{pq,r}. \quad (10)$$

By inspection, the 5th, 6th, 7th, and 8th terms of Eq. (10) are seen to vanish identically because they involve contractions of expressions that are antisymmetric in r and k with an expression that is symmetric in the same indices. The index permutation $[(m, p)(n, q)(k, r)]$, which is allowable inside the second square bracket in Eq. (10), shows that the 15th term is identically the negative of the 13th term, and that the 16th term is identically the negative of the 14th term, so that these four terms are also identically eliminated. The 9th and 10th terms of Eq. (10) can be seen to vanish because of the Maxwell equation (3), while the 11th and 12th terms vanish because of the Maxwell equation (2). Thus, only the first four terms of Eq. (10) survive, enabling that equation to be condensed to

$$4Z^{ijk}{}_{,k} = [g^{ir}(g^{kn}\epsilon^{jpmq} + g^{jq}\epsilon^{kpmn}) + g^{jr}(g^{kn}\epsilon^{ipmq} + g^{iq}\epsilon^{kpmn})]\phi_{mn}\phi_{pq,rk}. \quad (11)$$

The further reduction of this equation is greatly facilitated by the use of the following identity:

$$[g^{kn}\epsilon^{jpmq} - g^{km}\epsilon^{jpnq} - g^{jk}\epsilon^{mnpq} + g^{qk}\epsilon^{mnpj} + g^{pk}\epsilon^{mnjq}] = 0. \quad (12)$$

The proof of this identity is surprisingly simple. Inspection shows that the left-hand side of Eq. (12) is completely antisymmetric in the five free indices (m, n, p, q, j); it must therefore vanish in four dimensions, where at least two out of any set of five free indices must always be equal.

By contracting the identity (12) with $\phi_{pq,k}$, taking advantage of antisymmetries that exist, relabeling dummy indices, and rearranging terms, the following less obvious identity is derived:

$$(g^{kn}\epsilon^{ipmq} - g^{km}\epsilon^{ipnq})\phi_{pq,k} = g^{iq}\epsilon^{kpmn}\phi_{kp,q} - 2\epsilon^{mnpi}(g^{qk}\phi_{pq,k}). \quad (13)$$

The last term on the right-hand side of Eq. (13) vanishes because of the Maxwell equation (3); when this term is dropped from Eq. (13), the resulting weak identity can be differentiated with respect to x^r, and then contracted with ϕ_{mn}, to give the following weak identity:

$$g^{kn}\epsilon^{ipmq}\phi_{mn}\phi_{pq,rk} = \tfrac{1}{2}g^{iq}\epsilon^{kpmn}\phi_{mn}\phi_{kp,qr}. \quad (14)$$

Adding the term $[g^{iq}\epsilon^{kpmn}\phi_{mn}\phi_{pq,rk}]$ to both sides of Eq. (14) and rearranging the right-hand side, the following weak identity is next obtained:

$$(g^{kn}\epsilon^{ipmq} + g^{iq}\epsilon^{kpmn})\phi_{mn}\phi_{pq,rk} = \tfrac{1}{2}g^{iq}\epsilon^{kpmn}\phi_{mn}[\phi_{pq,k} + \phi_{qk,p} + \phi_{kp,q}]_{,r}. \quad (15)$$

However, the square bracket in Eq. (15) vanishes because of the Maxwell equation (2); the following weak identity has therefore been proved on the basis of Maxwell's equations:

$$(g^{kn}\epsilon^{ipmq} + g^{iq}\epsilon^{kpmn})\phi_{mn}\phi_{pq,rk} = 0. \quad (16)$$

This equation (together with the same equation with the free index j replaced by i) obviously suffices to prove the vanishing of the right-hand side of Eq. (11). This completes the proof of the divergence equation (6) on the basis of Maxwell's vacuum equations, and provides the foundation for the conservation law under discussion.

5. COMPONENTS OF THE DESCRIPTIVE TENSOR

Straightforward calculation from Eq. (4), with the free use of Maxwell's equations, indicates that the individual components Z^{ijk} of the descriptive tensor can be expressed fairly simply in terms of the electric and magnetic field vectors and their derivatives. The spatial density components Z^{ij0} are found to be given by the following formulas:

$$Z^{000} = [\mathbf{E}\cdot(\text{curl }\mathbf{E}) + \mathbf{H}\cdot(\text{curl }\mathbf{H})], \quad (17)$$

$$Z^{0b0} = \left[\mathbf{E}\times\frac{\partial\mathbf{E}}{\partial T} + \mathbf{H}\times\frac{\partial\mathbf{H}}{\partial T}\right]_{(b)}, \quad (18)$$

$$Z^{ab0} = \delta_{ab}[\mathbf{E}\cdot(\text{curl }\mathbf{E}) + \mathbf{H}\cdot(\text{curl }\mathbf{H})] - E_a(\text{curl }\mathbf{E})_{(b)} - H_a(\text{curl }\mathbf{H})_{(b)} - E_b(\text{curl }\mathbf{E})_{(a)} - H_b(\text{curl }\mathbf{H})_{(a)}. \quad (19)$$

Note that the quantity Z^{000} equals the trace of the matrix formed of the quantities Z^{ab0}. The flux components Z^{ijc} are found to be given by the following formulas:

$$Z^{00c} = Z^{0c0} - [\text{curl }(\mathbf{E}\times\mathbf{H})]_{(c)}. \quad (20)$$

$$Z^{0bc} = Z^{bc0} + \epsilon_{cde}[\tfrac{1}{2}(\mathbf{E}^2 + \mathbf{H}^2)\delta_{bd} - (E_bE_d + H_bH_d)]_{,e}, \quad (21)$$

$$Z^{abc} = \delta_{ab}Z^{00c} + (H_aE_{b,c} - E_aH_{b,c} + H_bE_{a,c} - E_bH_{a,c}). \quad (22)$$

The original conservation equation (1) is seen to be represented by the particular case $i=j=0$ of Eq. (6).

6. PROPERTIES OF THE DESCRIPTIVE TENSOR

A. Independence of Stress-Energy

The tensor Z^{ijk}, according to its defining equation (4), is bilinear in the electromagnetic field and its first partial derivatives. As such, it is similar in structure to tensors that can be constructed from the first partial derivatives of the components of the conventional stress-energy tensor T_{mn}. The tensor Z^{ijk} is independent of the stress-energy tensor, however, in the sense that the components of Z^{ijk} cannot be represented as linear combinations of the derivatives $T_{mn,p}$, taken with constant coefficients, even when the Maxwell equations are freely used. This can be seen particularly clearly in the case of the components Z^{000} and Z^{ab0}, although the proof of this is not displayed here.

Earlier formulas that contained fewer terms than Eq. (4) were considered for the definition of the tensor Z^{ijk}, but were rejected because detailed examination revealed that the individual components of the tensor contained extraneous terms that were identically conserved independently of Maxwell's equations, or that were expressible in terms of the first derivatives of the stress-energy tensor. The majority of the extraneous terms of the second type and, it is believed, all the extraneous terms of the first type, have been eliminated by covariant subtractions. These subtractions necessitated the present lengthy form of Eq. (4), but led to the recognition of the symmetry expressed by Eq. (5), and gave the simple component expressions displayed in Eqs. (17)–(22). In Eq. (4), the last four terms, taken together, are not only expressible completely in terms of stress-energy derivatives, but even have a vanishing contribution to the divergence $Z^{ijk}{}_{,k}$ independently of the Maxwell equations; the subtraction of these four terms in Eq. (4) is nevertheless desirable because it frees the tensor components Z^{ijk} of a great many stress-energy derivatives whose presence is otherwise implied, but implied much less obviously, by the first four terms of Eq. (4).

The tensor Z^{ijk} has been normalized to give the component Z^{000} the value specified by Eq. (17), modulo the Maxwell equations.

The extent of the subtractions of stress–energy derivatives that have been made in arriving at the present form for Eq. (4) can be largely understood by examining the following rearranged form of Eq. (4):

$$Z^{ijk} = [\tfrac{1}{2}g^{ir}(g^{kn}\epsilon^{jpmq} + g^{jq}\epsilon^{kpmn})\phi_{mn}\phi_{pq,r} - 2\pi(g^{im}\epsilon^{jknp} - g^{jm}\epsilon^{kinp} + g^{km}\epsilon^{ijnp})T_{mn,p}], \quad (23)$$

in which T_{mn} stands for the conventional stress–energy tensor of the electromagnetic field,

$$T_{mn} = (1/4\pi)(\delta^r_m\delta^s_n - \tfrac{1}{4}g^{rs}g_{mn})\phi_{rp}g^{pq}\phi_{qs}. \quad (24)$$

In the formulation of the tensor Z^{ijk} given by Eqs. (4) or (23), the only remaining terms that its components contain which are identifiable as being proportional to stress–energy derivatives $T_{mn,p}$ are the curl of the Poynting vector, appearing in Eq. (20) and implicitly in Eq. (22), and the Maxwell stress gradients appearing in Eq. (21). These terms affect the localization of the fluxes of the new conserved quantities, but not the localization of their spatial densities. Upon closer examination, all of these residual flux terms that involve stress–energy derivatives are seen to be curl terms whose 3-divergences vanish identically; they therefore do not contribute to the total efflux integrals F^{ij} defined by Eq. (8), and thus have no effect on the rates of flow of the new conserved quantities over extended regions of space. These curl terms have identically vanishing instantaneous values in the important case of a time-periodic plane-wave field of arbitrary type of polarization, further supporting the conclusion that their presence is completely inessential. The curl terms in question may not be arbitrarily dropped from their respective equations, being required from the standpoint of covariance, but their elimination may be sought by means of some further covariant subtraction process.

B. Vanishing of Contractions

No nonvanishing 4-vectors can be constructed from the descriptive tensor Z^{ijk} by contracting it with the usual constant tensors. Thus, the contraction $\epsilon_{ijkm}Z^{ijk}$ vanishes identically because of the symmetry property expressed by Eq. (5); the contraction $g_{ij}Z^{ijk}$ can be shown to vanish because of the Maxwell equations (2) and (3), by direct calculation from Eq. (4); finally, the contractions $g_{mn}Z^{imn} = g_{mn}Z^{min}$ also vanish because of the Maxwell equations (2) and (3), as can be proved by proceeding from Eq. (4) with the aid of the identity expressed by Eq. (12). The inability of simple contractions to nontrivially lower the valence of the tensor Z^{ijk} implies that the same means are also incapable of lowering the tensor valence of the basic divergence equation (6).

C. Conservation Symmetries

In stress–energy theory, the fact is familiar that the vector flux of energy is proportional to the spatial density of momentum. In the case of the new conserved quantities under discussion, a larger but analogous set of symmetries exists. Thus, with reference to the formulas (18)–(21), the following relationships are found to hold (neglecting the curl terms of flux discussed in Sec. 6A above): The vector flux of the (0, 0)th conserved quantity (described by the components Z^{00b}) is proportional to the 3-vector formed from the spatial densities of the three (0, b)th conserved quantities (described by the components Z^{0b0}); but, in turn, the components of the vector fluxes of the (0, b)th conserved quantities (described by the components Z^{0bc}) are proportional to the spatial densities of the (b, c)th conserved quantities (described by the components Z^{bc0}).

7. PHYSICAL DIMENSIONS OF THE CONSERVED QUANTITIES

The ten conserved extensive quantities Z^{ij} defined by Eq. (7) all have units of dynes, and are presumably dynamical quantities of some sort. If the definition of the descriptive tensor Z^{ijk} were augmented by a dimensional factor equal to the velocity of light, then the conserved quantities Z^{ij} would have the dimensions of ergs per second. This very crudely suggests that the Z^{ij} might provide a measure of some sort of activity in the field, a suggestion that finds support in the fact that the densities of the new conserved quantities all vanish in a static field [see Eqs. (17)–(19), modulo Maxwell's equations].

Without the introduction of dimensional factors more arbitrary than the velocity of light, the units of the conserved quantities Z^{ij} cannot be brought into coincidence with those of action per unit time or of angular momentum. This, together with the distinctness of the new conserved quantities from stress–energy, discussed previously, and the unfamiliar form of the new conservation laws, suggests that these conserved quantities may form a fundamentally new physical entity not heretofore known.

If so, then because of the ubiquitous nature of electromagnetism in physics, these quantities could be expected to occur in other branches of physical theory, just as do energy and momentum.

Pending the satisfactory physical interpretation of the new conserved quantities, economy of expression will be facilitated by assigning them convenient identifying names; the ten conserved extensive quantities Z^{ij} defined by Equation (7) will hereby be collectively called the "zilch" of the electromagnetic field, and a particular one labeled by the indices (i, j) will be referred to as the "ij-zilch" of the field.

8. RETROGRADE FLOW OF ZILCH

It is instructive to calculate the zilch density tensor Z^{ijk} in the special case of a time-periodic, plane-wave, vacuum electromagnetic field of arbitrary type of polarization. Consider the wave field to propagate in the $+z$ direction, and employ complex phasor notation in which $\partial/\partial T = +j\beta$, where β is the propagation constant of the wave. The components of the electromagnetic field can then be expressed as

$$E_x = H_y = A \exp(-j\beta z), \tag{25a}$$

$$E_y = -H_x = B \exp(-j\beta z), \tag{25b}$$

$$E_z = H_z = 0, \tag{25c}$$

where A and B are arbitrary complex coefficients. With the aid of Eqs. (17)–(22), the time-averaged values of the components Z^{ijk} can be computed to be the following (the bar denotes the time average):

$$\overline{Z^{000}} = [j\beta(A^*B - AB^*)], \tag{26a}$$

$$\overline{Z^{0b0}} = \overline{Z^{00b}} = \delta_3^b \overline{Z^{000}}, \tag{26b}$$

$$\overline{Z^{bc0}} = \overline{Z^{0bc}} = \delta_3^b \delta_3^c \overline{Z^{000}}, \tag{26c}$$

$$\overline{Z^{abc}} = \delta_3^a \delta_3^b \delta_3^c \overline{Z^{000}}. \tag{26d}$$

Thus, in the case under consideration, and referring exclusively to time averages, only the 00-, 03-, and 33-zilches may have nonvanishing densities and fluxes, and their fluxes are all aligned parallel to the z axis. Finally, in the units used (namely, dyn/cm^3 for spatial densities, and dyn/cm^2/light-cm for flux components), all nonvanishing spatial densities and flux components have a common real value, equal to $[j\beta(A^*B - AB^*)]$.

In the case of a linearly polarized wave, A/B is real, and $(A^*B - AB^*)$ vanishes. Thus, zilch is not transported by linearly polarized waves. In the case of a right-circularly polarized wave, $A = +jB$, and $[j\beta(A^*B - AB^*)] = 2\beta |B|^2 > 0$; in the case of a left-circularly polarized wave, $A = -jB$, whereupon $[j\beta(A^*B - AB^*)] = -2\beta |B|^2 < 0$; thus, a nonvanishing flow of zilch accompanies any circularly polarized wave, but the direction of this flow reverses with the screw sense of the wave. Another unusual property of this flow is that its rate is linearly proportional to the frequency of oscillation of the field.

Unlike energy and momentum, which are always transported in the direction of propagation of the wave field, zilch can evidently be transported either in this direction or in the opposite (or retrograde) direction, depending upon the sense of circular polarization of the wave. This behavior of zilch flow is somewhat similar to what would be expected for quantities representing an intrinsic spin of the field, and is suggestive of a possible direction for the physical interpretation of zilch. Certainly, the occurrence of this similarity in what is strictly a classical field theory would appear to merit further investigation.

9. SUMMARY

The existence of ten new conserved quantities, defined for the electromagnetic field and apparently unrelated to stress–energy, has been mathematically demonstrated. The new conserved quantities have been demonstrated to possess flow properties that are remarkably different from those of energy and momentum. The problem of the physical interpretation of these new quantities is raised, and the possibility is suggested that they occur in other areas of physical theory as well as in electromagnetism. The nature of the group-invariance properties that the new conservation laws may imply also deserves investigation.

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