Remarks on Lightlike Continuous Spin and Spacelike Representations of the Poincaré Group

A. Chakrabarti
Centre de Physique Théoreque de l'Ecole Polytechnique 17, rue Descartes, 75, Paris V, France
(Received 23 June 1970)

Certain classes of unitary representations of the lightlike continuous spin and the spacelike cases are constructed. The generators in these representations involve operators forming the "intrinsic" algebras (i.e., commuting with the orbital parts) E_3 and $O(3,1)$ for $P^2 = 0$ and $P^2 < 0$, respectively. The parallel construction for $P^2 > 0$ involving an intrinsic O_4 algebra is indicated. Equivalence relations with certain other forms are given through a unitary transformation. The physical significance of the "translation" generators of E_3 is brought out in terms of the projections of **W** orthogonal to **P**. Corresponding results for the $O_{(3,1)}$ and $O_{(4)}$ algebras are given. For the continuous-spin case, these operators are shown to provide a basis with extremely simple transformation properties, related to a certain symmetric toplike behavior even under Lorentz transformations. With a view to future use, the matrix elements of **W** on the energy-rotation basis are calculated in a unified manner for all the three cases, $P^2 \gtrless 0$. A deformation formula leading from zero-mass continuous-spin representations to spacelike ones is studied. Certain types of nonunitary representations are briefly introduced at the end.

1. INTRODUCTION

Zero-mass, continuous-spin, and imaginary-mass representations of the Poincaré group and the corresponding basis functions have recently become of interest in connection with crossed-channel partial-wave analysis (see some of the sources quoted in Ref. 1). Also speculations have been made about the possible existence of faster-than-light particles. In this paper we will discuss certain types of representations for the above-mentioned cases, their relations through a deformation formula, and the matrix elements of certain interesting operators on the bases introduced. Though in this article we will be mainly interested in the cases $P^2 \leqslant 0$, the parallel results for $P^2 > 0$ will be indicated wherever necessary. In particular, the matrix elements of **W** on the energy-angular momentum basis are given in a form valid for all the three cases. These results will be used in a separate article,[1] to calculate the transformation coefficients connecting the momentum and Lorentz basis, in a unified fashion for all the three cases, namely, for positive-, zero-, and imaginary-mass representations. These latter results are, in turn, of interest for analysis in "Lorentz partial waves" of scattering amplitudes for particles with spin. But, apart from such applications, certain operator structures and symmetrical and simple properties exhibited by the formalism seem to the present author to be intrinsically attractive.

2. CONSTRUCTION OF THE REPRESENTATIONS

Elsewhere[2] we have discussed how, starting with the postulated forms (Sec. 4 of Ref. 2)

$$\mathbf{M} = -i\mathbf{P} \times \frac{\partial}{\partial \mathbf{P}} + \mathbf{S}, \quad \mathbf{N} \mp -iP^0 \frac{\partial}{\partial \mathbf{P}} + \mathcal{T} \tag{2.1}$$

where

$$\mathcal{T} \cdot \mathbf{P} = \mathbf{P} \cdot \mathcal{T} = 0, \tag{2.1'}$$

one can discuss, in a unified manner, the behavior of spin for the positive-mass and the zero-mass discrete-spin cases. The simplest solution for these two cases are

$$\mathcal{T} = (\mathbf{S} \times \mathbf{P})/(P^0 + \epsilon m), \qquad m \geqslant 0, \tag{2.2}$$

S being the usual irreducible $(2S+1)$-dimensional spin matrices and ϵ being the sign of the energy.[3] It was also shown in Ref. 2 that a unitary transformation by the operator

$$U = \exp(i\{P^1 S^2 - P^2 S^1\}/[(P_1)^2 + (P_2)^2]^{1/2}\}\theta), \tag{2.3}$$

where

$$\theta = \tan^{-1}\{[(P_1)^2 + (P_2)^2]^{1/2}/P^3\}, \tag{2.3'}$$

leads to a representation for the zero-mass discrete-spin case, where among the three components of **S** now only S_3 appears in the transformed generators. [This is obtained here as a particular case of (2.18)–(2.21) by putting $T^1 = T^2 = 0$.] This corresponds to a diagonalization of the helicity

$$U(\mathbf{S} \cdot \mathbf{P}/|\mathbf{P}|)U^{-1} = S_3, \tag{2.4}$$

which is an invariant for such representations.

The condition, implied in (2.1) and (2.1'),

$$\begin{aligned} \mathbf{N} \cdot \mathbf{P} + \mathbf{P} \cdot \mathbf{N} &= -iP^0\left(\mathbf{P} \cdot \frac{\partial}{\partial \mathbf{P}} + \frac{\partial}{\partial \mathbf{P}} \cdot \mathbf{P}\right) \\ &= -iP^0\left(2\mathbf{P} \cdot \frac{\partial}{\partial \mathbf{P}} + 3\right) \\ &= -iP^0\left(2|\mathbf{P}|\frac{\partial}{\partial |\mathbf{P}|} + 3\right), \end{aligned} \tag{2.5}$$

corresponds to the property that the spin index σ of the state $|p, \sigma\rangle$ is invariant under a Lorentz transformation collinear with the initial momentum **p**. This corresponds directly to a basic property of "physical" spin for real particles. Moreover, here and in Ref. 1 we will find it very useful to consider (for the general case, including continuous-sping and spacelike ones) the action of the operator $(\mathbf{N} \cdot \mathbf{P} + \mathbf{P} \cdot \mathbf{N})$ on the states

$$\left| \begin{matrix} p^0 \mu \\ j j_3 \end{matrix} \right\rangle$$

diagonalizing the energy (p_0), the angular momentum (j, j_3), and the helicity (μ). For this purpose also it is good to have (2.5) built into the representation of the generators for all cases: This is

a criterion of simplicity assuring that, at least for Lorentz transformations collinear to the initial momentum, our representations will behave like zero-spin ones. Also we would like to be able to consider pure spatial rotations in a uniform fashion for all cases, including spacelike representations. So we propose to search for representations of the generators of the form (2.1) and (2.1′) for lightlike (continuous-spin) and spacelike cases. We can always diagonalize helicity afterwards through the transformation (2.3). But, in our opinion, a symmetrical treatment of the rotation generators as in (2.1) suggests constructions for **N** which, as will be seen, bring directly into evidence certain interesting operator structures. The significance of this statement will be clearer later on.

We know that, for zero-mass continuous-spin representations discovered by Wigner, we have the little-group algebra E_2, with the generators satisfying

$$[S^3, T^1] = iT^2, \quad [S^3, T^2] = -iT^1, \quad [T^1, T^2] = 0, \tag{2.6}$$

and that, for imaginary mass, we have the little group $SU(1,1)$, with

$$[S^3, K^1] = iK^2, \quad [S^3, K^2] = -iK^1, \quad [K^1, K^2] = -iS^3. \tag{2.7}$$

However, in our case, the symmetrical appearance of the three components of **S** in **M** in (2.1) suggests the possibility of a rotationally symmetric appearance (in **N**) of the generators (**S**, **T**) of E_3 and (**S**, **K**) of 0(3, 1) respectively, for $P^2 = 0$ and $P^2 < 0$, commuting with the orbital parts and satisfying

$$[S^i, S^j] = i\epsilon_{ijk}S^k, \quad [S^i, T^j] = i\epsilon^{ijk}T^k, \quad [T^i, T^j] = 0, \tag{2.8}$$

and

$$[S^i, S^j] = i\epsilon_{ijk}S^k, \quad [S^i, K^j] = i\epsilon_{ijk}K^k, \quad [K^i, K^j] = -i\epsilon_{ijk}S^k. \tag{2.9}$$

[We will, however, demonstrate unitary equivalence of these representations to those in which the usual little-group generators alone appear. See (2.18)–(2.21).]

Again the condition (2.1′) suggests that we try such combination as

$$(\mathbf{S}\times\mathbf{P}), \quad (\mathbf{S}\times\mathbf{P})\times\mathbf{P}, \quad (\mathbf{T}\times\mathbf{P}), \quad (\mathbf{T}\times\mathbf{P})\times\mathbf{P}, \quad (\mathbf{K}\times\mathbf{P}), \quad (\mathbf{K}\times\mathbf{P})\times\mathbf{P}. \tag{2.10}$$

The simplest solutions satisfying

$$[N^i, N^j] = i\epsilon_{ijk}M^k$$

turn out to be (including ϵ, the sign of the energy as indicated in Ref. 3)

$$\text{(a)} \quad \mathbf{N} = -iP^0\frac{\partial}{\partial\mathbf{P}} + \frac{1}{\mathbf{P}^2}(P^0\mathbf{S} + \epsilon\mathbf{T})\times\mathbf{P}, \quad P^2 = 0, \tag{2.11}$$

$$\mathbf{N} = -iP^0\frac{\partial}{\partial\mathbf{P}} + \frac{1}{\mathbf{P}^2}(P^0\mathbf{S} + \epsilon m\mathbf{K})\times\mathbf{P}, \quad P^2 = -m^2, \tag{2.12}$$

$$\text{(b)} \quad \mathbf{N} = -iP^0\frac{\partial}{\partial\mathbf{P}} + \frac{1}{\mathbf{P}^2}[P^0\mathbf{S} + |\mathbf{P}|^{-1}(\mathbf{T}\times\mathbf{P})]\times\mathbf{P}, \quad P^2 = 0 \tag{2.13}$$

$$\mathbf{N} = -iP^0\frac{\partial}{\partial\mathbf{P}} + \frac{1}{|\mathbf{P}|^2}\times[P^0\mathbf{S} + |\mathbf{P}|^{-1}m(\mathbf{K}\times\mathbf{P})]\times\mathbf{P}, \quad P^2 = -m^2. \tag{2.14}$$

The hermiticity of (**S**, **T**) and (**S**, **K**) guarantees that of **N** and hence the unitarity of the representations.

Other more complicated solutions can be found, but they do not seem to be of particular interest. {The Casimir operators of E_3 [or 0(3, 1)] appearing above can not be expressed in terms of the generators (P, **N**, **M**) and hence have no direct significance for the Poincaré group. The utility of the spinor representations for neutrinos shows that in certain cases it may be of interest to introduce a larger "intrinsic" algebra than is required by the structure of the little group. We apply this lesson here and interpret afterwords **T** and **K**.}

For $\epsilon = \pm 1$, we note that

$$e^{[-i\epsilon(\mathbf{S}\cdot\mathbf{P}/|\mathbf{P}|)\theta]}\left(\epsilon\mathbf{T}\times\frac{\mathbf{P}}{|\mathbf{P}|}\right)e^{[i\epsilon(\mathbf{S}\cdot\mathbf{P}/|\mathbf{P}|)\theta]} = \left(\epsilon\frac{\mathbf{T}\times\mathbf{P}}{|\mathbf{P}|}\right)\cos\theta + \left(\mathbf{T}\times\frac{\mathbf{P}}{|\mathbf{P}|}\right)\times\frac{\mathbf{P}}{|\mathbf{P}|}\sin\theta. \tag{2.15}$$

We have of course, an exactly similar formula for **K**.

Using (2.15) and the fact that $(\mathbf{S}\cdot\mathbf{P}/|\mathbf{P}|$ commutes with the rest of **N** in (2.11) and (2.12) (and, of course, with **M**), we see that (2.11) and (2.12) can, respectively, be transformed to (2.13) and (2.14)[4] putting in (2.15)

$$\theta = \pi/2 \tag{2.16}$$

(for other values of θ we get intermediate types of representations).

Let us also note that changing the last relation of Eq. (2.9) to

$$[K^i, K^j] = i\epsilon_{ijk}K^k, \tag{2.17}$$

i.e., considering the generators of 0(4) rather than 0(3,1), we obtain, in (2.12) and (2.14), representations for the timelike case with

$$P^2 = m^2 > 0. \tag{2.17′}$$

This shows that all the three types ($P^2 \gtrless 0$) can be cast into closely similar forms. However, for $P^2 > 0$, (2.2) provides a simpler solution and, moreover, the forms (2.12), (2.14) become singular for the rest frame

$$\mathbf{p} = 0.$$

Introducing now the transformation U [Eq. (2.3)], diagonalizing the helicity operator, we obtain for $\mathbf{M}$ [which is always as in (2.1)]

$$\mathbf{M}_{\mathrm{tr}} = UMU^{-1} = -i\mathbf{P} \times \frac{\partial}{\partial \mathbf{P}} + \zeta,$$

where

$$\zeta = (P^1, P^2, (\mathbf{P}^2)^{1/2}) S^3/[(\mathbf{P}^2)^{1/2} + P^3]. \quad (2.18)$$

For (2.11) we obtain (using $P^0/\mathbf{P}^2 = 1/P^0$ for $P^2 = 0$)

$$\mathbf{N}_{\mathrm{tr}} = -iP^0 \frac{\partial}{\partial \mathbf{P}} + \eta + \epsilon \frac{1}{\mathbf{P}^2} \chi, \quad (2.19)$$

where

$$\eta = (-P^2, P^1, 0)\, S^3/[(\mathbf{P}^2)^{1/2} + P^3] \quad (2.20)$$

and

$$\chi^1 = T^2P^3 + (P^1T^1 + P^2T^2)P^2/[(\mathbf{P}^2)^{1/2} + P^3],$$
$$\chi^2 = T^1P^3 - (P^1T^1 + P^2T^2)P^2/[(\mathbf{P}^2)^{1/2} + P^3],$$
$$\chi^3 = (T^1P^2 - T^2P^1). \quad (2.21)$$

We have an exactly similar form (except for a factor $|p^0|/|\mathbf{P}|$ before η and the substitution $\mathbf{T} \to m\mathbf{K}$) corresponding to the transformation of (2.12). [In order to exhibit the property indicated in Ref. 3, separate determinations of the sign of the square root $(\mathbf{p}^2)^{1/2}$ is to be used according to the sign of ϵ. We do not propose to enter into these details as we will not make any use of the transformed representations.]

The transformed versions (always with the same U) of (2.13) and (2.14) correspond to the forms given by Moses[5] (except for his conventions regarding ϵ), and so we refer to his results. Moses has calculated the corresponding finite transformation formulas and utilized such representations for the reduction of direct products. He has also considered the relation of such representations with the canonical form (2.2) for the positive-mass case.

Let us now consider in more detail the role of the operators $\mathbf{T}$ and $\mathbf{K}$. We note that in (2.18)–(2.21), only the generators of E_2 [Eq. (2.6)] (S^3, T^1, T^2) appear, whereas in (2.1) and (2.11) we have all the six generators ($\mathbf{S}, \mathbf{T}$) of E_3 [(2.8)]. The situation is similar for the case $p^2 = -m^2$, only the subgroup generators (2.7) remaining out of the six of (2.9). Let us, however, note that in (2.11)–(2.14), $\mathbf{T}$ and $\mathbf{K}$ appear only in the combinations

$$(\mathbf{T} \times \mathbf{P}), \quad (\mathbf{K} \times \mathbf{P}).$$

Thus only the components

$$\tilde{\mathbf{T}} = \mathbf{T} - (\mathbf{T}\cdot\mathbf{P}/|\mathbf{P}|)(\mathbf{P}/|\mathbf{P}|) \quad (2.22)$$

and

$$\tilde{\mathbf{K}} = \mathbf{K} - (\mathbf{K}\cdot\mathbf{P}/|\mathbf{P}|)(\mathbf{P}/|\mathbf{P}|) \quad (2.22')$$

orthogonal to $\mathbf{P}$ *enter into play.*

The significance of $\tilde{\mathbf{T}}$ and $\tilde{\mathbf{K}}$ becomes clearer on considering, along with P^μ, the other two fundamental 4-vectors of the Poincaré group, namely,

$$W^\mu = (P\cdot M^*)^\mu = -i[P^\mu, \mathbf{N}\cdot\mathbf{M}] \quad (2.23)$$

and

$$G^\mu = \tfrac{1}{2}(P\cdot M + M\cdot P)^\mu = -\tfrac{1}{2}i[P^\mu, (\mathbf{N}^2 - \mathbf{M}^2)]. \quad (2.23')$$

[M is the antisymmetric tensor $M^{\mu\nu}$ or $(\mathbf{N}, \mathbf{M})$ and M^* is its dual or $(-\mathbf{M}, \mathbf{N})$.]

More explicitly, we have

$$W = [\mathbf{P}\cdot\mathbf{M}, P^0\mathbf{M} - \mathbf{P} \times \mathbf{N}] \quad (2.24)$$

and

$$G = \tfrac{1}{2}[(\mathbf{P}\cdot\mathbf{N}, P^0\mathbf{N} + \mathbf{P} \times \mathbf{M}) + (\mathrm{H.c.})], \quad (2.25)$$

so that

$$\mathbf{P} \times \mathbf{W} = P^0[\mathbf{G} - (\mathbf{P}/P^0)G^0] - P^2\mathbf{N}. \quad (2.26)$$

From (2.1) for all the representations considered,

$$W^0 = \mathbf{P}\cdot\mathbf{M} = \mathbf{P}\cdot\mathbf{S}. \quad (2.27)$$

From (2.11) we obtain for $P^2 = 0$

$$\tilde{\mathbf{W}} = \mathbf{W} - (P^0W^0/\mathbf{P}^2)\mathbf{P} = \mathbf{W} - (W^0/P^0)\mathbf{P} = -\epsilon\tilde{\mathbf{T}} \quad (2.28)$$

and

$$(\mathbf{P}/|\mathbf{P}|) \times \mathbf{W} = \epsilon(\mathbf{G} - G^0\mathbf{P}/P^0)$$
$$= -\epsilon(\mathbf{P}/|\mathbf{P}|) \times \mathbf{T}$$
$$= -\epsilon(\mathbf{P}/|\mathbf{P}|) \times \tilde{\mathbf{T}}. \quad (2.29)$$

(The negative signs of $-\tilde{\mathbf{T}}$ can be absorbed in the construction of the generators if so desired. See Ref. 4).

In the corresponding results obtained from (2.73), the roles of $\mathbf{T}$ and $\mathbf{P} \times \mathbf{T}$ are interchanged as compared to (2.28) and (2.29).

We have, of course, an analogous result in terms of $m\mathbf{K}$ for $p^2 = -m^2$.

Thus, we see that $\tilde{\mathbf{T}}$ and $\mathbf{P}/|\mathbf{P}| \times \tilde{\mathbf{T}}$ correspond to the two projections of $\mathbf{W}$ orthogonal to $\mathbf{P}$. These projections have particularly interesting properties (see the following sections), and one of the aims in constructing the preceeding representations was to exhibit them explicitly in the generators themselves in a symmetrical fashion. In the transformed representations such as (2.19), these features are much less evident.

Let us finally note that, using (2.11) or (2.13), we obtain

$$W^2 = -(\tilde{\mathbf{T}})^2 = [(\mathbf{P}/|\mathbf{P}|) \times \tilde{\mathbf{T}}]^2 = -[\mathbf{T}^2 - (\mathbf{T}\cdot\mathbf{P}/|\mathbf{P}|)^2], \quad (2.30)$$

and similarly [(2.12) or (2.14)] we obtain

$$W^2 = m^2\{(\mathbf{S}\cdot\mathbf{P}/|\mathbf{P}|)^2 - [\mathbf{K}^2 - (\mathbf{K}\cdot\mathbf{P}/|\mathbf{P}|)^2]\}. \quad (2.31)$$

For the corresponding helicity diagonalized representations, these become, respectively,

$$UW^2U^{-1} = -(T_1^2 + T_2^2) \quad (2.30')$$
$$= m^2(S_3^2 - K_1^2 - K_2^2).$$

These are the familiar invariants of the corresponding little groups.

3. SPECIAL FEATURES OF THE CONTINUOUS-SPIN CASE

We now propose to study in more detail, for the case

$$P^2 = 0, \quad W^2 = -\tau^2,$$

the properties of the operators

$$\tilde{\mathbf{W}} = \mathbf{W} - (W^0/P^0)\mathbf{P} \quad (3.1)$$

and

$$\tilde{\mathbf{G}} = \mathbf{G} - G^0\mathbf{P}/P^0 = (\mathbf{P}/P^0) \times \tilde{\mathbf{W}} \quad (3.2)$$

Let us first note that the commutators of $\mathbf{P}$ (or $\mathbf{P}/P^0$), $\tilde{\mathbf{W}}$ and $\mathbf{M}$, close to form an algebra,

$$[M^i, P^j] = i\epsilon_{ijk}P^k, \quad [M^i, \tilde{W}^j] = i\epsilon_{ijk}\tilde{W}^k,$$
$$[P^i, P^j] = 0, \quad [\tilde{W}^i, \tilde{W}^j] = 0, \quad [P^i, \tilde{W}^j] = 0. \quad (3.3)$$

We will call this algebra $E_3^{(2)}$, the index (2) indicating a doubling of the usual triplet of the translation generators of the Euclidean algebra E^3. This algebra has three Casimir operators:

$$\mathbf{P}^2, \tilde{\mathbf{W}}^2, \text{ and } \mathbf{P}\cdot\tilde{\mathbf{W}} \quad (3.4)$$

among which only the particular case corresponding to the zero value of the third one, namely,

$$\mathbf{P}\cdot\tilde{\mathbf{W}} = 0,$$

along with

$$\mathbf{P}^2 = \mathbf{p}^2, \quad \text{say, and} \quad \tilde{\mathbf{W}}^2 = -W^2 = \tau^2, \quad (3.5)$$

is relevant for our present purposes [see, however (A18)]. (All the generators of the above $E_3^{(2)}$ commute with P^0).

The matrix element of $\tilde{\mathbf{W}}$ acting on the basis diagonalizing the E_3 subalgebra of $(\mathbf{P}, \mathbf{M})$ can be obtained directly by using (3.3) and (3.5). This aspect is discussed in the following section. [Since the last term of (3.2) can be used to obtain the action of G on this basis, we need not separately consider the enlarged algebra including G. See (A18).]

Let us consider now the effect of pure Lorentz transformations. We have

$$[i\chi\hat{n}\cdot\mathbf{N}, \mathbf{P}/P^0] = -\chi(\hat{n} \times \mathbf{P}/P^0) \times \mathbf{P}/P^0, \quad (3.6)$$

$$[i\chi\hat{n}\cdot\mathbf{N}, \tilde{\mathbf{W}}] = -\chi(\hat{n} \times \mathbf{P}/P^0) \times \tilde{\mathbf{W}}. \quad (3.7)$$

For $\mathbf{G}$, again we have a similar formula. *Thus it is seen that the three constant length and mutually orthogonal operators*

$$\mathbf{P}/P^0, \quad \tilde{\mathbf{W}}, \quad \text{and} \quad \tilde{\mathbf{G}},$$

with

$$(\mathbf{P}/P^0)^2 = 1, \quad \tilde{\mathbf{W}}^2 = \tau^2 = \tilde{\mathbf{G}}^2, \quad (3.8)$$

and

$$\mathbf{P}\cdot\tilde{\mathbf{W}} = \mathbf{P}\cdot\tilde{\mathbf{G}} = \tilde{\mathbf{W}}\cdot\tilde{\mathbf{G}} = 0,$$

rotate as rigidly fixed axes not only under rotations, but under pure Lorentz transformations as well. Under the latter, the rotations are, of course, determined by those of $\mathbf{P}$ about the axes $\hat{n} \times \mathbf{P}$. [The angle of rotation is given, for example, by formula (A19) of Ref. 3]. Thus a "symmetric top-like" behavior (with two axes $\tilde{\mathbf{W}}$ and $\tilde{\mathbf{G}}$ of equal length) is generalized under the whole Lorentz group.

A more explicitly four-dimensional point of view in constructing projections of W, which include (3.1), is as follows.

Using

$$P^2 = 0$$

and

$$W \wedge W = i(P \wedge W)^*, \quad (3.9)$$

i.e.,

$$[W^\mu, W^\nu] = i\epsilon_{\mu\nu\rho\delta}(P^\rho W^\delta - P^\delta W^\rho),$$

one can show that the components of

$$W_{(n)} = \left(W - \frac{W\cdot n}{P\cdot n}P\right), \quad (3.10)$$

n being any c-number 4-vector, commute, namely

$$W_{(n)} \wedge W_{(n)} = 0. \quad (3.11)$$

Of these four components only two are independent, since

$$P\cdot W_{(n)} = 0 = n\cdot W_{(n)}. \quad (3.12)$$

Also

$$W_{(n)}\cdot W_{(n)} = W^2. \quad (3.13)$$

Moreover, as a consequence of (3.11), the components of the tensor

$$P \wedge W_{(n)} = P \wedge W \tag{3.14}$$

commute mutually.

For

$$n = (1,0),$$

we get

$$W_{(n)} = (0, \tilde{\mathbf{W}}). \tag{3.15}$$

The choice

$$n = (1,0,0,1) \tag{3.16}$$

would correspond more directly to the operators of the little group E_2.[6]

Let us now consider the basis $|p,\tau\rangle$, such that

$$\begin{aligned} P^\mu |p,\tau\rangle &= p^\mu |p,\tau\rangle, \\ \tilde{\mathbf{W}} |p,\tau\rangle &= \tau |p,\tau\rangle, \end{aligned} \tag{3.17}$$

with

$$\mathbf{p}\cdot\boldsymbol{\tau} = 0.$$

Corresponding to the eigenvalues of P^μ, (3.18)

$$p_{(0)} = (\omega, 0, 0, \omega),$$

we have from (3.1)

$$\begin{aligned} \tilde{W}^1_{(0)} &= \omega(M^1 + N^2) = \omega\pi^1, \quad \text{say,} \\ \tilde{W}^2_{(0)} &= \omega(M^2 + N^1) = \omega\pi^2, \quad \text{say,} \\ \tilde{W}^3_{(0)} &= 0. \end{aligned} \tag{3.19}$$

As is well known (M^3, π^1, π^2) constitute the usual little group E_2 for lightlike momentum.

Thus, we see that for $p_{1,2} = 0$, the $|p,\tau\rangle$ basis coincides with $|p,\pi\rangle$ basis, which diagonalizes the continuous generators of the usual little group.[7] We can, of course, construct, at will, operators which coincide with π_1 and π_2 for $\mathbf{p}$ parallel to the z axis, having other null components or not. Among these, $\tilde{\mathbf{W}}$ corresponds to a maximal simplicity in the following sense. In considering the transformation properties of the momentum states we have in any case to take into account the parameters corresponding to the transformation undergone by p^μ. For states labeled by the eigenvalues of $P^0, \mathbf{p}, \tilde{\mathbf{W}}$, the above-mentioned parameters are all that we need, since, as we pass to other frames, τ rotates as if rigidly attached to $\mathbf{p}$.

Thus we have the extremely simple transformation property that for any transformation Λ of HLG (homogeneous Lorentz group) such that the direction $\hat{p}$ or $(\equiv \mathbf{p}/|\mathbf{p}|)$ undergoes a rotation, R,

$$U(\Lambda)|p^0,\hat{p},\tau\rangle = |p^{0\prime},\hat{p}',\tau'\rangle, \tag{3.20}$$

where

$$\hat{p}' = R\cdot\hat{p} \quad \text{and} \quad \tau' = R\cdot\tau.$$

The necessary group properties are satisfied without even additional phase factors. In this sense, the simplicity achieved is comparable to that of the zero-spin case. Our basis states are, however, more singular due to the presence of continuous parameters corresponding to a rotation 0 to 2π in a plane orthogonal to $\mathbf{p}$. It is convenient to parametrize the states by starting from one basic configuration, say,

$$\mathbf{p}_{(0)} = |\mathbf{p}|(0,0,1) \tag{3.21}$$

and

$$\tau_{(0)} = \tau(1,0,0).$$

The general states can then be labeled as

$$\left|\begin{matrix} p^0\tau \\ \Omega \end{matrix}\right\rangle, \tag{3.22}$$

where

$$\Omega \equiv (\varphi, \theta, \psi)$$

corresponds to the rotation $R(\varphi,\theta,\psi)$ such that

$$R(\varphi,\theta,\psi)(\mathbf{p}_{(0)},\tau_{(0)}) = (\mathbf{p},\tau). \tag{3.23}$$

Unlike the zero- or the discrete-spin case, we have to consider explicitly not only θ, φ (sufficing for $\mathbf{p}$) but also ψ, since we have something like a rigid body rotation. We adopt the invariant normalization

$$\left\langle\begin{matrix} p^{0\prime}\tau' \\ \Omega \end{matrix}\middle|\begin{matrix} p^0\tau \\ \Omega \end{matrix}\right\rangle = \frac{2}{p^{0}\tau}\delta(|\mathbf{p}'|-|\mathbf{p}|)\delta(\Omega'-\Omega)\delta(\tau'-\tau), \tag{3.24}$$

the corresponding completeness relation being

$$I = \int d\tau\, d|\mathbf{p}|\, d\Omega \left(\frac{\tau p^0}{2}\right) \left|\begin{matrix} p^0\tau \\ \Omega \end{matrix}\right\rangle \left\langle\begin{matrix} p^0\tau \\ \Omega \end{matrix}\right|, \tag{3.25}$$

where

$$\begin{aligned} \delta(\Omega - \Omega') &= \frac{8\pi^2}{\sin\theta}\,\delta(\varphi-\varphi')\delta(\theta-\theta')\delta(\psi-\psi') \\ \text{and} \quad d\Omega &= (1/8\pi^2)\sin\theta d\varphi\, d\theta\, d\Omega. \end{aligned} \tag{3.26}$$

In Ref. 1, we will use systematically the energy angular momentum states $\left|\begin{matrix} p^0\mu \\ jj_3 \end{matrix}\right\rangle$, such that

$$\begin{aligned} &(P^0, \mathbf{M}\cdot\mathbf{P}/|\mathbf{P}|, \mathbf{M}^2, M_3)\left|\begin{matrix} p^0\mu \\ jj_3 \end{matrix}\right\rangle \\ &\quad = (p^0, \mu, j(j+1), j_3)\left|\begin{matrix} p^0\mu \\ jj_3 \end{matrix}\right\rangle. \end{aligned} \tag{3.27}$$

Using the results of the following section [and (3.27)] regarding the matrix elements of $\mathbf{P}$ and

$\tilde{\mathbf{W}}$ on the basis $\left|\begin{matrix} p^0\mu \\ jj_3 \end{matrix}\right\rangle$, we can show that [consistent with (3.24)]

$$\left\langle \tau' \begin{matrix} p_0'\mu \\ jj_3 \end{matrix} \middle| \begin{matrix} p_0\tau \\ \Omega \end{matrix} \right\rangle = \frac{2}{p_0\tau}\,\delta(p_0' - p_0)\delta(\tau' - \tau)\left(\frac{2j+1}{8\pi^2}\right)^{1/2} \times \mathfrak{D}^j_{j_3\mu}(\varphi,\theta,\psi) \tag{3.28}$$

(corresponding to the symmetric toplike behavior of $|\mathbf{p},\tau\rangle$). This result differs from that for the usual momentum-helicity ket through the factor

$$(2\pi)^{-1/2}e^{-i\psi\mu}.$$

4. MATRIX ELEMENTS OF $\tilde{\mathbf{W}}$ ON (p_0,μ,j,j_3) BASIS (ROTATION-INVARIANT HELICITY LADDER OPERATORS)

We will use these matrix elements in the following section [as in (3.27)]. In Ref. 1, extensive use was made of the operators

$$\tilde{\mathbf{W}}\cdot\mathbf{M} \quad \text{and} \quad \mathbf{P}\times\tilde{\mathbf{W}}\cdot\mathbf{M}, \tag{4.1}$$

where

$$\tilde{\mathbf{W}} = \left(\mathbf{W} - \frac{P^0W^0}{|\mathbf{P}|^2}\,\mathbf{P}\right).$$

These operators commute with P^0 and $\mathbf{M}$, but change the helicity values (μ) by ±1. Hence, combining these two as in (4.6), we obtain "helicity ladder operators" commuting with P^0 and $\mathbf{M}$. The derivation of the matrix elements of $\mathbf{W}$ in Appendix A holds for all the cases ($P^2 \gtrless 0$).

For zero mass we have the matrix elements of the $E_3^{(2)}$ algebra (3.3). For positive mass m, we could have considered the algebra formed by $\mathbf{M},\mathbf{P},\mathbf{S}$, where

$$\mathbf{S} = (1/m)[\mathbf{W} - (W^0/P^0 + m)\mathbf{P}].$$

However, in order to treat all cases in a uniform fashion, we write the matrix elements as follows:

$$\begin{aligned}\tilde{W}^3\left|\begin{matrix} p^0\mu \\ jj_3 \end{matrix}\right\rangle &= \frac{[(j+1)^2 - j_3^2]^{1/2}}{(j+1)[(2j+1)(2j+3)]^{1/2}}\left[\alpha_{(+)}\{(j+\mu+2)(j+\mu+1)\}^{1/2}\left|\begin{matrix} p^0\,\mu+1 \\ j+1j_3 \end{matrix}\right\rangle\right.\\ &\left. - \alpha_{(-)}\{(j-\mu+2)(j-\mu+1)\}^{1/2}\left|\begin{matrix} p^0\,\mu-1 \\ j+1j_3 \end{matrix}\right\rangle\right] - \frac{j_3}{j(j+1)}\left[\alpha_{(+)}\{(j-\mu)(j+\mu+1)\}^{1/2}\left|\begin{matrix} p^0\,\mu+1 \\ jj_3 \end{matrix}\right\rangle\right.\\ &\left. + \alpha_{(-)}\{(j+\mu)(j-\mu+1)\}^{1/2}\left|\begin{matrix} p^0\,\mu-1 \\ jj_3 \end{matrix}\right\rangle\right] + \frac{[j^2 - j_3^2]^{1/2}}{j[(2j-1)(2j+1)]^{1/2}}\\ &\times\left[-\alpha_{(+)}\{(j-\mu)(j-\mu-1)\}^{1/2}\left|\begin{matrix} p^0\,\mu+1 \\ j-1j_3 \end{matrix}\right\rangle + \alpha_{(-)}\{(j+\mu)(j+\mu-1)\}^{1/2}\left|\begin{matrix} p^0\,\mu-1 \\ j-1j_3 \end{matrix}\right\rangle\right],\end{aligned} \tag{4.2}$$

where

$$\alpha_{(\pm)} = \tfrac{1}{2}[-W^2 - P^2\mu(\mu\pm1)]^{1/2}. \tag{4.3}$$

The action of the other components of $\tilde{\mathbf{W}}$ can be obtained as usual by commuting $\tilde{\mathbf{W}}^3$ with $(M_1 \pm iM_2)$. From these results we obtain

$$\tilde{\mathbf{W}}\cdot\mathbf{M}\left|\begin{matrix} p^0\mu \\ jj_3 \end{matrix}\right\rangle = -\left[\alpha_{(+)}\{(j-\mu)(j+\mu+1)\}^{1/2}\left|\begin{matrix} p^0\,\mu+1 \\ jj_3 \end{matrix}\right\rangle + \alpha_{(-)}\{(j+\mu)(j-\mu+1)\}^{1/2}\left|\begin{matrix} p^0\,\mu+1 \\ jj_3 \end{matrix}\right\rangle\right] \tag{4.4}$$

and

$$\begin{aligned}\frac{\mathbf{P}}{|\mathbf{P}|}\times\tilde{\mathbf{W}}\cdot\mathbf{M}\left|\begin{matrix} p^0\mu \\ jj_3 \end{matrix}\right\rangle &= i\left[\frac{\mathbf{P}\cdot\mathbf{M}}{|\mathbf{P}|},\tilde{\mathbf{W}}\cdot\mathbf{M}\right]\left|\begin{matrix} p^0\mu \\ jj_3 \end{matrix}\right\rangle = -i\left[\alpha_{(+)}\{(j-\mu)(j+\mu+1)\}^{1/2}\left|\begin{matrix} p^0\,\mu+1 \\ jj_3 \end{matrix}\right\rangle\right.\\ &\left. - \alpha_{(-)}\{(j+\mu)(j-\mu+1)\}^{1/2}\left|\begin{matrix} p^0\,\mu-1 \\ jj_3 \end{matrix}\right\rangle\right].\end{aligned} \tag{4.5}$$

Hence the helicity ladder operators (commuting with P^0 and $\mathbf{M}$) are seen to be

$$[\tilde{\mathbf{W}} \mp i(\mathbf{P}/|\mathbf{P}|)\times\tilde{\mathbf{W}}]\cdot\mathbf{M}. \tag{4.6}$$

Let us now note that for

(a) $P^2 = m^2$, $W^2 = -m^2S(S+1)$,
$2\alpha_{(\pm)} = m[S(S+1) - \mu(\mu\pm1)]^{1/2}$, (4.7)

(b) $P^2 = 0$, $W^2 = -\tau^2$, $2\alpha_{(\pm)} = \tau$, (4.8)

(c) $P^2 = -m^2$, $W^2 = m^2K(K+1)$,
$2\alpha_{(\pm)} = m[-K(K+1) + \mu(\mu\pm1)]^{1/2}$
$= im[K(K+1) - \mu(\mu\pm1)]^{1/2}$, (4.9)

where, for example, for the principal series of $SU(1,1)$,

$$K = (-\tfrac{1}{2} + i\eta) \text{ or } K(K+1) = -(\tfrac{1}{4} + \eta^2), \quad (4.10)$$

and for the discrete series (with $n = 1, 2, \cdots$)

$$K = -n/2 \text{ or } K(K+1) = n/2(n/2-1), \quad \text{with } |\mu| \geq n/2. \quad (4.11)$$

These are the cases we need in Ref. 1.

5. DEFORMATION OF CONTINUOUS SPIN TO SPACELIKE REPRESENTATIONS

This type of deformations have already been introduced in Sec. 4 of Ref. 8. Here we will consider it in more detail.

Let us start with a representation with

$$P^2 = 0, \quad W^2 = -\tau^2. \quad (5.1)$$

Then, using the definition (2.23') of G^μ, we can show that each of the two 4-vectors,

$$\hat{P}^\mu_{(\pm)} = (\pm)\, G^\mu + \eta P^\mu, \quad (5.2)$$

satisfy, along with $(\mathbf{N}, \mathbf{M})$, a Poincaré algebra. The arbitrary parameter η has to be real for $\hat{P}$ to be Hermitian. Moreover,

$$\hat{P}^2_{(\pm)} = -\tau^2, \quad (5.3)$$

and

$$\hat{W}^2_{(\pm)} = -\tau^2(\tfrac{1}{4} + \eta^2) = \tau^2(-\tfrac{1}{2} + i\eta)(-\tfrac{1}{2} + i\eta + 1), \quad (5.4)$$

where $\hat{W}$ has been defined as in (2.23) in terms of $\hat{P}$. Thus we are led to a spacelike representation with the continuous-spin parameter playing the role of the mass and the deformation parameter η corresponding to that of the unitary principal series representation of the little group $SU(1,1)$.

Corresponding to the ambiguity of sign in (5.2), the operators $\hat{P}'_{(\pm)}$ can be related through a kind of time reversal by choosing to define this operation through the auxiliary operators P^μ, as $T(p^0, \mathbf{p})T^{-1} = (p^0, -\mathbf{p})$. But, also,

$$\hat{P}^\mu_{(+,\eta)} = -\hat{P}^\mu_{(-,-\eta)}. \quad (5.5)$$

Since the representations $\pm\eta$ of $SU(1,1)$ are equivalent, and both signs of energy are included for spacelike representations, diagonalizing $\hat{P}_{(+)}$ or $\hat{P}_{(-)}$, we obtain the same irreducible basis.

From now on, we will consider only one sign (+) for the sake of simplicity and write $\hat{P}^\mu_{(+)}$ as $\hat{P}^\mu$. We would now like to derive the transformation coefficients

$$\left\langle \begin{matrix} \hat{p}_0 \hat{\mu} \\ j j_3 \end{matrix} \middle| \begin{matrix} p_0 \mu \\ j j_3 \end{matrix} \right\rangle.$$

We propose to do this in two steps.

Let us first consider the intermediate basis

$$\left| \begin{matrix} \hat{p}_0 \mu \\ j j_3 \end{matrix} \right\rangle.$$

This is possible since $(\mathbf{N}\cdot\mathbf{P} + \mathbf{P}\cdot\mathbf{N})$, appearing in $\hat{P}^0$, commutes with μ. In fact, using (2.11) or (2.13), we have

$$p_0 \left\langle \begin{matrix} \hat{p}_0 \mu \\ j j_3 \end{matrix} \middle| \begin{matrix} p_0 \mu \\ j j_3 \end{matrix} \right\rangle = [-i(p_0^2 \partial_{0} + \tfrac{3}{2} p_0) + \eta p_0] \left\langle \begin{matrix} \hat{p}_0 \mu \\ j j_3 \end{matrix} \middle| \begin{matrix} p_0 \mu \\ j j_3 \end{matrix} \right\rangle, \quad (5.6)$$

or

$$\left\langle \begin{matrix} \hat{p}_0 \mu \\ j j_3 \end{matrix} \middle| \begin{matrix} p_0 \mu \\ j j_3 \end{matrix} \right\rangle = C(\hat{p}_0) p_0^{-(3/2 + i\eta)} e^{-i p_0/p_0}. \quad (5.7)$$

(For the sake of simplicity we consider only positive p_0, $\epsilon = 1$.)

In order to determine $C(\hat{p}_0)$, let us first note that due to the presence of both signs of the energy we have for spacelike representations the completeness relation (limiting ourselves to a fixed η and τ for the moment)

$$I = \sum_\mu \int d^4\hat{p}\, \delta(\hat{p}^2 + \tau^2) |\hat{p}\,\mu\rangle\langle\mu\hat{p}\,| = \sum_\mu \int_0^\infty d|\hat{\mathbf{p}}| \frac{\hat{\mathbf{p}}^2}{2|\hat{p}_0|} \int d\Omega \sum_{\epsilon=\pm 1} \left| \begin{matrix} \epsilon, |\hat{\mathbf{p}}| \\ \mu, \Omega \end{matrix} \right\rangle \left\langle \begin{matrix} \epsilon, |\hat{\mathbf{p}}| \\ \mu, \Omega \end{matrix} \right| = \sum_\mu \int_0^\infty d|\hat{p}_0| \frac{|\hat{\mathbf{p}}|}{2} \int d\Omega \left[\sum_{\epsilon=\pm 1} \left| \begin{matrix} \epsilon, |\hat{\mathbf{p}}| \\ \mu, \Omega \end{matrix} \right\rangle \left\langle \begin{matrix} \epsilon, |\hat{\mathbf{p}}| \\ \mu, \Omega \end{matrix} \right| \right]$$

[μ or $\hat{\mu}$ can be used and $\Omega = \Omega(\theta, \varphi)$]. (5.8)

The corresponding relation for the rotational basis is obtained on replacing the Ω-integration by sums of (j, j_3). Inserting this latter relation in

$$\frac{2\delta(p_0' - p_0)}{p_0} \delta_{\mu'\mu} = \left\langle \begin{matrix} p_0' \mu' \\ j j_3 \end{matrix} \middle| I \middle| \begin{matrix} p_0 \mu \\ j j_3 \end{matrix} \right\rangle$$

and, using (5.7), we obtain (apart from a phase)

$$C_{(\pm)}(\hat{p}_0) = (2/\pi|\hat{\mathbf{p}}|)^{1/2}. \quad (5.9)$$

This corresponds to the normalization

$$\left[\left\langle \tau \begin{matrix} \hat{p}_0' \mu' \\ j' j_3' \end{matrix} \middle| \begin{matrix} \hat{p}_0 \mu_\tau \\ j j_3 \end{matrix} \right\rangle + \left\langle \tau \begin{matrix} -\hat{p}_0' \mu' \\ j' j_3' \end{matrix} \middle| \begin{matrix} -\hat{p}_0 \mu_\tau \\ j j_3 \end{matrix} \right\rangle \right] = \delta_{\mu\mu'} \delta_{jj'} \delta_{j_3 j_3'} \times [2/(\hat{p}_0^2 + \tau^2)^{1/2}] \delta(\hat{p}_0' - \hat{p}_0). \quad (5.10)$$

The consistency can be verified by inserting the completeness relation for the p^0 states in (5.10). In considering a larger space by including a factor $\delta(\eta' - \eta)$ in (5.10), we should remember the equivalence of η and $-\eta$, and hence restrict the range of η to zero and positive, or negative values only.

Let us now consider the passage to the states

$$\left|\begin{matrix}\hat{p}_0\hat{\mu}\\ jj_3\end{matrix}\right\rangle$$

corresponding to the diagonalization of $\hat{\mathbf{P}}\cdot\mathbf{M}/|\hat{\mathbf{P}}|$. We have

$$\hat{\mathbf{P}}\cdot\mathbf{M} = (\mathbf{G}+\eta\mathbf{P})\cdot\mathbf{M},$$

$$= \left(\mathbf{G} - G^0\frac{\mathbf{P}}{P^0}\right)\cdot\mathbf{M} + (G^0+\eta P^0)\frac{\mathbf{P}\cdot\mathbf{M}}{P^0}, \quad (5.11)$$

$$= \frac{\mathbf{P}}{P^0}\times\tilde{\mathbf{W}}\cdot\mathbf{M} + \hat{P}_0\frac{\mathbf{P}\cdot\mathbf{M}}{P^0}. \quad (5.12)$$

Hence, using (4.5), we have

$$\frac{\hat{\mathbf{P}}\cdot\mathbf{M}}{|\hat{\mathbf{P}}|}\left|\begin{matrix}\hat{p}_0\mu\\ jj_3\end{matrix}\right\rangle = -\frac{i}{2}\sin\hat{\theta}\left([(j-\mu)(j+\mu+1)]^{1/2}\times\left|\begin{matrix}\hat{p}_0\mu+1\\ jj_3\end{matrix}\right\rangle - [(j+\mu)(j-\mu+1)]^{1/2}\left|\begin{matrix}\hat{p}_0\mu-1\\ jj_3\end{matrix}\right\rangle\right) + \cos\hat{\theta}\mu\left|\begin{matrix}\hat{p}_0\mu\\ jj_3\end{matrix}\right\rangle, \quad (5.13)$$

where, using $\hat{\mathbf{p}}^2 = \hat{p}_0^2 + \tau^2$, we have defined

$$\sin\hat{\theta} = \tau/|\hat{\mathbf{p}}| \text{ and } \cos\hat{\theta} = \hat{p}_0/|\hat{\mathbf{p}}|. \quad (5.14)$$

Hence, we obtain,

$$\left|\begin{matrix}\hat{p}_0\hat{\mu}\\ jj_3\end{matrix}\eta\right\rangle = \sum_\mu\left|\begin{matrix}\hat{p}_0\mu\\ jj_3\end{matrix}\eta\right\rangle\mathfrak{D}^j_{\mu\hat{\mu}}(o,-\hat{\theta},-\pi/2). \quad (5.15)$$

Thus, finally,

$$\left|\begin{matrix}\hat{p}_0\hat{\mu}\\ jj_3\end{matrix}\eta\right\rangle = (2\pi|\hat{\mathbf{p}}|)^{-1/2}\sum_\mu\int_0^\infty dp^0\, p_0^{-(1/2-i\eta)}\, e^{i\hat{p}_0/p_0}\times\mathfrak{D}^j_{\mu\hat{\mu}}(o,-\hat{\theta},-\pi/2)\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\tau\right\rangle,\ \hat{p}_0^2 = -\tau^2+\mathbf{p}^2. \quad (5.16)$$

We would like to add that for the discrete series (see 4.11), or the supplementary series of spacelike representations, we have to replace η in (5.2) by $\pm i(K+1/2)$. A pair of such nonunitary representations can be used to define a scalar product exactly as for the spinor representation; namely, we define the scalar product either as

$$_{\mp i(K+1/2)}\langle|\rangle_{\pm i(K+1/2)}, \quad (5.17)$$

or by doubling the components by coupling the two types (just as for the Dirac equation) and introducing a metric

$$\left|\begin{matrix}I\\ I\end{matrix}\right|. \quad (5.18)$$

Again, defining

$$\hat{P}^\mu_{(\pm)} = \pm iG^\mu + \tfrac{1}{2}(2S+1)P^\mu, \quad (5.19)$$

we get such a pair of timelike representations [$P^2 = \tau^2$ and $W^2 = -\tau^2 S(S+1)$]. Scalar products can again be defined exactly as for the preceding case.

6. A CLASS OF NONUNITARY SPACELIKE REPRESENTATIONS

So far we have mainly considered unitary representations (except at the end of Sec. 5).

For $P^2 = -m^2$, an interesting class of nonunitary representations can be obtained by constructing [in closest possible analogy with (2.2)] the generators as

$$\mathbf{M} = -i\mathbf{P}\times\frac{\partial}{\partial\mathbf{P}} + \mathbf{S},$$
$$\mathbf{N}_{(\pm)} = -iP^0\frac{\partial}{\partial\mathbf{P}} + \frac{\mathbf{S}\times\mathbf{P}}{P^0\pm im}. \quad (6.1)$$

A scalar product can be defined exactly as for (5.17) or (5.18), namely as

$$_{(\mp)}\langle|\rangle_{(\pm)} \text{ or through a metric } \left|\begin{matrix}I\\ I\end{matrix}\right|, \quad (6.2)$$

where the I is now $(2S+1)$-dimensional unit matrix. From (6.1), we obtain

$$W^2 = m^2S(S+1). \quad (6.3)$$

Thus W is now a timelike vector.

These representations can be transformed to the spinor representations through a generalization of the canonical transformation treated elsewhere,[9] since in this case the Lorentz transformation reducing $\mathbf{P}$ to rest is a complex one.

Such representations may be of interest in considering exchanges of particles of definite spin S [we have $-W^2/P^2 = S(S+1)$ exactly as for real spin-S particles] and spacelike momenta.

APPENDIX

From the known results of the E_3 algebra (the general case $I0_n$ is discussed in Ref. 10), we can, using suitable phase conventions, write down the matrix elements

$$M^3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle = j_3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle,\quad (M^1\pm iM^2)\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle = [(j\mp j_3)\pm(j\pm j_3+1)]^{1/2}\left|\begin{matrix}p^0\mu\\ j\pm j_3\pm 1\end{matrix}\right\rangle, \quad (A1)$$

and

$$P^3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle = \frac{|\mathbf{p}|}{(j+1)}\left[\frac{(j+1)^2-\mu^2}{(2j+1)(2j+3)}\right]^{1/2}[(j+1)^2-j_3^2]^{1/2}\left|\begin{matrix}p^0\mu\\ j+1\,j_3\end{matrix}\right\rangle$$

$$+|\mathbf{p}|\frac{\mu j_3}{j(j+1)}\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle+\frac{|\mathbf{p}|}{j}\left[\frac{(j^2-\mu^2)}{(2j-1)(2j+1)}\right]^{1/2}[j^2-j_3^2]^{1/2}\left|\begin{matrix}p^0\mu\\ j-1\,j_3\end{matrix}\right\rangle. \tag{A2}$$

The matrix elements of $(P_1 \pm iP_2)$ are obtained on commuting P_3 with $(M_1 \pm iM_2)$.

In order now to obtain the matrix elements of $\mathbf{W}$ on this basis, we will utilize the basic relations

$$\begin{aligned}&\mathbf{W}\times\mathbf{W} = i(P^0\mathbf{W}-W^0\mathbf{P}),\\ &\mathbf{P}\cdot\mathbf{W} = P^0W^0 = P^0\mathbf{P}\cdot\mathbf{M},\\ &[P^i, W^j]=0,\\ &\mathbf{W}^2 = -W^2+W_0^2 = -W^2+(\mathbf{P}\cdot\mathbf{M})^2,\end{aligned} \tag{A3}$$

and others obtainable from them.

Thus, for example, using

$$[\mathbf{P}\cdot\mathbf{M},[\mathbf{P}\cdot\mathbf{M},\mathbf{W}]] = \mathbf{P}^2\mathbf{W}-P^0W^0\mathbf{P}, \tag{A4}$$

we obtain easily

$$[1-(\mu'-\mu)^2]\left\langle\begin{matrix}p^0\mu'\\ j'j_3\end{matrix}\right|W^3\left|\begin{matrix}p_0\mu\\ jj_3\end{matrix}\right\rangle$$

$$=\delta_{\mu'\mu}\left(\frac{p_0\mu}{|\mathbf{p}|}\right)\left\langle\begin{matrix}p^0\mu\\ j'j_3\end{matrix}\right|P^3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle. \tag{A5}$$

Hence

$$\left\langle\begin{matrix}p^0\mu\\ j'j_3\end{matrix}\right|W^3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle = \frac{p^0\mu}{|\mathbf{p}|}\left\langle\begin{matrix}p^0\mu\\ j'j_3\end{matrix}\right|P^3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle, \tag{A6}$$

and other nonvanishing matrix elements correspond to

$$\mu' = \mu\pm 1. \tag{A7}$$

(*We see at once that by replacing* $\mathbf{W}$ *by* $\tilde{\mathbf{W}}$ *the term* $\mu'=\mu$ *disappears and the other two are unaffected.*)

Again utilizing the relation

$$[[\mathbf{P}\cdot\mathbf{M}, W^3], P^3] = 0\,, \tag{A8}$$

we obtain

$$\sum_{\mu'j'j''}(\mu'-\mu)\left[\left\langle\begin{matrix}p^0\mu'\\ j''j_3\end{matrix}\right|W^3\left|\begin{matrix}p^0\mu\\ j'j_3\end{matrix}\right\rangle\left\langle\begin{matrix}p^0\mu\\ j'j_3\end{matrix}\right|P^3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle\right.$$

$$\left.-\left\langle\begin{matrix}p^0\mu'\\ j''j_3\end{matrix}\right|P^3\left|\begin{matrix}p^0\mu'\\ j'j_3\end{matrix}\right\rangle\left\langle\begin{matrix}p^0\mu'\\ j'j_3\end{matrix}\right|W^3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle\right]=0. \tag{A9}$$

This leads to simple recursion relations which enable us to factor out completely the j dependence of the matrix elements of W, by starting with the form (corresponding to the usual Wigner–Eckart factorization)

$$W^3\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle = \sum_{\mu'=\mu,\mu\pm1}\left[\left\langle\begin{matrix}p^0\mu'\\ j+1\end{matrix}\right|W\left|\begin{matrix}p^0\mu\\ j\end{matrix}\right\rangle[(j+1)^2-j_3^2]\right.$$

$$\times\left|\begin{matrix}p^0\mu'\\ j+1\,j_3\end{matrix}\right\rangle+\left\langle\begin{matrix}p^0\mu'\\ j\end{matrix}\right|W\left|\begin{matrix}p^0\mu\\ j\end{matrix}\right\rangle j_3\left|\begin{matrix}p^0\mu'\\ jj_3\end{matrix}\right\rangle$$

$$\left.+\left\langle\begin{matrix}p^0\mu'\\ j-1\end{matrix}\right|W\left|\begin{matrix}p^0\mu\\ j\end{matrix}\right\rangle[j^2-j_3^2]^{1/2}\left|\begin{matrix}p^0\mu'\\ j-1\,j_3\end{matrix}\right\rangle\right]. \tag{A10}$$

For $\mu'=\mu$ we have already the relation (A6).

For $\mu'=\mu\pm1$, we obtain from (A9), with a consistent choice of phases,

$$\left\langle\begin{matrix}p^0\ \mu\pm1\\ j+1\end{matrix}\right|W\left|\begin{matrix}p^0\mu\\ j\end{matrix}\right\rangle = \mp\frac{[(j\pm\mu+2)(j\pm\mu+1)]^{1/2}}{(j+1)[(2j+1)(2j+3)]^{1/2}}$$

$$\times\left\langle\begin{matrix}p^0\\ \mu\pm1\end{matrix}\right\|W\left\|\begin{matrix}p^0\\ \mu\end{matrix}\right\rangle,$$

$$\left\langle\begin{matrix}p^0\ \mu\pm1\\ j-1\end{matrix}\right|W\left|\begin{matrix}p^0\mu\\ j\end{matrix}\right\rangle \tag{A11}$$

$$=\pm\frac{[(j\mp\mu)(j\mp\mu-1)]^{1/2}}{j[(2j-1)(2j+1)]^{1/2}}\left\langle\begin{matrix}p^0\\ \mu\pm1\end{matrix}\right\|W\left\|\begin{matrix}p^0\\ \mu\end{matrix}\right\rangle,$$

$$\left\langle\begin{matrix}p^0\ \mu\pm1\\ j\end{matrix}\right|W\left|\begin{matrix}p^0\mu\\ j\end{matrix}\right\rangle$$

$$=\frac{[(j\mp\mu)(j\pm\mu+1)]^{1/2}}{j(j+1)}\left\langle\begin{matrix}p^0\\ \mu\pm1\end{matrix}\right\|W\left\|\begin{matrix}p^0\\ \mu\end{matrix}\right\rangle.$$

Now, using the relation

$$[[\mathbf{P}\cdot\mathbf{M}, W^3], W^3] = W^0P^2-P^0P^3W^3+W^0P_3^2 \tag{A12}$$

and considering, for example, the element

$$\left\langle\begin{matrix}p^0\mu\\ j+2j_3\end{matrix}\right|[[\mathbf{P}\cdot\mathbf{M}, W^3], W^3]\left|\begin{matrix}p^0\mu\\ jj_3\end{matrix}\right\rangle,$$

we finally obtain

$$\left\langle\begin{matrix}p^0\\ \mu\end{matrix}\right\|W\left\|\begin{matrix}p^0\\ \mu-1\end{matrix}\right\rangle\left\langle\begin{matrix}p^0\\ \mu-1\end{matrix}\right\|W\left\|\begin{matrix}p^0\\ \mu\end{matrix}\right\rangle-\left\langle\begin{matrix}p^0\\ \mu\end{matrix}\right\|W\left\|\begin{matrix}p^0\\ \mu+1\end{matrix}\right\rangle$$

$$\times\left\langle\begin{matrix}p^0\\ \mu+1\end{matrix}\right\|W\left\|\begin{matrix}p^0\\ \mu\end{matrix}\right\rangle=\tfrac{1}{2}(p_0^2-\mathbf{p}^2)\mu=\tfrac{1}{2}p^2\mu. \tag{A13}$$

Hence

$$\left\langle {p^0 \atop \mu} \middle\| W \middle\| {p^0 \atop \mu+1} \right\rangle \left\langle {p^0 \atop \mu+1} \middle\| W \middle\| {p^0 \atop \mu} \right\rangle = C - (\tfrac{1}{4})p^2\mu(\mu+1). \quad \text{(A14)}$$

The parameter c is obtained from the relation

$$\mathbf{W}^2 = W_0^2 - W^2, \quad \text{(A15)}$$

giving

$$C = -\tfrac{1}{4}W^2. \quad \text{(A16)}$$

Thus

$$\left\langle {p^0 \atop \mu} \middle\| W \middle\| {p^0 \atop \mu \pm 1} \right\rangle \left\langle {p^0 \atop \mu \pm 1} \middle\| W \middle\| {p^0 \atop \mu} \right\rangle = \tfrac{1}{4}\left[-W^2 - P^2\mu(\mu \pm 1)\right]. \quad \text{(A17)}$$

Putting all the foregoing results together, we obtain finally (4.2).

The above results, put together, give the matrix elements of $\tilde{\mathbf{W}}$ given in (4.2). For $p^2 = 0$ and $\mathbf{W}^2 = \tau^2$ [(4.8)], $(\mathbf{M}, \mathbf{P}, \tilde{\mathbf{W}})$ form the $E_3^{(2)}$ algebra (3.3). If we want to include a third triplet of "translations" (say $\mathbf{V}$) to form (in an obvious notation) an $E_3^{(3)}$ algebra, its matrix elements will be given by those of

$$|\mathbf{V}|\left[\alpha(\mathbf{P}/|\mathbf{P}|) + \beta(\tilde{\mathbf{W}}/\tau) + \gamma(\mathbf{P}/|\mathbf{P}|) \times \tilde{\mathbf{W}}/\tau\right], \quad \text{(A18)}$$

where (α, β, γ) are suitable direction cosines. Putting $\gamma = 0$ and $\alpha = \cos\theta, \beta = \sin\theta$, $(\mathbf{M}, \mathbf{P}, \mathbf{V})$ constitute a general representation of $E_3^{(2)}$, with $\mathbf{P}\cdot\mathbf{V} \neq 0$. Its matrix elements can be written down combining (A1), (A2), and (4.2).

---

[1] A. Chakrabarti, J. Math. Phys. 12, 1822 (1971).
[2] A. Chakrabarti, J. Math. Phys. 7, 949 (1966).
[3] In this paper and also in Ref. 1, ϵ is introduced in such a fashion that M and N both remain invariant under the reflection $P^\mu \to -P^\mu$. The relation of this feature to the crossing properties are discussed in the introduction and Sec. 2D of A. Chakrabarti, J. Math. Phys. 11, 1085 (1970).
[4] In fact, since, for $P^2 = -m^2$, ϵ is not well-defined for $p^0 = 0$, the form (2.14) seems to be more suitable for this case. We have introduced ϵ in (2.11) and (2.12) in order to ensure the property indicated in Ref. 3, though the computation relations are independent of its presence. Besides this, it should be noted that the liberty in choosing a phase factor ± 1 in the representations of T and K introduces corresponding ambiguities of sign.
[5] H. E. Moses, J. Math. Phys. 9, 2039 (1968). It is also of interest to compare our representations for $P^2 < 0$ with those not satisfying the basic condition given by our Eq. (2.5). Thus, for example, compare the corresponding representation of Iu. M. Shirokov, Zh. Eksp. Teor. Fiz. 33, 1196 (1957) [Sov. Phys. JETP 6, 919 (1958)]. The continuous spin representations were introduced in the fundamental paper of Wigner [Ann. Math. (N.Y.) 40, 149 (1939)].
[6] A. Chakrabarti, thesis, University of Paris 1965.
[7] The connection between the bases $|p, \pi\rangle$ and $|p, \mu\rangle$, μ being the discrete eigenvalues of M_3, is given by $\langle\mu|\pi\rangle = (2\pi)^{-1/2} e^{-i\mu\phi}$, where $\pi = \pi(\cos\phi, \sin\phi)$. Strictly speaking, we should use the notation $|[\pi]\rangle$ in order to indicate that half-integral values of μ are included as well. The same holds for the notation τ. This need, however, cause no confusion.
[8] A. Chakrabarti, M. Lévy-Nahas, and R. Sénéor, J. Math. Phys. 9, 1274 (1968).
[9] A. Chakrabarti, J. Math. Phys. 4, 1215 (1963); 5, 1747 (1964) (Appendix A).
[10] A. Chakrabarti, J. Math. Phys. 9, 2087 (1968).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Lorentz Basis of the Poincaré Group. II

A. Chakrabarti
Centre de Physique Théorique de l'Ecole Polytechnique 17, rue Descartes, 75, Paris V, France
(Received 23 June 1970)

The transformation coefficients connecting the momentum and Lorentz bases of the unitary representations of the Poincaré group are derived for timelike, lightlike, and spacelike momenta ($P^2 \gtrless 0$) and for arbitrary spin (i.e., for general values of W^2) in each case.

1. INTRODUCTION

We propose to study in the following sections the transformation coefficients connecting the momentum and the Lorentz basis[1] of the unitarity representations of the Poincaré group. We will make a detailed study of the following cases:

(a) lightlike continuous spin:

$$P^2 = 0, \quad W^2 = -\tau^2 < 0; \quad (1.1)$$

(b) timelike nonzero spin:

$$P^2 = m^2 > 0, \quad W^2 = -m^2 s(s+1), \quad s = \tfrac{1}{2}, 1, \cdots; \quad (1.2)$$

(c) spacelike:

$$P^2 = -m^2 < 0, \quad W^2 = m^2 k(k+1), \quad (1.3)$$

where either

$$k = -\tfrac{1}{2} + i\eta, \quad \eta \text{ real},$$

or $k = -n, \quad n = \tfrac{1}{2}, 1, \ldots$.

(We exclude the case $-\tfrac{1}{2} < k < 0$.)

The zero-mass discrete spin ($P^2 = 0 = W^2$) has already been studied in Ref. 1 and the relatively simple positive-mass zero-spin ($s = 0$) case will be briefly treated in Appendix B.

Hence

$$\left\langle {p^0 \atop \mu} \middle\| W \middle\| {p^0 \atop \mu+1} \right\rangle \left\langle {p^0 \atop \mu+1} \middle\| W \middle\| {p^0 \atop \mu} \right\rangle = C - (\tfrac{1}{4})p^2\mu(\mu+1). \quad \text{(A14)}$$

The parameter c is obtained from the relation

$$\mathbf{W}^2 = W_0^2 - W^2, \quad \text{(A15)}$$

giving

$$C = -\tfrac{1}{4}W^2. \quad \text{(A16)}$$

Thus

$$\left\langle {p^0 \atop \mu} \middle\| W \middle\| {p^0 \atop \mu \pm 1} \right\rangle \left\langle {p^0 \atop \mu \pm 1} \middle\| W \middle\| {p^0 \atop \mu} \right\rangle = \tfrac{1}{4}\left[-W^2 - P^2\mu(\mu \pm 1)\right]. \quad \text{(A17)}$$

Putting all the foregoing results together, we obtain finally (4.2).

The above results, put together, give the matrix elements of $\tilde{\mathbf{W}}$ given in (4.2). For $p^2 = 0$ and $\mathbf{W}^2 = \tau^2$ [(4.8)], $(\mathbf{M}, \mathbf{P}, \tilde{\mathbf{W}})$ form the $E_3^{(2)}$ algebra (3.3). If we want to include a third triplet of "translations" (say $\mathbf{V}$) to form (in an obvious notation) an $E_3^{(3)}$ algebra, its matrix elements will be given by those of

$$|\mathbf{V}|\left[\alpha(\mathbf{P}/|\mathbf{P}|) + \beta(\tilde{\mathbf{W}}/\tau) + \gamma(\mathbf{P}/|\mathbf{P}|) \times \tilde{\mathbf{W}}/\tau\right], \quad \text{(A18)}$$

where (α, β, γ) are suitable direction cosines. Putting $\gamma = 0$ and $\alpha = \cos\theta, \beta = \sin\theta$, $(\mathbf{M}, \mathbf{P}, \mathbf{V})$ constitute a general representation of $E_3^{(2)}$, with $\mathbf{P}\cdot\mathbf{V} \neq 0$. Its matrix elements can be written down combining (A1), (A2), and (4.2).

---

[1] A. Chakrabarti, J. Math. Phys. 12, 1822 (1971).
[2] A. Chakrabarti, J. Math. Phys. 7, 949 (1966).
[3] In this paper and also in Ref. 1, ϵ is introduced in such a fashion that M and N both remain invariant under the reflection $P^\mu \to -P^\mu$. The relation of this feature to the crossing properties are discussed in the introduction and Sec. 2D of A. Chakrabarti, J. Math. Phys. 11, 1085 (1970).
[4] In fact, since, for $P^2 = -m^2$, ϵ is not well-defined for $p^0 = 0$, the form (2.14) seems to be more suitable for this case. We have introduced ϵ in (2.11) and (2.12) in order to ensure the property indicated in Ref. 3, though the computation relations are independent of its presence. Besides this, it should be noted that the liberty in choosing a phase factor ± 1 in the representations of T and K introduces corresponding ambiguities of sign.
[5] H. E. Moses, J. Math. Phys. 9, 2039 (1968). It is also of interest to compare our representations for $P^2 < 0$ with those not satisfying the basic condition given by our Eq. (2.5). Thus, for example, compare the corresponding representation of Iu. M. Shirokov, Zh. Eksp. Teor. Fiz. 33, 1196 (1957) [Sov. Phys. JETP 6, 919 (1958)]. The continuous spin representations were introduced in the fundamental paper of Wigner [Ann. Math. (N.Y.) 40, 149 (1939)].
[6] A. Chakrabarti, thesis, University of Paris 1965.
[7] The connection between the bases $|p, \pi\rangle$ and $|p, \mu\rangle$, μ being the discrete eigenvalues of M_3, is given by $\langle\mu|\pi\rangle = (2\pi)^{-1/2} e^{-i\mu\phi}$, where $\pi = \pi(\cos\phi, \sin\phi)$. Strictly speaking, we should use the notation $|[\pi]\rangle$ in order to indicate that half-integral values of μ are included as well. The same holds for the notation τ. This need, however, cause no confusion.
[8] A. Chakrabarti, M. Lévy-Nahas, and R. Sénéor, J. Math. Phys. 9, 1274 (1968).
[9] A. Chakrabarti, J. Math. Phys. 4, 1215 (1963); 5, 1747 (1964) (Appendix A).
[10] A. Chakrabarti, J. Math. Phys. 9, 2087 (1968).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Lorentz Basis of the Poincaré Group. II

A. Chakrabarti
Centre de Physique Théorique de l'Ecole Polytechnique 17, rue Descartes, 75, Paris V, France
(Received 23 June 1970)

The transformation coefficients connecting the momentum and Lorentz bases of the unitary representations of the Poincaré group are derived for timelike, lightlike, and spacelike momenta ($P^2 \gtrless 0$) and for arbitrary spin (i.e., for general values of W^2) in each case.

1. INTRODUCTION

We propose to study in the following sections the transformation coefficients connecting the momentum and the Lorentz basis[1] of the unitarity representations of the Poincaré group. We will make a detailed study of the following cases:

(a) lightlike continuous spin:

$$P^2 = 0, \quad W^2 = -\tau^2 < 0; \quad (1.1)$$

(b) timelike nonzero spin:

$$P^2 = m^2 > 0, \quad W^2 = -m^2 s(s+1), \quad s = \tfrac{1}{2}, 1, \cdots; \quad (1.2)$$

(c) spacelike:

$$P^2 = -m^2 < 0, \quad W^2 = m^2 k(k+1), \quad (1.3)$$

where either

$$k = -\tfrac{1}{2} + i\eta, \quad \eta \text{ real},$$

or $k = -n, \quad n = \tfrac{1}{2}, 1, \ldots$.

(We exclude the case $-\tfrac{1}{2} < k < 0$.)

The zero-mass discrete spin ($P^2 = 0 = W^2$) has already been studied in Ref. 1 and the relatively simple positive-mass zero-spin ($s = 0$) case will be briefly treated in Appendix B.

The techniques and results of two previous papers[1,2] will be used throughout.

One of the interests of the basis functions we will calculate as the transformation coefficients is the possibility of their use in generalized partial-wave analysis of scattering amplitudes for particles with spin. For particles of zero spin the results of Vilenkin and Smorodinsky[3] and Winternitz *et al.*[4] generalize the expansions in terms of the representations of little groups[5] for different types of momentum transfer in the crossed channels. (References to many important papers on crossed-channel partial-wave analysis will be found in Refs. 4 and 6.) The timelike case is of course relevant for the direct channel also.

For the cases where particles with spin are involved, basis functions corresponding to more general representations of the Lorentz group are needed. One way of constructing basis functions which have mass and spin quantum numbers associated with them is to calculate the transformation coefficients for the different cases indicated at the beginning [(a), (b), and (c)]. For the timelike case with spin (m, s) this problem has been discussed by several authors.[7-9] A common feature of the above works[7-9] is the use of covariant spinor representations for the momentum basis. In our opinion this is not the best approach since it obscures a very simple and fundamental relationship which is at once evident when one uses the canonical basis.[2] This is shown below.

Using the canonical basis, let us write (considering positive energy for the time being)

$$U(\Lambda_{(p)})\,|p, s_3\rangle = |p_{(0)}, s_3\rangle, \tag{1.4}$$

where

$$p_{(0)} = (m, 0, 0, 0)$$

and $\Lambda_{(p)}$ is the pure Lorentz transformation reducing the particle to rest.[10]

Let us now consider the Lorentz basis (which diagonalizes the rotation subgroup). The required transformation coefficient is

$$\begin{aligned}
&\left\langle \begin{matrix} p, s_3 \\ [m, s] \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} [m, s] \right\rangle \\
&\quad \times \left\langle \begin{matrix} p, s_3 \\ [m, s] \end{matrix} \middle| U^{-1}(\Lambda_{(p)})\, U(\Lambda_{(p)}) \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} \right\rangle \\
&\quad = \sum_{j' j_3'} \left\langle \begin{matrix} p_{(0)} s_3 \\ [m, s] \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ j' j_3' \end{matrix} [m, s] \right\rangle \\
&\quad \times \left\langle [m, s] \begin{matrix} \lambda j_0 \\ j' j_3' \end{matrix} \middle| U(\Lambda_{(p)}) \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} [m, s] \right\rangle \\
&\quad = \left\langle \begin{matrix} p_{(0)}, s_3 \\ [m, s] \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ s s_3 \end{matrix} [m, s] \right\rangle \mathfrak{D}^{\lambda j_0}_{s s_3, j j_3}(\Lambda_{(p)}),
\end{aligned} \tag{1.5}$$

where $\mathfrak{D}^{\lambda j_0}(\Lambda_{(p)})$ denotes the finite Lorentz transformation matrix corresponding to $\Lambda_{(p)}$[11] and is obtained from a study of the homogeneous Lorentz group (HLG) only.

Had we used spinor representations, the action of $U(\Lambda_{(p)})$ would have given a superposition of states, and the essential simplicity of (1.4) and (1.5) would have been lost.

The factor $\left\langle p_{(0)}, s_3 \middle| \begin{matrix} \lambda j_0 \\ s s_3 \end{matrix} \right\rangle$ turns out to be quite simple. In fact, using our methods, we can show quite easily (Appendix C) that, with our conventions, one obtains

$$\left\langle p_{(0)}, s_3 \middle| \begin{matrix} \lambda j_0 \\ s s_3 \end{matrix} \right\rangle = a_{(m,s)} e^{i\pi j_0}, \tag{1.6}$$

where $a_{(m,s)}$ depends only on m and s. The phase factor can, of course, be absorbed by a change of convention and $a_{(m,s)}$ can be determined through normalization conditions.

We will, however, give a self-contained derivation of the complete result for the timelike case using our methods since it permits certain simplifications [see the remarks following (1.16)] and permits direct comparison with lightlike and spacelike cases.

It is somewhat surprising that the finite Lorentz transformations[12-15] using the rotational basis and the Lorentz basis functions for real particles with spin[7-9] have been studied as two separate problems, though the direct proportionality of the solutions is evident for the spin-zero case.

For the lightlike and spacelike cases a factorization similar to that of (1.5) is obtained if one uses Lorentz bases which diagonalize the E_2 and $SU(1, 1)$ subgroups, respectively (see Sec. 6). The E_2 subgroup is constituted by the generators $(M^1 + N^2, M^2 - N^1, M^3)$ and the $SU(1, 1)$ subgroup by (N^1, N^2, M^3). The unitarity representations of these subgroups will be supposed to be known, and certain points concerning the Lorentz bases which diagonalize them will be briefly discussed in Sec. 6. But, in this paper, we will be mainly concerned with the so-called canonical Lorentz basis which diagonalizes the rotation subgroup $SU(2)$ and which has been studied in Ref. 1. The diagonalization of the E_2 subgroup has not yet proved to be particularly useful. The diagonalization of $SU(1, 1)$ has been much studied in view of their connection with complex angular momentum and Regge poles.[15-19] However, the $SU(1, 1)$ partial-wave analysis[20] gives only the background and the non-sense terms (of the Regge formalism for particles with spin) and not the sense terms which are, after all, the most interesting ones. These have to be introduced by making other arbitrary assumptions.

Hence the identification of the sequences of singularities obtained on diagonalizing the $SU(1, 1)$ subgroup in the Lorentz basis with the Regge poles themselves is a somewhat arbitrary assertion.

In view of such facts direct passage via the respective little groups for the different types of momentum transfer should not be considered as the one and only interesting way. Other possibilities should be explored. For expansion in generalized partial waves, the essential formal properties of the basis functions to be used are their orthogonality and completeness relations. It is not obligatory to expand first in terms of the little group representations and then generalize.[21] Whatever be the nature of the momentum transfer, the rotation subgroup has always a clear physical significance. As has been discussed at length in Ref. 2, the three cases $p^2 \gtrless 0$ can be discussed in a unified and fruitful manner by starting with the same representation of the $SU(2)$ subgroup for each case. So, in this paper, we make a unified study of all the cases using always the canonical Lorentz basis. We will, so far as this article is concerned, make no attempt to study explicitly the possible applications of the basis functions constructed, but will limit our study to their formal derivations.

The other two subgroups are, however, not to be neglected and certain important results concerning them already emerge as by-products of our solutions, namely, the transformation coefficients between the Lorentz bases diagonalizing the subgroups $SU(2)$, $SU(1,1)$, and $E(2)$, respectively (see Sec. 6).

Now that we have explained what we intend to do and why, let us briefly indicate how we propose to do it. As already stated, the necessary techniques are contained in Refs. 1 and 2. However, for the Lorentz basis we will (considering fixed values of P^2 and W^2) now use the normalization

$$\left\langle \begin{matrix} \lambda' j_0' \\ j' j_3' \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} \right\rangle = \delta_{j_3 j_3'} \delta_{j j'} \delta_{j_0 j_0'} \delta(\lambda - \lambda')(j_0^2 + \lambda^2)^{-1} . \tag{1.7}$$

With this convention and considering different possible values of P^2 and the sign of $P^0 (\epsilon = \pm 1)$, we will write the matrix elements of P^0 as

$$P^0 \left| \begin{matrix} \lambda & j_0 \\ j j_3 \end{matrix} \right\rangle = C_\lambda^{j_0+1, j_0} [(j - j_0)(j + j_0 + 1)]^{1/2} \left| \begin{matrix} \lambda & j_0 + 1 \\ j j_3 \end{matrix} \right\rangle + C_\lambda^{j_0-1, j_0} [(j + j_0)(j - j_0 + 1)]^{1/2} \left| \begin{matrix} \lambda & j_0 - 1 \\ j j_3 \end{matrix} \right\rangle$$

$$+ C_{j_0}^{\lambda+i, \lambda} [(j + i\lambda)(j - i\lambda + 1)]^{1/2} \left| \begin{matrix} \lambda + i & j_0 \\ j j_3 \end{matrix} \right\rangle + C_{j_0}^{\lambda-i, \lambda} [(j - i\lambda)(j + i\lambda + 1)]^{1/2} \left| \begin{matrix} \lambda - i & j_0 \\ j j_3 \end{matrix} \right\rangle, \tag{1.8}$$

where

$$C_\lambda^{j_0 \pm 1, j_0} = \frac{\epsilon e^{\pm i\varphi}}{2(j_0^2 + \lambda^2)} [-W^2 - P^2 j_0(j_0 \pm 1)]^{1/2}, C_{j_0}^{\lambda \pm i, \lambda} = \frac{\epsilon e^{\pm i\varphi'}}{2(j_0^2 + \lambda^2)} [-W^2 - P^2 i\lambda(i\lambda \mp 1)]^{1/2}, \tag{1.9}$$

φ and φ' being phase factors to be chosen suitably.[22] The matrix elements of $W^0 (= \mathbf{p}\cdot\mathbf{M})$ and $G^0 = \frac{1}{2}(\mathbf{N}\cdot\mathbf{P} + \mathbf{P}\cdot\mathbf{N})$ can be obtained from (1.8) by commuting P^0 with the two Casimir operators of the HLG, namely, $\mathbf{N}\cdot\mathbf{M}$ and $\frac{1}{2}(\mathbf{N}^2 - \mathbf{M}^2)$, respectively.[1]

As for the momentum basis, the following main results will be taken from Ref. 2. For all the cases $(p^2 \gtrless 0)$ one can use the momentum helicity basis and its angular decomposition defined as (with μ as the helicity eigenvalue)

$$|p, \mu\rangle = \sum_{j j_3} \left(\frac{2j+1}{4\pi}\right)^{1/2} \mathfrak{D}^j_{j_3 \mu}(\varphi, \theta, -\varphi) \left| \begin{matrix} p^0 \mu \\ j j_3 \end{matrix} \right\rangle, \quad (\mathbf{p} : |\mathbf{p}|, \theta, \varphi) . \tag{1.10}$$

Hence it is sufficient for us to calculate

$$\left\langle \begin{matrix} p^0 \mu \\ j' j_3' \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} \right\rangle = \left\langle \begin{matrix} p_0 \mu \\ j j_3 \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} \right\rangle \delta_{j j'} \delta_{j_3 j_3'} \tag{1.11}$$

when

$$\left\langle p, \mu \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} \right\rangle = \left(\frac{2j+1}{4\pi}\right)^{1/2} \mathfrak{D}^{j*}_{j_3 \mu}(\varphi, \theta, -\varphi) \times \left\langle \begin{matrix} p^0 \mu \\ j j_3 \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} \right\rangle . \tag{1.12}$$

Defining

$$\tilde{\mathbf{W}} = [\mathbf{W} - (P^0 W^0 / \mathbf{P}^2)\mathbf{P}],$$

we have

$$\tfrac{1}{2}(\tilde{\mathbf{W}}\cdot\mathbf{M} \mp i(\mathbf{P}/|\mathbf{P}|) \times \tilde{\mathbf{W}}\cdot\mathbf{M}) \left| \begin{matrix} p^0 \mu \\ j j_3 \end{matrix} \right\rangle$$

$$= -\alpha_{(\pm)} [(j \mp \mu)(j \pm \mu + 1)]^{1/2} \left| \begin{matrix} p^0 \mu \pm 1 \\ j j_3 \end{matrix} \right\rangle, \tag{1.13}$$

where

$$\alpha_{(\pm)} = (e^{\pm i\varphi}/2)[-W^2 - P^2 \mu(\mu \pm 1)]^{1/2} \tag{1.14}$$

and φ is a constant arbitrary phase factor which we will choose by convention so as to make our solutions symmetrical with respect to an interchange of μ and $j_0 (\mu \rightleftharpoons j_0)$.

As shown in Ref. 2, representations can be constructed in a unified fashion for all the cases $(p^2 \gtrless 0)$ such that

$$G^0 = \tfrac{1}{2}(\mathbf{N}\cdot\mathbf{P} + \mathbf{P}\cdot\mathbf{N})$$

$$= -iP^0 \left(\mathbf{P}\cdot\frac{\partial}{\partial \mathbf{P}} + \frac{\partial}{\partial \mathbf{P}}\cdot\mathbf{P}\right)$$

$$= -iP^0 \left(2|\mathbf{P}|\frac{\partial}{\partial |\mathbf{P}|} + 3\right). \tag{1.15}$$

(That is, no extra terms due to spin appear in G^0.)

This relation will be used concerning the action of G^0 on the momentum basis.

We will also use a deformation formula (Ref. 2, Sec. 5) to give an alternative derivation for the spacelike case in terms of the zero-mass continuous-spin solution.

Indeed we have preferred to start with the lightlike case since in many respects it is the simplest one[23] and provides a useful check on the properties of the solutions for the cases

$$P^2 = m^2, \quad W^2 = -m^2 s(s+1),$$

and

$$P^2 = -m^2, \quad W^2 = -m^2(\tfrac{1}{4} + \eta^2),$$

since these must reduce to the continuous-spin solution under suitable limiting conditions.

For each case we first use the matrix elements of the operators

$$P^0, \quad W^0, \quad \tilde{\mathbf{W}}\cdot\mathbf{M}, \quad \mathbf{P}\times\tilde{\mathbf{W}}\cdot\mathbf{M},$$

to obtain difference equations in the parameters μ, j_0, λ. For the limiting values $\pm j$ of μ (or $\pm s$ for $p^2 > 0, j \geq s$) we are able to obtain simple difference equations in j_0 or λ which can be solved immediately.[24] Then the actions of the operators $(P_1 \pm iP_2)$ and G^0 are used successively to extract the remaining dependence on j and p^0 (or $|\mathbf{p}|$ for a given ϵ).

The final step consists (apart from fixing a *constant* normalization factor) in obtaining a solution for an arbitrary value of μ within its range. It is shown that in our formalism this can be reduced to the solution of a difference equation of the type (starting from $\mu = j$, for example)

$$(j_0 + i\lambda)B^{j\mu-1}_{\lambda j_0} + (\mu - i\lambda)B^{j\mu}_{\lambda j_0+1} + (\mu + j_0)B^{j\mu}_{\lambda+i,j} = (\eta x)^{1/2}(j_0 + i\lambda)(\mu - i\lambda)(\mu + j_0)B^{j\mu}_{\lambda j_0},$$

$$\eta = +1, 0, -1 \text{ for } p^2 \gtrless 0, \text{ respectively,} \quad (1.16)$$

where $B^{jj}_{\lambda j_0}$ is already explicitly known. As will be seen, one can write down the solution without undue difficulty. In order to compare with known things,[25] we may consider our solution for the timelike case (4.42).

Indeed, certain results, though concerning the HLG only, can sometimes by obtained in a more convenient form in the context of the larger Poincaré group, since we can use operators to vary not only jj_3 (as does N) but also λ and j_0. This gives a wider choice of recursion relations and we can pick out the most convenient ones. In our opinion, the forms of the finite Lorentz transformation matrix and of the transformation coefficients between the Lorentz bases diagonalizing the rotation and the other two subgroups $[E_2, SU(1,1)]$ that can be obtained as by-products from our solutions are examples of the above-mentioned fact.

It may be noted that our systematic use of the matrix elements of the operators such as P^0 and W^0 permits us to avoid complicated differential difference equations[26] and simplifies considerably our work. We are, of course, obliged to use rather unconventional formal manipulations involving the variations $(\lambda \pm i)$. Matrix elements of this type have been repeatedly discovered and discussed by different authors.[27] However one may choose to interpret them, as has already been emphasized in Ref. 1, they can be used directly as a quite efficient formal tool in certain types of calculations. For simple cases (e.g., the case of zero-spin, zero-mass discrete spin, and finite Lorentz transformation matrix for certain limiting values of the parameters) the known results obtained by other methods can be reproduced fairly effortlessly. But they also enable us to tackle the more complicated cases with relative ease and in a unified fashion. In this paper we content ourselves with exploiting to the full their effectiveness in formal calculations, without attempting rigorous mathematical justifications of the steps involved.

2. CALCULATIONS OF THE COEFFICIENTS $\left\langle \begin{matrix} p^0\mu \\ jj_3 \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ jj_3 \end{matrix} \right\rangle$: RECURSION RELATIONS FOR μ, j_0, AND λ (GENERAL CASE)

Let us introduce for the time being the compact notations [see (1.8)]

$$[j_0 \pm 1] = \left\langle \begin{matrix} \lambda\, j_0 \pm 1 \\ jj_3 \end{matrix} \middle| P^0 \middle| \begin{matrix} \lambda j_0 \\ jj_3 \end{matrix} \right\rangle \left\langle \begin{matrix} p^0\mu \\ jj_3 \end{matrix} \middle| \begin{matrix} \lambda\, j_0 \pm 1 \\ jj_3 \end{matrix} \right\rangle$$

and (2.1)

$$[\lambda \pm i] = \left\langle \begin{matrix} \lambda \pm i\, j_0 \\ jj_3 \end{matrix} \middle| P^0 \middle| \begin{matrix} \lambda j_0 \\ jj_3 \end{matrix} \right\rangle \left\langle \begin{matrix} p^0\mu \\ jj_3 \end{matrix} \middle| \begin{matrix} \lambda \pm i\, j_0 \\ jj_3 \end{matrix} \right\rangle .$$

Then, considering the action of P^0 on the two sides of $\left\langle \begin{matrix} p^0\mu \\ jj_3 \end{matrix} \middle| P^0 \middle| \begin{matrix} \lambda j_0 \\ jj_3 \end{matrix} \right\rangle$, we obtain

$$p^0 \left\langle \begin{matrix} p^0\mu \\ jj_3 \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ jj_3 \end{matrix} \right\rangle = \{[j_0 + 1] + [j_0 - 1]\} + \{[\lambda + i] + [\lambda - i]\}. \quad (2.2)$$

The matrix elements of W^0 [Eq. (2.23) of Ref. 1] give us

$$|\mathbf{p}| \mu \left\langle \begin{matrix} p^0\mu \\ jj_3 \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ jj_3 \end{matrix} \right\rangle = i\lambda\{[j_0 + 1] - [j_0 - 1]\} - j_0\{[\lambda + i] - [\lambda - i]\}. \quad (2.3)$$

Similarly, using the operator $\tilde{\mathbf{W}}\cdot\mathbf{M}$, we have[2]

$$-\left[\alpha_{(+)}\{(j-\mu)(j+\mu+1)\}^{1/2}\left\langle {}^{p\ 0}_{jj_3}{}^{\mu+1}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle + \alpha_{(-)}\{(j+\mu)(j-\mu+1)\}^{1/2}\left\langle {}^{p^0\,\mu-1}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle\right]$$

$$= -p_0\mu^2\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle + (i\lambda)^2\{[j_0+1]+[j_0-1]\} + j_0^2\{[\lambda+i]+[\lambda-i]\} \tag{2.4}$$

$$= -p_0(\mu^2-j_0^2)\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle - (j_0^2+\lambda^2)\{[j_0+1]+[j_0-1]\} \tag{2.5}$$

$$= -p_0(\mu^2+\lambda^2)\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle + (j_0^2+\lambda^2)\{[\lambda+i]+[\lambda-i]\}, \tag{2.6}$$

where we have used (2.2) in deriving (2.5) and (2.6). Again using the operator $\mathbf{P}\times\tilde{\mathbf{W}}\cdot\mathbf{M}^2$ and simplifying the rhs as before by using (2.2) and (2.3), we obtain finally

$$\left[\alpha_{(+)}\{(j-\mu)(j+\mu+1)\}^{1/2}\left\langle {}^{p^0\mu+1}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle - \alpha_{(-)}\{(j+\mu)(j-\mu+1)\}^{1/2}\left\langle {}^{p^0\mu-1}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle\right]$$

$$= |\mathbf{p}|\left(\frac{j_0}{i\lambda}\right)(\mu^2+\lambda^2)\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle + \left(\frac{\mu}{i\lambda}\right)(j_0^2+\lambda^2)\{[\lambda+i]-[\lambda-i]\} \tag{2.7}$$

$$= |\mathbf{p}|\left(\frac{i\lambda}{j_0}\right)(\mu^2-j_0^2)\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle + \left(\frac{\mu}{j_0}\right)(j_0^2+\lambda^2)\{[j_0+1]-[j_0-1]\}. \tag{2.8}$$

(For zero value of j_0 or λ we cannot, of course, put it in the denominator. This need, however, cause no confusion.)

Hence, separating the values $(\mu\pm1)$, we can write

$$2\alpha_{(\pm)}\{(j\mp\mu)(j\pm\mu+1)\}^{1/2}\left\langle {}^{p^0\mu\pm1}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle$$

$$= \left(p_0 \pm |\mathbf{p}|\frac{j_0}{i\lambda}\right)(\mu^2+\lambda^2)\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle + (j_0^2+\lambda^2)$$

$$\times\{(-1\pm\mu/i\lambda)[\lambda+i]+(-1\mp\mu/i\lambda)[\lambda-i]\} \tag{2.9}$$

$$= \left(p_0 \pm |\mathbf{p}|\frac{i\lambda}{j_0}\right)(\mu^2-j_0^2)\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{j_0\lambda}_{jj_3}\right\rangle + (j_0^2+\lambda^2)$$

$$\times\{(1\pm\mu/j_0)[j_0+1]+1\mp\mu/j_0)[j_0-1]\}. \tag{2.10}$$

Let us now consider the expression

$$(j_0+\epsilon i\lambda)\alpha_{(-)}\{(j+\mu)(j-\mu+1)\}^{1/2}\left\langle {}^{p^0\mu-1}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle. \tag{2.11}$$

From (2.9) and (2.10), noting the relation

$$(i\lambda p_0-|\mathbf{p}|j_0)(\mu^2+\lambda^2)+\epsilon(j_0p_0-|\mathbf{p}|i\lambda)(\mu^2-j_0^2)$$
$$= (\epsilon p_0-|\mathbf{p}|)\{j_0(\mu^2+\lambda^2)+\epsilon i\lambda(\mu^2-j_0^2)\}$$
$$-(j_0^2+\lambda^2)(j_0-\epsilon i\lambda)\epsilon p_0 \tag{2.12}$$

and using the expression for

$$(\epsilon p_0-|\mathbf{p}|)\mu\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle$$

as obtained from (2.2) and (2.3), we get after some simplifications the result

$$2(j_0+\epsilon i\lambda)\alpha_{(-)}\{(j+\mu)(j-\mu+1)\}^{1/2}\left\langle {}^{p^0\mu-1}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle$$
$$= (\epsilon p_0-|\mathbf{p}|)\{j_0(\mu^2+\lambda^2)+\epsilon i\lambda(\mu^2-j_0^2)$$
$$+\mu(j_0^2+\lambda^2)\}\left\langle {}^{p^0\mu}_{jj_3}\middle|{}^{j_0\lambda}_{jj_3}\right\rangle - 2\epsilon\{(\mu-\epsilon i\lambda)$$
$$\times[j_0+1]+(\mu+j_0)[\lambda+i\epsilon]\}. \tag{2.13}$$

This expression will turn out to be quite useful later on. An analogous expression can be written with $\left\langle {}^{p^0\mu+1}_{jj_3}\middle|{}^{\lambda j_0}_{jj_3}\right\rangle$ on the left.

Up to this point we have treated the three cases ($P^2 \gtrless 0$) in a unified fashion. Now it becomes more convenient to separate them in order to bring out the particular features for each case and to compare them eventually.

3. THE LIGHTLIKE CONTINUOUS-SPIN CASE

Let us now consider the case $P^2=0$, $W^2=-\tau^2$.

Variation of j_0 and λ (for $\mu=j$)

Let us define (considering for the present a fixed value of τ)

$$\left\langle {}^{p^0\mu}_{jj^3}\middle|{}^{\lambda j_0}_{jj^3}\tau\right\rangle = [(j+\mu)!(j-\mu)!(j+j_0)!$$
$$\times(j-j_0)!(j+i\lambda)!(j-i\lambda)!]^{-1/2}A^{j\mu}_{\lambda j_0}(p_0,\tau)$$
$$\text{always } (z)! = \Gamma(z+1). \tag{3.1}$$

(We will sometimes drop certain indices, when there is no risk of confusion.) Now, putting $\mu=j$ in (2.9) and (2.10), we get finally (corresponding to $\mu+1=j+1$ on the left)

$$0 = [\epsilon(2|\mathbf{p}|/\tau)(j_0+\epsilon i\lambda)A^{jj_0}_{\lambda j_0} + A^{jj}_{\lambda+ij_0} - A^{jj}_{-ij_0}] \tag{3.2}$$

and

$$0 = (j^2 - j_0^2)[(2|\mathbf{p}|/\tau)(j_0 + i\epsilon\lambda)A^{jj}_{\lambda j_0} + A^{jj}_{\lambda j_0+1} - A^{jj}_{\lambda j_0-1}]. \quad (3.3)$$

The solution of (3.2) and (3.3) satisfying the proper symmetry and (as will be shown below) proper normalization conditions turns out to be in terms of the modified Bessel functions of the third kind,[28]

$$A^{jj}_{\lambda j_0}(p_0,\tau) = e^{i\pi j_0} K_{j_0+i\epsilon\lambda}(\tau/|\mathbf{p}|) F_j(p_0,\tau). \quad (3.4)$$

In an analogous manner, putting $j_0 = j$, one can show that

$$A^{j\mu}_{\lambda j}(p_0,\tau) = e^{i\pi\mu} K_{\mu+i\lambda}(\tau/|\mathbf{p}|) F_j(p_0,\tau). \quad (3.5)$$

The same F_j in (3.4) and (3.5) guarantees the symmetry

$$A^{j\alpha}_{\lambda\beta} = A^{j\beta}_{\lambda\alpha} \quad (3.6)$$

(α and β being possible values of j_0 and μ). The values for $\mu = -j$ (or $j_0 = -j$) can be taken to be consistent with the symmetry condition

$$A^{j\mu}_{\lambda j_0} = A^{j-\mu}_{\lambda -j_0}. \quad (3.7)$$

We also have the symmetry

$$A^{jj}_{\lambda j_0} = (\pm) A^{jj}_{-\lambda -j_0}, \qquad A^{j\mu}_{\lambda j} = (\pm) A^{j\mu}_{-\lambda j_0}, \quad (3.8)$$

the positive and the negative signs corresponding, respectively, to integral and half-integral values of j. These again will hold for general values of μ and j_0.

The fundamental symmetry relation

$$K_\nu(z) = K_{-\nu}(z)$$

makes the foregoing results evident.

We will now extract successively the j and p_0 dependence of $F_j(p_0,\tau)$ in (3.4) and (3.5).

Variations of j

Using the matrix elements of $P_\pm (= P^1 \pm iP^2)$ on the energy rotation states (Ref. 2, Appendix), we obtain (for $j_3 = j$)

$$-2|\mathbf{p}|\left[\frac{j^2-\mu^2}{(2j)(2j+1)}\right]^{1/2}\left\langle {p^0 \mu \atop jj} \middle| {\lambda j_0 \atop jj}\right\rangle = \left\langle {p^0 \mu \atop j-1\, j-1} \middle| P_- \middle| {\lambda j_0 \atop jj}\right\rangle. \quad (3.9)$$

Now using the matrix elements of P_- on the Lorentz basis[1] we obtain finally for $\mu = j-1$, $j_0 = j$

$$A^{j-1}_{\lambda,j-1}(p_0,\tau) = -i\frac{2p^0}{\tau}\frac{1}{(2j-1)(2j)} A^{j,j-1}_{\lambda,j}(p_0,\tau) \quad (3.10)$$

or, from (3.5),

$$F_{j-1}(p_0,\tau) = \left(-i\frac{2p_0}{\tau}\right)\{(2j-1)(2j)\}^{-1} F_j(p_0,\tau). \quad (3.11)$$

Hence

$$F_j(p_0,\tau) = (2j)!\left(-i\frac{2p_0}{\tau}\right)^{-j} F(p_0,\tau), \text{ say} \quad (3.12)$$

($p_0 = \epsilon|\mathbf{p}|$ for zero mass).

Variation of $|\mathbf{p}|$

We now utilize the basic relation (1.15):

$$2G^0 = -i[P^0, (\mathbf{N}^2 - \mathbf{M}^2)] = (\mathbf{N}\cdot\mathbf{P} + \mathbf{P}\cdot\mathbf{N}) = -iP^0\left(2|\mathbf{p}|\frac{\partial}{\partial|\mathbf{p}|} + 3\right) \quad (3.13)$$

and the matrix elements of G^0 on the Lorentz basis [Eq. (4.3) of Ref. 1]. After some simplifications we obtain

$$\frac{2|\mathbf{p}|}{\tau}(j_0^2 + \lambda^2)\left(|\mathbf{p}|\frac{\partial}{\partial|\mathbf{p}|} + 1\right) A^{j\mu}_{\lambda j_0}(p_0) = j_0[(j-j_0)A^{j\mu}_{\lambda j_0+1}(p_0) - (j+j_0)A^{j\mu}_{\lambda j_0-1}] - i\lambda[(j+i\lambda)A^{j\mu}_{\lambda+ij_0}(p_0) - A^{j\mu}_{\lambda-ij_0}(p_0)(j-i\lambda)]. \quad (3.14)$$

Putting $\mu = j$, we obtain, finally,

$$\frac{2|\mathbf{p}|}{\tau}\left[|\mathbf{p}|\frac{\partial}{\partial|\mathbf{p}|} + (j+1)\right] A^{jj}_{\lambda j_0}(p_0,\tau) = A^{jj}_{\lambda+ij_0}(p_0,\tau) + A^{jj}_{\lambda-ij_0}(p_0,\tau). \quad (3.15)$$

Hence, using (3.14), (3.12), (3.15), and the well-known relation[29]

$$-2K'_\nu(z) = K_{\nu-1}(z) + K_{\nu+1}(z),$$

we obtain

$$F_j(p_0,\tau) = (2j)!\left(-i\frac{2p^0}{\tau}\right)^{-(j+1)} C(\tau). \quad (3.16)$$

The constant $C(\tau)$ will be determined through normalization conditions. (For $P^2 = 0$, the operator $\mathbf{N}\cdot\mathbf{M}$ can also be used conveniently for varying $|\mathbf{p}|$.)

Descent from $\mu = j$

From (2.13) (with $P^2 = 0$), (3.1), and the further definition

$$A^{j\mu}_{\lambda j_0}(p_0,\tau) = \{(j+\mu)!(j-j_0)!(j+i\epsilon\lambda)!\} B^{j\mu}_{\lambda j_0}(p_0,\tau), \quad (3.17)$$

we obtain the quite simple relation

$$(j_0 + i\epsilon\lambda)B^{j\mu-1}_{\lambda j_0} + (\mu - i\epsilon\lambda)B^{j\,\mu}_{\lambda\ j_0+1} + (\mu + j_0)B^{j\ \ \mu}_{\lambda+i\epsilon\, j_0} = 0. \quad (3.18)$$

Let us consider an integer n such that

$$\mu = j - n \geq j_0.$$

It can be shown that by applying (3.18) n times we obtain

$$B^{jj-n}_{\lambda j_0} = (-1)^n \sum_{a=0}^{n} \frac{n!}{a!b!} \frac{(j - i\epsilon\lambda)!(j + j_0)!(j_0 + i\epsilon\lambda - b - 1)!}{(j - i\epsilon\lambda - a)!(j + j_0 - b)!(j_0 + i\epsilon\lambda + a)!}(j_0 + i\epsilon\lambda + \alpha - b)B^{jj}_{\lambda+i\epsilon b, j_0+a},$$

with $a + b = n = j - \mu$. (3.19)

Hence, for $\mu \geq j_0$,

$$A^{j\mu}_{\lambda j_0} = [(-1)^{j-\mu}/(2j)!]\{(j + \mu)!(j - \mu)!(j + j_0)!(j - j_0)!(j + i\lambda)!(j - i\lambda)!\} \times \sum_{a=0}^{j=\mu} \frac{(j_0 + \epsilon i\lambda - b - 1)!(j_0 + \epsilon i\lambda + a - b)A^{jj}_{j_0+a,\lambda+i\epsilon b}}{a!(j + j_0 - b)!(j - j_0 - a)!(j + i\epsilon\lambda - b)!(j - i\epsilon\lambda - a)!(j_0 + i\epsilon\lambda + a)!},$$

with $a + b = j - \mu$, (3.20)

where due to the factors $(j + j_0 - b)!$, $(j - j_0 - a)!$ in the denominator the summation is restricted to

$$(j - j_0) \geq a, (j + j_0) \geq b. \quad (3.21)$$

For $\mu \leq j_0$ we can utilize the symmetry condition (3.6)

$$A^{j\alpha}_{\lambda\beta} = A^{j\beta}_{\lambda\alpha}.$$

The solutions for $A^{j\mu}_{\lambda j_0}$ obtained by starting from other boundary values ($\mu = -j$ or $j_0 = \pm j$) turn out to be equivalent, as they should.

Final Expression

As is shown in Appendix A, the normalization constant in (3.16) is given by

$$C(\tau) = 4/\sqrt{\pi}\tau. \quad (3.22)$$

Thus finally, we can write (for $\mu \geq j_0$)

$$\left\langle \tau \begin{matrix} p^0\mu \\ jj_3 \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ jj_3' \end{matrix} \tau \right\rangle = \delta_{jj'}\delta_{j_3 j_3'}(4/\sqrt{\pi})(i\tau/2p_0)^{(j+1)}\{(j + \mu)!(j - \mu)!(j + j_0)!(j - j_0)!(j + i\lambda)!(j - i\lambda)!\}^{1/2} \times (-1)^{j-\mu+j_0}\sum_{a=0}^{j=\mu} \frac{(-1)^a(j_0 + i\epsilon\lambda - b - 1)!(j_0 + i\epsilon\lambda + a - b)K_{j_0+i\lambda+a-b}(\tau/|\mathbf{p}|)}{a!b!(j + j_0 - b)!(j - j_0 - a)!(j + i\epsilon\lambda - b)!(j - i\epsilon\lambda - a)!(j_0 + i\epsilon\lambda + a)!},$$

$$j + j_0 \geq b, \quad j - j_0 \geq a; \quad a + b = j - \mu. \quad (3.23)$$

The formula (3.23) along with the symmetry relation (3.6) gives the complete solution. If we want to consider a larger space including all possible values of τ, we have to add a factor $\tau^{-1}\delta(\tau - \tau')$ for a set corresponding to τ'.

4. THE TIMELIKE CASE

Let us now consider the case

$$P^2 = m^2 > 0, \quad W^2 = -m^2 s(s + 1).$$

To start with, we define (considering fixed m and s)

$$\left\langle m, s \begin{matrix} p^0\mu \\ jj_3 \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ jj_3 \end{matrix} m, s \right\rangle = \left[\frac{(j + \mu)!(j - \mu)!(j + j_0)!(j - j_0)!(j + i\lambda)!(j - i\lambda)!}{(s + \mu)!(s - \mu)!(s + j_0)!(s - j_0)!(s + i\lambda)!(s - i\lambda)!}\right]^{-1/2} A^{j\mu}_{\lambda j_0}(p_0; m, s). \quad (4.1)$$

We have to consider two cases separately in using (2.9) and (2.10).

Case 1, $j \geq s$: Putting $\mu = s$ in (2.9) and (2.10), we obtain

$$\{(2\epsilon/m)(p_0 i\lambda + |\mathbf{p}|j_0)A^{js}_{\lambda+j_0} + (j + i\lambda)A^{js}_{\lambda+ij_0} - (j - i\lambda)A^{js}_{\lambda ij_0}\} = 0, \quad (4.2)$$

$$(s^2-j_0^2)\{(2\epsilon/m)(p_0j_0+|\mathbf{p}|i\lambda)A^{js}_{\lambda j_0}+(j-j_0)A^{js}_{\lambda j_0+1}-(j+j_0)A^{js}_{\lambda j_0-1}\}=0. \quad (4.3)$$

Case 2, $j \leq s$: Putting $\mu = j$ in (2.9) and (2.10), we obtain

$$\{(2\epsilon/m)(p_0 i\lambda+|\mathbf{p}|j_0)A^{jj}_{\lambda j_0}+(s+i\lambda)A^{jj}_{\lambda+ij_0}-(s-i\lambda)A^{jj}_{\lambda-ij_0}\}=0, \quad (4.4)$$

$$(j^2-j_0^2)\{(2\epsilon/m)(p_0j_0+|\mathbf{p}|i\lambda)A^{jj}_{\lambda j_0}+(s-j_0)\times A^{jj}_{\lambda j_0+1}-(s+j_0)A^{jj}_{\lambda j_0-1}\}=0. \quad (4.5)$$

(Analogous equations can be written for $j_0 = s$ or $j_0 = j$, and the symmetry $\mu \rightleftharpoons j_0$ is always present.)

A special situation occurs for the simplest case, namely $s = 0$. The complete solution for zero spin is briefly derived in Appendix B. Let us now concentrate on the case $s > 0$.

For the sake of the definiteness, we will consider for the present only the positive energy case ($\epsilon = +1$). It is not difficult to see that, as in Sec. 3, a change of sign of p^0 is associated with the substitution $\lambda \to -\lambda$.

For $s > 0$ ($j_0 \neq 0$), it is convenient to introduce the variable

$$x = e^{-2\zeta}, \quad 0 \leq x \leq 1,$$

where

$$p_0 = m\cosh\zeta, \quad |\mathbf{p}| = m\sinh\zeta. \quad (4.6)$$

Case 2, $j \leq s$[30]: Substituting in Eqs. (4.4) and (4.5), in order to eliminate the factors $x^{\pm 1/2}$ which appear, we define

$$A^{jj}_{\lambda j_0}(x) = x^{\pm 1/2(j_0+i\lambda)}\mathfrak{F}^{j(\pm)}_{\lambda j_0}(x). \quad (4.7)$$

We obtain for $\mathfrak{F}^{(+)}$

$$[(j_0+i\lambda)-x(j_0-i\lambda)]\mathfrak{F}^{(+)}_{\lambda j_0}+(s+i\lambda)\mathfrak{F}^{(+)}_{\lambda+ij_0}\times -x(s-i\lambda)\mathfrak{F}^{(+)}_{\lambda-ij_0}=0, \quad (4.8)$$

$$(j^2-j_0^2)\{[(j_0+i\lambda)+x(j_0-i\lambda)]\mathfrak{F}^{(+)}_{\lambda j_0}+x(s-j_0)\times \mathfrak{F}^{(+)}_{\lambda j_0+1}-(s+j_0)\mathfrak{F}^{(+)}_{\lambda j_0-1}\}=0. \quad (4.9)$$

Similarly,

$$[(j_0+i\lambda)-x(j_0-i\lambda)]\mathfrak{F}^{(-)}_{\lambda j_0}+x(s+i\lambda)\mathfrak{F}^{(-)}_{\lambda+ij_0}-(s-i\lambda)\mathfrak{F}^{(-)}_{\lambda-ij_0}=0, \quad (4.10)$$

$$(j^2-j_0^2)\{[(j_0+i\lambda)+x(j_0-i\lambda)]\mathfrak{F}^{(-)}_{\lambda j_0}+(s-j_0)\mathfrak{F}^{(-)}_{\lambda j_0+1}-x(s+j_0)\mathfrak{F}^{(-)}_{\lambda j_0-1}\}=0. \quad (4.11)$$

These equations correspond to well-known recursion relations for hypergeometric functions or polynomials,[31] except for an additional change of sign for the variations $\lambda \to \lambda \pm i$.

As will be seen more explicitly later on, the symmetry $(\lambda, j_0) \to (-\lambda, -j_0)$, and more particularly the required limiting form (as $m \to 0$, $s \to \infty$, such that $ms \to \tau$) corresponding to the result of Sec. 3, namely

$$e^{i\pi j_0}K_{j_0+i\lambda}(\tau/p_0),$$

leads us to the solution[32]

$$A^{jj}_{\lambda j_0}(x) = [x^{-1/2(j_0+i\lambda)}F(-s-j_0,-s-i\lambda;-2s;1-x) - x^{1/2(j_0+i\lambda)}F(-s+j_0,-s+i\lambda;-2s;1-x)] \times e^{i\pi j_0}\csc\{\pi(j_0+i\lambda)\}\mathfrak{F}^j_{(m,s)}(x). \quad (4.12)$$

In the above formula, the hypergeometric polynomials are defined to be

$$F(-s\mp j_0,-s\mp i\lambda;-2s;1-x) = \sum_{n=0}^{s\pm j_0}\frac{(-s\mp j_0)_n(-s\mp i\lambda)_n}{(-2s)_n n!}(1-x)^n, \quad (4.13)$$

where

$$(a)_n = a(a+1)\cdots(a+n-1) = \Gamma(a+n)/\Gamma(a).$$

We can express the solutions also in terms of hypergeometric polynomials in x or in terms of Jacobi polynomials. We will use these forms later on. *It will then also be seen that the symmetry conditions implied in (4.12) lead automatically to solutions regular at $x = 1$ or $|\mathbf{p}| = 0$.*

Symmetry relations of the type (3.6)–(3.8) hold again, *and we could, in particular, have written an exactly similar formula for $j_0 = j$ by interchanging μ and j_0 in (4.12).*

Variation of j: Using the matrix elements of $P_\pm$ (as in Sec. 3) we obtain

$$(-i2|\mathbf{p}|/m)\{(2j-1)(2j)(s+j)\}^{-1}A^{jj-1}_{\lambda j} = A^{j-1j-1}_{\lambda j-1}. \quad (4.14)$$

Hence (using the solution corresponding $j_0 = j$),

$$\mathfrak{F}^j_{(m,s)}(x) = (-i(2|\mathbf{p}|/m)^{-j}(2j)!(s+j)!\,\mathfrak{F}_{(m,s)}(x) = x^{(1/2)j}(1-x)^{-j}e^{i(\pi/2)j} \quad (4.15)$$

$$\times (s+j)!(2j)!\mathfrak{F}_{(m,s)}(x). \quad (4.16)$$

Variation of x: Using the matrix elements of G_0, we obtain (as in Sec. 3)

$$(j_0^2+\lambda^2)(2p_0/m)[(|\mathbf{p}|^2/p_0)\partial_0+1]A^{j\mu}_{\lambda j_0}(x) = (j_0^2+\lambda^2)x^{-1/2}[-2x(1-x)\partial_x+(1+x)]A^{j\mu}_{\lambda j_0}(x) = j_0[(s-j_0)(j-j_0)A^{j\mu}_{\lambda j_0+1}-(s+j_0)(j+j_0) \times A^{j\mu}_{\lambda j_0-1}]-i\lambda[(s+i\lambda)(j+i\lambda)A^{j\mu}_{\lambda+ij_0} - (s-i\lambda)(j-i\lambda)A^{j\mu}_{\lambda-ij_0}]. \quad (4.17)$$

As a generalization of (3.16), one may assume a solution of the form

$$\mathfrak{F}_{(m,s)}(x) = x^{\alpha}(1-x)^{\beta}C_{(m,s)}. \tag{4.18}$$

Substituting in (4.17), cancelling some common powers of x, and then comparing the coefficients of $(1-x)^n$ on both sides, we obtain

$$\alpha = \tfrac{1}{2}, \quad \beta = s-1. \tag{4.19}$$

Thus, finally, for $j \leq s$,

$$\begin{aligned} A^{jj}_{\lambda j_0}(x) &= C_{(m,s)} e^{i(\pi/2)j} \cdot e^{i\pi j_0} \csc\{\pi(j_0 + i\lambda)\} \\ &\times (s+j)!\,(2j)!\,x^{(1/2)(j+1)}(1-x)^{-s-j-1} \\ &\times [x^{-(1/2)(j_0+i\lambda)}F(-s-j_0,-s-i\lambda;-2s;1-x) \\ &- x^{(1/2)(j_0+i\lambda)}F(-s+j_0,-s+i\lambda;-2s;1-x)]. \end{aligned} \tag{4.20}$$

The correspondence with Ströms formula[33] is evident. We may note the following useful alternative forms of the hypergeometric polynomials in (4.20). We have

$$\begin{aligned} &F(-s \mp j_0, s \mp i\lambda; -2s; 1-x) \\ &\quad = C_{(\mp)}F(-s \mp j_0, -s \mp i\lambda, 1 \mp j_0 \mp i\lambda; x), \end{aligned} \tag{4.21}$$

where

$$C_{(\pm)} = (s \pm j_0)!\,(s \pm i\lambda)!/(2s)!\,(\pm j_0 \pm i\lambda)!. \tag{4.22}$$

Again in terms of the Jacobi polynomials we can write

$$\begin{aligned} &F(-s \pm j_0, -s \pm i\lambda; (-2s); 1-x) \\ &\quad = \frac{(s+j_0)!\,(s-j_0)!}{(2s)!} \\ &\quad \times (1-x)^{s \mp j_0} P^{(\mp j_0 \pm i\lambda, \pm j_0 \mp i\lambda)}_{s \mp j_0}\left(\frac{1+x}{1-x}\right), \end{aligned} \tag{4.23}$$

where

$$(1+x)/(1-x) = \coth \xi. \tag{4.24}$$

Using (4.1), (4.20), and (4.23), we obtain (for $j \leq s$ and $\epsilon = 1$)

$$\begin{aligned} \mathfrak{F}^{\lambda j_0}_{jj_s}(x,m) &\equiv \left\langle m, s; {}^{p\,0j}_{jj_3} \middle| {}^{\lambda j_0}_{jj_3}; m, s \right\rangle = \frac{C_{(m,s)}}{(2s)!}\, e^{i(\pi/2)j + i\pi j_0} \csc\{\pi(j_0 + i\lambda)\} \\ &\times \left[\frac{(2j)!\,(s+j)!\,(s+j_0)!\,(s-j_0)!}{(s-j)!\,(j+j_0)!\,(j-j_0)!\,(j+i\lambda)!\,(j-i\lambda)!\,(s+i\lambda)!\,(s-i\lambda)!}\right]^{1/2} x^{(1/2)(j+1)}(1-x)^{-j-1} \\ &\left[x^{-(1/2)(j_0+\lambda)}(1-x)^{j_0} P^{(j_0-i\lambda,-j_0+i\lambda)}_{s+j_0}\left(\frac{1+x}{1-x}\right) - x^{(j_0+i\lambda)/2}(1-x)^{-j_0} P^{(j_0+i\lambda,-j_0-i\lambda)}_{s-j_0}\left(\frac{1+x}{1-x}\right)\right]. \end{aligned} \tag{4.25}$$

As compared to the formula (A19) of Ref. 14 [including the additional phase factor given following (A19)], the rhs of (4.25) is of the form[34]

$$\{(2j+1)(2s+1)\}^{-1/2} \frac{C_{(m,s)}}{\pi(2s)!}\, e^{i\pi(s+j_0)} d^{\lambda j_0}_{jj_s}(x), \tag{4.26}$$

where $$d^{\lambda j_0}_{jj_s}(1) = \delta_{js}. \tag{4.27}$$

Limit to Zero Mass Continuous Spin and Normalization

Let us now consider the limiting form when

$$m \to 0 \text{ and } s \to \infty, \text{ such that } ms \to \tau. \tag{4.28}$$

The condition (4.28) implies

$$sx^{1/2} \to (\tau/2p_0). \tag{4.29}$$

From (4.1), (4.20), using (4.21), (4.22) taking the term by term limit and noting that[35]

$$\lim_{|z| \to \infty} \Gamma(z+\alpha) = z^{\alpha}\Gamma(z), \tag{4.30}$$

we obtain, finally (in terms of the results of Sec. 3, with $\epsilon = 1$),

$$\begin{aligned} &\lim \left\langle m, s; {}^{p_0 j}_{jj_3} \middle| {}^{\lambda j_0}_{jj_3} m, s \right\rangle \\ &\quad = \left[\lim \frac{C_{(m,s)}m}{(2s)!\,2\sqrt{\pi}}\right] \left\langle \tau {}^{p^0\mu}_{jj_3} \middle| {}^{\lambda j_0}_{jj_3} \tau \right\rangle. \end{aligned} \tag{4.31}$$

Hence the correct limiting behavior is obtained:

$$C_{(m,s)} = 2\sqrt{\pi}/m(2s)!. \tag{4.32}$$

Such a determination of $C_{(m,s)}$ is not quite unambiguous. However, since our normalization condition is (for fixed m, s, j, j_3)

$$\begin{aligned} &\sum_{\mu} \int_0^{\infty} \frac{d|\mathbf{p}|\mathbf{p}^2}{2p^0} \left\langle {}^{\lambda' j_0}_{jj_3} \middle| {}^{p^0\mu}_{jj_3} \right\rangle \left\langle {}^{p^0\mu}_{jj_3} \middle| {}^{\lambda j_0}_{jj_3} \right\rangle \\ &\quad = m^2 \sum_{\mu} \int_0^1 \frac{(1-x)^2}{16x^2}\, dx \left\langle {}^{\lambda' j_0'}_{jj_3} \middle| {}^{x\mu}_{jj_3} \right\rangle \left\langle {}^{x\mu}_{jj_3} \middle| {}^{\lambda j_0}_{jj_3} \right\rangle \\ &\quad = (j_0^2 + \lambda^2)^{-1} \delta_{j_0 j_0'} \delta(\lambda - \lambda'). \end{aligned} \tag{4.33}$$

Comparing with the corresponding formula (A18) of Ref. 14, and using (4.26) (it is sufficient for our present purpose to consider the simplest case

with $j=0$), we obtain

$$(m^2/4\pi)\{CC^*/[(2s)!]^2\}=1. \tag{4.34}$$

Hence (4.32) does indeed give the correct normalization, with the constant phase factor chosen to agree with our convention in Sec. 3.

Case 1, $j \geq s > 0$: It is not difficult to verify that, in this case,

$$\begin{aligned} A^{js}_{\lambda j_0}(x) &= C_{(m,s)} e^{i(\pi/2)j + i\pi j_0}(j+s)!(2j)! \\ &\times \csc\{\pi(j_0+i\lambda)\} x^{(s+1)/2}(1-x)^{-j-s-1} \\ &\times [x^{-(1/2)(j_0+i\lambda)} F(-j-j_0,-j-i\lambda;2j;1-x) \\ &- x^{(j_0+i\lambda)/2} F(-j+j_0,-j^0+i\lambda;-2j;1-x)]. \end{aligned} \tag{4.35}$$

The treatment of Eqs. (4.2), (4.3), and (4.17) is evidently symmetric with that of the previous case and so presents no problem. There still remains to determine a factor depending (apart from m and s) only on j, which according to (4.35) should turn out to be

$$\mathfrak{F}_j = C_{(m,s)} e^{i(\pi/2)j}(j+s)!(2j)!. \tag{4.36}$$

Since now

$$-s \leq \mu, j_0 \leq s,$$

and we have again to vary j (and not s), the situation here is not quite symmetric with respect to the previous case. Using the matrix elements of P_- and putting $\mu = s$, we obtain

$$\begin{aligned} (-i2|\mathbf{p}|/m)A^{js}_{\lambda j_0} &= (j_0^2+\lambda^2)^{-1}(j^2+\lambda^2) \\ &\times [(j-j_0)(j-j_0-1)(s-j_0)A^{j-1\,s}_{\lambda j_0+1} + (j+j_0) \\ &\times (j+j_0-1)(s+j_0)A^{j-1\,s}_{\lambda j_0-1}] + (j^2-j_0^2)[(j+i\lambda) \\ &\times (j+i\lambda-1)(s+i\lambda)A^{j-1\,s}_{\lambda+i\,s} + (j-i\lambda) \\ &\times (j-i\lambda-1)(s-i\lambda)A^{j-1\,s}_{\lambda-ij_0}]. \end{aligned} \tag{4.37}$$

Cancelling the common factors of x on comparing the coefficients of $(1-x)^0$ on both sides, we obtain

$$\mathfrak{F}_j = i(2j-1)(2j)(s+j)\mathfrak{F}_{j-1}. \tag{4.38}$$

This verifies (4.36) and hence (4.35). The constant $C_{(m,s)}$ is, of course, the same as in (4.32), ensuring consistency at $j=s$.

Hence finally, using the definition (4.25), we obtain

$$\mathfrak{F}^{\lambda j_0}_{\alpha\alpha\beta}(x) = e^{i\pi(\alpha-\beta)/2}\mathfrak{F}^{\lambda j_0}_{\beta\,\alpha\alpha}, \tag{4.39}$$

where α and β are possible values of j and s.

Descent from $\mu = j$ or s: From (2.13) (with $\epsilon = 1$), defining

$$\begin{aligned} A^{j\mu}_{\lambda j_0} &= (s+\mu)!(s-j_0)!(s+i\lambda)!(j+\mu)! \\ &\times (j-j_0)!(j+i\lambda)!B^{j\mu}_{\lambda j_0}, \end{aligned} \tag{4.40}$$

we obtain

$$\begin{aligned} &(j_0+i\lambda)B^{j\mu-1}_{\lambda j_0} + (\mu-i\lambda)B^{j\mu}_{\lambda j_0+1} + (\mu+j_0)B^{j\mu}_{\lambda+i j_0} \\ &\quad = x^{1/2}(j_0+i\lambda)(\mu-i\lambda)(\mu+j_0)B^{j\mu}_{\lambda j_0}. \end{aligned} \tag{4.41}$$

This is a generalization of (3.18).

For $j \leq s$ and $\mu \geq j_0$, the solution is found to be

$$\begin{aligned} B^{j\mu}_{\lambda j_0} &= e^{i\pi(j-\mu)}(j-\mu)!(j-i\lambda)!(j+j_0)! \\ &\times \left[\sum_{r=0}^{j-\mu} \frac{(-1)^r x^{r/2}}{r!}\left(\sum_{a=0}^{j-\mu-r} f^{j,r}_{a,b} B^{jj}_{\lambda+i\,b,\,j_0+a}\right)\right], \end{aligned} \tag{4.42}$$

where

$$a+b = (j-\mu-r) \tag{4.42'}$$

and

$$f^{j,r}_{a,b} = \frac{(j_0+i\lambda-b-1)!(j_0+i\lambda+a-b)}{a!b!(j_0-i\lambda-a-r)!(j+j_0-b-r)!(j_0+i\lambda+a)!}. \tag{4.42''}$$

As usual the sum is restricted to nonnegative values of $(j+j_0-b-r)$. Similarly, for $j \geq s$,

$$\begin{aligned} B^{j\mu}_{\lambda j_0} &= e^{i\pi(s-\mu)}(s-\mu)!(s-i\lambda)!(s+j_0)! \\ &\times \left[\sum_{r=0}^{s-\mu} \frac{(-1)^r x^{r/2}}{r!}\left(\sum_{a=0}^{s-\mu-r} f^{s,r}_{a,b} B^{js}_{j_0+a,\lambda+ib}\right)\right], \end{aligned} \tag{4.43}$$

where $a+b = s-\mu-r$.

For $\mu < j_0$, we can as before use the symmetry

$$A^{j\alpha}_{\lambda\beta} = A^{j\beta}_{\lambda\alpha}.$$

Final Expression

Putting together the foregoing results, we obtain, for $j \leq s$ and $\mu \geq j_0$ ($\epsilon = 1$),

$$\mathfrak{F}^{\lambda j_0}_{j\mu s}(x) \equiv \left\langle m, s\, p^0\mu \middle| \lambda j_0 m, s \right\rangle_{jj_3} = \frac{2(2s)!}{\sqrt{\pi}m} \exp[i(\tfrac{3}{2}\pi)j + i\pi(j_0-\mu)] \left[\frac{(s+\mu)!(s-j_0)!(s+i\lambda)!}{(s-\mu)!(s+j_0)!(s-i\lambda)!}\right]^{1/2}$$

$$\times[(j+\mu)!(j-\mu)!(j+j_0)!(j-j_0)!(j+i\lambda)!(j-i\lambda)!]^{1/2}x^{(j+1)/2}(1-x)^{-j-s-1}\sum_{r=0}^{j-\mu}\frac{(-1)^r x^{r/2}}{r!}$$

$$\times\sum_{a=0}^{j-\mu-r}\left(\frac{(-1)^a(j_0+i\lambda-b-1)!(j_0+i\lambda+a-b)!(-j_0-i\lambda-a+b)!}{a!b!(j-i\lambda-a-r)!(j+j_0-b-r)!(j_0+i\lambda+a)!(j-j_0-a)!(j+i\lambda-b)!}\right.$$

$$\left.\times\frac{1}{(s-j_0-a)!(s+i\lambda-b)!}\right)[x^{-(j_0+i\lambda+a-b)/2}F(-s-j_0-a,-s-i\lambda+b;-2s;1-x)$$

$$-x^{(j_0+i\lambda+a-b)/2}F(-s+j_0+a,-s+i\lambda-b;-2s;1-x)],\quad a+b=j-\mu-r. \tag{4.44}$$

The above expression, coupled with the symmetries

$$\mathfrak{F}^{\lambda\alpha}_{j\beta s}(x)=\mathfrak{F}^{\lambda\beta}_{j\alpha s}(x)=\mathfrak{F}^{\lambda-\alpha}_{j-\beta s}(x) \tag{4.45}$$

and

$$\mathfrak{F}^{\lambda j_0}_{\alpha\mu\beta}(x)=e^{(i\pi/2)(\alpha-\beta)}\mathfrak{F}^{\lambda j_0}_{\beta\mu\alpha}(x), \tag{4.46}$$

completes the solution.

5. THE SPACELIKE CASE

Let $P^2=-m^2<0$ and $W^2=m^2K(K+1)$. Let us first consider the case

$$K=-\tfrac{1}{2}+i\eta,\quad \eta \text{ real}$$

A. Application of a Deformation Formula

One solution is immediately obtained by using the deformation formula of Ref. 2 (Sec. 5) and the results of the Sec. 3 of this article.

Replacing m for the moment by τ, we obtain, *in the notation of Ref. 2* ($\hat{p}^2=-\tau^2$), with

$$\sin\hat{\theta}=\tau/|\hat{\mathbf{p}}|,\quad \cos\hat{\theta}=\hat{p}_0/|\hat{\mathbf{p}}|; \tag{5.1}$$

$$\left\langle\begin{matrix}\hat{p}_0\hat{\mu}\\ jj_3\end{matrix}\middle|\begin{matrix}\lambda j_0\\ jj_3\end{matrix}\right\rangle=(2\pi|\hat{\mathbf{p}}|)^{-1/2}\sum_\mu\mathfrak{D}^{j*}_{\mu\hat{\mu}}(0,-\hat{\theta},-\pi/2)$$

$$\times\int_0^\infty d|\mathbf{p}_0|e^{-i}(|\hat{p}_0|/|p_0|)|p_0|^{-(1/2+i\eta)}\left\langle\begin{matrix}p^0\mu\\ jj_3\end{matrix}\middle|\begin{matrix}\lambda j_0\\ jj_3\end{matrix}\right\rangle. \tag{5.2}$$

We have chosen to integrate over positive or negative p^0 states accordingly as $\hat{p}_0$ is positive or negative. This displays directly the necessary symmetry relations $(\hat{p}_0,\lambda\rightleftharpoons-\hat{p}_0,-\lambda)$. The orthogonality and normalization properties are obtained at once from the results of Appendix A of this paper and those of Sec. 5 of Ref. 2.

The integral in (5.2) over the p^0-dependent terms can be carried out easily. Thus, for example, considering the case $\hat{p}_0>0$ and using (3.23) for the terms in (5.2) with $\mu\geq j_0$, we can write the integral as

$$I=\int_0^\infty dp_0 p_0^{-(j+i\eta+3/2)}e^{-i\hat{p}_0/p_0}K_{j'_0+i\lambda}(\tau/p_0),$$

$$j'_0=j_0+a-b,\quad a+b=j-\mu. \tag{5.3}$$

Using the appropriate formula for Laplace transforms,[36] we obtain, in terms of Legendre functions, for all a, b, and for

$$\mu\pm j_0>-\tfrac{1}{2}, \tag{5.4}$$

$$I=(\pi/2\tau)^{1/2}(|\hat{\mathbf{p}}|)^{-(j+i\eta)}\Gamma(j-j'_0+\tfrac{1}{2}i(\eta-\lambda))$$

$$\times\Gamma(j+j'_0+\tfrac{1}{2}i(\eta+\lambda))\ P^{-(j+i\eta)}_{-1/2+j'_0+i\lambda}(i\hat{p}_0/\tau). \tag{5.5}$$

The other values of μ, j_0 can be treated using the necessary symmetry relations $[\mu\rightleftharpoons j_0,(\mu,j_0)\rightleftharpoons(-\mu,-j_0)]$ for the last factor in (5.2).

The integral I can also be expressed in terms of hypergeometric functions by treating (5.3) as a Mellin transform. The resulting formula is then more complicated.

Analogous treatment can be given for $K=-n$ (and even for the timelike case), introducing the nonunitary representations discussed at the end of Sec. 5 of Ref. 2. Since, as has been noted in Ref. 2, such nonunitarity representations come in pairs, permitting the construction of scalar products, suitable orthogonality and completeness relations for the corresponding transformation coefficients can also be found. Due to this fact, such nonunitarity representations might be useful. We will not, however, discuss them in this paper.

B. Direct Method and Continuation of the Solution for $P^2>0$

We can, of course, also solve directly the recursion relations implied by our matrix elements for the spacelike case. In order to bring out most clearly the relation with solution for the timelike case (and with the continuous-spin case as a limiting form), let us adopt the following phase conventions [writing in (1.8) and (1.9) $(P^2)^{1/2}=im$]:

$$C^{j_0\pm1j_0}=\frac{im}{(j_0^2+\lambda^2)}[(K\mp j_0)(K\pm j_0+1)]^{1/2}, \tag{5.6}$$

$$C^{\lambda\pm i\lambda}_{j_0}=\frac{im}{(j_0^2+\lambda^2)}[(K\pm i\lambda)(K\mp i\lambda+1)]^{1/2}.$$

Similarly we put

$$\alpha_{(\pm)}=im[(K\mp\mu)(K\pm\mu+1)]^{1/2} \tag{5.6'}$$

in the formulas of Sec. 2.[37] Note that $C^{j_0\pm1j_0}$ and

$\alpha^{(\pm)}$ are real. For the energy and momentum we use the parametrization

$$p_0 = m \sinh\zeta, \qquad |\mathbf{p}| = m \cosh\zeta \tag{5.7}$$

and $x = e^{-2\xi}$ such that positive values of p^0 correspond to $0 < x < 1$ and the negative values to $1 < x < \infty$.

The solutions of the recursion relations can now be obtained in a fashion quite analogous to that for the timelike case. Thus, for example, defining

$$\left\langle m, K \begin{matrix} p^0 \mu \\ j j_3 \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ j j_3 \end{matrix} m, K \right\rangle = \left[\frac{(j+\mu)!(j-\mu)!(j+j_0)!(j-j_0)!(j+i\lambda)!(j-i\lambda)!}{(K+\mu)!(K-\mu)!(K+j_0)!(K-j_0)!(K+i\lambda)!(K-i\lambda)!} \right]^{-1/2} A^{j\mu}_{\lambda j_0}(p^0, K), \tag{5.8}$$

we obtain

$$\begin{aligned} A^{jj}_{\lambda j_0}(x) = {} & [(2\pi)^{1/2}/im] e^{-i\pi(j+1)} (2j)!(K+j)!\, x^{(j+1)/2} (1+x)^{-K-j-1} e^{i\pi j_0} \csc[\pi(j_0 + i\lambda)] \\ & \times \left[(-x)^{(j+i\lambda)/2} \frac{(K-j_0)!(K-i\lambda)!}{(-j_0-i\lambda)!} F(-K-j_0, -K-i\lambda; 1-j_0-i\lambda; -x) \right. \\ & \left. - (-x)^{(j_0+i\lambda)/2} \frac{(K+j_0)!(K+i\lambda)!}{(j_0+i\lambda)!} F(-K+j_0, -K+i\lambda; 1+j_0+i\lambda; -x) \right], \quad p_0 \geq 0 \text{ and } -x = e^{i\pi x} \end{aligned} \tag{5.9}$$

and, putting $y = 1/x = e^{2\xi}$,

$$\begin{aligned} A^{jj}_{\lambda j_0}(x) = {} & [(2\pi)^{1/2}/m e^{-i\pi(j+1)} (2j)!(K+j)!\, y^{(j+1)/2} (1+y)^{-K-j-1} e^{i\pi j_0} \csc[\pi(j_0 - i\lambda)] \\ & \times \left[(-y)^{(j_0-i\lambda)/2} \frac{(K-j_0)!(K+i\lambda)!}{(-j_0+i\lambda)!} F(-K-j_0, -K+i\lambda; 1-j_0+i\lambda; -y) - (-y)^{(j_0-i\lambda)/2} \right. \\ & \left. \times \frac{(K+j_0)!(K-i\lambda)!}{(j_0-i\lambda)!} F(-K+j_0, -K-i\lambda; 1+j_0-i\lambda; -y) \right] \quad p_0 \leq 0 \text{ when } x \geq 1 \text{ and } y \leq 1. \end{aligned} \tag{5.9'}$$

The expression (5.9′) can be shown to be the analytic continuation of (5.9) for $x > 1$.[38] Moreover, since the arguments of the hypergeometric functions are negative in (5.9) and (5.9′), integral representations (with suitable chosen contours) can be introduced, valid for all positive values of x (or y).

The final constant factors in (5.9) and (5.9′) have been chosen, as in Sec. 4, by considering the limiting forms that should give the zero-mass continuous-spin solutions. (But we have included an extra factor $1/\sqrt{2}$ to take account of presence of both signs of the energy.)

In comparing the limiting forms, it should be noted that our phase conventions correspond to the case $m \to 0$ (when $x \to 0$), $|\mathbf{K}| \to \infty$

such that

$$iKx^{1/2} \to \tau/2\,|\mathbf{p}|. \tag{5.10}$$

A change $im \to -im$ in (5.6) corresponds to a change $ix^{1/2} \to -ix^{1/2}$ (or $iy^{1/2} \to -iy^{1/2}$) in (5.9) [or (5.9′)] and $iK \to -iK$ in (5.10). That is (for $\tau > 0$) the two cases correspond to the choice of negative and positive η, respectively.

Let us note that the solutions [(5.8)–(5.10)] are obtained from the corresponding solutions for $P^2 > 0$, apart possibly from a constant factor to be adjusted suitably, through the substitutions [using the relation (4.21)]

$$m \to im, \qquad x^{1/2} \to ix^{1/2}, \qquad S \to K = -\tfrac{1}{2} + i\eta. \tag{5.10'}$$

(The introduction of y for $p_0 < 0$ amounts finally to a mere change of notation.)

Indeed it is not difficult to verify that considered as a function of the above-mentioned parameters, the solution obtained in Sec. 4 can be continued analytically in the corresponding complex planes (orienting suitably certain branch cuts) starting from the initial real values (satisfying $m > 0$, $0 < x < 1$, $s \geq |j_0|, |\mu|$) to the final values indicated in (5.10′). This relation holds for general μ values. We have to use the solutions (for $P^2 > 0$) with $\mu = \pm j$ as a starting point.

Let us, however, point out in more detail the different possible recursion relations for μ.

For $\epsilon = 1$, defining

$$\begin{aligned} A^{j\mu}_{\lambda j_0} = {} & \{(K+\mu)!(K \mp j_0)!(K \pm i\lambda)!(j+\mu)! \\ & \times (j \mp j_0)!(j \pm i\lambda)!\} B^{j\mu}_{\lambda j_0}, \end{aligned} \tag{5.11}$$

we obtain from (2.13) (and analogous equations that can be constructed)

$$(\pm j_0 \pm i\lambda)B^{j\mu-1}_{\lambda j_0} + (\mu \mp i\lambda)B^{j\mu}_{\lambda j_0\pm 1} + (\mu \pm j_0)B^{j\mu}_{\lambda \pm ij_0} = (-x)^{1/2}(\pm j_0 \pm i\lambda)(\mu \pm i\lambda)(\mu \pm j_0)B^{j\mu}_{\lambda j_0}. \quad (5.12)$$

[The factor $e^{i\pi/2}x^{1/2}$ on the right changes to $e^{-i\pi/2}x^{1/2}$ for the alternative phase convention indicated following (5.10).]

For $\epsilon = -1$, we have to substitute in (5.11) and (5.12)

$$x \to x^{-1} = y \quad \text{and} \quad \lambda \to -\lambda \quad (5.13)$$

in the coefficients, and the variation in λ becomes $B^{j\mu}_{\lambda - ij_0}$ [see (2.13)].

If we want to start with the limiting value $\mu = -j$, it can be shown [starting with equations analogous to (2.13) with the $(\mu + 1)$ amplitude on the left] that, on defining

$$A^{j\mu}_{\lambda j_0} = \{(K-\mu)!(K \mp j_0)!(K \mp i\lambda)!(j-\mu)! \times (j \mp j_0)!(j \mp i\lambda)!\}\tilde{B}^{j\mu}_{\lambda j_0}, \quad (5.14)$$

one obtains (for $\epsilon = 1$)

$$(\pm j_0 \mp i\lambda)\tilde{B}^{j\mu+1}_{\lambda j_0} + (-\mu \pm i\lambda)\tilde{B}^{j\mu}_{\lambda j_0\pm 1} + (-\mu \pm j_0)\tilde{B}^{j\mu}_{\lambda \pm ij_0} = (-x)^{1/2}(\pm j_0 \mp i\lambda)(-\mu \pm i\lambda)(-\mu \pm j_0)\tilde{B}^{j\mu}_{\lambda j_0}. \quad (5.15)$$

For $\epsilon = -1$, we have again to make the substitution (5.13).

The solution of (5.12)(with the upper signs) is obtained from (4.42) through the substitution

$$x^{1/2} \to (-x)^{1/2}. \quad (5.16)$$

The solutions for the other cases considered in (5.11) and (5.14) follow from quite evident symmetries.

First expressing $A^{j\mu}_{\lambda j_0}(x)$ in terms of $A^{j\pm j}_{\lambda j_0}(x)$ through solutions of (5.12) or (5.15) and then utilizing (5.9), (5.9′) (and analogous solutions for $A^{j-j}_{\lambda j_0}$) and finally (5.8), we get the required results.

Thus, for example, for $\epsilon = 1$ and $\mu \geq j_0$, starting from $\mu = j$, we obtain

$$\left\langle m, K \left| \begin{matrix} p^0 \mu \\ jj_3 \end{matrix} \right| \begin{matrix} \lambda j_0 \\ jj_3 \end{matrix} m, K \right\rangle = \frac{-\sqrt{2}}{im\sqrt{\pi}} \left[\frac{(K+\mu)!(K-j_0)!(K+i\lambda)!}{(K-\mu)!(K+j_0)!(K-i\lambda)!}\right]^{1/2} \left[\frac{(j+\mu)!(j-\mu)!(j+j_0)!}{(j-j_0)!(j+i\lambda)!(j-i\lambda)!}\right]^{1/2}$$
$$\times e^{i\pi(j_0-\mu)}x^{1/2(j+1)}(1+x)^{-j-K-1}\sum_{r=0}^{j-\mu}\frac{(-1)^r(-x)^{r/2}}{r!}$$
$$\times \sum_{a=0}^{j-\mu-r}\frac{(-1)^a(j_0+i\lambda-b-1)!}{a!b!(j-i\lambda-a-r)!(j+j_0-b-r)!(j_0+i\lambda+a)!(j-j_0-a)!(j+i\lambda-b)!}$$
$$\times (-x)^{-(j_0+i\lambda+a-b)/2}\frac{(K-i\lambda+b)!}{(K+i\lambda+b)!}(j_0+i\lambda+a-b)!\,F(-K-j_0-a,-K-i\lambda$$
$$+ b; 1+j_0+i\lambda; -x) - (x)^{(j_0+i\lambda+a-b)/2}\frac{(K+j_0+a)!}{(K-j_0-a)!}(-j_0-i\lambda-a+b)!$$
$$\times F(-K+j_0+a,-K+i\lambda-b,1-j_0-i\lambda;-x). \quad (5.17)$$

(The solution for $P^2 > 0$ can also be written in a closely similar form.)

The other cases can be obtained from (5.17) using the symmetry relations (repeatedly pointed out) which can be written symbolically as

$$(\mu, j_0) \rightleftharpoons (j_0, \mu) \quad \text{and} \quad (\mu, j_0) \rightleftharpoons (-\mu, -j_0).$$

For $p_0 < 0$, we have to make the substitutions

$$x \to y\,(=x^{-1}) \quad \text{and} \quad \lambda \to -\lambda.$$

We have not derived the normalization properties of the solutions of this subsection by direct calculation. This is one of the aspects in which our results remain incomplete.

In order to study thoroughly the relation of the two solutions given in subsections 5A and 5B, respectively, we should examine explicitly, among other things, the action, on the $(\hat{p}_0, \hat{\mu}, jj_3)$ basis of 5A, of $\mathbf{N}, \hat{\mathbf{W}}^0, \hat{\mathbf{G}}^0$ [the latter two operators being obtained by commuting $\hat{P}_0$ with $\mathbf{N}\cdot\mathbf{M}$ and $\frac{1}{2}(\mathbf{N}^2 - \mathbf{M}^2)$, respectively]. This we will not attempt to do. Let us note, however, that the deformation formula [Ref. 2, Eq. (5.2)]

$$\hat{P} = G + \eta P \quad \text{with} \quad K = -\tfrac{1}{2} + i\eta$$

corresponds to the matrix elements of $\hat{P}_0$ with [compare (5.6)]

$$C^{j_0\pm 1 j_0}_{\lambda} = \mp i(j_0 \pm K \pm 1)\tau/(j_0^2 + \lambda^2), \quad \hat{p}^2 = -\tau^2,$$
$$C^{\lambda \pm i\lambda}_{j_0} = \pm(i\lambda \mp K \mp 1)\tau/(j_0^2 + \lambda^2). \quad (5.18)$$

The conventions

$$\hat{\mathbf{P}} = G - \eta p \quad \text{or} \quad K = -\tfrac{1}{2} - i\eta$$

correspond to a substitution $(K+1) \to -K$ in (5.18).

Such an alternative form (5.18), which still conserves the Hermiticity of the matrix elements $j_0 \to j_0 \pm 1$ of the energy operator, is only possible for the case $\mathrm{Re}K = -\frac{1}{2}$.

A similar remark applies the matrix elements of $\tilde{\mathbf{W}}$ and its reduced elements $\alpha_{(\pm)}$.

C. $K = -n$

Let us now consider the case

$$K = -n, \quad n = \tfrac{1}{2}, 1, \tfrac{3}{2}, \cdots .$$

Now the values of j, μ, and j_0 are restricted to $j \geq |\mu|$, $|j_0| \geq n$, all being integral or half-integral accordingly as n. Subject to this restriction, for each value of μ, j_0 can be positive or negative and vice versa, giving four possible cases.

The case $n = \frac{1}{2}$ (which can be obtained in the limit as $\eta \to 0$ from the previous case) is exceptional. Its contribution in the crossed-channel partial-wave analysis, according to formalism of Ref. 5, vanishes [due to a factor $(2K+1)$]. For this case, W^2 $[=m^2K(K+1)]$ is negative, while, for $n = 1$, W^2 is zero (which is, hence, also somewhat special) and is positive for $n = \frac{3}{2}$ onwards. We will give only a somewhat brief and incomplete discussion of these cases.

Let us examine what happens if we substitute formally $K = -n$ in the solution (5.8), for $\mu = j$, where $A^{jj}_{\lambda j_0}$ is given by (5.9) (for $p_0 > 0$). The first (second) term of (5.9) has a pole for $j_0 \geq n$ $(j_0 \leq -n)$ which cancels exactly the zero due to the factor

$$[(K+\mu)!(K-\mu)!(K+j_0)!(K-j_0)!]^{-1/2}$$

and thus survives, the hypergeometric function reducing to a polynomial. The other term no longer contributes.

Starting with the case $p_0 > 0$, $\mu \geq n$, writing

$$\begin{aligned}[(K \mp j_0)!/(K-\mu)!]^{1/2} &= [(-n-\mu+1)(-n-\mu+2)\cdots(-n \mp j_0)]^{1/2} \\ &= e^{i\pi/2\,(\mu \mp j_0)}[(n+\mu-1)!/(n \pm j_0 - 1)!]^{1/2}\end{aligned} \tag{5.19}$$

for $j > 0$ and $j_0 < 0$, respectively, let us write the solution thus obtained from (5.8) and (5.9) for $\mu = j$ (including some modifications to be explained below) as

$$\left\langle n\, {}^{p^0 j}_{jj_3} \,\middle|\, {}^{\lambda j_0}_{jj_3}\, n \right\rangle = \frac{2e^{-i(\pi/2)j+i\pi j_0}(\pm j_0 \pm i\lambda - 1)![(2j)!(j-n)!(-n \mp i\lambda)!(n+j-1)!]^{1/2}}{\sqrt{\pi}m[(j+j_0)!(j-j_0)!(j+i\lambda)!(j-i\lambda)!(-n \pm i\lambda)!(n \pm j_0 - 1)!(-n \pm j_0)!]^{1/2}}$$
$$\times x^{(j \mp j_0 \mp i\lambda+1)/2}(1+x)^{-j+n-1}F(n \mp j_0, n \mp i\lambda; 1 \mp j_0 \mp i\lambda; -x). \tag{5.20}$$

The upper or lower signs are to be used for $j_0 \geq n$ and $j_0 \leq -n$, respectively.)

In writing (5.20) we have not only introduced an extra factor $\sqrt{2}$ [since now only one term (5.9) survives] but, what is more important, *we have suppressed a factor* $e^{\mp\pi\lambda/2}$ (which is, however, essential for $K = -\frac{1}{2} + i\eta$) in order to assure a certain normalization property to be discussed below [see (5.2) and (5.24)]. It can be shown that (5.20) (and its analog for $p_0 < 0$) satisfies the required recursion relations, provided we modify the matrix elements of P_0 by substituting for $C^{\lambda \pm i\lambda}_{j_0}$ [defined in (5.6)], $\tilde{C}^{\lambda \pm i\lambda}_{j_0}$ defined as (see Ref. 22)

$$\tilde{C}^{\lambda+i\lambda}_{j_0} = \mp \epsilon i C^{\lambda+i\lambda}_{j_0}, \quad \tilde{C}^{\lambda-i\lambda}_{j_0} = \pm \epsilon i C^{\lambda-i\lambda}_{j_0}. \tag{5.21}$$

The upper or lower signs are to be used for $j_0 \geq n$ and $j_0 \leq -n$, respectively. (The matrix elements can be given a more symmetrical appearance by introducing corresponding modifications of phase factors for the $j_0 \to j_0 \pm 1$ and $\mu \to \mu \pm 1$ matrix elements. But this is not essential.)

We will not write the general solution separately for different possible values of μ and j_0. It is sufficient to note that they are obtained by suppressing a factor $e^{-\pi\lambda/2}$ (or $e^{\pi\lambda/2}$) in the surviving term of (5.17) (on putting $K = -n$) and then applying the usual symmetry properties if necessary.

As regards the normalization property of the solutions thus obtained, it is convenient to start by considering one of the simplest cases, say

$$j = n = \mu = j_0. \tag{5.22}$$

It is quite easy to verify from (5.20) that [consistent with Eq. (5.10) of Ref. 2]

$$\int_0^\infty d|p_0| \frac{|\mathbf{p}|}{2}\left[\sum_{\epsilon=\pm 1} \left\langle {}^{\lambda' n}_{nj_3} \,\middle|\, {}^{|p_0|n}_{nj_3}\, \epsilon \right\rangle \left\langle \epsilon \,\middle|\, {}^{|p_0|n}_{nj_3} \,\middle|\, {}^{\lambda n}_{nj_3} \right\rangle\right] = \frac{\delta(\lambda'-\lambda)}{(n^2+\lambda^2)} \tag{5.23}$$

and

$$\sum_{\epsilon=\pm1}\int_0^\infty d\lambda \left\langle {\epsilon \atop nj_3} \middle| p_0' \middle|^n {\lambda n \atop nj_3} \right\rangle \left\langle {\lambda n \atop nj_3} \middle| p_0 \middle|^n {\epsilon \atop nj_3} \right\rangle = \frac{2\delta(p_0'-p_0)}{|\mathbf{p}|} = \frac{2\delta(\xi-\xi')}{m^2\cosh^2\xi}. \tag{5.24}$$

(The left-hand side is symmetric in $\pm\lambda$ and we have adopted the convention of integrating over the positive values.)

Evidently this property cannot be obtained without such a modification as (5.21).

In view of certain ambiguities, it would have been desirable to derive the normalization properties for general j values by direct calculation. Unfortunately, we have been unable to find a suitably simple technique permitting this.

One can, of course, avoid (for the case $K=-n$) gamma functions with negative integer arguments from the beginning by modifying (5.8) suitably for the different cases involved. Thus, for example, for $\mu, j_0 \geq n$, one can start with the definition (possible also, of course, for $K=-\frac{1}{2}+i\eta$)

$$[(j+\mu)!(j-\mu)!(j-j_0)!(j-j_0)!(j+i\lambda)! \times (j-i\lambda)!]^{1/2} \left\langle {p^0\mu \atop jj_3} \middle| {\lambda j_0 \atop jj_3} \right\rangle = \left[\frac{(\mu-K-1)!(j_0-K-1)!(-i\lambda-K-1)!}{(\mu+K)!(j_0+K)!(-i\lambda+K)!}\right]^{1/2} A^{j\mu}_{\lambda j}. \tag{5.25}$$

The solutions obtained present, in their turn, other problems to start with. It should also be noted that for $K=-n$, the limiting values $\pm n$ of μ or j_0 can also be used as starting points of corresponding recursion relations. We will not enter, in this paper, into a discussion of all these different aspects.

6. DIAGONALIZATION OF THE SUBGROUPS $SU(1,1)$ AND $E(2)$

So far we have always considered bases which diagonalize the rotation or $SU(2)$ subgroup of the HLG. Let us now discuss certain aspects of the bases which diagonalize the subgroups $SU(1,1)$ and $E(2)$, respectively. We will not attempt a thorough study of these cases, but only briefly indicate certain important features.

We can, of course, obtain the required results for the Poincaré group by combining our foregoing results with the transformation coefficients relating the three bases

$$\left|{\lambda j_0 \atop jj_3}\right\rangle, \quad \left|{\lambda j_0 \atop Kj_3}\right\rangle, \quad \text{and} \quad \left|{\lambda j_0 \atop \rho j_3}\right\rangle, \tag{6.1}$$

which diagonalize the subgroups $SU(2)$, $SU(1,1)$, and $E(2)$, respectively.

These transformation coefficients (involving only the HLG and not the Poincaré group) have been studied from various points of view.[15,16,18] They can also be obtained in fairly convenient forms (and except for a factor) as particular cases of our preceding results for the lightlike and spacelike cases, respectively. (See the final remarks of this section.) This, however, is not the most direct way.

Another point of view is to obtain factorized expressions just as in (1.5) by diagonalizing the $SU(1,1)$ subgroup for spacelike momenta and the $E(2)$ subgroup for lightlike momenta, respectively. The finite Lorentz transformation matrix (corresponding to each of the bases) appearing as a factor has been studied by several authors.[19,39,40]

Exactly as for the timelike case, we obtain for the spacelike one (starting for simplicity *with the original 3-momentum* $\mathbf{p}$ *parallel to the* z *axis* when M_3 and the helicity operator have the same eigenvalue)

$$\left\langle {p\mu \atop K} \middle| {\lambda j_0 \atop K'\mu} \right\rangle \approx \left\langle {p_{(0)}\mu \atop K} \middle| {\lambda j_0 \atop K\mu} \right\rangle \mathfrak{D}^{\lambda j_0}_{K\mu K'}, \ [\Lambda(p)], \tag{6.2}$$

where

$$\Lambda_{(p)}\cdot p = (0,0,0,m) \equiv p_{(0)},$$

and $\mathfrak{D}^{\lambda j_0}_{K\mu K'}[\Lambda_{(p)}]$ is the finite Lorentz transformation matrix corresponding to the pure Lorentz transformation $\Lambda_{(p)}$ (parallel to the z axis) acting on the basis $\left|{\lambda j_0 \atop K'\mu}\right\rangle$ diagonalizing the $SU(1,1)$ subgroup. *[It is further being supposed that the spacelike representation satisfies (1.15) as in Ref. 2.]*

For the lightlike case, starting with an arbitrary direction of momentum, we need essentially evaluate the matrix elements of a finite rotation which brings $\mathbf{p}$ in the z direction such that finally

$$p = (w,0,0,w), \quad \text{say.} \tag{6.3}$$

The effect of a further Lorentz transformation parallel to the z axis, reducing p to

$$p_{(0)} \equiv (1,0,0,1) \tag{6.4}$$

is trivial (multiplication by a factor ω^{-1}). The remaining unknown factor can thus be taken to be (with $\rho=\tau$ for $W^2=-\tau^2, P^2=0$, and $p^0_{(0)}=1$)

$$\left\langle {p_{(0)}\mu \atop \tau} \middle| {\lambda j_0 \atop \tau\mu} \right\rangle \tag{6.5}$$

This factor and the corresponding one in (6.2) may be determined, except for a phase factor, through suitable normalization conditions.

A systematic study of these bases, using techniques similar to those used in this paper, may

be attempted by first obtaining the matrix elements of P^3 and $(P^0 - P^3)$ acting on the $\left|\begin{matrix}\lambda j_0\\ K j_3\end{matrix}\right\rangle$ and $\left|\begin{matrix}\lambda j_0\\ \rho j_3\end{matrix}\right\rangle$ bases, respectively.

To evaluate the matrix elements of P^3, one can start with the relations [compare with Eqs. (2.7) and (2.11) of Ref. 1, replacing μ^2 by P^2], valid for the general case

$$\{N^3[N^3, P^3]\} = -P^3,$$
$$\{P^3, [P^3, (\mathbf{N}^2 - \mathbf{M}^2)]\} = -2[(P^3)^2 + P^2], \quad (6.6)$$
$$\{P^3, [P^3, \mathbf{N}\cdot\mathbf{M}]\} = 0.$$

The corresponding relations for $(P^0 - P^3)$ are

$$[N^3, (P^0 - P^3)] = i(P^0 - P^3),$$
$$\{(P^0 - P^3), [P^0 - P^3), (\mathbf{N}^2 - \mathbf{M}^2)]\} = -2(P^0 - P^3)^2,$$
$$\{(P^0 - P^3), [(P^0 - P^3), \mathbf{N}\cdot\mathbf{M}]\} = 0. \quad (6.7)$$

In this article we will not enter into the details of these aspects. Let us only briefly mention that a preliminary study indicates that the matrix elements of P^3 on the $\left|\begin{matrix}\lambda j_0\\ K j_3\end{matrix}\right\rangle$ basis can be given a form fairly similar (in terms of K) to those of P^0 on the $\left|\begin{matrix}\lambda j_0\\ j j_3\end{matrix}\right\rangle$ basis, and that those of $(P^0 - P^3)$ on the $\left|\begin{matrix}\lambda j_0\\ p j_3\end{matrix}\right\rangle$ basis are simple, being obtained by replacing the j-dependent factors of the matrix elements of P^0 just by ρ (the same factor ρ appearing in all the four matrix elements). Such results are consistent with the solutions for the "$P_{(0)}$ transformation coefficients" [which appear in (6.2) and (6.5) quite analogous to that appearing in Appendix C], namely a phase factor multiplied by a constant factor. This phase factor may, however, be modified, depending on the precise phase conventions adopted for the matrix elements. It is needless to emphasize that such results depend on the assumed formal validity of certain manipulations. Several special features arise, particularly for the spacelike case.

Let us finally come back to the problem of transformations among the bases. We would like to indicate the precise consequences of our phase conventions [in subsections 5B and 5C] for the spacelike case on the representations of the little group $SU(1, 1)$ corresponding to (6.2) with $p_{(0)} = (0, 0, 0, m)$. It is easily seen that

$$\left\langle\begin{matrix}p_{(0)}\mu\\ K\end{matrix}\middle|\begin{matrix}\lambda j_0\\ j j_3\end{matrix} K\right\rangle \approx (2j+1)^{1/2}\left\langle K\begin{matrix}p_{(0)} j_3\\ j j_3\end{matrix}\middle|\begin{matrix}\lambda j_0\\ j j_3\end{matrix} K\right\rangle \delta_{\mu j_3} \quad (6.8)$$

is proportional to

$$\left\langle\begin{matrix}\lambda j_0\\ K j_3\end{matrix}\middle|\begin{matrix}\lambda j_0\\ j j_3\end{matrix}\right\rangle. \quad (6.9)$$

[We will not attempt to determine, in this paper, the exact factor of proportionality. It does not affect the results (6.10) and (6.11).]

By considering the matrix elements of $(N_1 \pm iN_2)$ on the bra and ket, respectively, it can be shown (most easily on considering the states with $j_3 = \pm j$) by using the solutions obtained in subsections 5B and 5C that our conventions correspond to the results (apart from the evident one for M_3)

$$\left\langle\begin{matrix}\lambda j_0\\ K j_3 \pm 1\end{matrix}\middle| N_\pm \middle|\begin{matrix}\lambda j_0\\ K j_3\end{matrix}\right\rangle = \pm[(K \mp j_3)(K \pm j_3 + 1)]^{1/2}$$
$$\text{for } K = -\tfrac{1}{2} + i\eta, \quad (6.10)$$

and

$$\left\langle\begin{matrix}\lambda j_0\\ K j_3 \pm 1\end{matrix}\middle| N_\pm \middle|\begin{matrix}\lambda j_0\\ K j_3\end{matrix}\right\rangle = \mp i[j_3 \mp K)(j_3 \pm K \pm 1)]^{1/2}$$
$$\text{for } K = -n. \quad (6.11)$$

Thus, in both cases, our conventions lead to purely imaginary Hermitic matrix elements.

Similarly from our corresponding results for the lightlike case, it can be shown that our conventions correspond to the results

$$\left\langle\begin{matrix}\lambda j_0\\ \rho j_3 \pm 1\end{matrix}\middle|(M_\pm \mp iN_\pm)\middle|\begin{matrix}\lambda j_0\\ \rho j_3\end{matrix}\right\rangle = -\rho. \quad (6.12)$$

Certain other more complicated related results can also be obtained from our solutions. In this article, however, we limit our discussion to the preceeding brief remarks.

APPENDIX A: NORMALIZATION OF THE TRANSFORMATION COEFFICIENTS ($P^2 = 0$, $W^2 = -\tau^2$)

The normalization of the states are defined to be (considering a space corresponding to a fixed value of τ)

$$\left\langle \tau\ \begin{matrix}\lambda' j_0'\\ j' j_3'\end{matrix}\middle|\begin{matrix}\lambda j_0\\ j j_3\end{matrix}\ \tau\right\rangle = (j_0^2 + \lambda^2)^{-1}\delta(\lambda' - \lambda)\delta_{j_0' j_0}\delta_{j' j}\delta_{j_3' j_3}$$
$$j_0 = -j, +1, \cdots, j,\ 0 \leq \lambda < \infty, \quad (A1)$$

and

$$\left\langle \tau\ \begin{matrix}p_0'\mu'\\ j' j_3'\end{matrix}\middle|\begin{matrix}p_0\mu\\ j j_3\end{matrix}\ \tau\right\rangle = 2p_0^{-1}\delta(p_0' - p_0)\delta_{\mu'\mu}\delta_{j' j}\delta_{j_3' j_3}. \quad (A2)$$

Inserting the completeness relation corresponding to (A2) in (A1), we obtain

$$\sum_\mu \int_0^\infty d|\mathbf{p}|\,\frac{|\mathbf{p}|}{2}\left\langle\begin{matrix}\lambda' j_0'\\ j j_3\end{matrix}\middle|\begin{matrix}p^0\mu\\ j j_3\end{matrix}\right\rangle\left\langle\begin{matrix}p^0\mu\\ j j_3\end{matrix}\middle|\begin{matrix}\lambda j_0\\ j j_3\end{matrix}\right\rangle$$
$$= (j_0^2 + \lambda^2)^{-1}\,\delta(\lambda' - \lambda)\delta_{j_0' j_0}. \quad (A3)$$

The general expression obtained by substituting (3.23) in (A3) is complicated. *But, since $C(\tau)$ is independent of j, it is sufficient for our purpose to take the simplest case, namely, $j = 0$.*

Let us, however, write a somewhat more general expression by putting (for arbitrary j) $j_0' = j_0 = j$. Let us also consider in particular the case $\epsilon = +1$, since the other case can be treated exactly the same.

We obtain the condition

$$\{(j+i\lambda-1)!(j-i\lambda-1)!\}\delta(\lambda'-\lambda) = \sum_{\mu}\int_0^\infty dp_0\,\frac{p_0}{2}\left(\frac{\tau}{2p_0}\right)^{2(j+1)} C(\tau)C^*(\tau) \times K_{\mu+i\lambda}\left(\frac{\tau}{p_0}\right)K_{\mu-i\lambda}\left(\frac{\tau}{p_0}\right)K_{\mu-i\lambda'}\left(\frac{\tau}{p_0}\right) \times (2j)!\{(j+\mu)!(j-\mu)!\}^{-1}. \quad \text{(A4)}$$

Now

$$\int_0^\infty dp_0\,\frac{p_0}{2}\left(\frac{\tau}{2p_0}\right)^{2(j+1)} K_{\mu+i\lambda}\left(\frac{\tau}{p_0}\right)K_{\mu-i\lambda'}\left(\frac{\tau}{p_0}\right) = \frac{\tau^2}{2^{(2j+3)}}\int_0^\infty dx\, x^{(2j-1)}K_{\mu+i\lambda}(x)\,K_{\mu-i\lambda'}(x). \quad \text{(A5)}$$

Via the formulas[41]

$$K_{\mu+i\lambda}(x)\,K_{\mu-i\lambda'}(x) = 2\int_0^\infty K_{i(\lambda+\lambda')}(2x\cosh t) \times \cosh[2\mu+i(\lambda-\lambda')t]\,dt \quad \text{(A6)}$$

and

$$\int_0^\infty K_{i(\lambda+\lambda')}(2x\cosh t)x^{2j-1}\,dx = 2^{(2j-2)}(2\cosh t)^{-2j} \times \Gamma\left(j+i\,\frac{(\lambda+\lambda')}{2}\right)\Gamma\left(j-i\,\frac{(\lambda+\lambda')}{2}\right), \quad \text{(A7)}$$

the rhs of (A5) becomes finally

$$\frac{\tau^2}{2^{2(j+2)}}\Gamma\left(j+i\frac{(\lambda+\lambda')}{2}\right)\Gamma\left(j-i\frac{(\lambda+\lambda')}{2}\right) \times \left[\int_0^\infty dt\,\frac{\cosh(2\mu t)}{(\cosh t)^{2j}}\cos(\lambda-\lambda')t + (\text{a part antisymmetric in }\mu)\right]. \quad \text{(A8)}$$

Evidently, we can neglect the part antisymmetric in μ in view of the summation over μ in (A4). Moreover,

$$\frac{(2j)!}{2^{(2j)}}\sum_{\mu=-j}^{j}\frac{\cosh(2\mu t)}{(j+\mu)!(j-\mu)!} = (\cosh t)^{2j}. \quad \text{(A9)}$$

Thus, finally, (A4) reduces to

$$\delta(\lambda'-\lambda) = C(\tau)C^*(\tau)\tfrac{1}{16}\tau^2 \times \frac{\Gamma(j+i(\lambda+\lambda')/2)\Gamma(j-i(\lambda+\lambda')/2)}{\Gamma(j+i\lambda)\Gamma(j-i\lambda)} \times \int_0^\infty \cos(\lambda'-\lambda)\,t\,dt \quad \text{(A10)}$$

$$= C(\tau)C^*(\tau)\tfrac{1}{16}\tau^2\pi\delta(\lambda'-\lambda). \quad \text{(A11)}$$

Hence, except for a constant (arbitrary) phase factor,

$$C(\tau) = 4/\sqrt{\pi}\,\tau. \quad \text{(A12)}$$

Having once determined $C(\tau)$ as above, we can indeed reverse the procedure and utilize (A3) to assert the general result for the sum and integral of the special functions involved.

We would like at this stage to draw attention to the consequences of the fact that the representations (j_0, λ) and $(-j_0, -\lambda)$ of HLG are equivalent [compare Ref. 1, Eqs. (3.31), (3.32)].

For $j = 0 = \mu = j_0$, using the symmetry

$$K_{i\lambda'}(x) = K_{-i\lambda'}(x),$$

we can also obtain finally $\delta(\lambda+\lambda')$ on the rhs of (A11). This ambiguity corresponds to the equivalence of the representations $(0, \lambda)$ and $(0, -\lambda)$.

For $j = \frac{1}{2}$, if we fix $j_0 = +\frac{1}{2}$ (say), then the above feature is naturally no longer present. But it appears (as may easily be verified) when we test the orthogonality of the states

$$j_0 = \pm\tfrac{1}{2} \quad \text{and} \quad j_0' = \mp\tfrac{1}{2},$$

respectively.

We will exclude such ambiguities by fixing the ranges of j_0 and λ as in (A1).

Our normalization must be consistent with the completeness relation

$$\mathrm{I} = \sum_{j_0 j j_3}\int_0^\infty d\lambda\,(j_0^2+\lambda^2)\left|\begin{matrix}\lambda j_0\\ j j_3\end{matrix}\right\rangle\left\langle\begin{matrix}\lambda j_0\\ j j_3\end{matrix}\right|. \quad \text{(A13)}$$

A simple check is provided by inserting (A13) in (A2) for the case $j = 0$.

Using the value (A12), we obtain finally the consistency condition

$$\int_0^\infty \frac{d\lambda}{\Gamma(i\lambda)\Gamma(-i\lambda)}K_{i\lambda}\left(\frac{\tau}{p_0}\right)K_{i\lambda}\left(\frac{\tau}{p_0'}\right) = \tfrac{1}{2}\pi\,p_0\delta(p_0-p_0'). \quad \text{(A14)}$$

The lhs is

$$\frac{1}{\pi}\int_0^\infty \lambda\sinh(\pi\lambda)\,K_{i\lambda}\left(\frac{\tau}{p_0}\right)K_{i\lambda}\left(\frac{\tau}{p_0}\right)d\lambda. \quad \text{(A15)}$$

Using[42]

$$\frac{2}{\pi}\int_0^\infty K_{ix}(a)K_{ix}(b)\cosh[(\pi-\varphi)x]\,dx = K_0[(a^2+b^2-2ab\cos\varphi)^{1/2}], \quad \text{(A16)}$$

we obtain (putting $a = \tau/p_0$, $b = \tau/p_0'$

$$\frac{1}{\pi}\int_0^\infty \lambda\sinh(\pi\lambda)K_{i\lambda}(a)K_{i\lambda}(b)\,d\lambda = -\tfrac{1}{2}\lim_{\varphi\to 0}\frac{\partial}{\partial\varphi}K_0[(a^2+b^2-2ab\cos\varphi)^{1/2}] = -\tfrac{1}{2}\lim_{\varphi\to 0}K_0'[(a^2+b^2-2ab\cos\varphi)^{1/2}] \times \frac{ab\sin\varphi}{(a^2+b^2-2ab\cos\varphi)^{1/2}}$$

$$= \frac{(ab)^{1/2}}{2} \lim_{(ab)^{1/2}\varphi \to 0} \frac{(ab)^{1/2}\varphi}{(a-b)^2 + ab\varphi^2}$$

(using [43] the explicit expression for K_0)

$$= \tfrac{1}{2}\, a\pi\delta(a-b) = \tfrac{1}{2}\,\pi p_0\,\delta(p_0' - p_0). \qquad \text{(A17)}$$

This verifies (A14).

Again we can assert the corresponding general formula (arbitrary j) on the basis of our group theoretical results.

APPENDIX B: SOLUTION FOR $P^2 = m^2$, $W^2 = 0$

In this case only Eq. (4.2) need be considered, with

$$\left\langle \begin{matrix} p\,0\,0 \\ j j_3 \end{matrix} \middle| \begin{matrix} 0\lambda \\ j j_3 \end{matrix} \right\rangle = [(i\lambda)!(-i\lambda)!(j+i\lambda)!(j-i\lambda)!]^{-1/2} A^{j_0}_{\lambda_0}(p_0) \qquad \text{(B1)}$$

(since $s = 0 = \mu = j_0$).

[In this case (4.2) can be directly obtained from (2.2).]

For $j_0 = 0$, (4.2) corresponds to a recurrence relation for the Legendre functions[44] and we obtain

$$A^j_\lambda(p_0 \sim P^{-j-1/2}_{i\lambda-1/2}(\epsilon p_0/m). \qquad \text{(B2)}$$

Using successively the matrix elements of $(P_1 \pm iP_2)$ and G_0 (as in Sec. 3) and the relevant recursion relations of the Legendre functions,[45] we obtain the respective factors

$$(e^{i\epsilon\pi/2j})(j+i\lambda)!(j-i\lambda)! \quad \text{and} \quad |\mathbf{p}|^{-1/2}. \qquad \text{(B3)}$$

The final normalization constant $(2/m)^{1/2}$ is obtained at once on using a property of the Legendre function proved by Joos [Ref. 7, Eq. (4.15)].

Finally we obtain

$$\left\langle m \begin{matrix} p_0 \\ j j_3 \end{matrix} \middle| \begin{matrix} \lambda \\ j j_3 \end{matrix} m \right\rangle = \frac{e^{i\epsilon\pi/2j}}{m} \left[\frac{(j+i\lambda)!(j-i\lambda)!}{(i\lambda)!(-i\lambda)!}\right]^{1/2} \left(\frac{2m}{|\mathbf{p}|}\right)^{1/2} P^{-j-1/2}_{i\lambda-1/2}\left(\frac{ep_0}{m}\right).$$

This formula coincides (except for a factor λ^{-1} arising from a different normalization for the Lorentz basis) with the one found by Joos in a different fashion [Ref. 7, Eq. (4.18)].

APPENDIX C

In this appendix we consider the transformation coefficient to the Lorentz basis corresponding to the rest frame of the timelike momenta, namely,

$$\left\langle \begin{matrix} 0, s^3 \\ [m, s] \end{matrix} \middle| \begin{matrix} \lambda j_0 \\ s s_3 \end{matrix} \right\rangle, \qquad \text{(C1)}$$

This is, of course, a very simple particular case of the solution found in Sec. 4. We study it separately to show clearly how our methods permit a simple study of the factorized structure (1.5). It can be shown easily that it is independent of S_3 and we will write it briefly as

$$\langle \lambda j_0 \rangle_{(0)}. \qquad \text{(C2)}$$

Using the matrix elements of P^0, we obtain

$$m\langle \lambda j_0 \rangle_{(0)} = [m/2(j_0^2 + \lambda^2)] \times [A_{j_0+1} + A_{j_0-1} + B_{\lambda+i} + B_{\lambda-i}], \qquad \text{(C3)}$$

where

$$A_{j_0\pm1} = (S \mp j_0)(S \pm j_0 + 1)\langle \lambda j_0 \pm 1 \rangle_{(0)}$$

and

$$B_{\lambda\pm i} = (S \pm i\lambda)(S \mp i\lambda + 1)\langle \lambda \pm i j_0 \rangle_{(0)}. \qquad \text{(C4)}$$

Similarly, using the matrix element of W^0, we obtain

$$0 = i\lambda\{A_{j_0+1} - A_{j_0-1}\} - j_0\{B_{\lambda+i} - B_{\lambda-i}\}. \qquad \text{(C5)}$$

Finally, using the matrix elements of G^0, we obtain

$$3m\langle \lambda j_0 \rangle_{(0)} = \{(2j_0+1)A_{j_0+1} - (2j_0-1)A_{j_0-1}\} - \{(2i\lambda - 1)B_{\lambda+i} - (2i\lambda+1)B_{\lambda-i}\}. \qquad \text{(C6)}$$

Combining (C3)–(C6), we obtain

$$(S-j_0)(S+j_0+1)[\langle \lambda\ j_0+1\rangle_{(0)} + \langle \lambda\ j_0\rangle_{(0)}] = (S-j_0+1)(S+j_0)[\langle \lambda\ j_0\rangle_{(0)} + \langle \lambda\ j_0-1\rangle_{(0)}] \qquad \text{(C7)}$$

and

$$(S+i\lambda)(S-i\lambda+1)[\langle \lambda + ij_0\rangle_{(0)} - \langle \lambda j_0\rangle_{(0)}] = -(S+i\lambda+1)(S-i\lambda)[\langle \lambda j_0\rangle_{(0)} - \langle \lambda - ij_0\rangle_{(0)}]. \qquad \text{(C8)}$$

The boundary condition

$$|j_0| \leq S$$

gives at once

$$\langle \lambda j_0 \rangle_{(0)} = \langle \lambda S \rangle_{(0)} e^{\pm i\pi j_0}. \qquad \text{(C9)}$$

Also, from (C3), (C7), and (C8), one finally obtains

$$\langle \lambda, S \rangle_{(0)} = \langle \lambda + i, s \rangle_{(0)}.$$

Hence the solution satisfying the boundary and suitable normalization condition can be taken to be, say,

$$\langle \lambda j_0 \rangle_{(0)} = \mathfrak{A}_{(m,s)} e^{i\pi j_0}, \qquad \text{(C10)}$$

where $\mathfrak{A}_{(m,s)}$ may depend only on m and s.

[1] A. Chakrabarti, M. Levy-Nahas, and R. Seneor, J. Math. Phys. **9**, 1274 (1968), Paper I.
[2] A. Chakrabarti, J. Maths. Phys. **12**, 1813 (1971).
[3] N. Ya. Vilenkin and Ya. A. Smorodinsky, Zh. Eksp. Teor. Fiz. **46**, 1793 (1964) [Sov. Phys. JETP **19**, 1209 (1964)].
[4] P. Winternitz, Ya. A. Smorodinsky, and M. B. Sheftel, Sov. J. Nucl. Phys. **7**, 785 (1968)
[5] J. Strahdee, J. F. Boyce, R. Delbourgo, and A. Salam, ICTP, Preprint IC/67/9, 1967.
[6] G. Feldman and P. T. Malhews, Ann. Phys. (N.Y.) **55**, 506 (1969).
[7] H. Joos, Fortschr. Phys. **10**, 65 (1962).
[8] M. A. Liberman, Ya. A. Smorodinsky, and M. B. Sheftel, Sov. J. Nucl. Phys. **7**, 146, (1968).
[9] W. Rühl, CERN, Preprint TH. 1016-CERN, 1969.
[10] If we use the helicity basis, we have to replace $\Lambda(p)$ by a rotation bringing **p** along the z axis, followed by a pure Lorentz transformation to the rest frame.
[11] The summation over j', j_3' disappears since $|p_{(0)}, S_3\rangle$ is also an eigenstate of $\mathbf{M}^2$ and M^3 and with eigenvalues $S(S+1)$ and S_3, respectively.
[12] S. Ström, Arkiv Fysik **29**, 467 (1965).
[13] Dao Vong Duc and Nguyen Van Hieu, Ann. Inst. Henri Poincaré **6**, 17 (1967).
[14] A. Sebestyen, K. Szegö, and K. Toth, Forschr. Phys. **17**, 167 (1969).
[15] J. Sciarrino and M. Toller, J. Math. Phys. **8**, 1252 (1967).
[16] S. Ström, Arkiv Fysik **34**, 215 (1967).
[17] N. Mukunda, J. Math. **9**, 50 (1968).
[18] R. Delbourgo, K. Koller, and N. Matanta, Nuovo Cimento **52A**, 1254 (1967).
[19] N. W. Macfadyen, Nuovo Cimento **62A**, 925 (1969); Cambridge University Preprint DAMPT 69/8, 1969; Maths. Phys. **12**, 492 (1971).
[20] J. F. Boyce, J. Math. Phys. **8**, 675 (1967). Other important sources are quoted in this paper.
[21] The O-system expansion of Ref. 4 can, for example, be adopted for all values of P^2.
[22] It is to be noted that due to the peculiar nature of the variations $(\lambda \pm i)$ an alteration in the choice of the phase factor φ' is nontrivial. Hence working rules concerning this choice have to be evolved by carefully examining the properties of the results obtained. For $P^2 \geq 0$ we will always choose $\varphi = \varphi' = 0$. The necessary conventions for the spacelike case are explained in Sec. 5.
[23] Though the ranges of μ and j_0 which are finite $(-s \leq \mu, j_0 \leq s)$ for the timelike case increase along with j for the zero-mass continuous-spin one, each term is individually more simple for the later case.
[24] The general equations can finally be given a form symmetric in μ and j_0, and one can equally well start from a limiting value of j_0.
[25] The variation of certain corresponding parameters from their limiting values in Refs. 12 and 8 causes considerable complications, and the general solutions are not written explicitly. In Ref. 7 Joos has to introduce summations over 6-j symbols with complex coefficients. The unsolved differential difference equations of Ref. 14 are not so convenient either. It may be said that the general solution obtained in Ref. 13 is a fairly symmetric one and simpler in the sense that x $(x = e^{-2\zeta}$, where $p_0 = m\cosh\zeta)$ does not appear in the coefficients of the hypergeometric functions involved. But, on the other hand, even for the limiting values of m (replacing our μ) the solution (4.11) of Ref. 13 still involves [unlike (4.20)] a summation over one parameter and in general contains a much larger number of terms than our solution, which, moreover, involves only hypergeometric polynomials and not general hypergeometrical functions. The symmetry properties of our solution are also simpler.
[26] A single derivative appears in extracting the final p^0 dependence by using G^0. But this turns out to be quite simple.
[27] To the present authors knowledge the first explicit use is found in H. Joos, Revista Univ. Mat. Arg. **18**, 119 (1958). For a discussion in the context of $SU(1,1)$ one may consult G. Lindblad and B. Nagel, Ann. Inst. Henré Poincaré **13**, 27 (1970). Several other sources are quoted in this paper and in Ref. 1.
[28] A. Erdelyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 2, p. 79, Eq. (25).
[29] Ref. 28, Vol. 2, p. 79, Eq. (26).
[30] We have preferred to start with the case which leads to zero-mass continuous-spin representations in the limit.
[31] Ref. 28, Vol. 1, p. 103, Eqs. (28) and (29).
[32] The factor $\csc\{\pi(j_0 + i\lambda)\}$ of 4.12) appears in the definition of $K_{j_0+i\lambda}$.
[33] Ref. 12, Eq. (3.4).
[34] Compare Eqs. (1.5) and (1.12) with **p** parallel to the z axis.
[35] Ref. 28, Vol. 1, p. 47 (5).
[36] A. Erdelyi *et al.*, *Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. 1, p. 198 (27).
[37] The phase convention for $\alpha_{(\pm)}$ is chosen to as to ensure the symmetry $\mu \rightleftharpoons j_0$ of the solutions.
[38] Ref. 28, Vol. 1, p. 63 (17).
[39] S. J. Chang and L. O'Raifeartaigh, J. Math. Phys. **10**, 21 (1969).
[40] G. J. Iverson and G. Mack, ICTP, Preprint IC/69/53, 1969.
[41] Ref. 28, Vol. 2, p. 54. Eq. (39); p. 51, Eq. (27).
[42] Ref. 28, Vol. 2, p. 55, Eq. (42).
[43] Ref. 28, Vol. 2, p. 9, Eq. (38).
[44] Ref. 28, Vol. 1, p. 160, Eq. (2).
[45] Ref. 28, Vol. 1, p. 161, Eqs. (5), (6), and (10).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Polynomial Expansion Method for Problems Involving a Relativistic Maxwellian Distribution

Keiichi Nishimura
Lawrence Radiation Laboratory, University of California, Livermore, California
(Received 29 March 1971)

With the aim of extending the Sonine polynomial expansion method to the region of relativistic Maxwellian distribution functions, a new set of polynomials has been introduced in terms of their orthogonality equation. Their coefficients have been derived and tabulated as functions of the temperature for several lowest orders.

I. INTRODUCTION

The Sonine–Laguerre polynomials $S_m^{(a)}(x)$ are popular in plasma physics as well as in the molecular theory of gases and liquids because of their orthogonality condition

$$\int_0^\infty x^a e^{-x} S_m^{(a)}(x) S_{m'}^{(a)}(x)\, dx \propto \delta_{mm'}. \tag{1}$$

The advantage provided by this orthogonality condition becomes apparent if one makes the substitution $x = mv^2/2kT$, where $mv^2/2$ is the kinetic energy of a plasma particle or a molecule of the gas or the liquid and kT is the temperature of the system in units of energy. Then the weight function of the orthogonality equation contains what essentially is a Maxwellian distribution function

[1] A. Chakrabarti, M. Levy-Nahas, and R. Seneor, J. Math. Phys. **9**, 1274 (1968), Paper I.
[2] A. Chakrabarti, J. Maths. Phys. **12**, 1813 (1971).
[3] N. Ya. Vilenkin and Ya. A. Smorodinsky, Zh. Eksp. Teor. Fiz. **46**, 1793 (1964) [Sov. Phys. JETP **19**, 1209 (1964)].
[4] P. Winternitz, Ya. A. Smorodinsky, and M. B. Sheftel, Sov. J. Nucl. Phys. **7**, 785 (1968)
[5] J. Strahdee, J. F. Boyce, R. Delbourgo, and A. Salam, ICTP, Preprint IC/67/9, 1967.
[6] G. Feldman and P. T. Malhews, Ann. Phys. (N.Y.) **55**, 506 (1969).
[7] H. Joos, Fortschr. Phys. **10**, 65 (1962).
[8] M. A. Liberman, Ya. A. Smorodinsky, and M. B. Sheftel, Sov. J. Nucl. Phys. **7**, 146, (1968).
[9] W. Rühl, CERN, Preprint TH. 1016-CERN, 1969.
[10] If we use the helicity basis, we have to replace $\Lambda(p)$ by a rotation bringing **p** along the z axis, followed by a pure Lorentz transformation to the rest frame.
[11] The summation over j', j_3' disappears since $|p_{(0)}, S_3\rangle$ is also an eigenstate of $\mathbf{M}^2$ and M^3 and with eigenvalues $S(S+1)$ and S_3, respectively.
[12] S. Ström, Arkiv Fysik **29**, 467 (1965).
[13] Dao Vong Duc and Nguyen Van Hieu, Ann. Inst. Henri Poincaré **6**, 17 (1967).
[14] A. Sebestyen, K. Szegö, and K. Toth, Forschr. Phys. **17**, 167 (1969).
[15] J. Sciarrino and M. Toller, J. Math. Phys. **8**, 1252 (1967).
[16] S. Ström, Arkiv Fysik **34**, 215 (1967).
[17] N. Mukunda, J. Math. **9**, 50 (1968).
[18] R. Delbourgo, K. Koller, and N. Matanta, Nuovo Cimento **52A**, 1254 (1967).
[19] N. W. Macfadyen, Nuovo Cimento **62A**, 925 (1969); Cambridge University Preprint DAMPT 69/8, 1969; Maths. Phys. **12**, 492 (1971).
[20] J. F. Boyce, J. Math. Phys. **8**, 675 (1967). Other important sources are quoted in this paper.
[21] The O-system expansion of Ref. 4 can, for example, be adopted for all values of P^2.
[22] It is to be noted that due to the peculiar nature of the variations $(\lambda \pm i)$ an alteration in the choice of the phase factor φ' is nontrivial. Hence working rules concerning this choice have to be evolved by carefully examining the properties of the results obtained. For $P^2 \geq 0$ we will always choose $\varphi = \varphi' = 0$. The necessary conventions for the spacelike case are explained in Sec. 5.
[23] Though the ranges of μ and j_0 which are finite $(-s \leq \mu, j_0 \leq s)$ for the timelike case increase along with j for the zero-mass continuous-spin one, each term is individually more simple for the later case.
[24] The general equations can finally be given a form symmetric in μ and j_0, and one can equally well start from a limiting value of j_0.
[25] The variation of certain corresponding parameters from their limiting values in Refs. 12 and 8 causes considerable complications, and the general solutions are not written explicitly. In Ref. 7 Joos has to introduce summations over 6-j symbols with complex coefficients. The unsolved differential difference equations of Ref. 14 are not so convenient either. It may be said that the general solution obtained in Ref. 13 is a fairly symmetric one and simpler in the sense that x $(x = e^{-2\zeta}$, where $p_0 = m\cosh\zeta)$ does not appear in the coefficients of the hypergeometric functions involved. But, on the other hand, even for the limiting values of m (replacing our μ) the solution (4.11) of Ref. 13 still involves [unlike (4.20)] a summation over one parameter and in general contains a much larger number of terms than our solution, which, moreover, involves only hypergeometric polynomials and not general hypergeometrical functions. The symmetry properties of our solution are also simpler.
[26] A single derivative appears in extracting the final p^0 dependence by using G^0. But this turns out to be quite simple.
[27] To the present authors knowledge the first explicit use is found in H. Joos, Revista Univ. Mat. Arg. **18**, 119 (1958). For a discussion in the context of $SU(1,1)$ one may consult G. Lindblad and B. Nagel, Ann. Inst. Henré Poincaré **13**, 27 (1970). Several other sources are quoted in this paper and in Ref. 1.
[28] A. Erdelyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 2, p. 79, Eq. (25).
[29] Ref. 28, Vol. 2, p. 79, Eq. (26).
[30] We have preferred to start with the case which leads to zero-mass continuous-spin representations in the limit.
[31] Ref. 28, Vol. 1, p. 103, Eqs. (28) and (29).
[32] The factor $\csc\{\pi(j_0 + i\lambda)\}$ of 4.12) appears in the definition of $K_{j_0+i\lambda}$.
[33] Ref. 12, Eq. (3.4).
[34] Compare Eqs. (1.5) and (1.12) with **p** parallel to the z axis.
[35] Ref. 28, Vol. 1, p. 47 (5).
[36] A. Erdelyi *et al.*, *Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. 1, p. 198 (27).
[37] The phase convention for $\alpha_{(\pm)}$ is chosen to as to ensure the symmetry $\mu \rightleftharpoons j_0$ of the solutions.
[38] Ref. 28, Vol. 1, p. 63 (17).
[39] S. J. Chang and L. O'Raifeartaigh, J. Math. Phys. **10**, 21 (1969).
[40] G. J. Iverson and G. Mack, ICTP, Preprint IC/69/53, 1969.
[41] Ref. 28, Vol. 2, p. 54. Eq. (39); p. 51, Eq. (27).
[42] Ref. 28, Vol. 2, p. 55, Eq. (42).
[43] Ref. 28, Vol. 2, p. 9, Eq. (38).
[44] Ref. 28, Vol. 1, p. 160, Eq. (2).
[45] Ref. 28, Vol. 1, p. 161, Eqs. (5), (6), and (10).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Polynomial Expansion Method for Problems Involving a Relativistic Maxwellian Distribution

Keiichi Nishimura
Lawrence Radiation Laboratory, University of California, Livermore, California
(Received 29 March 1971)

With the aim of extending the Sonine polynomial expansion method to the region of relativistic Maxwellian distribution functions, a new set of polynomials has been introduced in terms of their orthogonality equation. Their coefficients have been derived and tabulated as functions of the temperature for several lowest orders.

I. INTRODUCTION

The Sonine–Laguerre polynomials $S_m^{(a)}(x)$ are popular in plasma physics as well as in the molecular theory of gases and liquids because of their orthogonality condition

$$\int_0^\infty x^a e^{-x} S_m^{(a)}(x) S_{m'}^{(a)}(x)\, dx \propto \delta_{mm'}. \tag{1}$$

The advantage provided by this orthogonality condition becomes apparent if one makes the substitution $x = mv^2/2kT$, where $mv^2/2$ is the kinetic energy of a plasma particle or a molecule of the gas or the liquid and kT is the temperature of the system in units of energy. Then the weight function of the orthogonality equation contains what essentially is a Maxwellian distribution function

which in most cases serves as the zeroth-order distribution function $f_0(v)$. The perturbed distribution function may be written, for example, in the form $f_0(v)[1 + \varphi(v)]$, and we expand the function $\varphi(v)$ as $\sum b_r S_r^{(a)}(mv^2/2kT)$. We then linearize the equation involving the distribution function, and the result is an expression of the form

$$f_0(v)\sum b_r S_r^{(a)}(mv^2/2kT) = \text{a known expression.} \quad (2)$$

The set of expansion coefficients b_r will be obtained by multiplying (2) with $s_{r'}^{(a)}(mv^2/2kT)$ and then integrating it.[1]

In recent years, however, increasing attention has been given to high-temperature plasmas owing to their importance in astrophysics as well as in controlled thermonuclear research. When there is a significant number of electrons with kinetic energies comparable to the rest energy, a relativistic description becomes necessary for the electrons. In an unperturbed system, a relativistic Maxwellian distribution function must be used for $f_0(v)$, and hence the expansion method can no longer be carried out in terms of the Sonine polynomials. The purpose of this paper is to introduce a new set of polynomials which will play, for relativistic plasmas, the role played by the Sonine polynomials for a nonrelativistic Maxwellian distribution. In Sec. II, the problem will be more clearly defined and the expression for the polynomials will be derived. In Sec. III, we will show by a direct method that our new polynomials approach the form of the Sonine polynomials in the low-temperature limit. Finally, in Sec. IV, a numerical table of the coefficients will be given for several of the lowest orders of the polynomials.

II. THE NEW POLYNOMIALS

Let $X_m^{(a)}(x)$ be the desired polynomials; our first step is to establish an orthogonality condition which should be satisfied by them. We know that the relativistic Maxwellian distribution function is of the form $\exp\{mc^2[1 - (1 - v^2/c^2)^{-1/2}]/kT\}$, where mc^2 is the rest energy of the electron. Comparing this form with (1), we can write the orthogonality condition for the $X_m^{(a)}$ as follows:

$$\int_0^1 x^a \exp\left(\frac{1-(1-x)^{-1/2}}{t}\right) \times X_m^{(a)}(x)X_{m'}^{(a)}(x)\,dx = N_m^{(a)}\delta_{mm'}, \quad (3)$$

where the dimensionless parameter t is essentially the temperature of the system measured in units of the electron rest energy and $N_m^{(a)}$ is a normalization constant. It should be remembered at this point that the polynomials $X_m^{(a)}(x)$ will eventually depend on t. Note also that a is nonnegative, while m, being the order of the polynomial, must be a positive integer on zero.

We will start by writing

$$X_m^{(a)}(x) = \sum_{p=0}^{m} c(a,m,p)x^p, \quad (4)$$

where

$$c(a,m,m) \neq 0. \quad (5)$$

We substitute (4) into (3) and, changing variables, obtain

$$2\int_0^\infty (1+x)^{-3}e^{-x/t}\sum_{p=0}^{m}\sum_{p'=0}^{m'} c(a,m,p)c(a,m',p') \times [1-(1+x)^{-2}]^{a+p+p'}dx = N_m^{(a)}\delta_{mm'}. \quad (6)$$

For convenience, we define a set of functions g by

$$g_b(t) = 2\int_0^\infty (1+x)^{-3}e^{-x/t}[1-(1+x)^{-2}]^b dx. \quad (7)$$

The $g_b(t)$ functions can be evaluated by a binomial expansion and a change of variables. We obtain

$$g_b(t) = 2e^{-t}\Gamma(1+b)\sum_{p=0}^{\infty}\frac{(-1)^p E_{2p+3}(1/t)}{p!\,\Gamma(1+b-p)}, \quad (8)$$

where the E's are the exponential integral functions defined by[2]

$$E_n(z) = \int_1^\infty y^{-n}e^{-zy}\,dy, \qquad n = 0, 1, 2, \cdots. \quad (9)$$

Hereafter, the argument of the g functions will be dropped for convenience, but it is understood to be the parameter t.

With the use of (7), the orthogonality condition (6) is simplified into the form

$$\sum_{p=0}^{m}\sum_{p'=0}^{m'} c(a,m,p)c(a,m',p')g_{a+p+p'} = N_m^{(a)}\delta^{mm'}, \quad (10)$$

from which we immediately obtain, by setting $m = m' = 0$,

$$c(a,0,0) = (1/g_a)^{1/2}. \quad (11)$$

The higher-order coefficients can be obtained in an ascending order from (10) by the following procedure. Suppose now that we want the $m + 1$ coefficients $c(a,m,p)$, where $p = 0, 1, \ldots, m$, knowing all the lower-order coefficients. We then set $m = m$ in (10) and vary m' from 0 to m. The $m + 1$ equations thus generated are

$$\sum_{p=0}^{m}\sum_{p'=0}^{m'} c(a,m,p)c(a,m',p')g_{a+p+p'} = 0, \qquad m' = 0, 1, \cdots, m-1 \quad (12)$$

and

$$\sum_{p=0}^{m}\sum_{p'=0}^{m} c(a,m,p)c(a,m,p')g_{m+p+p'} = N_m^{(a)}. \quad (13)$$

We simplify (12) as follows. First, we consider the equation with $m' = 0$, which, by (5), can be reduced to

$$\sum_{p=0}^{m} c(a,m,p)g_{a+p} = 0. \quad (14)$$

Next, (14) is multiplied by $c(a,1,0)$ and substracted

from the second ($m' = 1$) of (12). The result is

$$\sum_{p=0}^{m} c(a,m,p) g_{a+p+1} = 0. \tag{15}$$

By repeating this procedure, the set of m equations (12) are simplified now to read

$$\sum_{p=0}^{m} c(a,m,p) g_{a+p+m'} = 0, \qquad m' = 0,1,\cdots,m-1, \tag{16}$$

This set of equations is first solved for the m ratios defined by

$$c'(a,m,p) = c(a,m,p)/c(a,m,m), \qquad p = 0,1,\cdots,m-1 \tag{17}$$

by the standard determinantal method. For this purpose, we define an $m \times m$ symmetric matrix $\mathsf{M}^{(m)}$ whose ij component is given by

$$M_{ij}^{(m)} = g_{a+i+j-2}, \quad i,j = 1,2,\cdots,m. \tag{18}$$

Furthermore, we define two m-component column matrices $\mathsf{C}^{(m)}$ and $\mathsf{G}^{(m)}$ whose pth components are given by

$$C_p^{(m)} = c'(a,m,p-1) \tag{19}$$

and

$$G_p^{(m)} = g_{a+p+m-1}, \tag{20}$$

respectively, so that (16) may now be written in a matrix form as

$$\mathsf{M}^{(m)}\mathsf{C}^{(m)} = -\mathsf{G}^{(m)}. \tag{21}$$

This matrix equation can be solved by the standard method if $\det\mathsf{M}^{(m)} \neq 0$. Let $\hat{M}_{ij}^{(m)}$ be the cofactor of the determinant of the matrix $\mathsf{M}^{(m)}$ corresponding to the ij component. Then the ij component of the inverse matrix of $\mathsf{M}^{(m)}$ is $\hat{M}_{ij}^{(m)}/\det\mathsf{M}^{(m)}$. Using this inverse matrix on (21) and equating the $(p+1)$st components of both sides, we obtain

$$c'(a,m,p) = C_{p+1}^{(m)} = -(\det\mathsf{M}^{(m)})^{-1} \times \sum_{j=1}^{m} \hat{M}_{p+1,j}^{(m)} M_{m+1,j}^{(m+1)}. \tag{22}$$

In the last line above, we used the relation

$$G_j^{(m)} = M_{m+1,j}^{(m+1)}. \tag{23}$$

Now it should be noted that the summation on the last line of (22) represents the determinant of an $m \times m$ matrix formed by replacing the $(p+1)$st column of $\mathsf{M}^{(m)}$ by the $(m+1)$st column of $\mathsf{M}^{(m+1)}$ with its bottom element removed. If we move this inserted column to the right-hand end, the determinant will change its sign $m-p-1$ times and the resultant matrix will be equal to the minor of $\det\mathsf{M}^{(m+1)}$ corresponding to the $(p+1, m+1)$ element. Remembering the relation between the cofactor and the minor of a determinant, we can write (22) as

$$c'(a,m,p) = \hat{M}_{p+1,m+1}^{(m+1)}/\det\mathsf{M}^{(m)}. \tag{24}$$

Our final step is to divide (13) by $[c(a,m,m)]^2$ and combine it with (24):

$$\begin{aligned} N_m^{(a)}[c(a,m,m)]^{-2} &= \sum_{p=0}^{m} c'(a,m,p) \sum_{p=0}^{m} c'(a,m,p') M_{p'+1,p+1}^{(m+1)} \\ &= (\det\mathsf{M}^{(m)})^{-1} \sum_{p=0}^{m} c'(a,m,p) \sum_{p'=0}^{m} \hat{M}_{p'+1,m+1}^{(m+1)} \\ &\quad \times M_{p'+1,p+1}^{(m+1)} \\ &= \det\mathsf{M}^{(m+1)}/\det\mathsf{M}^{(m)}. \end{aligned} \tag{25}$$

For convenience, we will define

$$\det\mathsf{M}^{(0)} = 1. \tag{26}$$

Then we can combine (24) and (25) and write in a simple form

$$c(a,m,p) = \hat{M}_{p+1,m+1}^{(m+1)} [N_m^{(a)}/(\det\mathsf{M}^{(m)}\det\mathsf{M}^{(m+1)})]^{1/2} \tag{27}$$

for $m = 0, 1, 2, \cdots$ and $p = 0, 1, \cdots, m$.

III. ASYMPTOTIC BEHAVIOR

As mentioned earlier, the parameter t will eventually play the role of kT/mc^2. Thus the nonrelativistic limit of our formalism will be reached by making t approach zero. In this section, this limit will be considered analytically. For convenience of presentation, however, we will assume a to be an integer and write it as n.

First, we will study the nonrelativistic limit of the g functions. As can be seen in (7), only the region of small x contributes to the integral if t is nearly zero. Then the remaining factors in the integrand may be expanded in power series of x, and the integration can be performed term by term, yielding

$$\lim_{t\to 0} g_n(t) = 2n! \sum_{p=0}^{n} \sum_{m=0}^{\infty} \frac{(-1)^{p+m}(2p+m+2)!\, t^{m+1}}{p!(n-p)!(2p+2)!}. \tag{28}$$

We will now use the lemma

$$\sum_{p=0}^{n} \frac{(-1)^p (2p+m+2)!}{p!(n-p)!(2p+2)!} = \begin{cases} 0 \text{ if } n > m \\ (-2)^n \text{ if } n = m \end{cases} \tag{29}$$

so that

$$\lim_{t\to 0} g_n(t) = (2t)^{n+1} n! \tag{30}$$

The above lemma may be proved by taking the mth derivative of $x^{m+2}(1-x^2)^n$. This is done first by the binomial expansion of the second factor.

Next we use the formula for taking the derivative of a product. After equating the two results, we set $x = 1$ to obtain (29).

We consider next the nonrelativistic limit of $\det \mathsf{M}^{(m)}$. By combining (18) and (30), we see that the ij element of $\det \mathsf{M}^{(m)}$ will be $(2t)^{n+i+j-1}(n + i + j - 2)!$ in this limit. This determinant can easily be evaluated by the standard method. First, we factor out $(2t)^{n+k}$ from the kth row and $(2t)^{k-1}$ from the kth column ($k = 1, 2, \cdots, m$). The ij element of the remaining determinant is $(n + 1 + j - 2)!$, and by repeating the well-known procedure of extracting a factor from a row and subtracting it from another row we can make all the elements of the determinant vanish below the principal diagonal. Thus we obtain

$$\lim_{t\to 0} \det \mathsf{M}^{(m)} = (2t)^{m^2+mn} \prod_{q=0}^{m-1} [q!(n+q)!]. \quad (31)$$

Finally, we calculate the nonrelativistic limit of $\hat{M}^{(m+1)}_{p+1,m+1}$, which, by definition, is $(-1)^{m+p}$ times the determinant of the matrix made from $\mathsf{M}^{(m+1)}$ by deleting the $(p + 1)$st row and the $(m + 1)$st column. To evaluate this determinant, we add to it at the bottom a row which was originally deleted from $\mathsf{M}^{(m+1)}$ and onto the extreme right-hand side a column whose elements are all zero except that the bottom element is 1. The value of the determinant remains unchanged by such additions. We next interchange rows $(m - p)$ times so that the added row will appear at the $(p + 1)$st place. We then repeat the same simplifying procedure described above. Paying special attention to see how the last column changes as subtractions of rows are repeated, we eventually obtain

$$\lim_{t\to 0} \hat{M}^{(m+1)}_{p+1,m+1} = \frac{(-1)^{m-p}(2t)^{mn+m^2+m-p} \prod_{q=0}^{m} [q!(n+q)!]}{(m-p)!\,p!\,(n+p)!}. \quad (32)$$

Using the nonrelativistic limits (31) and (32), we obtain

$$\lim_{t\to 0} X^{(n)}_m(x) = \left(\frac{m!(n+m)!N^{(n)}_m}{(2t)^{n+1}} \right)^{1/2} \times \sum_{p=0}^{m} \frac{(-1)^{m-p}(x/2t)^p}{(m-p)!p!(n+p)!}. \quad (33)$$

It should be observed that the above summation is of the form of $M(-m, n + 1, x/2t)$, where M is the hypergeometric function.[2] This function is also related to the Sonine polynomials by

$$M(-m, n+1, x) = [m!n!/(n+m)!]S^{(n)}_m(x). \quad (34)$$

Hence,

$$\lim_{t\to 0} X^{(n)}_m(x) = (-1)^m \left(\frac{m!N^{(n)}_m}{(n+m)!(2t)^{n+1}} \right)^{1/2} S^{(n)}_m\left(\frac{x}{2t}\right). \quad (35)$$

This asymptotic form is also true for nonintegral values of n except that the factorials must be replaced by gamma functions with appropriate arguments.

Before leaving this section, let us consider the other asymptotic region of t becoming infinitely large, though a plasma with a temperature much greater than the electron rest energy is not a practical problem at present.

When t is infinitely large, the exponential factor of (3) may be deleted and the weight function of the orthogonality equation becomes simply x^a. Hence, in this limit, our polynomials will take the form of $G_m(a + 1, a + 1, x)$, where the Jacobi polynomials $G_m(p, q, x)$ are, aside from a normalization factor, given by[2]

$$\sum_{m'=0}^{m} (-1)^{m'} \binom{m}{m'} \frac{\Gamma(p+m+m')x^{m'}}{\Gamma(q+m')}. \quad (36)$$

IV. TABULATION

Since the nonrelativistic limit is more of interest to us than the extremely relativistic limit, the normalization constant $N^{(a)}_m$ will be determined so that the deviation of the $X^{(a)}_m(x)$ from the Sonine polynomials will be shown most clearly as t increases from zero. We choose

$$N^{(a)}_m = m!(2t)^{a+2m+1}\Gamma(a+m+1) \quad (37)$$

in view of (33) and (35), so that

$$\lim_{t\to 0} c(a, m, m) = 1. \quad (38)$$

Further, we note in (35) that the argument of the Sonine polynomials is not x but $x/2t$ in the nonrelativistic limit. For this reason, we will rewrite (4) as

$$X^{(a)}_m(x) = (2t)^m c(a, m, m) \sum_{p=0}^{m} \tilde{c}(a, m, p)\left(\frac{x}{2t}\right)^p, \quad (39)$$

where

$$\tilde{c}(a, m, p) = (2t)^{p-m} c'(a, m, p). \quad (40)$$

Obviously, $\tilde{c}(a, m, m) = 1$. Hence, for the purpose of characterizing the polynomials it will be sufficient to tabulate $c(a, m, m)$ and $\tilde{c}(a, m, p)$, where $p = 0, 1, \cdots, m - 1$.

In the actual evaluation of these coefficients as functions of t, the first step is to integrate (7) numerically to obtain the g functions. The $g^{(t)}_b$ with smaller b are found to approach their asymptotic form (30) much faster than those with larger b. At $t = 0.01$, the ratio of $g^{(t)}_b$ to its nonrelativistic limit is 0.97 for $b = 0$, but it is 0.18 for $b = 10$. At $t = 0.001$, it is 0.997 for $b = 0$, while it is still as low as 0.82 for $b = 10$.

TABLE I. Coefficients of the derived polynomials as defined in the text. The number at the right in parentheses indicates the power of ten by which that entry should be multiplied.

t	$c(0,0,0)$	$c(0,1,0)$	$\bar{c}(0,1,0)$	$c(0,2,2)$	$\bar{c}(0,2,1)$	$\bar{c}(0,2,0)$	$c(0,3,3)$	$\bar{c}(0,3,2)$	$\bar{c}(0,3,1)$	$\bar{c}(0,3,0)$
0	1.00	1.00	−1.00	1.00	−4.00	2.00	1.00	−9.00	1.80(1)	−6.00
0.001	1.00	1.01	−9.94(−1)	1.03	−3.95	1.96	1.1	−8.8	1.7(1)	−5.7
0.002	1.00	1.02	−9.88(−1)	1.06	−3.90	1.92	1.1	−8.7	1.7(1)	−5.5
0.005	1.01	1.05	−9.71(−1)	1.15	−3.78	1.81	1.3	−8.3	1.5(1)	−4.9
0.01	1.01	1.10	−9.44(−1)	1.30	−3.58	1.65	1.6	−7.7	1.3(1)	−4.0
0.02	1.03	1.21	−8.96(−1)	1.63	−3.25	1.39	2.5	−6.7	1.1(1)	−2.9
0.05	1.07	1.53	−7.80(−1)	2.83	−2.58	9.14(−1)	6.5	−5.0	6.0	−1.3
0.1	1.13	2.07	−6.47(−1)	5.54	−1.95	5.44(−1)	1.9(1)	−3.6	3.1	−5.1(−1)
0.2	1.24	3.23	−4.90(−1)	1.38(1)	−1.34	2.67(−1)	8.2(1)	−2.3	1.3	−1.5(−1)
0.5	1.50	7.25	−2.92(−1)	6.54(1)	−7.08(−1)	7.87(−2)	8.6(2)	−1.2	3.5(−1)	2.1(−2)
1	1.83	1.55(1)	−1.79(−1)	2.61(2)	−4.05(−1)	2.64(−2)	6.5(3)	−6.4(−1)	1.1(−1)	−3.7(−3)
t	$c(\frac{1}{2},0,0)$	$c(\frac{1}{2},1,1)$	$\bar{c}(\frac{1}{2},1,0)$	$c(\frac{1}{2},2,2)$	$\bar{c}(\frac{1}{2},2,1)$	$\bar{c}(\frac{1}{2},2,0)$	$c(\frac{1}{2},3,3)$	$\bar{c}(\frac{1}{2},3,2)$	$\bar{c}(\frac{1}{2},3,1)$	$\bar{c}(\frac{1}{2},3,0)$
0	1.00	1.00	−1.50	1.00	−5.00	3.75	1.00	−1.05(1)	2.63(1)	−1.31(1)
0.001	1.00	1.01	−1.49	1.03	−4.93	3.66	1.1	−1.0(1)	2.5(1)	−1.3(1)
0.002	1.01	1.03	−1.48	1.07	−4.87	3.57	1.1	−1.0(1)	2.5(1)	−1.2(1)
0.005	1.01	1.07	−1.45	1.18	−4.69	3.34	1.4	−9.6	2.2(1)	−1.0(1)
0.01	1.03	1.14	−1.40	1.37	−4.42	3.00	1.8	−8.8	1.9(1)	−8.4
0.02	1.05	1.29	−1.31	1.79	−3.97	2.48	2.8	−7.7	1.5(1)	−5.8
0.005	1.13	1.74	−1.11	3.41	−3.09	1.57	8.1	−5.6	8.1	−2.5
0.1	1.25	2.55	−8.95(−1)	7.37	−2.30	8.99(−1)	2.7(1)	−4.0	4.1	−9.6(−1)
0.2	1.46	4.44	−6.56(−1)	2.09(1)	−1.55	4.24(−1)	1.3(2)	−2.5	1.7	−2.7(−1)
0.5	2.00	1.19(1)	−3.76(−1)	1.20(2)	−8.07(−1)	1.20(−1)	1.7(3)	−1.3	4.4(−1)	−3.6(−2)
1	2.75	2.95(1)	−2.24(−1)	5.59(2)	−4.57(−1)	3.91(−1)	1.5(4)	−6.9(−1)	1.3(−1)	−6.2(−3)
t	$c(1,0,0)$	$c(1,1,1)$	$\bar{c}(1,1,0)$	$c(1,2,2)$	$\bar{c}(1,2,1)$	$\bar{c}(1,2,0)$	$c(1,3,3)$	$\bar{c}(1,3,2)$	$\bar{c}(1,3,1)$	$\bar{c}(1,3,0)$
0	1.00	1.00	−2.00	1.00	−6.00	6.00	1.00	−1.20(1)	3.60(1)	−2.40(1)
0.001	1.00	1.02	−1.98	1.04	−5.91	5.84	1.1	−1.2(1)	3.5(1)	−2.3(1)
0.002	1.01	1.04	−1.97	1.08	−5.83	5.70	1.1	−1.2(1)	3.3(1)	−2.2(1)
0.005	1.02	1.09	−1.91	1.21	−5.59	5.28	1.4	−1.1(1)	3.0(1)	−1.9(1)
0.01	1.04	1.18	−1.84	1.45	−5.24	4.69	1.9	−1.0(1)	2.6(1)	−1.5(1)
0.02	1.09	1.37	−1.70	1.99	−4.67	3.80	3.2	−8.6	1.9(1)	−1.0(1)
0.05	1.21	2.00	−1.41	4.12	−3.57	2.31	1.0(1)	−6.2	1.0(1)	−4.1
0.1	1.41	3.19	−1.11	9.95	−2.61	1.28	3.9(1)	−4.3	5.2	−1.5
0.2	1.77	6.19	−7.91(−1)	3.18(1)	−1.74	5.83(−1)	2.1(2)	−2.8	2.1	−4.2(−1)
0.5	2.77	1.98(1)	−4.39(−1)	2.21(2)	−8.90(−1)	1.59(−1)	3.4(3)	−1.4	5.2(−1)	−5.3(−2)
1	4.33	5.70(1)	−2.57(−1)	1.21(3)	−5.00(−1)	5.09(−2)	3.5(4)	−7.4(−1)	1.6(−1)	−6.9(−3)
t	$c(\frac{3}{2},0,0)$	$c(\frac{3}{2},1,1)$	$\bar{c}(\frac{3}{2},1,0)$	$c(\frac{3}{2},2,2)$	$\bar{c}(\frac{3}{2},2,1)$	$\bar{c}(\frac{3}{2},2,0)$	$c(\frac{3}{2},3,3)$	$\bar{c}(\frac{3}{2},3,2)$	$\bar{c}(\frac{3}{2},3,1)$	$\bar{c}(\frac{3}{2},3,0)$
0	1.00	1.00	−2.50	1.00	−7.00	8.75	1.00	−1.35(1)	4.73(1)	−3.94(1)
0.001	1.01	1.02	−2.47	1.05	−6.89	8.49	1.1	−1.3(1)	4.5(1)	−3.7(1)
0.002	1.01	1.04	−2.45	1.10	−6.78	8.25	1.2	−1.3(1)	4.4(1)	−3.5(1)
0.005	1.03	1.11	−2.38	1.25	−6.48	7.59	1.5	−1.2(1)	3.9(1)	−3.0(1)
0.01	1.07	1.23	−2.27	1.54	−6.03	6.67	2.0	−1.1(1)	3.3(1)	−2.4(1)
0.02	1.13	1.48	−2.08	2.19	−5.33	5.30	3.6	−9.5	2.4(1)	−1.6(1)
0.05	1.31	2.31	−1.68	5.04	−4.01	3.11	1.3(1)	−6.8	1.3(1)	−6.1
0.1	1.62	4.03	−1.29	1.34(1)	−2.90	1.67	5.6(1)	−4.7	6.2	−2.2
0.2	2.21	8.72	−9.03(−1)	4.87(1)	−1.90	7.40(−1)	3.5(2)	−3.0	2.5	−5.8(−1)
0.5	3.98	3.33(1)	−4.88(−1)	4.10(2)	−3.62(−1)	1.95(−1)	6.7(3)	−1.4	6.1(−1)	−7.0(−2)
1	7.11	1.12(2)	−2.82(−1)	2.63(3)	−5.36(−1)	6.16(−2)	8.3(4)	−7.9(−1)	1.8(−1)	−1.2(−2)
t	$c(2,0,0)$	$c(2,1,1)$	$\bar{c}(2,1,0)$	$c(2,2,2)$	$\bar{c}(2,2,1)$	$\bar{c}(2,2,0)$	$c(2,3,3)$	$\bar{c}(3,3,2)$	$\bar{c}(2,3,1)$	$\bar{c}(2,3,0)$
0	1.00	1.00	−3.00	1.00	−8.00	1.20(1)	1.00	−1.50(1)	6.00(1)	−6.00(1)
0.001	1.01	1.03	−2.96	1.06	−7.86	1.16(1)	1.1	−1.5(1)	5.7(1)	−5.6(1)
0.002	1.02	1.05	−2.93	1.11	−7.72	1.12(1)	1.2	−1.4(1)	5.5(1)	−5.4(1)
0.005	1.04	1.14	−2.83	1.29	−7.35	1.03(1)	1.5	−1.3(1)	4.9(1)	−4.5(1)
0.01	1.09	1.28	−2.69	1.62	−6.81	8.92	2.2	−1.2(1)	4.1(1)	−3.5(1)
0.02	1.18	1.59	−2.44	2.43	−5.97	6.97	4.1	−1.0(1)	3.0(1)	−2.2(1)
0.05	1.44	2.70	−1.93	6.19	−4.42	3.96	1.7(1)	−7.3	1.5(1)	−8.4
0.1	1.89	5.14	−1.46	1.82(1)	−3.15	2.07	7.9(1)	−5.0	7.2	−2.9
0.2	2.82	1.25(1)	−9.98(−1)	7.54(1)	−2.04	8.91(−1)	5.8(2)	−3.1	2.9	−7.5(−1)
0.5	5.92	5.69(1)	−5.28(−1)	7.69(2)	−1.02	2.29(−1)	1.3(4)	−1.5	6.8(−1)	−8.8(−2)
1	1.21(1)	2.22(2)	−3.02(−1)	5.78(3)	−5.67(−1)	7.13(−2)	2.0(5)	−8.2(−1)	2.1(−1)	−1.5(−2)

Table I–(continued)

t	$c(\frac{5}{2},0,0)$	$c(\frac{5}{2},1,1)$	$\tilde{c}(\frac{5}{2},1,0)$	$c(\frac{5}{2},2,2)$	$\tilde{c}(\frac{5}{2},2,1)$	$\tilde{c}(\frac{5}{2},2.0)$	$c(\frac{5}{2},3,3)$	$\tilde{c}(\frac{5}{2},3,2)$	$\tilde{c}(\frac{5}{2},3,1)$	$\tilde{c}(\frac{5}{2},3,0)$
0	1.00	1.00	−3.50	1.00	−9.00	1.58(1)	1.00	−1.65(1)	7.43(1)	−8.66(1)
0.001	1.01	1.03	−3.45	1.06	−8.83	1.52(1)	1.1	−1.6(1)	7.1(1)	−8.1(1)
0.002	1.02	1.07	−3.41	1.13	−8.66	1.47(1)	1.2	−1.6(1)	6.8(1)	−7.6(1)
0.005	1.06	1.17	−3.28	1.29	−8.21	1.33(1)	1.6	−1.5(1)	6.0(1)	−6.3(1)
0.01	1.12	1.34	−3.09	1.73	−7.57	1.14(1)	2.4	−1.3(1)	4.9(1)	−4.8(1)
0.02	1.24	1.73	−2.78	2.72	−6.58	8.78	4.7	−1.1(1)	3.6(1)	−3.0(1)
0.05	1.60	3.18	−2.16	7.63	−4.81	4.83	2.2(1)	−7.8	1.8(1)	−1.1(1)
0.1	2.25	6.63	−1.60	2.50(1)	−3.39	2.46	1.2(2)	−5.3	8.3	−3.7
0.2	3.67	1.80(1)	−1.08	1.17(2)	−2.17	1.04	9.4(2)	−3.3	3.2	−9.2(−1)
0.5	9.02	9.85(1)	−5.62(−1)	1.45(3)	−1.08	2.60(−1)	2.7(4)	−1.6	7.6(−1)	−1.1(−1)
1	2.11(1)	4.47(2)	−3.18(−1)	1.28(4)	−5.94(−1)	8.00(−2)	4.6(5)	−8.5(−1)	2.2(−1)	−1.7(−2)
t	$c(3.0,0)$	$c(3,1,1)$	$\tilde{c}(3,1,0)$	$c(3,2,2)$	$\tilde{c}(3,2,1)$	$\tilde{c}(3,2,0)$	$c(3,3,3)$	$\tilde{c}(3,3,2)$	$\tilde{c}(3,3,1)$	$\tilde{c}(3,3,0)$
0	1.00	1.00	−4.00	1.00	−1.00(1)	2.00(1)	1.00	−1.80(1)	9.00(1)	−1.20(2)
0.001	1.02	1.04	−3.91	1.07	−9.79	1.92(1)	1.1	−1.8(1)	8.6(1)	−1.1(2)
0.002	1.03	1.08	−3.88	1.14	−9.59	1.85(1)	1.2	−1.7(1)	8.1(1)	−1.0(2)
0.005	1.08	1.20	−3.73	1.38	−9.07	1.67(1)	1.7	−1.6(1)	7.1(1)	−8.6(1)
0.01	1.15	1.41	−3.49	1.84	−8.31	1.42(1)	2.6	−1.4(1)	5.8(1)	−6.5(1)
0.02	1.31	1.89	−3.11	3.05	−7.17	1.07(1)	5.4	−1.2(1)	4.2(1)	−4.0(1)
0.05	1.80	3.78	−2.38	9.54	−5.17	5.73	2.8(1)	−8.3	2.0(1)	−1.4(1)
0.1	2.71	8.65	−1.74	3.45(1)	−3.60	2.85	1.6(2)	−5.6	9.3	−4.5
0.2	4.88	2.64(1)	−1.15	1.84(2)	−2.29	1.17	1.5(3)	−3.4	3.6	−1.1
0.5	1.41(1)	1.78(2)	−5.90(−1)	2.76(3)	−1.12	2.89(−1)	5.3(4)	−1.6	8.3(−1)	−1.3(−1)
1	3.81(1)	9.14(2)	−3.31(−1)	2.84(4)	−6.18(−1)	8.79(−2)	1.1(6)	−8.9(−1)	2.4(−1)	−2.0(−2)

When the $g_b^{(t)}$ are evaluated, these values are directly substituted into (18), and so on. The results are tabulated in Table I for some low integral and half-odd integral values of a. The entries corresponding to $t = 0$ are by the nonrelativistic formulas given in Sec. III.

Finally it should be pointed out that a very careful evaluation of the g functions is essential in calculating these coefficients. This is especially true for higher-order (i.e., large m) terms. This is why only two significant figures are given for $m = 3$ in Table I.

* Work performed under the auspices of the U.S. Atomic Energy Commission.

[1] For a discussion of the Sonine polynomial expansion method, see, for example, J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1954).

[2] See, for example, *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1965).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Point Charge in the Vicinity of a Schwarzschild Black Hole*

Jeffrey M. Cohen
Institute for Advanced Study, Princeton, New Jersey 08540
and
Robert M. Wald†
Joseph Henry Physical Laboratory, Princeton University, Princeton, New Jersey 08540
(Received 1 February 1971)

The electrostatic field of a point charge at rest in Schwarzschild space is derived. The solution is used to study the problem of a point charge slowly lowered into a nonrotating black hole. We find that the electric field of the charge remains well behaved as the charge is lowered and that all the multipole moments except the monopole fade away. We conclude that a Reissner–Nordstrom black hole is produced.

I. INTRODUCTION

If a body with a small charge is dropped into a static black hole,[1,2] a number of different outcomes seem plausible[3,4] as the body approaches the event horizon: (i) The body's electromagnetic field may create a sufficiently large stress energy that it may destroy the event horizon or make it singular; (ii) the event horizon will not be destroyed. If the latter outcome holds, the resultant metric would be the Reissner–Nordstrom metric if the topology of the event horizon does not change. This conclusion can be drawn from a theorem provided by Israel[5]: The Reissner–Nordstrom solution is the only static, asymptotically flat, electrovac solution of Einstein's equations for which the surfaces $g_{00} = \text{const}$ are closed and simply connected and the event horizon $g_{00} = 0$ is regular. Thus, if the event horizon is not destroyed and retains the properties given in Israel's

Table I–(continued)

t	$c(\frac{5}{2},0,0)$	$c(\frac{5}{2},1,1)$	$\tilde{c}(\frac{5}{2},1,0)$	$c(\frac{5}{2},2,2)$	$\tilde{c}(\frac{5}{2},2,1)$	$\tilde{c}(\frac{5}{2},2.0)$	$c(\frac{5}{2},3,3)$	$\tilde{c}(\frac{5}{2},3,2)$	$\tilde{c}(\frac{5}{2},3,1)$	$\tilde{c}(\frac{5}{2},3,0)$
0	1.00	1.00	−3.50	1.00	−9.00	1.58(1)	1.00	−1.65(1)	7.43(1)	−8.66(1)
0.001	1.01	1.03	−3.45	1.06	−8.83	1.52(1)	1.1	−1.6(1)	7.1(1)	−8.1(1)
0.002	1.02	1.07	−3.41	1.13	−8.66	1.47(1)	1.2	−1.6(1)	6.8(1)	−7.6(1)
0.005	1.06	1.17	−3.28	1.29	−8.21	1.33(1)	1.6	−1.5(1)	6.0(1)	−6.3(1)
0.01	1.12	1.34	−3.09	1.73	−7.57	1.14(1)	2.4	−1.3(1)	4.9(1)	−4.8(1)
0.02	1.24	1.73	−2.78	2.72	−6.58	8.78	4.7	−1.1(1)	3.6(1)	−3.0(1)
0.05	1.60	3.18	−2.16	7.63	−4.81	4.83	2.2(1)	−7.8	1.8(1)	−1.1(1)
0.1	2.25	6.63	−1.60	2.50(1)	−3.39	2.46	1.2(2)	−5.3	8.3	−3.7
0.2	3.67	1.80(1)	−1.08	1.17(2)	−2.17	1.04	9.4(2)	−3.3	3.2	−9.2(−1)
0.5	9.02	9.85(1)	−5.62(−1)	1.45(3)	−1.08	2.60(−1)	2.7(4)	−1.6	7.6(−1)	−1.1(−1)
1	2.11(1)	4.47(2)	−3.18(−1)	1.28(4)	−5.94(−1)	8.00(−2)	4.6(5)	−8.5(−1)	2.2(−1)	−1.7(−2)
t	$c(3.0,0)$	$c(3,1,1)$	$\tilde{c}(3,1,0)$	$c(3,2,2)$	$\tilde{c}(3,2,1)$	$\tilde{c}(3,2,0)$	$c(3,3,3)$	$\tilde{c}(3,3,2)$	$\tilde{c}(3,3,1)$	$\tilde{c}(3,3,0)$
0	1.00	1.00	−4.00	1.00	−1.00(1)	2.00(1)	1.00	−1.80(1)	9.00(1)	−1.20(2)
0.001	1.02	1.04	−3.91	1.07	−9.79	1.92(1)	1.1	−1.8(1)	8.6(1)	−1.1(2)
0.002	1.03	1.08	−3.88	1.14	−9.59	1.85(1)	1.2	−1.7(1)	8.1(1)	−1.0(2)
0.005	1.08	1.20	−3.73	1.38	−9.07	1.67(1)	1.7	−1.6(1)	7.1(1)	−8.6(1)
0.01	1.15	1.41	−3.49	1.84	−8.31	1.42(1)	2.6	−1.4(1)	5.8(1)	−6.5(1)
0.02	1.31	1.89	−3.11	3.05	−7.17	1.07(1)	5.4	−1.2(1)	4.2(1)	−4.0(1)
0.05	1.80	3.78	−2.38	9.54	−5.17	5.73	2.8(1)	−8.3	2.0(1)	−1.4(1)
0.1	2.71	8.65	−1.74	3.45(1)	−3.60	2.85	1.6(2)	−5.6	9.3	−4.5
0.2	4.88	2.64(1)	−1.15	1.84(2)	−2.29	1.17	1.5(3)	−3.4	3.6	−1.1
0.5	1.41(1)	1.78(2)	−5.90(−1)	2.76(3)	−1.12	2.89(−1)	5.3(4)	−1.6	8.3(−1)	−1.3(−1)
1	3.81(1)	9.14(2)	−3.31(−1)	2.84(4)	−6.18(−1)	8.79(−2)	1.1(6)	−8.9(−1)	2.4(−1)	−2.0(−2)

When the $g_b^{(t)}$ are evaluated, these values are directly substituted into (18), and so on. The results are tabulated in Table I for some low integral and half-odd integral values of a. The entries corresponding to $t = 0$ are by the nonrelativistic formulas given in Sec. III.

Finally it should be pointed out that a very careful evaluation of the g functions is essential in calculating these coefficients. This is especially true for higher-order (i.e., large m) terms. This is why only two significant figures are given for $m = 3$ in Table I.

* Work performed under the auspices of the U.S. Atomic Energy Commission.

[1] For a discussion of the Sonine polynomial expansion method, see, for example, J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1954).

[2] See, for example, *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1965).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Point Charge in the Vicinity of a Schwarzschild Black Hole*

Jeffrey M. Cohen
Institute for Advanced Study, Princeton, New Jersey 08540
and
Robert M. Wald†
Joseph Henry Physical Laboratory, Princeton University, Princeton, New Jersey 08540
(Received 1 February 1971)

The electrostatic field of a point charge at rest in Schwarzschild space is derived. The solution is used to study the problem of a point charge slowly lowered into a nonrotating black hole. We find that the electric field of the charge remains well behaved as the charge is lowered and that all the multipole moments except the monopole fade away. We conclude that a Reissner–Nordstrom black hole is produced.

I. INTRODUCTION

If a body with a small charge is dropped into a static black hole,[1,2] a number of different outcomes seem plausible[3,4] as the body approaches the event horizon: (i) The body's electromagnetic field may create a sufficiently large stress energy that it may destroy the event horizon or make it singular; (ii) the event horizon will not be destroyed. If the latter outcome holds, the resultant metric would be the Reissner–Nordstrom metric if the topology of the event horizon does not change. This conclusion can be drawn from a theorem provided by Israel[5]: The Reissner–Nordstrom solution is the only static, asymptotically flat, electrovac solution of Einstein's equations for which the surfaces $g_{00} = \text{const}$ are closed and simply connected and the event horizon $g_{00} = 0$ is regular. Thus, if the event horizon is not destroyed and retains the properties given in Israel's

theorem,[5] a paradoxical situation arises since the nonspherical charge distribution occurring as the body approaches the horizon must give rise to a spherical electric field according to the theorem. The only escape from this outcome is for the horizon to become singular, be destroyed, or become multiply connected or disconnected.[6] If one of these latter possibilities were to occur, a static black hole could not be found in nature since (even if it were formed) a charged particle would fall in and destroy it.

The closely related problem of the magnetic field of a collapsing, nonrotating star has been treated by Ginzburg and Ozernoi[7] and Anderson and Cohen.[8] In this case, Israel's theorem implies that either (a) the magnetic field must prevent the formation of a nonsingular, topologically spherical event horizon (e.g., by becoming infinite at the horizon, thereby creating a singularity there) or (b) the collapsing star becomes a Schwarzschild black hole and the magnetic field goes to zero everywhere. Under the assumptions that the magnetic field is frozen in and that the collapse proceeds adiabatically, the above-cited authors find that the magnetic field tends to become compressed against the surface of the collapsing star as it approaches its Schwarzschild radius. Thus, the magnetic field a finite distance from the surface of the star tends to go to zero [thus supporting the likelihood of possibility (b)], but, on the other hand, the field tends to blow up at the Schwarzschild radius as the surface of the star reaches it [thus supporting possibility (a)]: The analysis, based on the assumption that the magnetic field has a negligible effect on the metric, becomes invalid at this final stage. Recently, de la Cruz, Chase, and Israel,[9] Anderson,[10] and Price[11] have considered other problems involving the fading out of multipole moments during gravitational collapse.

In this paper we consider the problem of a point charge slowly lowered into a Schwarzschild black hole as a simple example where the final outcome can be investigated. We find that, as the charge is brought near the horizon, the electrostatic field remains well behaved, while all the multipole moments, except the monopole, fade away, so that a Reissner–Nordstrom black hole is produced.

In Sec. II, an expression is obtained for the electrostatic field of a point test charge at rest in Schwarzschild space. In Sec. III this result is used to investigate the questions raised in the above paragraphs.

II. ELECTROSTATIC FIELD OF A POINT TEST CHARGE IN SCHWARZSCHILD SPACE

Maxwell's equation in curved space may be written in the form,[1]

$$4\pi j^{\mu} = F^{\nu\mu}_{\ ;\nu} = \frac{1}{(-g)^{1/2}} \frac{\partial}{\partial x^{\nu}} [(-g)^{1/2} F^{\nu\mu}], \tag{1}$$

$$F_{\mu\nu} = A_{\nu,\mu} - A_{\mu,\nu}, \tag{2}$$

where the semicolon denotes covariant derivative and the comma ordinary derivative. Combining these equations, we have,

$$4\pi j^{\mu} = \frac{1}{(-g)^{1/2}} \frac{\partial}{\partial x^{\nu}} \{(-g)^{1/2} g^{\nu\alpha} g^{\mu\beta} [A_{\beta,\alpha} - A_{\alpha,\beta}]\}. \tag{3}$$

Here we use the standard Schwarzschild coordinates, with the metric

$$dS^2 = -(1 - 2m/r)dt^2 + (1 - 2m/r)^{-1}dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2).$$

We are interested in the case of a point test charge held at rest at the point $r = b$, $\theta = 0$. (Here $b > 2m$ or the charge could not be held at rest.) We choose the charge to be sufficiently small that the interaction of the electrostatic field back on the metric is negligible. [Of course, once the calculations are completed, we must check that the electrostatic field (and hence the gravitational perturbation) calculated under this assumption is indeed small.] Since the field of the point charge (on the Z axis) must be static and axially symmetric, the components of the electromagnetic field will not be a function of time or φ. Since the spacelike components of the current vanish $j^i = 0, i = r, \theta, \varphi$, we may take $A_i = 0$ (no magnetic fields). Setting $A_0 = v$, we obtain as the only nontrivial equation ($\mu = t$)

$$-4\pi j^0 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial v}{\partial r}\right) + \frac{1}{1 - 2m/r} \frac{1}{r^2 \sin\theta} \times \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial v}{\partial \theta}\right). \tag{4}$$

If the angular part of the potential is expanded in Legendre polynomials in $\cos\theta$,

$$v(r, \theta) = \sum_{l=0}^{\infty} R_l(r) P_l(\cos\theta), \tag{5}$$

then in the source-free regions ($j^0 = 0$) the equation for $R_l(r)$ becomes

$$0 = \left(1 - \frac{2m}{r}\right) \frac{d}{dr} \left(r^2 \frac{dR_l}{dr}\right) - l(l+1)R_l(r). \tag{6}$$

The solutions of this equation have been obtained independently by Israel[5] and by Anderson and Cohen.[8] We use as the two linearly independent solutions of (6)

$$g_l(r) = \begin{cases} 1, & \text{for } l = 0, \\ \dfrac{2^l l!(l-1)!\, m^l}{(2l)!}(r - 2m) \dfrac{dP_l}{dr}\left(\dfrac{r}{m} - 1\right), & \text{for } l \neq 0, \end{cases} \tag{7a}$$

$$f_l(r) = -\frac{(2l+1)!}{2^l(l+1)!\,l!\,m^{l+1}}(r-2m)\frac{d}{dr}Q_l\left(\frac{r}{m}-1\right), \tag{7b}$$

where P_l and Q_l are the two types of Legendre functions.[8,12] We note the following properties of $f_l(r)$ and $g_l(r)$:

(I) For $l=0, g_0(r)=1$ (by definition) and $f_0(r)=1/r$.

(II) For all l, as $r\to\infty$, the leading term of $g_l(r)$ is r^l, while the leading term of $f_l(r) = 1/r^{l+1}$. (The normalization factors were chosen for just this reason.)

(III) As $r\to 2m, f_l(r)\to$ finite const, but df_l/dr blows up as $\ln(1-2mr^{-1})$ for $l\neq 0$. For $l\neq 0$, $g_l(r) = (r-2m)\times$ (polynomial in r), so, as $r\to 2m, g_l(r)\to 0$ as $(r-2m)$.

The above three properties of $f_l(r)$ and $g_l(r)$ are all that will be used in the following analysis. But for completeness we give analytic expressions for each term in the multipole expansion.

For a point charge at rest at $r=b$, $\theta=0$ we have $j^0 = \text{const}\times\delta(r-b)\delta(\cos\theta-1)$. [The normalization of these δ functions is

$$\int r^2\delta(r-b)dr = 1,\ \int\delta(\cos\theta-1)\sin\theta d\theta d\varphi = 1].$$

The constant is determined by the requirement that the total charge be e, where e is the conserved quantity given by (the standard method[13] of showing this for a bounded source is to integrate the conservation law $j^\mu_{;\mu}=0$ over all space-time and to use the curved space form of the divergence theorem)

$$e = \int j^0(-g)^{1/2}dr d\theta\varphi = \int j^0 r^2\sin\theta dr d\theta d\varphi. \tag{8}$$

Thus,

$$j^0 = e\delta(r-b)\delta(\cos\theta-1), \tag{9}$$

and Eq. (4) for this source becomes

$$-4\pi e\delta(r-b)\delta(\cos\theta-1) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial v}{\partial r}\right) + \frac{1}{1-2m/r}\frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial v}{\partial\theta}\right). \tag{10}$$

In the regions $r>b$ and $r<b$, j^0 vanishes and, consequently v satisfies the source-free equation (6), with the solution

$$v(r,\theta) = \begin{cases}\sum_{l=0}^{\infty}[A_l f_l(r) + A'_l g_l(r)]P_l(\cos\theta), & r>b,\\ \sum_{l=0}^{\infty}[B_l g_l(r) + B'_l f_l(r)]P_l(\cos\theta), & r<b,\end{cases} \tag{11}$$

The $g_l(r)$ blow up as r^l for $r\to\infty$ [property (II)], so that we must have $A'_l=0$. The constants B'_l can be determined by requiring that the invariant

$$\tfrac{1}{2}F_{\mu\nu}F^{\mu\nu} = \left(\frac{\partial v}{\partial r}\right)^2 + \frac{1}{r^2}\frac{1}{1-2m/r}\left(\frac{\partial v}{\partial\theta}\right)^2 \tag{12}$$

be finite as $r\to 2m$. From property (III) we see that although $f_l(r)$ remains finite at $r=2m$, it produces infinite fields for $l\neq 0$ at $r=2m$, unless we have $B'_l=0$. [$f_0(r)=r^{-1}$ does not produce infinite fields at $r=2m$, but is excluded since it represents an additional source at $r=0$. Note that we are assuming that for fixed b the field is finite at $r=2m$; we are not assuming that the field remains finite at $r=2m$ as $b\to 2m$. We will investigate this question later.] Thus, we have

$$v = \begin{cases}\sum_{l=0}^{\infty}A_l f_l(r)P_l(\cos\theta), & r>b,\\ \sum_{l=0}^{\infty}B_l g_l(r)P_l(\cos\theta), & r<b.\end{cases} \tag{13}$$

Continuity of v (and consequently of E_θ) at $r=b$ requires that

$$A_l f_l(b) = B_l g_l(b). \tag{14}$$

Thus, letting $C_l \equiv A_l/g_l(b) = B_l/f_l(b)$, we have

$$v = \begin{cases}\sum_{l=0}^{\infty}C_l g_l(b)f_l(r)P_l(\cos\theta), & r>b,\\ \sum_{l=0}^{\infty}C_l f_l(b)g_l(r)P_l(\cos\theta), & r<b.\end{cases} \tag{15}$$

We evaluate C_l by integrating Eq. (10) across the source as is often done with the flat space Maxwell equations. Writing $v=\sum_{l=0}^{\infty}R_l(r)P_l(\cos\theta)$, multiplying (10) by $P_l(\cos\theta)$, and integrating over θ, we get

$$-2e\delta(r-b) = \frac{2}{2l+1}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) - \frac{l(l+1)}{r^2(1-2m/r)}R_l(r)\right], \tag{16}$$

where we have used the following properties of Legendre functions: $P_l(1)=1$ and $\int_{-1}^{1}P_l(x)P'_l(x)dx = 2(2l+1)^{-1}\delta_{ll'}$. Multiplying by r^2 and integrating from $b-\epsilon$ to $b+\epsilon$, we get

$$-e = \frac{1}{2l+1}\left(b^2\frac{dR_l}{dr}\bigg|_{b+\epsilon} - b^2\frac{dR_l}{dr}\bigg|_{b-\epsilon}\right) = \frac{C_l}{2l+1}b^2\left(g_l(b)\frac{df_l}{dr}(b) - f_l(b)\frac{dg_l}{dr}(b)\right) = \frac{C_l}{2l+1}b^2W(g_l,f_l,b), \tag{17}$$

where $W(g_l,f_l,b)$ is the Wronskian of g_l and f_l at the point b. But the Wronskian $W\equiv(u_1u'_2-u_2u'_1)$

of two solutions u_1, u_2 of a differential equation of the form $u'' + p(x)u' + q(x)u = 0$ satisfies[14]

$$W(u_1, u_2, r) = W(u_1, u_2, r_0) \exp\left(-\int_{r_0}^{r} p(x)dx\right). \tag{18}$$

In the case of our Eq. (6), $p(x) = 2/x$, so that (18) yields

$$W(g_l, f_l, r) = W(g_l, f_l, r_0)\, r_0^2/r^2. \tag{19}$$

Thus there results,

$$r^2 W(g_l, f_l, r) = \text{const.} \tag{20}$$

We evaluate this constant by finding $W(g_l, f_l, r)$ for large values of r. By property (II) of the functions f_l and g_l, we have, for large r, $g_l(r) \sim r^l$ and $f_l(r) \sim 1/r^{l+1}$ so that for large r [and therefore, by (20), for all r], we have

$$r^2 W(g_l, f_l, r) = r^2\left(r^l[-(l+1)]\frac{1}{r^{l+2}} - l r^{l-1}\frac{1}{r^{l+1}}\right) \tag{21}$$

$$= -(2l+1). \tag{22}$$

Substitution of (22) in (17) gives the simple result

$$C_l = e. \tag{23}$$

Thus the field of a point charge is given by

$$v = \begin{cases} e\sum_{l=0}^{\infty} g_l(b) f_l(r) P_l(\cos\theta), & r > b, \\ e\sum_{l=0}^{\infty} f_l(b) g_l(r) P_l(\cos\theta), & r < b. \end{cases} \tag{24}$$

In the orthonormal frame $\omega^0 = (1 - 2m/r)^{1/2}dt$, $\omega^1 = dr(1 - 2m/r)^{-1/2}$, $\omega^2 = r d\theta$, $\omega^3 = r \sin\theta d\varphi$, the only nonvanishing components of the field tensor $F_{\mu\nu}$ are

$$F_{01} = -F_{10} = -\frac{\partial v}{\partial r},$$

$$F_{02} = -F_{20} = -r^{-1}\left(1 - \frac{2m}{r}\right)^{-1/2}\frac{\partial v}{\partial \theta}. \tag{25}$$

We note that [as seen from Eq. (24) with $r < b$ and property (III) of the functions g_l], for $b > r$ and r near $2m$, $F_{20} \sim 0[(1 - 2m/r)^{1/2}]$, while F_{10} remains finite, so that a stationary observer positioned at radius r with $b > r \approx 2m$ sees a radial electrostatic field. (No net flux enters the black hole, however, since as many flux lines exit the black hole from the side opposite the charge as enter from the side near the charge.) But if $r > b$ with r and b both near $2m$, the $l \neq 0$ contribution to the electrostatic field is mostly tangential because [as seen from Eq. (24) with $r > b$ and property (III) of the functions f_l] $F_{10}/F_{20} \sim (1 - 2m/r)^{1/2} \ln(1 - 2m/r) \to 0$; this phenomenon has been noted for the dipole case by Ginzburg and Ozernoi[7] and for the general case by Anderson and Cohen.[8] Nevertheless, the dominant contribution to the field in this case comes from the $l = 0$ term because the coefficients $g_l(b)$ of the higher multipole terms vanish like $(1 - 2m/b)$, so that the total electrostatic field is still mostly radial in this case. A plot of the field lines corresponding to the above solution will be given elsewhere by Wheeler and Ruffini [see also R. Hanni, Princeton junior paper (1971)].

III. ASYMPTOTIC FIELD OF A TEST CHARGE LOWERED INTO A SCHWARZSCHILD BLACK HOLE

As mentioned above, we chose the functions $g_l(r)$ for the region $r < b$, so that the electrostatic field of a test charge at $r = b$ is well behaved at the horizon. In doing this we have only assumed that a test charge placed at finite distance from the horizon does not produce infinite fields there. Now let us consider what happens if we lower a charge (sufficiently slowly so that our static results can be used) toward $r = 2m$. Does the electrostatic field tend to blow up at the horizon as $b \to 2m$, or will it remain finite there? We see from Eq. (24), with $r < b$ and property (III) of the functions g_l and f_l, that F_{01} and F_{02} both remain finite at $r = 2m$ as $b \to 2m$; we also see [using Eq. (24) with $r > b$] that F_{01} and F_{02} remain finite outside of the radius b of the charge as $b \to 2m$, since the logarithmic divergence of df_l/dr ($l \neq 0$) is now more than compensated by the linear decrease to zero of g_l ($l \neq 0$). Thus, the field remains well behaved as we slowly lower a charge toward the horizon, and we conclude that we do not drastically affect the horizon in this process.

On the other hand, let us examine the limiting value of the field seen by any observer at $r > 2m$ as $b \to 2m$. From Eq. (24) (with $r > b$) and the fact that, for $l \neq 0$, $g_l(b) \to 0$ as $b \to 2m$, we see that all the multipole contributions to v except the monopole go to zero as $b \to 2m$. Since $g_0 = 1$ and $f_0 = r^{-1}$, we have the result that for all $r > 2m$, $v(r, \theta) \to e/r$ as $b \to 2m$. Thus, although the charge distribution is highly asymmetrical as $b \to 2m$, the electrostatic potential approaches the spherically symmetric Reissner–Nordstrom value of e/r.

From the results of the above two paragraphs and our discussion in the Introduction, we conclude that as we slowly lower a test charge into a Schwarzschild black hole, we produce a Reissner–Nordstrom black hole.

ACKNOWLEDGMENTS

We are indebted to Professor J. A. Wheeler for suggesting this problem and for reporting the results of this manuscript at the Clifford Centennial, February, 1970. One of us (J.M.C.) wishes to thank Dr. C. Kaysen for his hospitality at the Institute for Advanced Study.

* Work supported in part by the National Science Foundation, under Grant Nos. GP-16147 and GP-7669.
† NSF Predoctoral Fellow.

1 J. A. Wheeler, *Geometrodynamics* (Academic, New York, 1962).
2 A. Einstein and N. Rosen, Phys. Rev. **48**, 731 (1935).
3 W. Israel, Nature **216**, 148 (1967); **216**, 312 (1967).
4 V. L. Ginzburg, *Quasi-Sellar Sources and Gravitational Collapse* (U. of Chicago P., Chicago, 1965), p. 283.
5 W. Israel, Commun. Math. Phys. **8**, 245 (1968). See also R. M. Wals, Phys. Rev. Letters **26**, 1653 (1971).
6 R. Gautreau and R. Hoffmann, Bull. Am. Phys. Soc. **15**, 1332 (1970).
7 V. L. Ginzburg and L. M. Ozernoi, Zh. Eksp. Teor. Fiz. **47**, 1030 (1964) [Sov. Phys. JETP **20**, 689 (1965)].
8 J. L. Anderson and J. M. Cohen, Astrophys. Space Sci., **9**, 146 (1970).
9 V. de la Cruz, J. E. Chase, and W. Israel, Phys. Rev. Letters **24**, 423 (1970).
10 J. L. Anderson, (unpublished).
11 R. Price, (unpublished); see also K. S. Thorne, (unpublished).
12 W. Magnus and F. Oberhettinger, *Special Functions of Mathematical Physics* (Chelsea, New York, 1949).
13 See, e.g., J. M. Cohen, J. Math. Phys. **9**, 905 (1968) and references cited therein.
14 G. Birkhoff and G. Rota, *Ordinary Differential Equations* (Ginn, New York, 1962).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Generalization of the Cook Formalism for Fock Space

F. E. Schroeck, Jr.
Departments of Physics and Mathematics, Florida Atlantic University, Boca Raton, Florida 33432
(Received 22 February 1971)

The Cook formalism for Fock space is extended by finding additional properties of the creation and annihilation operators and by giving a rigorous definition of the second-quantized form for n-body operators (for any n). Properties of these second-quantized operators are given, including an expansion in terms of the creation and annihilation operators.

I. INTRODUCTION

By requiring that creation and annihilation operators ("fields") create or annihilate particles with definite probability functions, Cook[1] was able to define rigorously the fields as linear operators on Fock space. He furthermore gave a rigorous definition of the second-quantized form for one-body operators and found certain relations between the operators and the fields. This formalism was not developed sufficiently for considering interactions between pairs of particles, an inherently two-body interaction. We extend Cook's result to handle this and other problems by defining the second-quantized form of n-body operators for any n. With this definition we establish certain properties of these operators, including expansions in terms of the fields. The results are then applied to several common interactions.

In Sec. II we define Fock space. In Sec. III we define the second-quantized forms of n-body operators and derive some important properties for them. In Sec. IV we review Cook's definitions of the fields and results, which we state without proof, as well as derive some new properties. In Sec. V we obtain expansions of the second-quantized n-body operators in terms of the fields. Finally, we analyze the free Hamiltonians, the Yukawa interaction, and the Coulomb interaction as examples of the method.

II. THE FOCK SPACE

Definition 1: Let $\mathfrak{K}^{(1)}$ denote a given complex Hilbert space. Let $\mathfrak{K}^{(n)}$ denote the n-fold tensor product of $\mathfrak{K}^{(1)}$ with itself. Let $\mathfrak{K}^{(0)}$ denote the one-dimensional Hilbert space of the complex numbers. Then we define

$$\mathfrak{F} = \sum_{n=0}^{\infty} \oplus \mathfrak{K}^{(n)}.$$

$\mathfrak{K}^{(1)}$ is the single-particle Hilbert space, $\mathfrak{K}^{(n)}$ the n-particle Hilbert space, and $\mathfrak{F}$ the Fock space.[2] We let $\mathfrak{j}$ denote the natural isomorphism $\mathfrak{j}: \mathfrak{K}^{(n)} \to 0 \oplus \cdots \oplus 0 \oplus \mathfrak{K}^{(n)} \oplus 0 \oplus \cdots$ of $\mathfrak{K}^{(n)}$ into $\mathfrak{F}$. We let $\{P_n\}$ denote the resolution of the identity corresponding to $P_n \mathfrak{F} = \mathfrak{j}\mathfrak{K}^{(n)}$.

III. SECOND QUANTIZATION OF N-BODY OPERATORS

Definition 2: Let A_i be densely defined, closed, linear transformations on the Hilbert spaces $\mathfrak{H}_i$. Then $A_1 \otimes \cdots \otimes A_n$ is the densely defined, closed, linear transformation on $\mathfrak{H}_1 \otimes \cdots \otimes \mathfrak{H}_n$ with domain $D(A_1) \otimes \cdots \otimes D(A_n)$ equal to the set of all h in $\mathfrak{H}_1 \otimes \cdots \otimes \mathfrak{H}_n$ such that there exists g in $\mathfrak{H}_1 \otimes \cdots \otimes \mathfrak{H}_n$ with $(g, \varphi_1 \otimes \cdots \otimes \varphi_n) = (h, A_1^\dagger \varphi_1 \otimes \cdots \otimes A_n^\dagger \varphi_n)$ for all φ_i in $D(A_i^\dagger)$, in which case $(A_1 \otimes \cdots \otimes A_n)h = g$.

In our case, all $\mathfrak{H}_i \equiv \mathfrak{K}^{(1)}$; we will denote the n-fold tensor product $A \otimes \cdots \otimes A$ by $A^{(n)}$ in $\mathfrak{K}^{(n)}$. If $\mathfrak{M}$ is any subset of $\mathfrak{K}^{(1)}$, we will denote the manifold in $\mathfrak{K}^{(n)}$ of all finite linear combinations of decomposable elements of $\mathfrak{K}^{(n)}$, all of whose product factors lie in $\mathfrak{M}$, by $\mathfrak{M}^{[n]}$. We will denote the identity operator on $\mathfrak{K}^{(1)}$ by I.

Definition 3: Let S_n denote the symmetric group on n objects. For every permutation $\pi \in S_n$, there corresponds a unitary operator U_π on $\mathfrak{K}^{(n)}$ uniquely defined as the bounded linear extension of the operator $U_\pi \psi_1 \otimes \cdots \otimes \psi_n = \psi_{\pi(1)} \otimes \cdots \otimes \psi_{\pi(n)}$ on decomposable tensors in $\mathfrak{K}^{(n)}$. The $n!$ dimensional ring $\mathcal{G}_n$ generated by the set $\{U_\pi\}$, with $U_\pi U_\varphi = U_{\varphi\pi}$, is isomorphic with the group algebra. Any linear operator A in $\mathfrak{K}^{(n)}$ will be called an n-body operator. We will now list a hierarchy of domain conditions which A might satisfy.

Definition 4: Let A be a densely defined, linear operator in $\mathfrak{K}^{(n)}$.

* Work supported in part by the National Science Foundation, under Grant Nos. GP-16147 and GP-7669.
† NSF Predoctoral Fellow.

1 J. A. Wheeler, *Geometrodynamics* (Academic, New York, 1962).
2 A. Einstein and N. Rosen, Phys. Rev. **48**, 731 (1935).
3 W. Israel, Nature **216**, 148 (1967); **216**, 312 (1967).
4 V. L. Ginzburg, *Quasi-Sellar Sources and Gravitational Collapse* (U. of Chicago P., Chicago, 1965), p. 283.
5 W. Israel, Commun. Math. Phys. **8**, 245 (1968). See also R. M. Wals, Phys. Rev. Letters **26**, 1653 (1971).
6 R. Gautreau and R. Hoffmann, Bull. Am. Phys. Soc. **15**, 1332 (1970).
7 V. L. Ginzburg and L. M. Ozernoi, Zh. Eksp. Teor. Fiz. **47**, 1030 (1964) [Sov. Phys. JETP **20**, 689 (1965)].
8 J. L. Anderson and J. M. Cohen, Astrophys. Space Sci., **9**, 146 (1970).
9 V. de la Cruz, J. E. Chase, and W. Israel, Phys. Rev. Letters **24**, 423 (1970).
10 J. L. Anderson, (unpublished).
11 R. Price, (unpublished); see also K. S. Thorne, (unpublished).
12 W. Magnus and F. Oberhettinger, *Special Functions of Mathematical Physics* (Chelsea, New York, 1949).
13 See, e.g., J. M. Cohen, J. Math. Phys. **9**, 905 (1968) and references cited therein.
14 G. Birkhoff and G. Rota, *Ordinary Differential Equations* (Ginn, New York, 1962).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Generalization of the Cook Formalism for Fock Space

F. E. Schroeck, Jr.
Departments of Physics and Mathematics, Florida Atlantic University, Boca Raton, Florida 33432
(Received 22 February 1971)

The Cook formalism for Fock space is extended by finding additional properties of the creation and annihilation operators and by giving a rigorous definition of the second-quantized form for n-body operators (for any n). Properties of these second-quantized operators are given, including an expansion in terms of the creation and annihilation operators.

I. INTRODUCTION

By requiring that creation and annihilation operators ("fields") create or annihilate particles with definite probability functions, Cook[1] was able to define rigorously the fields as linear operators on Fock space. He furthermore gave a rigorous definition of the second-quantized form for one-body operators and found certain relations between the operators and the fields. This formalism was not developed sufficiently for considering interactions between pairs of particles, an inherently two-body interaction. We extend Cook's result to handle this and other problems by defining the second-quantized form of n-body operators for any n. With this definition we establish certain properties of these operators, including expansions in terms of the fields. The results are then applied to several common interactions.

In Sec. II we define Fock space. In Sec. III we define the second-quantized forms of n-body operators and derive some important properties for them. In Sec. IV we review Cook's definitions of the fields and results, which we state without proof, as well as derive some new properties. In Sec. V we obtain expansions of the second-quantized n-body operators in terms of the fields. Finally, we analyze the free Hamiltonians, the Yukawa interaction, and the Coulomb interaction as examples of the method.

II. THE FOCK SPACE

Definition 1: Let $\mathfrak{K}^{(1)}$ denote a given complex Hilbert space. Let $\mathfrak{K}^{(n)}$ denote the n-fold tensor product of $\mathfrak{K}^{(1)}$ with itself. Let $\mathfrak{K}^{(0)}$ denote the one-dimensional Hilbert space of the complex numbers. Then we define

$$\mathfrak{F} = \sum_{n=0}^{\infty} \oplus \mathfrak{K}^{(n)}.$$

$\mathfrak{K}^{(1)}$ is the single-particle Hilbert space, $\mathfrak{K}^{(n)}$ the n-particle Hilbert space, and $\mathfrak{F}$ the Fock space.[2] We let $\mathfrak{j}$ denote the natural isomorphism $\mathfrak{j}: \mathfrak{K}^{(n)} \to 0 \oplus \cdots \oplus 0 \oplus \mathfrak{K}^{(n)} \oplus 0 \oplus \cdots$ of $\mathfrak{K}^{(n)}$ into $\mathfrak{F}$. We let $\{P_n\}$ denote the resolution of the identity corresponding to $P_n \mathfrak{F} = \mathfrak{j}\mathfrak{K}^{(n)}$.

III. SECOND QUANTIZATION OF N-BODY OPERATORS

Definition 2: Let A_i be densely defined, closed, linear transformations on the Hilbert spaces $\mathfrak{H}_i$. Then $A_1 \otimes \cdots \otimes A_n$ is the densely defined, closed, linear transformation on $\mathfrak{H}_1 \otimes \cdots \otimes \mathfrak{H}_n$ with domain $D(A_1) \otimes \cdots \otimes D(A_n)$ equal to the set of all h in $\mathfrak{H}_1 \otimes \cdots \otimes \mathfrak{H}_n$ such that there exists g in $\mathfrak{H}_1 \otimes \cdots \otimes \mathfrak{H}_n$ with $(g, \varphi_1 \otimes \cdots \otimes \varphi_n) = (h, A_1^\dagger \varphi_1 \otimes \cdots \otimes A_n^\dagger \varphi_n)$ for all φ_i in $D(A_i^\dagger)$, in which case $(A_1 \otimes \cdots \otimes A_n)h = g$.

In our case, all $\mathfrak{H}_i \equiv \mathfrak{K}^{(1)}$; we will denote the n-fold tensor product $A \otimes \cdots \otimes A$ by $A^{(n)}$ in $\mathfrak{K}^{(n)}$. If $\mathfrak{M}$ is any subset of $\mathfrak{K}^{(1)}$, we will denote the manifold in $\mathfrak{K}^{(n)}$ of all finite linear combinations of decomposable elements of $\mathfrak{K}^{(n)}$, all of whose product factors lie in $\mathfrak{M}$, by $\mathfrak{M}^{[n]}$. We will denote the identity operator on $\mathfrak{K}^{(1)}$ by I.

Definition 3: Let S_n denote the symmetric group on n objects. For every permutation $\pi \in S_n$, there corresponds a unitary operator U_π on $\mathfrak{K}^{(n)}$ uniquely defined as the bounded linear extension of the operator $U_\pi \psi_1 \otimes \cdots \otimes \psi_n = \psi_{\pi(1)} \otimes \cdots \otimes \psi_{\pi(n)}$ on decomposable tensors in $\mathfrak{K}^{(n)}$. The $n!$ dimensional ring $\mathcal{G}_n$ generated by the set $\{U_\pi\}$, with $U_\pi U_\varphi = U_{\varphi\pi}$, is isomorphic with the group algebra. Any linear operator A in $\mathfrak{K}^{(n)}$ will be called an n-body operator. We will now list a hierarchy of domain conditions which A might satisfy.

Definition 4: Let A be a densely defined, linear operator in $\mathfrak{K}^{(n)}$.

D_1: We will say that A has property D_1 if in each $\mathfrak{H}^{(m)}$, $m \geq n$,

$$\left(\sum_{\pi\in S_m} U_\pi (A \otimes I^{(m-n)}) U_\pi^{-1}\right)^\dagger$$

is densely defined.

D_2: We will say that A has property D_2, if in each $\mathfrak{H}^{(m)}$, $m \geq n$,
(a) there exists a dense domain $\mathfrak{M}_m$ such that

$$\mathfrak{M}_m \subseteq D(A \otimes I^{(m-n)}) \text{ and } U_\pi \mathfrak{M}_m = \mathfrak{M}_m \text{ for all } \pi \in S_m;$$

(b) there exists a dense domain $\mathfrak{N}_m$ such that

$$\mathfrak{N}_m \subseteq D(A^\dagger \otimes I^{(m-n)}) \text{ and } U_\pi \mathfrak{N}_m = \mathfrak{N}_m \text{ for all } \pi \in S_m.$$

D_3: We will say that A has property D_3 if there exist dense domains $\mathfrak{M}_0, \mathfrak{N}_0$ in $\mathfrak{H}^{(1)}$ such that $\mathfrak{M}_0^{[n]} \subseteq D(A)$ and $\mathfrak{N}_0^{[n]} \subseteq D(A^\dagger)$.

D_4: We will say that A is particle-symmetry preserving if

$$U_\pi A = A U_\pi \text{ for all } \pi \in S_n.$$

It is clear that D_3 implies D_2 implies D_1. We conjecture a relation between the particle-symmetry-preserving property and property D_2 and will outline this relation shortly. We also remark that any closed, bounded, linear operator in $\mathfrak{H}^{(n)}$ has property D_3, and any densely defined, closed, linear operator in $\mathfrak{H}^{(1)}$ has property D_2.

When the minimal closed, linear extension of an operator T exists, we shall denote it by $[T]^\sim$.

Definition 5: If A is any operator in $\mathfrak{H}^{(n)}$ satisfying D_1, then the second-quantized form of A, $\Omega(A; n)$, is the densely defined, closed, linear operator

$$\Omega(A; n) \equiv \sum_{m=0}^{\infty} \oplus \frac{1}{(m-n)!} \left[\sum_{\pi\in S_m} U_\pi (A \otimes I^{(m-n)}) U_\pi^{-1}\right]^\sim$$

on $\mathfrak{F}$, where the summand is defined to be the zero operator for $m < n$.

By property D_1,

$$\left[\sum_{\pi\in S_m} U_\pi (A \otimes I^{(m-n)}) U_\pi^{-1}\right]^\sim$$

exists. The special operator $\Omega(I; 1)$ exists and has the property $\Omega(I; 1)\psi = n\psi$ for all $\psi \in \mathfrak{H}^{(n)}$. $\Omega(I; 1)$ is called the number operator and is frequently denoted by N.

Let $\{E_\lambda^{(i)}\}$, $i = 1, \cdots, n$, be n spectral families in $\mathfrak{H}^{(1)}$, not necessarily commuting. Then

$$E_{\lambda_1, \cdots, \lambda_n} \equiv E_{\lambda_1}^{(1)} \otimes \cdots \otimes E_{\lambda_n}^{(n)}$$

is a spectral family on $\mathfrak{H}^{(n)}$, and any operator A,

$$A = \int \alpha(\lambda_1, \lambda_2, \cdots, \lambda_n) dE_{\lambda_1, \cdots, \lambda_n},$$

is a normal operator on $\mathfrak{H}^{(n)}$.[3] We will call such operators s-normal (simple, normal). An operator A will be called uniformly normal if it can be written in the form

$$A = \int \alpha(\lambda_1, \lambda_2, \cdots, \lambda_n) dE_{\lambda_1} \otimes \cdots \otimes E_{\lambda_n}$$

with respect to a single spectral family $\{E_\lambda\}$ in $\mathfrak{H}^{(1)}$, and we will say that $\{E_\lambda\}$ is a spectral family associated with A.

Lemma: For any $\pi \in S_n$,

$$U_\pi [E(1; \lambda_1) \otimes \cdots \otimes E(n; \lambda_n)] U_\pi^{-1} = E(\pi(1); \lambda_{\pi(1)}) \otimes \cdots \otimes E(\pi(n); \lambda_{\pi(n)}).$$

Proof: Since $E(1; \lambda_1) \otimes \cdots \otimes E(n; \lambda_n)$ is a bounded operator and since U_π is unitary, it suffices to show the result on decomposable tensors. Let $f_{\pi(1)} \otimes \cdots \otimes f_{\pi(n)}$ denote any decomposable tensor on $\mathfrak{H}^{(n)}$. Then

$$\begin{aligned} &U_\pi (E(1; \lambda_1) \otimes \cdots \otimes E(n; \lambda_n)) U_\pi^{-1} (f_{\pi(1)} \otimes \cdots \otimes f_{\pi(n)}) \\ &= U_\pi (E(1; \lambda_1) \otimes \cdots \otimes E(n; \lambda_n))(f_1 \otimes \cdots \otimes f_n) \\ &= U_\pi (E(1; \lambda_1) f_1 \otimes \cdots \otimes E(n; \lambda_n) f_n) \\ &= E(\pi(1); \lambda_{\pi(1)}) f_{\pi(1)} \otimes \cdots \otimes E(\pi(n); \lambda_{\pi(n)}) f_{\pi(n)} \\ &= (E(\pi(1); \lambda_{\pi(1)}) \otimes \cdots \otimes E(\pi(n); \lambda_{\pi(n)})) \\ &\quad \times (f_{\pi(1)} \otimes \cdots \otimes f_{\pi(n)}). \end{aligned}$$

Conjecture: Any s-normal particle-symmetry-preserving n-body operator is uniformly normal.

Plausibility proof: We have

$$\begin{aligned} U_\pi A U_\pi^{-1} &= \int \alpha(\lambda_1, \cdots, \lambda_n) dE(\pi(1); \lambda_{\pi(1)}) \otimes \cdots \\ &\quad \otimes E(\pi(n); \lambda_{\pi(n)}) \\ &= A = \int \alpha(\lambda_1, \cdots, \lambda_n) dE(1; \lambda_1) \otimes \cdots \\ &\quad \otimes E(n; \lambda_n). \end{aligned}$$

Since A commutes with

$$E_{\mu_1}^{(1)} \otimes I^{(n-1)}, I \otimes E_{\mu_2}^{(2)} \otimes I^{(n-2)}, \cdots, I^{(n-1)} \otimes E_{\mu_n}^{(n)},$$

it follows that all $E_{\mu_i}^{(i)}$ commute with all $E(\pi(j); \lambda_{\pi(j)})$ for all $\pi \in S_n$ wherever $\alpha(\lambda_1, \cdots, \lambda_n)$ is nonzero. For those λ_i where α vanishes, we may choose the $E_{\lambda_i}^{(i)}$ to be pairwise commuting since that does not effect the definition of A. We therefore obtain the $E_{\lambda_i}^{(i)}$ to be pairwise commuting so that they may be written as a function of a common spectral family $\{E_\mu\}$. A liberal sprinkling of the Radon–Nikodym theorem then yields

$$A = \int \alpha^1(\mu_1, \cdots, \mu_n)\, d\, E_{\mu_1} \otimes \cdots \otimes E_{\mu_n},$$

where α^1 is some function of α and the Radon–Nikodym derivatives. Furthermore, since $U_\pi A U_\pi^{-1} = A$ we have

$$\alpha^1(\mu_1, \cdots, \mu_n) = \alpha^1(\mu_{\pi(1)}, \cdots, \mu_{\pi(n)})$$

for all $\pi \in S_n$.

Lemma: Any uniformly normal n-body operator A has property D_2.

Proof: We may write $A = \int \alpha(\lambda_1, \cdots, \lambda_n) dE_{\lambda_1} \otimes \cdots \otimes E_{\lambda_n}$. Since A is densely defined and closed, α can be undefined at most on a subset Γ_0 of $R^{(n)}$ which is of measure zero with respect to $E_{\lambda_1} \otimes \cdots \otimes E_{\lambda_n}$. We define a representation of S_m in R^m by

$$V_\pi(x_1, \cdots, x_m) = (x_{\pi(1)}, \cdots, x_{\pi(m)})$$

on coordinates in R^m. Then

$$\Gamma_2^m = \bigcup_{\pi \in S_m} V_\pi(\Gamma_0 \otimes R^{(m-n)})$$

is a set of measure zero with respect to $E_{\lambda_1} \otimes \cdots \otimes E_{\lambda_m}$, $m \geq n$.

We define

$$\Delta_k = \left\{ \lambda \in R^{(m)} \sum_{\pi \in S_m} |\alpha(V_\pi(\lambda))| \leq k \right\}$$

$$E_{\Delta_k} = \int \epsilon(k, \lambda)\, dE_{\lambda_1} \otimes \cdots \otimes E_{\lambda_m},$$

where

$$\epsilon(k, \lambda) = \begin{cases} 1 & \text{if } \lambda \in \Delta_k \\ 0 & \text{otherwise} \end{cases}$$

Then $\{E_{\Delta_k}\}$ is a family of projections which converges strongly to the identity as $k \to \infty$.

Let $\mathfrak{M}_m$ denote the set of vectors f in $\mathfrak{H}^{(m)}$ such that there exists $k < \infty$ for which $E_{\Delta_k} f = f$. Then $\mathfrak{M}_m$ is dense in $\mathfrak{H}^{(m)}$ and

$$U_\pi \mathfrak{M}_m = \mathfrak{M}_m \subseteq D(A \otimes I^{(m-n)}) \quad \text{for all} \quad \pi \in S_m.$$

We similarly construct $\mathfrak{N}_m$.

Theorem 1: If A is a uniformly normal operator in $\mathfrak{H}^{(n)}$, then $\Omega(A; n)$ is normal and $\Omega(A; n)^\dagger = \Omega(A^\dagger; n)$.

Proof: Since the P_m reduce $\Omega(A; n)$, it suffices to prove the result on each $\mathfrak{H}^{(m)}$. It is trivial for $m < n$. For $m \geq n$ we have

$$U_\pi A \otimes I^{(m-n)} U_\pi^{-1}$$

$$= \int \alpha(\lambda_1, \cdots, \lambda_n)\, d E_{\lambda_{\pi(1)}} \otimes \cdots \otimes E_{\lambda_{\pi(m)}}$$

$$= \int \alpha(\lambda_{\pi^{-1}(1)}, \cdots, \lambda_{\pi^{-1}(n)})\, d E_{\lambda_1} \otimes \cdots \otimes E_{\lambda_m},$$

$$J_1 \equiv \frac{1}{(m-n)!} \left[\sum_{\pi^{-1} \in S_m} U_\pi^{-1} A \otimes I^{(m-n)} U_\pi \right]^\sim$$

$$= \frac{1}{(m-n)!} \left[\sum_{\pi \in S_m} \int \alpha(\lambda_{\pi(1)}, \cdots, \lambda_{\pi(n)}) d E_{\lambda_1} \otimes \cdots \otimes E_{\lambda_m} \right]^\sim$$

$$\subseteq \frac{1}{(m-n)!} \int \left[\sum_{\pi \in S_m} \alpha(\lambda_{\pi(1)}, \cdots, \lambda_{\pi(n)}) \right] \times d E_{\lambda_1} \otimes \cdots \otimes E_{\lambda_m} \equiv J_2.$$

J_2 is closed and normal.

We define $\Delta_k, \epsilon(k, \boldsymbol{\lambda}), E_{\Delta_k}$ as before. E_{Δ_k} commutes with J_2. Furthermore, $E_{\Delta_k} \mathfrak{H}^{(m)} \subseteq D(J_1)$. Pick $f \in D(J_2)$. Since

$$E_{\Delta_k} f \in D(J_1),$$

$$E_{\Delta_k} f \to f \quad \text{as} \quad k \to \infty,$$

$$J_1 E_{\Delta_k} f = J_2 E_{\Delta_k} f = E_{\Delta_k} J_2 f \to J_2 f \quad \text{as} \quad k \to \infty,$$

and J_1 is closed, it follows that $J_1 = J_2$. Thus $\Omega(A; n)$ is normal.

Furthermore,

$$J_2^\dagger = \frac{1}{(m-n)!} \int \sum_{\pi \in S_m} \alpha^*(\lambda_{\pi(1)}, \cdots, \lambda_{\pi(n)}) d E_{\lambda_1} \otimes \cdots \otimes E_{\lambda_n};$$

i.e., $\Omega(A; n)^\dagger = \Omega(A^\dagger; n)$.

Corollary 1: Let A, B be uniformly normal operators in $\mathfrak{H}^{(n)}$. Then A and B commute if and only if $\Omega(A; n)$ and $\Omega(B; n)$ commute.

Proof: Let $\{E_\lambda^A\}$ be a spectral family in $\mathfrak{H}^{(1)}$ associated with A, and $\{E_\mu^B\}$ one associated with B. Then $\Omega(A; n)$ commutes with $\Omega(B; n)$ iff $E_{\lambda_1}^A \otimes \cdots \otimes E_{\lambda_m}^A$ commutes with $E_{\mu_1}^B \otimes \cdots \otimes E_{\mu_m}^B$ iff A commutes with B.

Corollary 2: If A and B are linear transformations in $\mathfrak{H}^{(n)}$ satisfying condition D_1 such that $A \geq B$, and at least one is closed and bounded, then $\Omega(A; n) \geq \Omega(B; n)$.

Proof: $A \geq B$ implies $A - B \geq 0$ on $D(A) \cap D(B)$. Since one of A, B is closed and bounded, it follows that $A - B$ is a positive symmetric operator satisfying condition D_1. It follows that $A - B$ has at least one positive self-adjoint extension. Let one such extension be called $(A - B)'$. $(A - B)'$ automatically has property D_1 and $\Omega((A - B)'; n) \geq 0$. $\Omega(A; n) - \Omega(B; n)$ also has property D_1. We shall show $\Omega(A; n) - \Omega(B; n) \subseteq \Omega((A - B)'; n)$. Since the

P_m reduce these operators, it suffices to show the extension property in each $\mathfrak{K}^{(m)}$, $m \geq n$. Since the U_π are unitary operators, it suffices to show $(A-B)' \otimes I^{(m-n)} \supseteq A \otimes I^{(m-n)} - B \otimes I^{(m-n)}$. Let $f \in D(A \otimes I^{(m-n)} - B \otimes I^{(m-n)})$. Let $\varphi_1 \otimes \varphi_2 \in D(A^\dagger - B^\dagger) \otimes \mathfrak{K}^{(m-n)}$. Then

$$\begin{aligned}(\{A \otimes I^{(m-n)} - B \otimes I^{(m-n)}\}f, \varphi_1 \otimes \varphi_2) &= (f, \{A^\dagger - B^\dagger\}\varphi_1 \otimes \varphi_2) \\ &= (f, \{A-B\}^\dagger \varphi_1 \otimes \varphi_2)\end{aligned}$$

since one of A, B is bounded.

Since $(A-B) \subseteq (A-B)'$, then $[(A-B)']^\dagger \subseteq (A-B)^\dagger = A^\dagger - B^\dagger$. We may then restrict $\varphi_1 \otimes \varphi_2$ to $D((A-B)'^\dagger) \otimes \mathfrak{K}^{(m-n)}$, obtaining

$$\begin{aligned}(\{A \otimes I^{(m-n)} - B \otimes I^{(m-n)}\}f, \varphi_1 \otimes \varphi_2) &= (f, [(A-B)']^\dagger \varphi_1 \otimes \varphi_2) \\ &= (f, \{(A-B)' \otimes I^{(m-n)}\}^\dagger \varphi_1 \otimes \varphi_2)\end{aligned}$$

or $f \in D[(A-B)' \otimes I^{(m-n)}]$.

Theorem 2: Let A be any transformation in $\mathfrak{K}^{(n)}$ satisfying condition D_1. Let B_1, B_2 be any closed, bounded, linear transformations on $\mathfrak{K}^{(n)}$. Let $\overline{A}$ denote the symmetrized operator

$$\overline{A} = \frac{1}{n!} \sum_{\pi \in S_n} U_\pi A U_\pi^{-1}.$$

Then

(a) $\Omega(A; n) = \Omega(\overline{A}; n)$;
(b) $\Omega(\alpha A + \beta B; n) = [\alpha\Omega(A; n) + \beta\Omega(B; n)]^{\sim}$;
(c) for m, s integers, $m \geq s$,
$\Omega(A \otimes I^{(s)}; n+s) P_{n+m} = \frac{m!}{(m-s)!} \Omega(A; n) P_{n+m}$;
(d) $B_1 \geq B_2$ implies $\Omega(B_1; n) \geq \Omega(B_2; n)$;
(e) $\Omega(B; n)^\dagger = \Omega(B^\dagger; n)$;
(f) if A is any operator in $\mathfrak{K}^{(1)}$, then $D(\Omega(A; 1)) = \mathfrak{F}$ iff $A = 0$; if A is any positive, uniformly normal operator in $\mathfrak{K}^{(n)}$ satisfying D_3, then $D(\Omega(A; n)) = \mathfrak{F}$ iff $A = 0$;
(g) $[\Omega(B_1; n)\Omega(B_2; n)]^{\sim} = \left[\sum_{s=0}^{n} \frac{n!}{s!}\binom{n}{s} \Omega(\overline{B}_1 \otimes I^{(s)} \cdot I^{(s)} \otimes \overline{B}_2; n+s)\right]^{\sim}$;
(h) $[\Omega(B_1; n), \Omega(B_2; n)]^{\sim} = \left[\sum_{s=1} \frac{n!}{s!}\binom{n}{s} \Omega([\overline{B}_1 \otimes I^{(s)}, I^{(s)} \otimes \overline{B}_2]; n+s)\right]^{\sim}$.

Proof:

(a) A satisfies D_1 implies

$$\frac{1}{n!} \sum_{\pi \in S_n} U_\pi A U_\pi^{-1}$$

satisfies D_1. The rest follows from the rearrangement theorem for finite groups.

(b) Since B is bounded, we have $D(\alpha A + \beta B) = D(A)$, $\alpha A + \beta B$ satisfies D_1, and $\Omega(B; n)$ is bounded on each $\mathfrak{K}^{(n)}$. Thus $\Omega(\alpha A + \beta B; n)$ exists and $\Omega(\alpha A + \beta B; n) \supseteq \alpha\Omega(A; n) + \beta\Omega(B; n)$.

Pick $f \in D(\Omega(\alpha A + \beta B; n))$. Define

$$f_m = \sum_{s=0}^{m} P_s f.$$

Then f_m converges strongly to f and

$$\begin{aligned}s - \lim_{m\to\infty} [\alpha\Omega(A; n) + \beta\Omega(B; n)] f_m &= s - \lim_{m\to\infty} [\Omega(\alpha A + \beta B; n)] f_m \\ &= s - \lim_{m\to\infty} \sum_{s=0}^{m} P_s \Omega(\alpha A + \beta B; n) f \\ &= \Omega(\alpha A + \beta B; n) f.\end{aligned}$$

Hence $f \in D([\alpha\Omega(A; n) + \beta\Omega(B; n)]^{\sim})$.

(c) For $m \geq s$, we have

$$\begin{aligned}&\Omega(A \otimes I^{(s)}; n+s) P_{n+m} \\ &= \frac{1}{(m-s)!} \left(\sum_{\pi \in S_{n+m}} U_\pi A \otimes I^{(m)} U_\pi^{-1}\right) P_{n+m} \\ &= \frac{m!}{(m-s)!} \Omega(A; n) P_{n+m}.\end{aligned}$$

(d) This follows from Corollary 2.

(e) On each $\mathfrak{K}^{(m)}$, $m \geq n$,

$$\left[\sum_{\pi \in S_m} U_\pi B \otimes I^{(m-n)} U_\pi^{-1}\right]^{\sim} = \sum_{\pi \in S_m} U_\pi B \otimes I^{(m-n)} U_\pi^{-1}.$$

The result follows by taking adjoints.

(f) For the first result see Cook.[1]
Since A has property D_3, then for $A \neq 0$, there exists $\varphi \in \mathfrak{M}_0$, with

$$\|\varphi\| = 1, A \otimes I^{(m-n)} \varphi^{(m)} \neq 0,$$

where $\varphi^{(m)}$ equals the m-fold tensor product of φ with itself. Then

$$\Phi \equiv \sum_{m=1}^{\infty} \frac{1}{m} \varphi^{(m)} \in \mathfrak{F}.$$

Consider

$$\begin{aligned}\|\Omega(A; n)\Phi\|^2 &= \sum_{m=n}^{\infty} m^{-2}[(m-n)!]^{-2} \\ &\quad \times \sum_{\pi, \psi \in S_m} (U_\pi \overline{A} \otimes I^{(m-n)} U_\pi^{-1} \varphi^{(m)}, U_\psi \overline{A} \\ &\quad \otimes I^{(m-n)} U_\psi^{-1} \varphi^{(m)}) \\ &= \sum_{m=n}^{\infty} m^{-2} \frac{m!}{[(m-n)!]^2} \sum_{\pi \in S_m} (U_\pi \overline{A} \\ &\quad \otimes I^{(m-n)} U_\pi^{-1} \varphi^{(m)}, \overline{A} \otimes I^{(m-n)} \varphi^{(m)}).\end{aligned}$$

From the fact that A is uniformly normal it follows that $\overline{A} \otimes I^{(m-n)}$ commutes with $U_\pi \overline{A}$

$\otimes I^{(m-n)}U_\pi^{-1}$ for all $\pi \in S_m$. Thus all terms in the above sum are positive and

$$\|\Omega(A;n)\Phi\|^2 \geq \sum_{m=n}^{\infty} \frac{m!}{m^2[(m-n)!]^2} n!(m-n)! \times \|\overline{A} \otimes I^{(m-n)}\Phi^{(m)}\|^2 = n!\,\|\overline{A}\varphi^{(n)}\|^2 \sum_{m=n}^{\infty} \frac{m!}{m^2(m-n)!} = \infty.$$

(g) Since the P_m reduce Ω, it suffices to prove the result on each $\mathfrak{K}^{(m)}$:

$$\Omega(B_1;n)\Omega(B_2;n)P_m = [(m-n)!]^{-2} \sum_{\pi,\varphi \in S_m} U_\pi \overline{B}_1 \otimes I^{(m-n)}U_\pi^{-1} \times U_\varphi \overline{B}_2 \otimes I^{(m-n)}U_\varphi^{-1} = [(m-n)!]^{-2} \sum_{\pi \in S_m} U_\pi \overline{B}_1 \otimes I^{(m-n)} \times \left(\sum_{\psi \in S_m} U_\psi \overline{B}_2 \otimes I^{(m-n)} U_\psi^{-1}\right) U_\pi^{-1}.$$

Any permutation ψ which leaves $\overline{B}_2$ operating in the first n components of $\mathfrak{K}^{(m)} = \mathfrak{K}^{(n)} \otimes \mathfrak{K}^{(m-n)}$ gives an equal contribution to the above sum as does any other such ψ. In fact any ψ which leaves $\overline{B}_2$ operating on $n-r$ of the first n components of $\mathfrak{K}^{(m)}$ is equivalent to any other ψ which also leaves $\overline{B}_2$ operating on $n-r$ of the first n components of $\mathfrak{K}^{(m)}$. The number of ψ's of this kind is

$$\binom{n}{r}\binom{m-n}{r}(m-n)!n!$$

[the number of ways of picking, without regard to order, r objects out of n boxes, another r objects (spaces) out of $m-n$ boxes, interchanging the r objects with the r spaces, and then rearranging the two resulting sets of $n, m-n$ things]. Furthermore, one such ψ yields $\overline{B}_1 \otimes I^{(m-n)} \cdot I^{(r)} \otimes \overline{B}_2 \otimes I^{(m-n-r)}$ Thus

$$\Omega(B_1;n)\Omega(B_2;n)P_m = [(m-n)!]^{-2} \times \sum_{\pi \in S_m} \sum_{r=0}^{\min(n,m-n)} (m-n)!n!\binom{n}{r}\binom{m-n}{r} \times U_\pi\left[(\overline{B}_1 \otimes I^{(r)} \cdot I^{(r)} \otimes \overline{B}_2) \otimes I^{(m-n-r)}\right] U_\pi^{-1} = \sum_{r=0}^{\min(n,m-n)} \frac{n!}{(m-n)!}\binom{n}{r}\binom{m-n}{r}(m-n-r)! \times \Omega(\overline{B}_1 \otimes I^{(r)} \cdot I^{(r)} \otimes \overline{B}_2; n+r)P_m.$$

Since $\Omega(A;n+r)P_m = 0$ for $n+r > m$, i.e., $r > m-n$, we may replace the upper limit on the sum by n and the desired result follows.

(h) This result follows immediately from (g) by noting that

$$\sum_{\pi \in S_{n+r}} U_\pi(\overline{B}_2 \otimes I^{(r)} \cdot I^{(r)} \otimes \overline{B}_1)U_\pi^{-1} = \sum_{\pi \in S_{n+r}} U_\pi(I^{(r)} \otimes \overline{B}_2 \cdot \overline{B}_1 \otimes I^{(r)})U_\pi^{-1}$$

and

$$\sum_{\pi \in S_{2n}} U_\eta B_1 \otimes B_2 U_\pi^{-1} - \sum_{\varphi \in S_{2n}} U_\varphi B_2 \otimes B_1 U_\varphi^{-1} = 0.$$

IV. THE FIELDS

We shall review some of Cook's definitions and results which will either be expanded or will be of use in the next section. Cook's original work[1] should be consulted for additional results.

Definition 6: For every $f \in \mathfrak{K}^{(1)}$, we define the linear transformation $(f\otimes)$ on $\mathfrak{F}$ as the bounded linear extension of the operation $(f\otimes)\,|\,\psi_1 \otimes \cdots \otimes \psi_n = |\,f \otimes \psi_1 \otimes \cdots \otimes \psi_n$. Then $\|(f\otimes)\| = \|f\|$, and $(f\otimes)$ has the adjoint $(f\otimes)^\dagger$ equal to the bounded, linear extension of

$$(f\otimes)^\dagger\,|\,\psi_1 \otimes \cdots \otimes \psi_n = |\,(f,\psi_1)\psi_2 \otimes \cdots \otimes \psi_n$$

and

$$(f\otimes)^\dagger\,|\,\alpha = 0$$

for α in $\mathfrak{K}^{(0)}$.

Let G be an operator-valued function which assigns, for every $n = 1, 2, \cdots$, an operator G_n in $\mathfrak{S}_n$, with G_0 defined to be the identity. The creation and annihilation operators (fields), ω_G and $\omega_G^\dagger$, respectively, map $\mathfrak{K}^{(1)}$ into the set of all densely defined, closed, linear transformations on $\mathfrak{F}$ by

$$\omega_G(f) = \left(\sum_{n=0}^{\infty} \oplus G_n\right)(f\otimes),$$

$$\omega_G^\dagger(f) = \omega_G(f)^\dagger = \left[(f\otimes)^\dagger \sum_{n=0}^{\infty} \oplus G_n^\dagger\right]^-.$$

In particular we will discuss, among others, the cases where G projects onto the purely symmetric or purely antisymmetric spaces. We therefore consider the decomposition of $\mathfrak{F}$ into superselection sectors defined by particle symmetry. We recall that in each $\mathfrak{K}^{(m)}$ there is a resolution of the identity $I = \sum_\tau Q_\tau(m)$, where the $Q_\tau(m)$ are the orthogonal projections onto the Young shapes, labeled by τ (i.e., the irreducible representations of S_m). Let $t(m)$ denote any subset of the irreducible representations of S_m in $\mathfrak{K}^{(m)}$. Since $U_\pi\Omega(A;n)U_\pi^{-1}P_m = \Omega(A;n)P_m$ for all $\pi \in S_m$, it follows that any sum $T(m) \equiv \sum_{\tau \in t(m)} Q_\tau(m)$ is a projection which reduces $\Omega(A;n)P_m$. We define the projection T on $\mathfrak{F}$ by

$$T = \sum_{n=0}^{\infty} \oplus \sum_{\tau \in t(m)} Q_\tau(m)$$

for any set $\{t(m)\}$. Then T reduces $\Omega(A;n)$, and we write $T\Omega(A;n)T \equiv \Omega_T(A;n)$, $T\mathfrak{F} = \mathfrak{F}_T$. By choosing $G_m = T(m) =$ the identity, the projection onto the

antisymmetric component of $\mathfrak{K}^{(m)}$, or the projection onto the symmetric component of $\mathfrak{K}^{(m)}$, we obtain the unsymmetrized, Fermi, and Bose fields, respectively. We remark that although we shall treat only the Fermi and Bose cases, they are not the only cases of physical interest. For example, if $\mathfrak{K}^{(1)}$ is a tensor product space where some of the products are irrelevant to a particular physical situation, then other representations of S_m become relevant: In particle physics the configuration space part of $\mathfrak{K}^{(1)}$ may be neglected, the rest of $\mathfrak{K}^{(1)}$ being finite dimensional. The various irreducible representations in each $\mathfrak{K}^{(m)}$ are then identified as elementary particles. In the Wigner supermultiplet theory for nuclear physics, the configuration part of $\mathfrak{K}^{(1)}$ is also discarded but only after implying maximal antisymmetry of the remaining part. In this case only restricted types of representations of S_m are relevant. We believe that this formalism may be used for some problems of the above nature.

A. The Antisymmetric Case

We choose

$$G_n = Q_\alpha(n) = \frac{1}{n!} \sum_{\pi \in S_n} \sigma^\pi U_\pi,$$

where σ^π is the parity of the permutation π. $Q_\alpha(n)$ is the projection onto the antisymmetric component of $\mathfrak{K}^{(n)}$. We denote the corresponding $T = G$ by T_α and define $T_\alpha \mathfrak{F} = \mathfrak{F}_\alpha$, and $\omega_G(f) = \omega_{T_\alpha}(f) \equiv \omega_\alpha(f)$, $\omega^\dagger_{T_\alpha}(f) \equiv \omega^\dagger_\alpha(f)$. We restrict all operators to $\mathfrak{F}_\alpha$.

For any orthonormal basis $\{\varphi_i\}$ of $\mathfrak{K}^{(1)}$, we define an orthonormal basis $\{(\varphi_1^{n_1} \varphi_2^{n_2} \cdots)_\alpha\}$ of $\mathfrak{F}_\alpha$, where $n_i = 0$ or 1 and $\sum_i n_i < \infty$, by $(\varphi_1^{n_1} \varphi_2^{n_2} \cdots)_\alpha = \mathrm{i}\,[(\sum_i n_i)!]^{1/2} Q_\alpha(\sum_i n_i)\varphi_1 \otimes \cdots \otimes \varphi_1 \otimes \varphi_2 \otimes \cdots \otimes \varphi_2 \otimes \varphi_3 \cdots$, (the element φ_i appears n_i times in the tensor product). The definition of $(\varphi_1^{n_1} \varphi_2^{n_2} \cdots)_\alpha$ is extended so that the vector is zero if $n_k > 1$ or $n_k < 0$ for any k. We shall use the abbreviated notation of not listing φ_i if $n_i = 0$; thus

$$(\varphi_1{}^1 \varphi_2{}^1 \varphi_3{}^0 \varphi_4{}^0 \varphi_5{}^1 \cdots)_\alpha \equiv |\varphi_1, \varphi_2, \varphi_5, \cdots\rangle_\alpha.$$

Let $\varphi_{i_1}, \varphi_{i_2}, \cdots, \varphi_{i_n}$ be a selection from the basis such that $i_1 < i_2 < \cdots < i_n$. We observe that if π is a permutation of $(1, 2, \cdots, n)$, with parity σ^π, then

$$\omega_\alpha(\varphi_{i_{\pi(1)}})\,\omega_\alpha(\varphi_{i_{\pi(2)}}) \cdots \omega_\alpha(\varphi_{i_{\pi(n)}})\,|0\rangle = \sigma^\pi |\varphi_{i_1}, \cdots, \varphi_{i_n}\rangle_\alpha,$$

where $|0\rangle$ is a unit vector in $\mathfrak{K}^{(0)}$ (the vacuum state). By direct computation on the given basis it follows that $\omega_\alpha(\varphi)$ and $\omega^\dagger_\alpha(\varphi)$ are bounded linear transformations on $\mathfrak{F}_\alpha$ such that

$$\|\omega_\alpha(\varphi)\| = \|\omega^\dagger_\alpha(\varphi)\| = \|\varphi\|$$

and

$$\omega_\alpha(a\varphi + b\psi) = a\omega_\alpha(\varphi) + b\omega_\alpha(\psi),$$
$$\omega^\dagger_\alpha(a\varphi + b\psi) = a^* \omega^\dagger_\alpha(\varphi) + b^* \omega^\dagger_\alpha(\psi).$$

Lemma 1_α: For all $f \in \mathfrak{K}^{(1)}$

$$\omega_\alpha(f) = \text{uniform limit} \sum_{i=1}^{n} (f, \varphi_i)\omega_\alpha(\varphi_i) \text{ as } n \to \infty,$$

Proof:

$$\left\|\omega_\alpha(f) - \sum_{i=1}^{n} (f, \varphi_i)\omega_\alpha(\varphi_i)\right\| = \left\|\omega_\alpha\left(f - \sum_{i=1}^{n}(f, \varphi_i)\varphi_i\right)\right\| = \left\|f - \sum_{i=1}^{n}(f, \varphi_i)\varphi_i\right\|,$$

which is arbitrarily small for sufficiently large n since $\{\varphi_i\}$ is an orthonormal basis.

Definition 7: If $\psi_1, \psi_2 \in \mathfrak{K}^{(1)}$, then $\psi_1\psi_2^*$ is the bounded linear operator on $\mathfrak{K}^{(1)}$, defined by $(\psi_1\psi_2{}^*)\varphi = (\varphi, \psi_2)\psi_1$. We define the anticommutator $[A, B]_+ \equiv AB + BA$ wherever the right-hand side exists. I_α denotes the identity in $\mathfrak{F}_\alpha$.

With these definitions Cook obtains the following results:

(i) $\omega_\alpha(\varphi)\,\omega^\dagger_\alpha(\psi) = \Omega_\alpha(\varphi\psi^*; 1)$;
$\omega^\dagger_\alpha(\psi)\omega_\alpha(\varphi) = (\varphi, \psi)I_\alpha - \Omega_\alpha(\varphi\psi^*; 1)$;

(ii) $[\omega_\alpha(\varphi), \omega^\dagger_\alpha(\psi)]_+ = (\varphi, \psi) I_\alpha$;
$[\omega_\alpha(\varphi), \omega_\alpha(\psi)]_+ = [\omega^\dagger_\alpha(\varphi), \omega^\dagger_\alpha(\psi)]_+ = 0$;

(iii) The set $\{\omega_\alpha(\varphi_i)\}$ is irreducible on $\mathfrak{F}_\alpha$.

B. The Symmetric Case

We choose

$$G_n = Q_s(n) = \frac{1}{n!} \sum_{\pi \in S_n} U_\pi$$

which is the projection onto the symmetric component of $\mathfrak{K}^{(n)}$. We denote the corresponding $T = G$ by T_s, define $T_s\mathfrak{F} = \mathfrak{F}_s$, restrict all operators to $\mathfrak{F}_s$, and write

$$\omega_{T_s}(f) = \omega_s(f), \quad \omega^\dagger_{T_s}(f) = \omega^\dagger_s(f).$$

For an orthonormal basis $\{\varphi_i\}$ of $\mathfrak{K}^{(1)}$, we define an orthonormal basis $\{(\varphi_1^{n_1} \varphi_2^{n_2} \cdots)_s\}$ of $\mathfrak{F}_s$, where $n_i = 0, 1, 2, \cdots$, and $\sum_i n_i < \infty$, by

$$(\varphi_1^{n_1} \varphi_2^{n_2} \cdots)_s = \left[\left(\sum_i n_i\right)!/\prod_i (n_i!)\right]^{1/2} \times Q_s\left(\sum_i n_i\right)\varphi_1 \otimes \cdots \otimes \varphi_1 \otimes \varphi_2 \cdots \otimes \varphi_2 \otimes \varphi_3 \cdots$$

(each φ_1 appears n_i times in the tensor product). The definition is extended so that $(\varphi_1^{n_1} \varphi_2^{n_2} \cdots)_s$

is zero if any $n_i < 0$. We shall also use the notation of dropping φ_i from the list if $n_i = 0$:

$$(\varphi_1{}^3\varphi_2{}^0\varphi_3{}^1\varphi_4{}^2\cdots)_s \equiv |\varphi_1\varphi_1\varphi_1\varphi_3\varphi_4\varphi_4\cdots\rangle_s.$$

Let $\varphi_{i_1}, \varphi_{i_2}, \cdots, \varphi_{i_n}$ be any selection from the basis such that $i_1 \le i_2 \cdots \le i_n$, and such that φ_1 occurs n_1 times, etc. Let ψ be any permutation of $(1, 2, \cdots, n)$. Then we have

$$\omega_s(\varphi_{i_{\psi(1)}})\cdots\omega_s(\varphi_{i_{\psi(n)}})|0\rangle = \left[\prod_i (n_i)!\right]^{1/2} |\varphi_{i_1}, \cdots, \varphi_{i_n}\rangle_s.$$

For any subset S of $\mathfrak{K}^{(1)}$, let $[S]$ be the closed, linear manifold generated by S. Let $R[S]$ be the projection onto $[S]$. Cook obtains the following results: The $\omega_s(\varphi)$, $\omega_\alpha^\dagger(\varphi)$ are unbounded operators with domain $D(\omega_s(\varphi)) = D(\omega_\alpha^\dagger(\varphi)) = D(\Omega_s(R[\varphi]; 1)^{1/2})$. Let V_{φ_1} be the bounded, linear extension of the transformation $V_{\varphi_1}(\varphi_1^{n_1}\varphi_2^{n_2}\cdots)_s = (\varphi_1^{n_1}\varphi_2^{n_2}\cdots)_s$ of $\mathfrak{F}_s$. Then $V_{\varphi_1}^\dagger$ is the bounded linear extension of the operator

$$V_{\varphi_1}^\dagger(\varphi_1^{n_1}\varphi_2^{n_2}\cdots)_s = (\varphi_1^{n_1-1}\varphi_2^{n_2}\cdots)_s.$$

V_{φ_1} is an isometry of the range of $\Omega_s(R[\varphi_1]; 1)^{1/2}$, and

$$\|V_\varphi\| = \|V_\varphi^\dagger\| = \|\varphi\|.$$

Then the fields have polar decompositions:

$$\omega_s^\dagger(\varphi) = V_\varphi^\dagger \Omega_s(R[\varphi]; 1)^{1/2},$$

$$\omega_s(\varphi) = V_\varphi[\Omega_s(R[\varphi]; 1) + I_s]^{1/2},$$

where I_s denotes the identity in $\mathfrak{F}_s$.

Lemma 1$_s$: Let $\psi \in D(N_s^{1/2})$. Then

$$\omega_s(f)\psi = \lim_{n\to\infty} \sum_{i=1}^n (\varphi_i, f)\omega_s(\varphi_i)\psi.$$

Proof: Let

$$f_n = \sum_{i=1}^n (\varphi_i, f)\varphi_i.$$

Then

$$\begin{aligned}\|\omega_s(f) - \sum_{i=1}^n (\varphi_i, f)\omega_s(\varphi_i)\psi\| &= \|\omega_s\Big(f - \sum_{i=1}^n (\varphi_i, f)\varphi_i\Big)\psi\| \\ &= \|\omega_s(f - f_n)\psi\| \\ &= \|V_{f-f_n}\Omega_s(R[f-f_n]; 1)^{1/2}\psi\| \\ &= \|f - f_n\|\,\|\Omega_s(R[f-f_n]; 1)^{1/2}\psi\| \\ &\le \|f - f_n\|\,\|\Omega_s(I; 1)^{1/2}\psi\| \\ &= \|f - \sum_{i=1}^n (\varphi_i, f)\varphi_i\|\,\|N_s^{1/2}\psi\|,\end{aligned}$$

the inequality coming from Theorem 2(d). The right-hand side is arbitrarily small for sufficiently large n due to the completeness of $\{\varphi_i\}$.

Cook obtains the following results:

(i) $\omega_s(\psi)\omega_s^\dagger(\varphi)$ and $\omega_s^\dagger(\psi)\omega_s(\varphi)$ are densely defined linear operators with closures

$$(\omega_s(\psi)\omega_s^\dagger(\varphi))^\sim = \Omega_s(\psi\varphi^*; 1)$$
$$(\omega_s^\dagger(\psi)\omega_s(\varphi))^\sim = (\varphi, \psi)I_s + \Omega_s(\varphi\psi^*; 1),$$

to which the first is equal if and only if $\psi \neq 0$ or $\varphi = 0$, the second if and only if $\varphi = \lambda\psi$.

(ii) The brackets $[\omega_s(\varphi), \omega_s(\psi)]$, $[\omega_s^\dagger(\varphi), \omega_s^\dagger(\psi)]$, $[\omega_s^\dagger(\varphi), \omega_s(\psi)]$ are densely defined, linear transformations with the closures

$$([\omega_s(\varphi), \omega_s(\psi)])^\sim = 0 = ([\omega_s^\dagger(\varphi), \omega_s^\dagger(\psi)])^\sim$$
$$([\omega_s^\dagger(\varphi), \omega_s(\psi)])^\sim = (\psi, \varphi)I_s,$$

to which they are equal if and only if $\varphi = \psi = 0$.

(iii) If $\{\varphi_i\}$ is an orthonormal basis of $\mathfrak{K}^{(1)}$, then the set $\{\omega_s(\varphi_i)\}$ is irreducible on $\mathfrak{F}_s$.

V. EXPANSION OF N-BODY OPERATORS IN POLYNOMIALS OF THE FIELDS

Definition 8: Let A be any closed linear operator in a Hilbert space. A domain $D \subseteq D(A)$ is said to be a core for A if $[A|_D]^\sim = A$.

Theorem 3: Let A be a uniformly normal operator on $\mathfrak{K}^{(n)}$ possessing a core of the form $\mathfrak{M}^{[n]}$, where $\mathfrak{M}$ is the manifold generated by finite linear combinations of the elements of some basis $\{g_i\}$ of $\mathfrak{K}^{(1)}$. Let

$$D \equiv \sum_{m=0}^\infty + \mathfrak{M}^{[m]}$$

(no completion implied). Then for $T = T_\alpha$ or $T = T_s$ (the antisymmetric and symmetric cases),

$$\mathfrak{M}_T^{[m]} = T(m)\mathfrak{M}^{[m]}, \quad \text{and} \quad D_T = \sum_{m=0}^\infty + \mathfrak{M}_T^{[m]},$$

we have

$$\Omega_T(A; n) = \left[\sum_{i_1,\cdots,i_n;\, j_1,\cdots,j_n}^\infty (g_{i_1}\otimes\cdots\otimes g_{i_n}, A\, g_{j_1}\otimes\cdots\otimes g_{j_n})\, \omega_T(g_{i_1})\cdots\omega_T(g_{i_n})\,\omega_T^\dagger(g_{j_n})\cdots\omega_T^\dagger(g_{j_1})\,\Big|_{D_T}\right]^\sim.$$

Proof: Since $\Omega(A;n)$ exists and is normal, $\Omega_T(A;n)$ exists and is normal in $\mathfrak{F}_T$. Since the P_m reduce $\Omega_T(A;n)$, it suffices to prove the result in each $\mathfrak{K}^{(m)}$. Suppose we can prove the result on the domain $\mathfrak{M}_T^{[m]}$. Because $\mathfrak{M}^{[m]} = \mathfrak{M}^{[n]} \times \mathfrak{M}^{[m,n]}$ and $U_\pi \mathfrak{M}^{[m]} = \mathfrak{M}^{[m]}$, it follows that $\mathfrak{M}^{[m]}$ is a core for all $U_\pi A \otimes I^{(m-n)} U_\pi^{-1}$ for all $\pi \in S_m$. We also have

$$\left[\Omega_T(A;n)P_m\Big|_{\mathfrak{M}[m]}\right]^{\sim} = \left[\left(\sum_{\pi\in S_m} U_\pi A \otimes I^{(m-n)}U_\pi^{-1}\right)\Big|_{\mathfrak{M}[m]}\right]^{\sim} T(m)P_m \supseteq \sum_{\pi\in S_m}\left[\left(U_\pi A\otimes I^{(m-n)}U_\pi^{-1}\right)\Big|_{\mathfrak{M}[m]}\right]^{\sim} T(m)P_m$$

$$= \sum_{\pi\in S_m} U_\pi A\otimes I^{(m-n)}U_\pi^{-1}T(m)P_m$$

and

$$\left[\left(\sum_{\pi\in S_m} U_\pi A\otimes I^{(m-n)}U_\pi^{-1}\right)\Big|_{\mathfrak{M}[m]}\right]^{\sim} T(m)P_m \supseteq \left[\sum_{\pi\in S_m} U_\pi A\otimes I^{(m-n)}U_\pi^{-1}\right]^{\sim} T(m)P_m = \Omega_T(A;n)P_m\ .$$

Since $\Omega_T(A;n)P_m$ is normal in $P_m\,\mathfrak{F}_T$, it has no normal extensions. Therefore $\mathfrak{M}^{[m]}$ is a core for $\Omega_T(A;n)P_m$. It remains to show

$$\Omega_T(A;n)P_m\Big|_{\mathfrak{M}[m]} = \sum_{i_1,\cdots j_n,\, j_1,\cdots j_n}^{\infty} (g_{i_1}\otimes\cdots\otimes g_{i_n}, Ag_{j_1}\otimes\cdots\otimes g_{j_n})\,\omega_T(g_{i_1})\cdots\omega_T(g_{i_n})\cdots\omega_T^\dagger(g_{j_n})\cdots\omega_T^\dagger(g_{j_1})\Big|_{\mathfrak{M}_T[m]}.$$

Furthermore, since the decomposable elements of $\mathfrak{M}^{[m]}$ form a basis for $\mathfrak{K}^{(m)}$, it suffices to show the above as a bilinear form between properly symmetrized decomposable elements of $\mathfrak{M}^{[m]}$ of the form $|h_1,h_2,\cdots,h_m\rangle_T$, where the $h_1,\cdots,h_m$ are a selection from the basis $\{g_i\}$. We recall that for the symmetric and antisymmetric cases there are normalization factors $\mathfrak{O}_T(h_1,\cdots,h_m)$ such that

$$\omega_T(h_1)\cdots\omega_T(h_m)|0\rangle = \mathfrak{O}_T(h_1,\cdots,h_m)|h_1,\cdots,h_m\rangle_T$$

and defining $\sigma_T^\pi = I$ in the symmetric case, σ^π in the antisymmetric case, we have

$$|(m!)^{-1/2}\mathfrak{O}_T(h_1,\cdots,h_m)^{-1}\sum_{\pi\in S_m}\sigma_T^\pi U_\pi h_1\otimes\cdots\otimes h_m = |h_1,\cdots,h_n\rangle_T\ .$$

Let $|f_1,\cdots,f_m\rangle_T$ be another such element. Consider, for $m\geq n$, the matrix elements

$$J_{f,g} \equiv {}_T\langle f_1,\cdots,f_m| \sum_{i_1,\cdots,i_n,\, j_1,\cdots,j_n}^{\infty} (g_{i_1}\otimes\cdots\otimes g_{i_n}, Ag_{j_1}\otimes\cdots\otimes g_{j_n})\,\omega_T(g_{i_1})\cdots\omega_T(g_{i_n})$$

$$\times\,\omega_T^\dagger(g_{j_n})\cdots\omega_T^\dagger(g_{j_1})\,|h_1,\cdots,h_n\rangle_T.$$

Because the f_i, h_i were chosen from the basis $\{g_j\}$, the sums on $i_1,\cdots,i_n,j_1,\cdots,j_n$ have only a finite number of nonvanishing terms, so the sums are well defined. Thus, using the commutation relations, we obtain

$$J_{f,g} = \sum_{i_1,\cdots,i_n,\, j_1,\cdots,j_n} (g_{i_1}\otimes\cdots\otimes g_{i_n}, Ag_{j_1}\otimes\cdots\otimes g_{j_n})\mathfrak{O}_T(h_1,\cdots,h_m)^{-1}\mathfrak{O}_T(f_1,\cdots,f_m)^{-1}$$

$$\times\,\langle 0|\omega_T^\dagger(f_m)\cdots\omega_T^\dagger(f_1)\omega_T(g_{i_1})\cdots\omega_T(g_{i_n})\omega_T^\dagger(g_{j_n})\cdots\omega_T^\dagger(g_{j_1})\omega_T(h_1)\cdots\omega_T(h_m)|0\rangle$$

$$= \sum_{i_1,\cdots,i_n,\, j_1,\cdots,j_n} (g_{i_1}\otimes\cdots\otimes g_{i_n}, Ag_{j_1}\otimes\cdots\otimes g_{j_n})\mathfrak{O}_T(h_1,\cdots,h_m)^{-1}\mathfrak{O}_T(f_1,\cdots,f_m)^{-1}$$

$$\times\,\frac{1}{[(m-n)!]^2}\sum_{\pi,\varphi\in S_m}\sigma_T^\varphi(f_{\varphi(1)},g_{i_1})(f_{\varphi(2)},g_{i_2})\cdots(f_{\varphi(n)},g_{i_n})\sigma_T^\pi(g_{j_1},h_{\pi(1)})\cdots(g_{j_n},h_{\pi(n)})$$

$$\times\,\langle 0|\omega_T^\dagger(f_{\varphi(m)})\cdots\omega_T^\dagger(f_{\varphi(n+1)})\omega_T(h_{\pi(n+1)})\cdots\omega_T(h_{\pi(m)})|0\rangle.$$

Letting $\psi\in S_{m-n}$ be a permutation of the numbers $\pi(n+1),\ \cdots,\pi(n)$, we evaluate the last factor, the vacuum expectation, to be

$$\sum_{\psi\in S_{m-n}}\sigma_T^\psi(f_{\varphi(n+1)},h_{\psi(\pi(n+1))})\cdots(f_{\varphi(m)},h_{\psi(\pi(m))}).$$

We then have

$$J_{f,g} = \mathfrak{O}_T(h_1,\cdots,h_m)^{-1}\mathfrak{O}_T(f_1,\cdots,f_m)^{-1}\frac{1}{[(m-n)!]^2}\sum_{\pi,\varphi\in S_m}\sum_{\psi\in S_{m-n}}\sigma_T^{\varphi}\sigma_T^{\pi}$$
$$\times(f_{\varphi(1)}\otimes\cdots\otimes f_{\varphi(m)},\ A\otimes I^{(m-n)}h_{\pi(1)}\otimes\cdots\otimes h_{\pi(n)}\otimes h_{\psi(\pi(n+1))}\cdots\otimes h_{\psi(\pi(m))})$$
$$=\frac{m!}{[(m-n)!]}\ {}_T\langle f_1,\cdots,f_m|A\otimes I^{(m-n)}|h_1,\cdots,h_m\rangle_T$$
$$=\frac{1}{(m-n)!}\sum_{\pi\in S_m}{}_T\langle f_1,\cdots,f_m|U_\pi A\otimes I^{(m-n)}U_\pi^{-1}|h_1,\cdots,h_m\rangle_T$$
$$={}_T\langle f_1,\cdots,f_m|\Omega_T(A;n)|h_1,\cdots,h_m\rangle_T.$$

It follows that for all $\chi\in D_T$, the i sums in the expansion of $\Omega_T(A;n)\chi$ have only a finite number of nonzero terms, and the j sums converge since they are the basis expansion sums of the vector $\Omega_T(A;n)\chi$.

This theorem is augmented by recalling that any operator A in $\mathfrak{IC}^{(1)}$ is essentially self-adjoint if and only if it is symmetric and has a dense set of analytic vectors.[4] From this dense set construct an orthonormal basis $\{g_i\}$ of $\mathfrak{IC}^{(1)}$. Let $\mathfrak{M}$ denote the manifold of finite linear combinations of the basis. Then $\mathfrak{M}$ is dense in $\mathfrak{IC}^{(1)}$ and is a core for A. Furthermore if B is any densely defined, closed operator, then $B^\dagger B$ is self-adjoint and $D(B^\dagger B)$ is a core for B.[5]

VI. SOME PHYSICAL EXAMPLES

The free Hamiltonian $H_0^{(1)}$ is of the form of multiplication by either μ, or $\mu+|\mathbf{p}|^2/2m$, or $(\mu^2+|\mathbf{p}|^2)^{1/2}$, where $\mu\geq 0$ is the mass, and where $\mathfrak{IC}^{(1)}$ is the space of square-integrable functions over R^s with variable $\mathbf{p}=(p_1,\cdots,p_s)$. Thus $H_0^{(1)}$ is self-adjoint, and has property D_3; $\Omega(H_0^{(1)};1)$ is self-adjoint, and the harmonic oscillator functions provide a basis of $\mathfrak{IC}^{(1)}$ which generates a core for $H_0^{(1)}$.

The Yukawa interaction is given by the multiplication operator

$$(Y(f\otimes g))(x,y)=c\ e^{-\mu|x-y|}f(x)g(y),\qquad c>0,$$

in $\mathfrak{IC}^{(2)}$ for one space dimension ($\mathfrak{IC}^{(1)}=\mathfrak{L}^2(R^1)$), and by

$$(Y(f\otimes g))(\mathbf{x},\mathbf{y})=c(e^{-\mu|\mathbf{x}-\mathbf{y}|}/\mu|\mathbf{x}-\mathbf{y}|)f(\mathbf{x})g(\mathbf{y}),c>0,$$

in $\mathfrak{IC}^{(2)}$, for two and three space dimensions. $Y(|\mathbf{x}-\mathbf{y}|)$ is the Fourier transformation of the function $(\mu^2+|\mathbf{p}|^2)^{-1}$ which is bounded and square integrable. Thus $\Omega(Y;2)$ is self-adjoint. The tensor product of harmonic oscillator functions provides a basis of $\mathfrak{IC}^{(2)}$ which generates a core for Y. Y has property D_3.

The Coulomb interaction is given by the multiplication operator $(Af\otimes g)(\mathbf{x},\mathbf{y})=(c/|\mathbf{x}-\mathbf{y}|)$ $f(\mathbf{x})g(\mathbf{y})$, c either positive or negative. Thus A is self-adjoint, possesses property D_2, and $\Omega(A;2)$ is self-adjoint.

ACKNOWLEDGMENT

It is a pleasure to thank Dr. T. P. Schonbek for many discussions on the details of this work.

[1] J. M. Cook, Trans. Math. Soc. 74, 222 (1953).
[2] V. Fock, Z. Physik 75, 622 (1932).
[3] B. V. Sz. Nagy, *Spektraldarstellung Linearer Transformationen des Hilbertschen Raumes* (Springer-Verlag, Berlin, 1942).
[4] E. Nelson, Ann. Math. 7, 583 (1959).
[5] T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, New York, 1966), p. 275.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Some Exact Statistical Properties of Turbulent Kinematic Dynamo Equations

I. Lerche
Enrico Fermi Institute and Department of Physics, University of Chicago, Chicago, Illinois 60637
(Received 22 March 1971)

The *exact* statistical properties of solutions to two restricted turbulent kinematic dynamo problems are given and discussed in some detail. In view of the fact that all discussion and solutions of the turbulent kinematic dynamo equations given so far in the literature are approximate, we believe that the present paper, containing two exactly soluble turbulent dynamo problems, is of more than academic interest. The method of solution is rather general and may, perhaps, be of basic interest. Further, the exact statistical solutions, which admit of regenerative dynamo action, allow approximate solutions to be compared and contrasted with the exact solutions, thus outlining the regime of applicability of the approximate solutions.

I. INTRODUCTION

For many years now there has been considerable interest in mechanisms which maintain or regenerate large-scale magnetic fields in nature. One of the most attractive mechanisms for magnetic field regeneration is a kinematic dynamo, in which the velocity field is considered given and the resulting induction equation is to be solved for the space and time variations of the magnetic field. Since the velocity field is, in general, an arbitrary function of space and time, no general solution to the kinematic dynamo equation has yet been found. Special velocity fields which allow the induction equation to be solved exactly have, of course, been given (see the review by Roberts[1] for several such exactly soluble models).

It was recognized quite some time ago[2,3] that a turbulent velocity field, in combination with a large-scale ordered sheared velocity field, produced an extremely efficient kinematic dynamo. But in view of the complexity of the resulting equations (see, e.g., Lerche[4]) only approximate solutions have so far been given.

More recently[5-7] it has been pointed out that, even in the absence of large-scale ordered velocity fields, dynamo action is provided by turbulent velocity fields on their own, be they isotropic or not. Once again the complexity of the equations has been such that only approximate solutions have so far been given.

The purpose of the present paper is to present *exact* statistical solutions to the kinematic dynamo equations when the velocity field is completely turbulent. While the two types of turbulent velocity field to be considered are rather special, they nevertheless illustrate several points.

First, they demonstrate that a method exists for extracting exact statistical solutions from the turbulent kinematic dynamo equations. Second, the exact solutions obtained can be used as templates against which one can estimate the accuracy of any approximate treatment. Third, they illustrate the point that the exact statistical solutions have a character which is rather different from what one might expect from order-of-magnitude inspection of the relevant terms in the dynamo equations.

In Sec. II we set up the basic equations to be used in obtaining the exact statistical solutions, and we specify the two classes of velocity turbulence we shall be concerned with. In Secs. III and IV we obtain the exact statistical solutions to the dynamo equations under the two classes of velocity turbulence, and we discuss the normal-mode dispersion relation obtaining in each case for the ensemble average magnetic field.

Finally, in Sec. V we discuss the results obtained and suggest further lines of investigation if the method and results given here are to be more fully incorporated into the mainstream of present research efforts on the structure and properties of kinematic dynamo equations.

II. BASIC EQUATIONS

Consider an infinite medium of constant resistivity η, which is not undergoing either bulk convection or shear, so that only a turbulent velocity $\delta\mathbf{V}$ with zero mean is present. Then the magnetohydrodynamic equations for the vector potentional $\mathbf{A}$ are

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right) A_i = \epsilon_{ijk}\,\delta V_j(\mathbf{x}, t) B_k(\mathbf{x}, t), \tag{1}$$

with the magnetic field $\mathbf{B}$ given by

$$B_i(\mathbf{x}, t) = \epsilon_{ijk}\frac{\partial A_k}{\partial \mathbf{x}_j}. \tag{2}$$

For random velocities $\delta\mathbf{V}(\mathbf{x}, t)$, which are functions of both space and time, Eqs. (1) and (2) are, in general, difficult to solve. Under these conditions recourse is normally made to either the "short-sudden" approximation, first used by Parker[2] to discuss kinematic dynamo action, or the "long-slow" approximation, first used by Braginskii[3] in discussing kinematic dynamo action. (For a detailed mathematical description of the terms "short-sudden" and "long-slow" we refer the interested reader to Lerche,[4] where the nature and physical content of both approximations is spelled out.)

More generally, we would like to obtain exact solutions to Eqs. (1) and (2) so that they can be used as templates to measure the regime of validity of the approximations used in discussions of kinematic dynamo theory.[2-9] We have searched the literature, and to our knowledge there have so far been no exact solutions given to Eqs. (1) and (2) when $\delta\mathbf{V}$ is a random velocity field. The two situations investigated in this paper, while special, do constitute *exact* statistical solutions to Eqs. (1) and (2), and as such, they are useful (albeit special) templates

against which the approximate treatments can be compared. They also illustrate a general technique which may perhaps be employed under more general circumstances than considered here (see, e.g., Lerche and Parker[10] for a different application of the technique—but within the framework of kinematic dynamo theory).

The interesting problem at hand is the construction of exact solutions to Eqs. (1) and (2). We consider two special classes of random velocity:

Class I: We take $\delta\mathbf{V}$ to be a random function only of time and independent of any spatial coordinates. The basic equations take the form

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)A_i(\mathbf{x}, t) = \epsilon_{ijk}\epsilon_{klm}\delta V_j(t)\frac{\partial A_m}{\partial \mathbf{x}_l}(\mathbf{x}, t) \tag{3}$$

under

$$\delta\mathbf{V} = \delta\mathbf{V}(t).$$

Class II: We take $\delta\mathbf{V}$ to be a random function of only one spatial coordinate, say x, and independent of both time and the other two spatial coordinates. The basic equations take the form

$$\left(\frac{\partial}{\partial t} - \eta\nabla^2\right)A_i(\mathbf{x}, t) = \epsilon_{ijk}\epsilon_{klm}\delta V_j(x)\frac{\partial A_m}{\partial x_l}(\mathbf{x}, t), \tag{4}$$

under

$$\delta\mathbf{V} = \delta\mathbf{V}(x).$$

Since the exact solution to Eqs. (1) and (2) is somewhat easier to obtain under class I velocity turbulence than under class II motions, we consider it first.

III. RANDOM VELOCITY A FUNCTION OF TIME

Spatially Fourier transform Eq. (3) with

$$A_i(\mathbf{x}, t) \sim A_i(\mathbf{k}, t)\, e^{i\mathbf{k}\cdot\mathbf{x}} \tag{5}$$

Since Eq. (3) is linear and homogeneous in spatial variables, it suffices to consider only one mode as in Eq. (5). Then Eq. (3) takes the form

$$\frac{\partial A_i}{\partial t} = -\eta k^2 A_i + i\delta V_j(t)(k_i A_j - k_j A_i). \tag{6}$$

Let $\tau = t/T$, where T is the correlation time for $\delta\mathbf{V}$. Also write $\delta\mathbf{V} = \epsilon\delta\mathbf{v}$ so that $\langle\delta V^2\rangle = \epsilon^2$; i.e., we normalize the turbulent velocity field, and then Eq. (6) becomes

$$\frac{\partial A_i}{\partial \tau} = -\eta T k^2 A_i + iT\epsilon\delta v_j(k_i A_j - k_j A_i). \tag{7}$$

Now consider the probability $P(\tau, \mathbf{A}, \delta\mathbf{v})$ for finding the combination of values $\mathbf{A}, \delta\mathbf{v}$ at time τ. Let the probability of finding $\delta\mathbf{v}$ on its own be described by the operator field $\mathfrak{L}(\delta\mathbf{v})$. Then $P(\tau, \mathbf{A}, \delta\mathbf{v})$ satisfies the spatially homogeneous equation

$$\frac{\partial P}{\partial \tau} = \mathfrak{L}(\delta\mathbf{v})P - \frac{\partial}{\partial A_i}P\{-\eta T k^2 A_i + iT\epsilon\delta v_j(k_i A_j - k_j A_i)\}. \tag{8}$$

While Eq. (8) is quite general, it is difficult to proceed further until the statistical distribution of $\delta\mathbf{v}$ is given. For the remainder of this paper we shall take $\mathfrak{L}(\delta\mathbf{v})$ to represent a Gaussian velocity distribution in each component of $\delta\mathbf{v}$, with the same correlation time and intensity in each component. Then[11]

$$\mathfrak{L}(\delta\mathbf{v})P \equiv \frac{\partial}{\partial\delta v_i}(\delta v_i P) + \frac{\partial^2 P}{\partial\delta v_i^2}, \tag{9}$$

and Eq. (8) becomes

$$\frac{\partial P}{\partial \tau} = \frac{\partial}{\partial\delta v_i}(\delta v_i P) + \frac{\partial^2 P}{\partial\delta v_i^2} - \frac{\partial}{\partial A_i} \times \{P[-\eta T k^2 A_i + iT\epsilon\delta v_j(k_i A_j - k_j A_i)]\}. \tag{10}$$

The first terms on the right-hand side of Eq. (10) represent the assumption that the probability distribution over $\delta\mathbf{v}$ alone is the Gaussian $\exp(-\frac{1}{2}\delta v_i\delta v_i)$.

The initial values of $\mathbf{A}$ are sufficient to determine the solution of (10). Denote them by $\mathbf{A}(\mathbf{k}, 0)$, so that at $\tau = 0$ the probability distribution is

$$P(\tau = 0) = (2\pi)^{-3/2}\exp(-\tfrac{1}{2}\,\delta\mathbf{v}\cdot\delta\mathbf{v})\delta[\mathbf{A} - \mathbf{A}(\mathbf{k}, 0)]. \tag{11}$$

To proceed with the solution of Eq. (10), define the quantities

$$R_\alpha(\tau, \delta\mathbf{v}) = \int A_\alpha P\, d^3\mathbf{A}, \qquad \alpha = x, y, z,$$

so that the kth Fourier mode of the ensemble average vector potential $\langle\mathbf{A}\rangle$ is

$$\langle\mathbf{A}\rangle = \int R(\tau, \delta\mathbf{v})d^3\delta\mathbf{v}, \tag{12}$$

with

$$\langle\mathbf{B}\rangle = i\mathbf{k}\times\langle\mathbf{A}\rangle. \tag{13}$$

Then Eq. (8) yields

$$\frac{\partial R_\alpha}{\partial \tau} = \frac{\partial}{\partial\delta v_i}(\delta v_i R_\alpha) + \frac{\partial^2 R_\alpha}{\partial\delta v_i^2} - \eta k^2 T R_\alpha + iT\epsilon\delta v_j(k_\alpha R_j - k_j R_\alpha), \tag{14}$$

with the initial conditions

$$R_\alpha(\tau = 0, \delta\mathbf{v}) = A_\alpha(\mathbf{k}, 0)(2\pi)^{-3/2}\exp(-\tfrac{1}{2}\,\delta\mathbf{v}\cdot\delta\mathbf{v}). \tag{15}$$

The coefficients in Eq. (14) are independent of τ so that the solutions have an exponential time dependence $\exp(\sigma\tau)$. Note that all three ($\alpha = x, y, z$)

of Eq. (14) are homogeneous in **R**. Hence they have a solution if, and only if, some dispersion relation is satisfied. Our task is to obtain the dispersion relation.

It is convenient to expand **R** in the normal modes ψ_n of the homogeneous equation

$$\frac{d^2\psi_n}{dx^2} + \frac{d(x\psi_n)}{dx} + n\psi_n = 0, \tag{16}$$

which are

$$\psi_n(x) = \exp(-\tfrac{1}{2}x^2)\, H_n(2^{-1/2}x), \tag{17}$$

where H_n is the nth Hermite polynomial. Further, from the recurrence relation for Hermite polynomials we have

$$2^{1/2}x\psi_n(x) = \psi_{n+1}(x) + 2n\psi_{n-1}(x). \tag{18}$$

Then we write

$$R_\alpha(\tau, \delta\mathbf{v}) = e^{\sigma\tau} \sum_{n,m,l=0}^{\infty} C^{(\alpha)}_{nml}\, \psi_n(\delta v_x)\psi_m(\delta v_y)\psi_l(\delta v_z). \tag{19}$$

Insertion of Eq. (19) into Eq. (14) and equating coefficients of $\psi_n\psi_m\psi_l$ gives the three equations

$$\begin{aligned} C^{(\alpha)}_{nml}&[\sigma + (\eta k^2 T + n + m + l)] \\ &= iT\epsilon 2^{-1/2}\{k_\alpha[C^{(x)}_{n-1,m,l} + 2(n+1)C^{(x)}_{n+1,m,l} \\ &+ C^{(y)}_{n,m-1,l} + 2(m+1)C^{(y)}_{n,m+1,l} \\ &+ C^{(z)}_{n,m,l-1} + 2(l+1)C^{(y)}_{n,m,l+1}] \\ &- k_x[C^{(\alpha)}_{n-1,m,l} + 2(n+1)C^{(\alpha)}_{n+1,m,l}] \\ &- k_y[C^{(\alpha)}_{n,m-1,l} + 2(m+1)C^{(\alpha)}_{n,m+1,l}] \\ &- k_z[C^{(\alpha)}_{n,m,l-1} + 2(l+1)C^{(\alpha)}_{n,m,l+1}]\}, \\ &\alpha = x, y, z. \end{aligned} \tag{20}$$

It has been shown elsewhere[10] that the determinant of the coefficients of Eq. (20) gives the dispersion relation. The determinant is, as usual, infinite and divergent. However, expanding the determinant about the upper left-hand corner gives a series that is asymptotically convergent for small $T\epsilon k \ll 1$. [The reader who prefers to solve the homogeneous finite-difference equation (20) by the more rigorous differential equation method given in Lerche and Parker[10] is encouraged to do so. We point out here that for $T\epsilon k \ll 1$ the results from both the asymptotic determinant method and the differential equation method agree *exactly*.]

Start at the upper left-hand corner with the set of coefficients obeying $n + m + l = 0$; then add in the set obeying $n + m + l = 1$, etc. To order $n + m + l = 1$ the resulting equations are

$$(\sigma + \eta k^2 T) C^{(\alpha)}_{000} = iT\epsilon 2^{1/2}[k_\alpha(C^{(x)}_{100} + C^{(y)}_{010} + C^{(z)}_{001}) - (k_x C^{(\alpha)}_{100} + k_y C^{(\alpha)}_{010} + k_z C^{(\alpha)}_{001})], \tag{21}$$

$$C^{(\alpha)}_{100}(\sigma + 1 + \eta k^2 T) = iT\epsilon 2^{-1/2}(k_\alpha C^{(x)}_{000} - k_x C^{(\alpha)}_{000}), \tag{22}$$

$$C^{(\alpha)}_{010}(\sigma + 1 + \eta k^2 T) = iT\epsilon 2^{-1/2}(k_\alpha C^{(y)}_{000} - k_y C^{(\alpha)}_{000}), \tag{23}$$

$$C^{(\alpha)}_{001}(\sigma + 1 + \eta k^2 T) = iT\epsilon 2^{-1/2}(k_\alpha C^{(z)}_{000} - k_z C^{(\alpha)}_{000}). \tag{24}$$

Now the original free decay solution (valid when $\epsilon = 0$) is

$$\sigma = -\eta k^2 T. \tag{25}$$

The coefficients to order $n + m + l = 1$ give the first correction to the free decay rate as

$$\sigma = -\eta k^2 T - k^2 T^2 \epsilon^2 (\sigma + 1 + \eta k^2 T)^{-1}. \tag{26}$$

There is now an additional root

$$\sigma + 1 + \eta k^2 T = 0, \tag{27}$$

as follows from Eqs. (22) (with $\alpha = x$), (23) (with $\alpha = y$), and (24) (with $\alpha = z$).

Had we evaluated the determinant to order $n + m + l = 2$, there would appear still another root:

$$\sigma + 2 + \eta k^2 T = 0,$$

etc. The extra roots all converge to the original roots in the limit $T \to \infty$. The decay of these extra roots is faster than the original roots, so we will not consider them further in the present problem.

The modified free decay mode [Eq. (26)] is now

$$\sigma \simeq -k^2 T(\eta + \epsilon^2 T), \tag{28}$$

implying that the turbulent diffusivity brought about by the random (in time) velocity field *increases* the rate of decay of the *mean* magnetic *field* over that which would obtain in its absence. Note that this is by no means the same as the rate of decay of the mean magnetic *energy* being different in the presence of turbulent time-dependent velocity fluctuations and in their absence. In point of fact, the rate of decay of $\langle B^2 \rangle$ is at *precisely* the rate $2k^2\eta$ obtaining when $\epsilon = 0$. We refer the interested reader to Appendix A where we discuss this and other points which appear somewhat anomalous at first sight.

For the present, so as not to break the train of the argument, we content ourselves by noting that the corrections to the free decay mode, valid in $T\epsilon k \ll 1$, indicate that the mean magnetic field decays at a *faster* rate in the presence of velocity turbulence than in its absence.

IV. RANDOM VELOCITY A FUNCTION OF x

Spatially Fourier transform Eq. (4) in y and z with

$$\mathbf{A}(\mathbf{x}, t) \sim \mathbf{A}(\mathbf{k}, x) \exp(i\mathbf{k}_\perp \cdot \mathbf{x}_\perp + \sigma t),$$

where

$$\mathbf{x}_\perp = (o, y, z), \quad \mathbf{k}_\perp = (o, k_y, k_z),$$

to obtain

$$(\sigma + \eta k_\perp^2)A_i - \eta \frac{d^2 A_i}{dx^2} = \delta V_j(x)\left(\frac{\partial A_j}{\partial \kappa_i} - \frac{\partial A_i}{\partial \kappa_j}\right), \tag{29}$$

where

$$\frac{\partial}{\partial \kappa_i} \equiv \left(\frac{d}{dx}, ik_y, ik_z\right).$$

Let $X = x/L$, where L is the correlation length associated with $\delta\mathbf{V}$, and normalize $\delta\mathbf{V}$ to $\epsilon\delta\mathbf{v}$ so that $\langle \delta\mathbf{V}^2 \rangle = \epsilon^2$. Then, writing out the components of Eq. (29), we have

$$\Omega A_x - \eta L^{-2} \frac{d^2 A_x}{dX^2} = \epsilon\delta v_y\left(L^{-1}\frac{dA_y}{dX} - ik_y A_x\right) + \epsilon\delta v_z\left(L^{-1}\frac{dA_z}{dX} - ik_z A_x\right), \tag{30}$$

$$\Omega A_y - \eta L^{-2} \frac{d^2 A_y}{dX^2} = \epsilon\delta v_x\left(ik_y A_x - L^{-1}\frac{dA_y}{dX}\right) + \epsilon\delta v_z(ik_y A_z - ik_z A_y), \tag{31}$$

$$\Omega A_z - \eta L^{-2} \frac{d^2 A_z}{dX^2} = \epsilon\delta v_x\left(ik_z A_x - L^{-1}\frac{dA_z}{dX}\right) + \epsilon\delta v_y(ik_z A_y - ik_y A_z), \tag{32}$$

where

$$\Omega = \sigma + \eta k_\perp^2.$$

Note that Eqs. (30)–(32) are second order in X, and so each requires two boundary conditions for a deterministic solution. This is to be compared with the situation in Sec. III, where the vector equation (7) was first order and so required only three boundary conditions for a determined solution. We might expect that the extra degree of freedom here will complicate the probability equation governing the evolution of $\mathbf{A}(x)$, and this is in fact the case.[12]

Set

$$\alpha = \frac{dA_x}{dX}, \quad \beta = \frac{dA_y}{dX}, \quad \gamma = \frac{dA_z}{dX}, \tag{33}$$

when Eqs. (30)–(32) become

$$\frac{d\alpha}{dX} = \Omega L^2\eta^{-1}A_x - \epsilon L^2\eta^{-1}\delta v_y(\beta L^{-1} - ik_y A_x) - \epsilon L^2\eta^{-1}\delta v_z(\gamma L^{-1} - ik_z A_x), \tag{34}$$

$$\frac{d\beta}{dX} = \Omega L^2\eta^{-1}A_y - \epsilon L^2\eta^{-1}\delta v_x(ik_y A_x - \beta L^{-1}) - \epsilon L^2\eta^{-1}\delta v_z(ik_y A_z - ik_z A_y), \tag{35}$$

$$\frac{d\gamma}{dX} = \Omega L^2\eta^{-1}A_z - \epsilon L^2\eta^{-1}\delta v_x(ik_z A_x - \gamma L^{-1}) - \epsilon L^2\eta^{-1}\delta v_y(ik_z A_y - ik_y A_z). \tag{36}$$

Proceeding as in Sec. III we see that the probability $P(X, \delta\mathbf{v}, \mathbf{A}, d\mathbf{A}/dX)$ of finding the values $\delta\mathbf{v}$, $\mathbf{A}$, and $d\mathbf{A}/dX$ at position X satisfies the stationary probability equation

$$\begin{aligned}\frac{\partial P}{\partial X} = {} & \frac{\partial}{\partial \delta v_i}(\delta v_i P) + \frac{\partial^2 P}{\partial \delta v_i^2} - \frac{\partial}{\partial A_x}(\alpha P) - \frac{\partial}{\partial A_y}(\beta P) - \frac{\partial}{\partial A_z}(\gamma P) \\ & - \frac{\partial}{\partial \alpha}\{P[\Omega L^2\eta^{-1}A_x - \epsilon L^2\eta^{-1}(\beta L^{-1} - ik_y A_x)\delta v_y - \epsilon L^2\eta^{-1}(\gamma L^{-1} - ik_z A_x)\delta v_z]\} \\ & - \frac{\partial}{\partial \beta}\{P[\Omega L^2\eta^{-1}A_y - \epsilon L^2\eta^{-1}\delta v_x(ik_y A_x - \beta L^{-1}) - \epsilon L^2\eta^{-1}\delta v_z(ik_y A_z - ik_z A_y)]\} \\ & - \frac{\partial}{\partial \gamma}\{P[\Omega L^2\eta^{-1}A_z - \epsilon L^2\eta^{-1}\delta v_x(ik_z A_x - \gamma L^{-1}) - \epsilon L^2\eta^{-1}\delta v_y(ik_z A_y - ik_y A_z)]\},\end{aligned} \tag{37}$$

with the boundary conditions at $X = 0$,

$$P(X = 0) = (2\pi)^{-3/2}\exp(-\tfrac{1}{2}\delta v^2)\,\delta[\mathbf{A} - \mathbf{A}(\mathbf{k}, 0)]\,\delta\left[\left(\frac{d\mathbf{A}}{dX} - \frac{d\mathbf{A}}{dX}\Big|_{x=0}\right)\right]. \tag{38}$$

Define

$$R_\alpha = \int A_\alpha P d^3\mathbf{A}\, d\alpha\, d\beta\, d\gamma, \quad \alpha = x, y, z, \tag{39}$$

$$Q_\alpha = \int \frac{dA_\alpha}{dX} P d^3\mathbf{A}\, d\alpha\, d\beta\, d\gamma, \quad \alpha = x, y, z, \tag{40}$$

so that

$$\langle \mathbf{A} \rangle = \int \mathbf{R} d^3\delta\mathbf{v}, \langle d\mathbf{A}/dX \rangle = \int \mathbf{Q} d^3\delta\mathbf{v};$$

then from Eq. (37) we obtain the six linear coupled homogeneous equations:

$$\frac{\partial R_\alpha}{\partial X} = \frac{\partial}{\partial \delta v_i}(\delta v_i R_\alpha) + \frac{\partial^2 R_\alpha}{\partial \delta v_i^2} + Q_\alpha, \quad \alpha = x, y, z, \tag{41}$$

$$\frac{\partial Q_x}{\partial X} = \frac{\partial}{\partial \delta v_i}(\delta v_i Q_x) + \frac{\partial^2 Q_x}{\partial \delta v_i^2} + \Omega L^2 \eta^{-1} R_x - \epsilon L^2 \eta^{-1} [\delta v_y (L^{-1} Q_y - i k_y R_x) + \delta v_z (L^{-1} Q_z - i k_z R_x)], \tag{42}$$

$$\frac{\partial Q_y}{\partial X} = \frac{\partial}{\partial \delta v_i}(\delta v_i Q_y) + \frac{\partial^2 Q_y}{\partial \delta v_i^2} + \Omega L^2 \eta^{-1} R_y - \epsilon L^2 \eta^{-1} [\delta v_x (i k_y R_x - L^{-1} Q_y) + \delta v_z (i k_y R_z - i k_z R_y)], \tag{43}$$

$$\frac{\partial Q_z}{\partial X} = \frac{\partial}{\partial \delta v_i}(\delta v_i Q_z) + \frac{\partial^2 Q_z}{\partial \delta v_i^2} + \Omega L^2 \eta^{-1} R_z - \epsilon L^2 \eta^{-1} [\delta v_x (i k_z R_x - L^{-1} Q_z) + \delta v_y (i k_z R_y - i k_y R_z)]. \tag{44}$$

As in Sec. III we make use of the complete normal-mode set ψ_n to write

$$R_\alpha = e^{i\kappa x} \sum_{n,m,l=0}^{\infty} R_{nml}^{(\alpha)} \psi_n(\delta v_x) \psi_m(\delta v_y) \psi_l(\delta v_z), \tag{45a}$$

$$Q_\alpha = e^{i\kappa x} \sum_{n,m,l=0}^{\infty} Q_{nml}^{(\alpha)} \psi_n(\delta v_x) \psi_m(\delta v_y) \psi_l(\delta v_z). \tag{45b}$$

Inserting Eqs. (45) into Eqs. (41)–(44) and equating coefficients of $\psi_n \psi_m \psi_l$ gives

$$R_{nml}^{(\alpha)} (i\kappa + n + m + l) = Q_{nml}^{(\alpha)}, \quad \alpha = x, y, z, \tag{46}$$

$$Q_{nml}^{(x)}(i\kappa + n + m + l) = \Omega L^2 \eta^{-1} R_{nml}^{(x)} - \epsilon L^2 2^{-1/2} \eta^{-1} \{L^{-1}[Q_{n,m-1,l}^{(y)}] + 2(m+1) Q_{n,m+1,l}^{(y)}] - i k_y [R_{n,m-1,l}^{(x)} + 2(m+1) R_{n,m+1,l}^{(x)}] + L^{-1}[Q_{n,m,l-1}^{(z)} + 2(l+1) Q_{n,m,l+1}^{(z)}] - i k_z [R_{n,m,l-1}^{(x)} + 2(l+1) R_{n,m,l+1}^{(x)}]\}, \tag{47}$$

$$Q_{nml}^{(y)}(i\kappa + n + m + l) = \Omega L^2 \eta^{-1} R_{nml}^{(y)} - \epsilon L^2 2^{-1/2} \eta^{-1} \{i k_y [R_{n-1,m,l}^{(x)} + 2(n+1) R_{n+1,m,l}^{(x)}] - L^{-1} \times [Q_{n+1,m,l}^{(y)} + 2(n+1) Q_{n+1,m,l}^{(y)}] + i k_y [R_{n,m,l-1}^{(z)} + 2(l+1) R_{n,m,l-1}^{(z)}] - i k_z [R_{n,m,l+1}^{(y)} + 2(l+1) R_{n,m,l+1}^{(y)}]\}, \tag{48}$$

$$Q_{nml}^{(z)}(i\kappa + n + m + l) = \Omega L^2 \eta^{-1} R_{nml}^{(z)} - \epsilon L^2 2^{-1/2} \eta^{-1} \{i k_z [R_{n-1,m,l}^{(x)} + 2(n+1) R_{n+1,m,l}^{(x)}] - L^{-1}[Q_{n-1,m,l}^{(z)} + 2(n+1) Q_{n+1,m,l}^{(z)}] + i k_z [R_{n,m-1,l}^{(y)} + 2(m+1) R_{n,m+1,l}^{(y)}] - i k_y [R_{n,m-1,l}^{(z)} + 2(m+1) R_{n,m+1,l}^{(z)}]\}. \tag{49}$$

Note that Eqs. (46)–(49) are linear and homogeneous and so possess a solution if, and only if, a dispersion relation is satisfied. Once again our task is to obtain the dispersion relation. Again note that the determinant formed from the coefficients is infinite and divergent; but for $\epsilon L^2 (k_1^2 + \kappa^2 L^{-2})^{1/2} \ll \eta$ the determinant is asymptotically convergent. So we solve by iteration around the upper left-hand corner of the determinant. To order $n + m + l = 1$ we have

$$i\kappa R_{000}^{(\alpha)} = Q_{000}^{(\alpha)}, \quad \alpha = x, y, z, \tag{50}$$

$$(1 + i\kappa) R_{100}^{(\alpha)} = Q_{100}^{(\alpha)}, \quad \alpha = x, y, z, \tag{51}$$

$$(1 + i\kappa) R_{010}^{(\alpha)} = Q_{010}^{(\alpha)}, \quad \alpha = x, y, z, \tag{52}$$

$$(1 + i\kappa) R_{001}^{(\alpha)} = Q_{001}^{(\alpha)}, \quad \alpha = x, y, z, \tag{53}$$

$$i\kappa Q_{000}^{(x)} = \Omega L^2 \eta^{-1} R_{000}^{(x)} - \epsilon L^2 2^{1/2} \eta^{-1} \times (L^{-1} Q_{010}^{(y)} - i k_y R_{010}^{(x)} + L^{-1} Q_{001}^{(z)} - i k_z R_{001}^{(x)}), \tag{54}$$

$$i\kappa Q_{000}^{(y)} = \Omega L^2 \eta^{-1} R_{000}^{(y)} - \epsilon L^2 2^{1/2} \eta^{-1} \times [i k_y (R_{100}^{(x)} + R_{001}^{(z)}) - L^{-1} Q_{100}^{(y)} - i k_z R_{001}^{(y)}], \tag{55}$$

$$i\kappa Q_{000}^{(z)} = \Omega L^2 \eta^{-1} R_{000}^{(z)} - \epsilon L^2 2^{1/2} \eta^{-1} \times [i k_z (R_{100}^{(x)} + R_{010}^{(y)}) - L^{-1} Q_{100}^{(z)} - i k_y R_{010}^{(z)}], \tag{56}$$

$$(1 + i\kappa)Q^{(x)}_{100} = \Omega L^2\eta^{-1}R^{(x)}_{100}, \tag{57}$$

$$(1 + i\kappa)Q^{(x)}_{010} = \Omega L^2\eta^{-1}R^{(x)}_{010} - \epsilon L^2 2^{-1/2}\eta^{-1} \times (L^{-1}Q^{(y)}_{000} - ik_y R^{(x)}_{000}), \tag{58}$$

$$(1 + i\kappa)Q^{(x)}_{001} = \Omega L^2\eta^{-1}R^{(x)}_{001} - \epsilon L^2 2^{-1/2}\eta^{-1} \times (L^{-1}Q^{(z)}_{000} - ik_z R^{(x)}_{000}), \tag{59}$$

$$(1 + i\kappa)Q^{(y)}_{100} = \Omega L^2\eta^{-1}R^{(y)}_{100} - \epsilon L^2 2^{-1/2}\eta^{-1} \times (ik_y R^{(x)}_{000} - L^{-1}Q^{(y)}_{000}), \tag{60}$$

$$(1 + i\kappa)Q^{(y)}_{010} = \Omega L^2\eta^{-1}R^{(y)}_{010}, \tag{61}$$

$$(1 + i\kappa)Q^{(y)}_{001} = \Omega L^2\eta^{-1}R^{(y)}_{001} - \epsilon L^2 2^{-1/2}\eta^{-1} \times (ik_y R^{(z)}_{000} - ik_z R^{(y)}_{000}), \tag{62}$$

$$(1 + i\kappa)Q^{(z)}_{100} = \Omega L^2\eta^{-1}R^{(z)}_{100} - \epsilon L^2 2^{-1/2}\eta^{-1} \times (ik_z R^{(x)}_{000} - L^{-1}Q^{(z)}_{000}), \tag{63}$$

$$(1 + i\kappa)Q^{(z)}_{010} = \Omega L^2\eta^{-1}R^{(z)}_{010} - \epsilon L^2 2^{-1/2}\eta^{-1} \times (ik_z R^{(y)}_{000} - ik_y R^{(z)}_{000}), \tag{64}$$

$$(1 + i\kappa)Q^{(z)}_{001} = \Omega L^2\eta^{-1}R^{(z)}_{001}. \tag{65}$$

By inspection of Eqs. (50)–(65) we see that they consist of two decoupled sets of equations. The first set, obtained from equations (51), (53), (57), (61), and (65) has a solution if, and only if,

$$(1 + i\kappa)^2 = \Omega L^2\eta^{-1}, \tag{66}$$

which gives

$$\sigma = 2i\eta\kappa L^{-2} - \eta[k_\perp^2 + L^{-2}(\kappa^2 - 1)]. \tag{67}$$

This represents an additional mode which reduces to the original mode $\sigma = -\eta k_\perp^2$ in the limit $L \to \infty$. For finite L, $k_\perp L \ll 1$, and $\kappa < 1$, it represents a growing, progressive wave. Later we shall compare it with the original mode $\sigma = -\eta k_\perp^2$ as modified by the presence of the turbulent velocity field. Consider then the other modes. Assume that Eq. (67) is *not* satisfied. Then

$$R^{(x)}_{100} = R^{(y)}_{010} = R^{(z)}_{001} = Q^{(x)}_{100} = Q^{(y)}_{010} = Q^{(z)}_{001} \equiv 0,$$

and Eqs. (50)–(65) reduce to

$$D_0 R^{(x)}_{000} = -2i\Delta^2 D_1^{-1}[k_y(i\kappa L^{-1}R^{(y)}_{000} - ik_y R^{(x)}_{000}) + k_z(i\kappa L^{-1}R^{(z)}_{000} - ik_z R^{(x)}_{000})], \tag{68}$$

$$D_0 R^{(y)}_{000} = -2\Delta^2 D_1^{-1}[L^{-1}(1 + i\kappa)(ik_y R^{(x)}_{000} - i\kappa L^{-1}R^{(y)}_{000}) + ik_z(ik_y R^{(z)}_{000} - ik_z R^{(y)}_{000})], \tag{69}$$

$$D_0 R^{(z)}_{000} = -2\Delta^2 D_1^{-1}[L^{-1}(1 + i\kappa)(ik_z R^{(x)}_{000} - i\kappa L^{-1}R^{(z)}_{000}) + ik_y(ik_z R^{(y)}_{000} - ik_y R^{(z)}_{000})], \tag{70}$$

where

$$\Delta = \epsilon L^2/(2^{1/2}\eta), \quad D_1 = -\Omega L^2\eta^{-1} + (1 + i\kappa)^2 \ (\neq 0),$$

$$D_0 = -\Omega L^2\eta^{-1} - \kappa^2.$$

The determinant formed from the coefficients of $R^{(\alpha)}_{000}$ in Eqs. (68)–(70) is the dispersion relation to order $n + m + l = 1$, valid for $\Delta(k_\perp^2 + \kappa^2 L^{-2})^{1/2} \ll 1$.

For small values of $\Delta(k_\perp^2 + \kappa^2 L^{-2})^{1/2}$, the off-diagonal terms can be neglected in the determinant, and then we have three decoupled modes:

(a) $D_0 + 2\Delta^2 k_\perp^2 D_1^{-1} = 0$, for $R^{(x)}_{000}$, (71)

(b) $D_0 + 2\Delta^2 D_1^{-1}(k_z^2 + \kappa^2 L^{-2} - i\kappa L^{-2}) = 0$, for $R^{(y)}_{000}$, (72)

(c) $D_0 + 2\Delta^2 D_1^{-1}(k_y^2 + \kappa^2 L^{-2} - i\kappa L^{-2}) = 0$, for $R^{(z)}_{000}$. (73)

So what was a triply degenerate mode ($D_0^3 = 0$) in the absence of turbulent velocity fluctuations has the degeneracy lifted in the presence of velocity turbulence. Note further that it suffices to consider only the modes associated with $R^{(x)}_{000}$ and $R^{(y)}_{000}$ since the mode for $R^{(z)}_{000}$ is identical to that for $R^{(y)}_{000}$ with the replacement $k_y \to k_z$, $k_z \to k_y$.

A. The "Parallel" Mode ($R^{(x)}_{000}$)

From Eq. (71) we have

$$\sigma L^2\eta^{-1} + (k_\perp^2 L^2 + \kappa^2) = 2^{1/2}\epsilon^2 L^4 k_\perp^2 \eta^{-2} \times [(1 + i\kappa)^2 - \sigma L^2\eta^{-1} - k_\perp^2 L^2]^{-1}, \tag{74}$$

and, with $\epsilon L^2\eta^{-1}(k_\perp^2 + \kappa^2 L^{-2})^{1/2} \ll 1$, Eq. (74) is

$$\sigma L^2\eta^{-1} \simeq -(\kappa^2 + k_\perp^2 L^2) + 2^{1/2}\epsilon^2 L^4 k_\perp^2 \eta^{-2} \times (1 + 2i\kappa)^{-1}. \tag{75}$$

With $\kappa/L = k_\parallel$ and $k^2 = k_\perp^2 + k_\parallel^2$, we have

$$\sigma = -\eta[k^2 - 2^{1/2}\epsilon^2 L^2 k_\perp^2 \eta^{-2}(1 + 2ik_\parallel L)^{-1}], \tag{76}$$

which is valid when $\epsilon L^2 k \ll \eta$.

Consider Eq. (76) under the long-wavelength approximation $kL \ll 1$:

$$\sigma \simeq -\eta(k^2 - 2^{1/2}\epsilon^2 L^2 k_\perp^2 \eta^{-2}). \tag{77}$$

With $k_\perp = k \sin\theta$, Eq. (77) is

$$\sigma \simeq -\eta k^2(1 - 2^{1/2}\epsilon^2 L^2 \eta^{-2} \sin^2\theta). \tag{78}$$

Now note that if $\epsilon L 2^{1/4} > \eta$ (which from $\epsilon L^2 k \ll \eta$ implies $kL \ll 1$), then modes with $|\sin\theta| > \eta/(2^{1/4}\epsilon L)$ are growing and hence represent regenerative dynamo action. For $\epsilon L 2^{1/4} < \eta$, all parallel long-wavelength modes are degenerative. In mathematical respects Eq. (78) has a structure very similar to the Čerenkov radiation condition, where for $v > c/n$, radiation occurs for $\cos\theta > c/nv$, but for $v < c/n$, no radiation occurs.

B. The "Perpendicular" Modes $(R^{(y)}_{000}, R^{(z)}_{000})$

As remarked earlier it is sufficient to consider only one of the perpendicular modes. In particular, take Eq. (72). This gives (with $\epsilon L^2 k \ll \eta$)

$$\sigma = -\eta k^2 \left[1 - 2^{1/2}\epsilon^2 L^2 \eta^{-2}(1 + 2ik_{\parallel}L)^{-1} \times \left(1 - \frac{k_y^2}{k^2} - \frac{ik_{\parallel}}{k^2 L}\right)\right]. \tag{79}$$

Here there are two long-wavelength situations to investigate ($k_{\parallel} = 0$, $k_{\parallel} \neq 0$):

1. $k_{\parallel} = 0$

For $k_{\perp}L \ll 1$, Eq. (79) reduces to

$$\sigma = -\eta k_{\perp}^2 [1 - 2^{1/2}\epsilon^2 L^2 \eta^{-2}(1 - k_y^2/k_{\perp}^2)], \tag{80}$$

which with $k_y = k_{\perp}\cos\varphi$ and $k_z = k_{\perp}\sin\varphi$ gives regenerative modes when

$$\epsilon L 2^{1/4} > \eta, \tag{81a}$$

and

$$|\sin\varphi| > \eta/(2^{1/4}\epsilon L). \tag{81b}$$

2. $k_{\parallel} \neq 0$

For $kL \ll 1$, Eq. (79) reduces to

$$\sigma = -\eta k^2 [1 - 2^{1/2}\epsilon^2 L^2 \eta^{-2}(1 - \cos^2\varphi \sin^2\theta - ik_{\parallel}/k^2 L)]. \tag{82}$$

In this case σ has both real and imaginary parts given by

$$\mathrm{Im}(\sigma) = -k_{\parallel}\epsilon^2 2^{1/2} L \eta^{-1}, \tag{83a}$$

$$\mathrm{Re}(\sigma) = -\eta k^2 [1 - 2^{1/2}\epsilon^2 L^2 \eta^{-2}(1 - \cos^2\varphi \sin^2\theta)], \tag{83b}$$

corresponding to a progressive dynamo wave which propagates and grows if both $|\cos\varphi \sin\theta| < [1 - \eta^2 2^{-1/2}(\epsilon L)^{-2}]^{1/2}$ and inequality (81a) are satisfied, and which otherwise decays. The phase speed of the wave is $\epsilon^2 L 2^{1/2}/\eta$ in the positive x direction.

The perpendicular mode (73) has the same properties as the perpendicular mode given by (72) provided that $\cos\varphi$ ($\sin\varphi$) replaces $\sin\varphi$ ($\cos\varphi$) throughout.

Altogether, then, the long-wavelength ($kL \ll 1$) perpendicular modes give regenerative dynamo action whenever $\epsilon L^2 k \ll \eta$ and $\eta < \epsilon L 2^{1/4}$, and then there is a regenerative mode when either $|\sin\theta \sin\varphi|$ or $|\sin\theta \cos\varphi|$ is less than $[1 - \eta^2 2^{-1/2}(\epsilon L)^{-2}]^{1/2}$.

The long-wavelength parallel mode gives regenerative dynamo action when $|\sin\theta| > \eta/(2^{1/4}\epsilon L)$.

Consider now the "new" mode given by Eq. (67), which does not exist in the absence of a turbulent velocity field. When $kL \ll 1$, it satisfies

$$\sigma \simeq \eta L^{-2} + 2i\eta k_{\parallel} L^{-1}, \tag{84}$$

which is a progressive wave whose growth time is much faster than the unstable parallel and perpendicular modes if $\epsilon L k^2 \ll \eta$. If we set $\epsilon L k^2 = \eta$, which violates the conditions under which the growth rates were calculated, but which will serve to illustrate the point, the maximum growth rate of the parallel and perpendicular modes is $O(\eta L^{-2})$. This indicates that for high-intensity turbulence ($\epsilon L k^2 \gtrsim \eta$) the asymptotic solution to the finite-difference equations is probably becoming unreliable. However, it also illustrates that the growth of the new mode is faster than the growth of the modified original modes under weak velocity turbulence ($\epsilon L k^2 \lesssim \eta$).

But the new mode associated with $Q^{(x)}_{100}$, etc., does not contribute to either the ensemble average magnetic field or to the ensemble average vector potential, as can readily be seen by integrating Eq. (45) over velocity $d^3\delta\mathbf{v}$. Accordingly, we can ignore it for the remainder of this paper.

Altogether, then, it is the parallel and perpendicular modes which control the response of the mean magnetic field to the spatial velocity turbulence, and these admit of regenerative dynamo action under "weak" velocity turbulence.

V. DISCUSSION

In this paper we have set up *exact* statistical equations describing the evolution of a magnetic field under both resistive decay and turbulent velocity fluctuations in an infinite medium. It was shown that if the turbulent velocity was a function only of one spatial coordinate or of time alone, the equations could be solved statistically *exactly*. For weak turbulence we obtained the dispersion relations relating the growth of the ensemble average magnetic field to both the resistivity and the effective intensity of the velocity turbulence.

When the velocity turbulence is a function only of time, but isotropically distributed (at $t = 0$), we showed (Sec. III) that the mean magnetic field always decays *faster* than under resistivity alone. We pointed out (and prove in Appendix A) that this is *not* the same as stating that the mean magnetic energy is decaying faster than under free resistive decay. In fact, the mean magnetic energy

decays at just the free resistive decay rate (but see Appendix A).

When the velocity turbulence is a function only of x, we showed (Sec. IV) that the degeneracy in the dispersion of the modes describing the ensemble average magnetic is lifted under "weak" velocity turbulence. Further, in the limit of long wavelengths, we showed that there exist regenerative dynamo modes when the resistivity is sufficiently small (see also Appendix B).

We have done the present calculations for two reasons. First, because there are no *exact* statistical solutions available in the literature. So our computations, while specialized to specific dependences of the turbulent velocity field on coordinates and time, relieve this situation. They further indicate a general method which is, perhaps, capable of being used under wider classes of velocity turbulence than considered here. Second, the dispersion relations describing the normal modes of the ensemble average magnetic field indicate some unexpected properties which are not brought to light by considerations based on approximate treatments of the statistical kinematic dynamo equations. In particular, we believe that the anomalously rapid decay of the mean magnetic field under time-dependent velocity turbulence, and the Čerenkov-like structure of the normal modes of the mean magnetic field under space-dependent velocity turbulence, are phenomena deserving of a more detailed investigation than has been given in this first crude analysis of the *exact* statistical properties of the dynamo equations (1) and (2).

We would be extremely interested in seeing computations which make use of the statistical properties of the turbulence under physically more realistic approximations than we have done in this first demonstration of exact statistical solutions to the kinematic dynamo equations.

ACKNOWLEDGMENT

This work has been supported by the United States Air Force, Air Force Systems Command, under Contract No. F-19628-69-C-0041.

APPENDIX A

Consider Eq. (1) when $\delta\mathbf{V}$ is a random function of time. Take the curl of Eq. (1), giving

$$\frac{\partial \mathbf{B}}{\partial t} + (\delta\mathbf{V}(t)\cdot\nabla)\mathbf{B} = \eta\nabla^2\mathbf{B}. \tag{A1}$$

Take the spatial Fourier transform of Eq. (A1) with

$$\mathbf{B}(\mathbf{x}, t) \sim \mathbf{B}(\mathbf{k}, t)e^{i\mathbf{k}\cdot\mathbf{x}}$$

to obtain

$$\frac{\partial \mathbf{B}(\mathbf{k}, t)}{\partial t} + i\mathbf{k}\cdot\delta\mathbf{V}(t)\mathbf{B}(\mathbf{k}, t) = -\eta k^2\mathbf{B}(\mathbf{k}, t). \tag{A2}$$

To demonstrate that the energy stored in each mode $\mathbf{B}(\mathbf{k}, t)$ declines at the free decay rate, multiply Eq. (A2) by $\mathbf{B}(\mathbf{k}, t)^*$, complex conjugate the resulting equation, and then add to obtain

$$\frac{\partial |\mathbf{B}|^2}{\partial t} = -2\eta k^2 |\mathbf{B}|^2, \tag{A3}$$

where $|\mathbf{B}|^2 = \mathbf{B}(\mathbf{k}, t)\cdot\mathbf{B}(\mathbf{k}, t)^*$.

From Eq. (A3) we see that the energy $\propto|\mathbf{B}|^2$ stored in any mode declines as time progresses at a rate $2\eta k^2$. And this is true irrespective of the value of the random velocity $\delta\mathbf{V}(t)$.

On the other hand, consider now the behavior of $\mathbf{B}(\mathbf{k}, t)$. Equation (A2) has the solution

$$\mathbf{B}(\mathbf{k}, t) = \mathbf{B}(\mathbf{k}, o)\exp(-\eta k^2 t)\exp\left(i\int_o^t \mathbf{k}\cdot\delta\mathbf{V}(t')dt'\right), \tag{A4}$$

so that the phase of any mode of $\mathbf{B}(\mathbf{k}, t)$ is random when $\delta\mathbf{V}$ is random. If the probability of finding a particular velocity $\delta\mathbf{V}$ is Gaussian at $t = 0$ and thereafter satisfies a homogeneous probability equation of the Uhlenbeck and Ornstein[11] type, the mean value of

$$\exp\left(i\int_o^t \mathbf{k}\cdot\delta\mathbf{V}(t')dt'\right)$$

weighted with respect to the probability of finding $\delta\mathbf{V}$ is well known (see, e.g., Ref. 13) to be $\propto \exp(-k^2\epsilon^2 Tt)$ so that

$$\langle\mathbf{B}(\mathbf{k}, t)\rangle \propto \exp[-k^2 t(\eta + \epsilon^2 T)]. \tag{A5}$$

This behavior of the average magnetic field is precisely the same as the behavior of the randomly modulated simple harmonic oscillator. The increase in the damping rate over that obtaining in the absence of turbulent velocity fluctuations is due to phase incoherence.

It is also obvious by inspection of Eq. (A4) that

$$\mathbf{B}(\mathbf{k}, t)\cdot\mathbf{B}(\mathbf{k}, t)^* = \mathbf{B}(\mathbf{k}, o)\cdot\mathbf{B}(\mathbf{k}, o)^*\exp(-2\eta k^2 t),$$

which is independent of $\delta\mathbf{V}(t)$, so that once again we obtain the rate of decay of magnetic field energy progressing at the free decay rate.

This illustrates that the energy stored in the magnetic field is declining more slowly than the square of the mean field, indicating that, after a time $O[k^{-2}(\eta + \epsilon^2 T)^{-1}]$, the magnetic field is essentially all disordered. This type of phase interference damping occurs in nearly all random propagation problems and is to be ascribed to a phase interference similar to the Landau damping occurring in plasma physics problems (see, e.g., Ref. 14). An alternative way of picturing the damping is considering a set of waves which start in step. Then, as each wave moves under its velocity field, fiducial marks on each wave get out of step. After a time $O[k^{-2}(\eta + \epsilon^2 T)^{-1}]$, the fiducial marks are essentially nearly uniformly spread over a

wavelength so that the average field (proportional to the number of fiducial marks in step with each other) has declined. It is in this sense that the ensemble average field is said to damp.

APPENDIX B

The possibility exists that the exact statistical generation of dynamo action discussed in the text is due to sources and sinks of $\nabla\cdot\delta\mathbf{v}$ (but see Ref. 12). We demonstrate here that one obtains essentially the same regenerative dynamo action when the turbulent velocity field is incompressible. Let $\delta\mathbf{V} = (o, \delta v_y(x), \delta v_z(x))$, satisfying $\nabla\cdot\delta\mathbf{V} = 0$. Then, following the procedure outlined in the text, we obtain the equation for P, the probability of finding δv_y, δv_z, $\mathbf{A}$, and $d\mathbf{A}/dX$ at position X, as

$$\begin{aligned}\frac{\partial P}{\partial X} &= \frac{\partial}{\partial \delta v_y}(\delta v_y P) + \frac{\partial^2 P}{\partial \delta v_y^2} + \frac{\partial}{\partial \delta v_z}(\delta v_z P) + \frac{\partial^2 P}{\partial \delta v_z^2} \\ &- \frac{\partial}{\partial A_x}(L\alpha P) - \frac{\partial}{\partial A_y}(L\beta P) - \frac{\partial}{\partial A_z}(L\gamma P) \\ &- \frac{\partial}{\partial \alpha}\left[P\left(\frac{L}{\eta}(\sigma + \eta k_\perp^2)A_x - \frac{L\epsilon}{\eta}(\beta\delta v_y + \gamma\delta v_z)\right.\right. \\ &\left.\left. + i\frac{L\epsilon}{\eta}A_x(k_y\delta v_y + k_z\delta v_z)\right)\right] \\ &- \frac{\partial}{\partial \beta}\left[P\left(\frac{L}{\eta}(\sigma + \eta k_\perp^2)A_y - i\frac{\epsilon L}{\eta}\delta v_z(k_y A_z - k_z A_y)\right)\right] \\ &- \frac{\partial}{\partial \gamma}\left[P\left(\frac{L}{\eta}(\sigma + \eta k_\perp^2)A_z + i\frac{\epsilon L}{\eta}\delta v_y(k_y A_z - k_z A_y)\right)\right].\end{aligned} \tag{B1}$$

Define

$$\begin{aligned}R^{(\mu)} &= \int A_\mu P d^3\mathbf{A}\, d\alpha d\beta d\gamma, \\ Q^{(\mu)} &= \int(\alpha, \beta, \gamma)P d^3\mathbf{A}\, d\alpha d\beta d\gamma,\end{aligned} \tag{B2}$$

and, as in the text, write

$$R^{(\mu)} = e^{i\kappa X}\sum_{m,n=0}^{\infty} R_{nm}^{(\mu)}\psi_n(\delta v_y)\psi_m(\delta v_z), \tag{B3}$$

$$Q^{(\mu)} = e^{i\kappa X}\sum_{m,n=0}^{\infty} Q_{nm}^{(\mu)}\psi_n(\delta v_y)\psi_m(\delta v_z). \tag{B4}$$

Then, following the same procedure as outlined in the text, we obtain

$$(i\kappa + n + m)R_{nm}^{(\alpha)} = LQ_{nm}^{(\alpha)}, \qquad \alpha = x, y, z, \tag{B5}$$

$$\begin{aligned}(i\kappa + n + m)Q_{nm}^{(x)} &= (L/\eta)(\sigma + \eta k_\perp^2)R_{nm}^{(x)} - (L\epsilon/2^{1/2}\eta) \\ &\times [Q_{n-1,m}^{(y)} + 2(n+1)Q_{n+1,m}^{(y)}] \\ &- (L\epsilon/2^{1/2}\eta)[Q_{n,m-1}^{(z)} + 2(m+1)Q_{n,m+1}^{(z)}] \\ &+ (iL\epsilon/2^{1/2}\eta)\{k_y[R_{n-1,m}^{(x)} + 2(n+1)R_{n+1,m}^{(x)}] \\ &+ k_z[R_{n,m-1}^{(x)} + 2(m+1)R_{n,m+1}^{(x)}]\},\end{aligned} \tag{B6}$$

$$\begin{aligned}(i\kappa + n + m)Q_{nm}^{(y)} &= (L/\eta)(\sigma + \eta k_\perp^2)R_{nm}^{(y)} \\ &- (i\epsilon L/2^{1/2}\eta) \\ &\times [k_y(R_{n,m-1}^{(z)} + 2(m+1)R_{n,m+1}^{(z)}) \\ &- k_z(R_{n,m-1}^{(y)} + 2(m+1)R_{n,m+1}^{(y)})],\end{aligned} \tag{B7}$$

$$\begin{aligned}(i\kappa + n + m)Q_{nm}^{(z)} &= (L/\eta)(\sigma + \eta k_\perp^2)R_{nm}^{(z)} \\ &+ (i\epsilon L/2^{1/2}\eta) \\ &\times [k_y(R_{n-1,m}^{(z)} + 2(n+1)R_{n+1,m}^{(z)}) \\ &- k_z(R_{n-1,m}^{(y)} + 2(n+1)R_{n+1,m}^{(y)})].\end{aligned} \tag{B8}$$

As usual, the determinant of the coefficients gives the dispersion relation. It is infinite and divergent, but it is asymptotically convergent for small values of

$$L^2\epsilon\eta^{-1}(k_\perp^2 + \kappa^2 L^{-2})^{1/2} \ll 1.$$

Start at the upper left-hand corner of the determinant with the set of coefficients obeying $n + m = 0$, then add in the set with $n + m = 1$, etc. To order $n + m = 1$, we obtain two decoupled sets of equations; the first set from $Q_{01}^{(z)}$, $R_{01}^{(z)}$, $Q_{10}^{(y)}$, and $R_{10}^{(y)}$ have a solution if the dispersion relation

$$\eta(i\kappa + 1)^2 = L^2(\sigma + \eta k_\perp^2) \tag{B9}$$

is satisfied. This representa a "new" mode not encountered when $L^{-1} \to 0$. But $Q_{01}^{(z)}$, $R_{01}^{(z)}$, $R_{10}^{(y)}$ and $Q_{10}^{(y)}$ do not contribute to either the mean field $\langle\mathbf{A}\rangle$ or to $\langle d\mathbf{A}/dX\rangle$, as can be seen by integrating Eqs. (B3) and (B4) with respect to $d\delta v_y d\delta v_z$.

Consequently, we can neglect the new mode for the purposes of discussing the normal modes of the ensemble average magnetic field.

After some algebra the remaining set of equations reduces to (to order $n + m = 1$)

$$\begin{aligned}R_{10}^{(x)}&[(i\kappa + 1)^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] \\ &= (L\epsilon/2^{1/2}\eta)(ik_y R_{00}^{(x)} - i\kappa L^{-1}R_{00}^{(y)}),\end{aligned} \tag{B10}$$

$$\begin{aligned}R_{01}^{(x)}&[i\kappa + 1)^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] \\ &= (L\epsilon/2^{1/2}\eta)(ik_z R_{00}^{(x)} - i\kappa L^{-1}R_{00}^{(z)}),\end{aligned} \tag{B11}$$

$$\begin{aligned}R_{01}^{(y)}&[i\kappa + 1)^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] \\ &= -(i\epsilon L/2^{1/2}\eta)(k_y R_{00}^{(z)} - k_z R_{00}^{(y)}),\end{aligned} \tag{B12}$$

$$\begin{aligned}R_{10}^{(z)}&[(i\kappa + 1)^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] \\ &= (i\epsilon L/2^{1/2}\eta)(k_y R_{00}^{(z)} - k_z R_{00}^{(y)}),\end{aligned} \tag{B13}$$

$$\begin{aligned}R_{00}^{(x)}&[-\kappa^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] \\ &= (i\epsilon L 2^{1/2}/\eta)(k_y R_{10}^{(x)} + k_z R_{01}^{(x)}),\end{aligned} \tag{B14}$$

$$R_{00}^{(y)}[-\kappa^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] = i\epsilon(L2^{1/2}/\eta)k_z R_{01}^{(y)}, \quad \text{(B15)}$$

$$R_{00}^{(z)}[-\kappa^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] = (i\epsilon L2^{1/2}/\eta)k_y R_{10}^{(z)}. \quad \text{(B16)}$$

From Eqs. (B12) and (B13) we have

$$R_{01}^{(y)} + R_{10}^{(z)} = 0, \quad \text{(B17)}$$

which, when used in Eqs (B15) and (B16), gives

$$k_y R_{00}^{(y)} + k_z R_{00}^{(z)} = 0. \quad \text{(B18)}$$

This leads to the dispersion of $R_{00}^{(x)}$ being completely decoupled from the dispersion in $R_{00}^{(y)}$ and $R_{00}^{(z)}$. In the present, incompressible, case the dispersion relations for $R_{00}^{(x)}$ and for the coupled pair $R_{00}^{(y)}, R_{00}^{(z)}$ are the same:

$$\kappa^2 L^{-2} + L(\sigma + \eta k_\perp^2)/\eta = \epsilon^2 L^2 k_\perp^2 \eta^{-1} \times [(i\kappa + 1)^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2]^{-1}. \quad \text{(B19)}$$

With $k_\parallel = \kappa L^{-1}$ and $k^2 = k_\perp^2 + k_\parallel^2$, we obtain, in $kL \ll 1$, the approximate form of Eq. (B19) as

$$\sigma = -\eta k_\parallel^2 + (\epsilon^2 L^2 \eta^{-2} - 1)\eta k_\perp^2 (1 - 2ik_\parallel L). \quad \text{(B20)}$$

Note that Eq. (B20) has the same basic structure as Eq. (83b).

For $\epsilon L > \eta$, Eq. (B20) gives long-wavelength regenerative dynamo action when

$$k_\perp > k_\parallel (\epsilon^2 L^2 \eta^{-2} - 1)^{-1/2}, \quad \text{(B21)}$$

while for $\epsilon L < \eta$ all long-wavelength modes are degenerative.

This illustrates, by direct computation, that the exact statistical regenerative dynamo action computed in the text is *not* due to sources and sinks of $\nabla \cdot \delta\mathbf{V}$, for we obtain here essentially the same results using *incompressible* velocity turbulence as we obtained in the text using *compressible* velocity turbulence.

[1] P. H. Roberts, "Dynamo Theory," 1968 (unpublished).
[2] E. N. Parker, Astrophys. J. **122**, 293 (1955).
[3] S. I. Braginskii, Zh. Eksp. Teor. Fiz. **20**, 726 (1964) [Sov. Phys. JETP **47**, 1084 (1964)].
[4] I. Lerche, Astrophys. J. **166**, 627 (1971).
[5] M. Steenbeck, F. Krause, and K. H. Radler, Z. Naturforsch. **21**, 369 (1966).
[6] K. H. Moffatt, J. Fluid Mech. **41**, 435 (1970).
[7] I. Lerche, Astrophys. J. **166**, 639 (1971).
[8] E. N. Parker, Astrophys. J. **162**, 665 (1970).
[9] M. Steenbeck and F. Krause, Z. Naturforsch. **21**, 1285 (1966).
[10] I. Lerche and E. N. Parker, Astrophys. J. September (1971).
[11] G. E. Uhlenbeck and L. S. Ornstein, Phys. Rev. **36**, 823 (1936).
[12] It was pointed out by R. Jayanthan [Monthly Notices Roy. Astron. Soc. **138**, 477 (1968)] that axisymmetric fluid motions can give dynamo action on their own. But T. G. Cowling [Monthly Notices Roy. Astron. Soc. **140**, 547 (1968)] noted that such dynamo action depends on $\nabla \cdot \delta\mathbf{V} \neq O$ for its existence. It might be argued *a priori* that the same is true in the present case where $\nabla \cdot \delta\mathbf{V} \neq O$. In Appendix B we demonstrate that, under $\nabla \cdot \delta\mathbf{V} = O$, the basic equations give dynamo action essentially as described in this section. So the dynamo action discussed here is *not* dependent on the nonzero nature of $\nabla \cdot \delta\mathbf{V}$ for its existence. It is a property of the dynamo equations existing in essentially the same basic form under both $\nabla \cdot \delta\mathbf{V} \neq O$ and $\nabla \cdot \delta\mathbf{V} = O$.
[13] U. Frisch, in *Probabalistic Methods in Applied Mathematics*, edited by A. T. Barucha-Reid (Academic, New York, 1968), Vol. 1, p. 92.
[14] J. D. Jackson, J. Nucl. Energy **C1**, 178, (1960).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Eigenvalue Problems for Lagrangian Systems. V

E. M. Barston
Courant Institute of Mathematical Sciences, New York University, New York, New York 10012
(Received 19 March 1971)

Sufficient conditions for exponential instability are obtained for a class of infinite-dimensional gyroscopic Lagrangian systems. Applications are made to the problems of the stability of a rotating thin annular elastic disk and the stability of the steady flow of a one-dimensional warm electron plasma.

I. INTRODUCTION

In an earlier paper[1] we gave sufficient conditions (Theorems III and IV of Ref. 1) for exponential instability of the gyroscopic Lagrangian system

$$P\ddot{\xi} + A\dot{\xi} + H\xi(t) = 0 \quad (1)$$

for the finite-dimensional problem, i.e., for the case where H, iA, and P (>0) were linear Hermitian operators in a finite-dimensional Hilbert space E_n. In this article we extend these results to a certain class of infinite-dimensional systems, namely, the case where P (>0) and iA are Hermitian operators in a separable Hilbert space E, with H possessing a compact Hermitian inverse H^{-1} in E. The results we obtain are directly applicable to a large number of problems concerning the stability of rotating elastic bodies; as an example we consider the stability of a thin, rotating annular disk. We also briefly consider a simple but useful special case of Eq. (1) where P is a positive real-valued function of x for $a \leq x \leq b$, A is a real, formally antisymmetric first-order differential operator defined on a dense subspace of $E = L_2[a, b]$, H is a real second-order formally

$$R_{00}^{(y)}[-\kappa^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] = i\epsilon(L2^{1/2}/\eta)k_z R_{01}^{(y)}, \quad \text{(B15)}$$

$$R_{00}^{(z)}[-\kappa^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2)] = (i\epsilon L2^{1/2}/\eta)k_y R_{10}^{(z)}. \quad \text{(B16)}$$

From Eqs. (B12) and (B13) we have

$$R_{01}^{(y)} + R_{10}^{(z)} = 0, \quad \text{(B17)}$$

which, when used in Eqs (B15) and (B16), gives

$$k_y R_{00}^{(y)} + k_z R_{00}^{(z)} = 0. \quad \text{(B18)}$$

This leads to the dispersion of $R_{00}^{(x)}$ being completely decoupled from the dispersion in $R_{00}^{(y)}$ and $R_{00}^{(z)}$. In the present, incompressible, case the dispersion relations for $R_{00}^{(x)}$ and for the coupled pair $R_{00}^{(y)}, R_{00}^{(z)}$ are the same:

$$\kappa^2 L^{-2} + L(\sigma + \eta k_\perp^2)/\eta = \epsilon^2 L^2 k_\perp^2 \eta^{-1} \times [(i\kappa + 1)^2 L^{-1} - L\eta^{-1}(\sigma + \eta k_\perp^2]^{-1}. \quad \text{(B19)}$$

With $k_\parallel = \kappa L^{-1}$ and $k^2 = k_\perp^2 + k_\parallel^2$, we obtain, in $kL \ll 1$, the approximate form of Eq. (B19) as

$$\sigma = -\eta k_\parallel^2 + (\epsilon^2 L^2 \eta^{-2} - 1)\eta k_\perp^2 (1 - 2ik_\parallel L). \quad \text{(B20)}$$

Note that Eq. (B20) has the same basic structure as Eq. (83b).

For $\epsilon L > \eta$, Eq. (B20) gives long-wavelength regenerative dynamo action when

$$k_\perp > k_\parallel (\epsilon^2 L^2 \eta^{-2} - 1)^{-1/2}, \quad \text{(B21)}$$

while for $\epsilon L < \eta$ all long-wavelength modes are degenerative.

This illustrates, by direct computation, that the exact statistical regenerative dynamo action computed in the text is *not* due to sources and sinks of $\nabla \cdot \delta\mathbf{V}$, for we obtain here essentially the same results using *incompressible* velocity turbulence as we obtained in the text using *compressible* velocity turbulence.

[1] P. H. Roberts, "Dynamo Theory," 1968 (unpublished).
[2] E. N. Parker, Astrophys. J. **122**, 293 (1955).
[3] S. I. Braginskii, Zh. Eksp. Teor. Fiz. **20**, 726 (1964) [Sov. Phys. JETP **47**, 1084 (1964)].
[4] I. Lerche, Astrophys. J. **166**, 627 (1971).
[5] M. Steenbeck, F. Krause, and K. H. Radler, Z. Naturforsch. **21**, 369 (1966).
[6] K. H. Moffatt, J. Fluid Mech. **41**, 435 (1970).
[7] I. Lerche, Astrophys. J. **166**, 639 (1971).
[8] E. N. Parker, Astrophys. J. **162**, 665 (1970).
[9] M. Steenbeck and F. Krause, Z. Naturforsch. **21**, 1285 (1966).
[10] I. Lerche and E. N. Parker, Astrophys. J. September (1971).
[11] G. E. Uhlenbeck and L. S. Ornstein, Phys. Rev. **36**, 823 (1936).
[12] It was pointed out by R. Jayanthan [Monthly Notices Roy. Astron. Soc. **138**, 477 (1968)] that axisymmetric fluid motions can give dynamo action on their own. But T. G. Cowling [Monthly Notices Roy. Astron. Soc. **140**, 547 (1968)] noted that such dynamo action depends on $\nabla \cdot \delta\mathbf{V} \neq O$ for its existence. It might be argued *a priori* that the same is true in the present case where $\nabla \cdot \delta\mathbf{V} \neq O$. In Appendix B we demonstrate that, under $\nabla \cdot \delta\mathbf{V} = O$, the basic equations give dynamo action essentially as described in this section. So the dynamo action discussed here is *not* dependent on the nonzero nature of $\nabla \cdot \delta\mathbf{V}$ for its existence. It is a property of the dynamo equations existing in essentially the same basic form under both $\nabla \cdot \delta\mathbf{V} \neq O$ and $\nabla \cdot \delta\mathbf{V} = O$.
[13] U. Frisch, in *Probabalistic Methods in Applied Mathematics*, edited by A. T. Barucha-Reid (Academic, New York, 1968), Vol. 1, p. 92.
[14] J. D. Jackson, J. Nucl. Energy **C1**, 178, (1960).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Eigenvalue Problems for Lagrangian Systems. V

E. M. Barston
Courant Institute of Mathematical Sciences, New York University, New York, New York 10012
(Received 19 March 1971)

Sufficient conditions for exponential instability are obtained for a class of infinite-dimensional gyroscopic Lagrangian systems. Applications are made to the problems of the stability of a rotating thin annular elastic disk and the stability of the steady flow of a one-dimensional warm electron plasma.

I. INTRODUCTION

In an earlier paper[1] we gave sufficient conditions (Theorems III and IV of Ref. 1) for exponential instability of the gyroscopic Lagrangian system

$$P\ddot{\xi} + A\dot{\xi} + H\xi(t) = 0 \quad (1)$$

for the finite-dimensional problem, i.e., for the case where H, iA, and P (>0) were linear Hermitian operators in a finite-dimensional Hilbert space E_n. In this article we extend these results to a certain class of infinite-dimensional systems, namely, the case where P (>0) and iA are Hermitian operators in a separable Hilbert space E, with H possessing a compact Hermitian inverse H^{-1} in E. The results we obtain are directly applicable to a large number of problems concerning the stability of rotating elastic bodies; as an example we consider the stability of a thin, rotating annular disk. We also briefly consider a simple but useful special case of Eq. (1) where P is a positive real-valued function of x for $a \leq x \leq b$, A is a real, formally antisymmetric first-order differential operator defined on a dense subspace of $E = L_2[a, b]$, H is a real second-order formally

symmetric differential operator defined on a dense subspace of E, and $\xi = \xi(x, t)$ vanishes at the endpoints of $[a, b]$. The results obtained are used to discuss the stability of steady flow of a warm, one-dimensional, electron plasma.

II. SUFFICIENT CONDITIONS FOR INSTABILITY

The extension of previous finite-dimensional results (Theorems III and IV of Ref. 1) to the infinite-dimensional case is accomplished in the theorems of this section. The infinite-dimensional problems are effectively made finite-dimensional by means of the fact that a completely continuous (i.e., compact) operator can be uniformly approximated by a finite-dimensional operator.

Theorem 1: Assume the following hypothesis:

(a) Let Z be a compact subset of the complex plane.
(b) For each $\omega \in Z$, let C_ω be a linear, completely continuous operator on and into the separable Hilbert space E, with continuous ω dependence (in the operator norm topology) on Z.
(c) Let $\{\varphi_n\}_{n=1}^{\infty}$ be a complete orthonormal system in E, and let P_n be the projector onto the subspace E_n spanned by $\varphi_1, \varphi_2, \cdots, \varphi_n$.
(d) Suppose that given any $N > 0$, there exists an integer $n > N$, an $\alpha(n) \in Z$, and an $\eta(n) \in E_n$, $\eta \neq 0$, such that $\eta = P_n C_\alpha \eta$.

Conclusion: For some $\Omega \in Z$ and a nonzero $\zeta \in E$, we have $\zeta = C_\Omega \zeta$.

Proof: We first show that

$$\inf_{\omega \in Z,\ \xi \in E} \frac{\|(I - C_\omega)\xi\|}{\|\xi\|} = 0. \tag{2}$$

Let $\epsilon > 0$. The compactness of Z, the continuity of C_ω on Z, and the fact that C_ω is completely continuous for each $\omega \in Z$ imply the existence of a real number N_ϵ, with the following property: For all integers $m \geq N_\epsilon$ and all $\omega \in Z$, $\|P_m C_\omega P_m - C_\omega\| < \epsilon$. By Theorem 1(d) there exist $n > N_\epsilon$, $\alpha \in Z$, and $\eta \in E_n$, with $\|\eta\| = 1$ satisfying the equation $(I - P_n C_\alpha)\eta = 0$. Now

$$\inf_{\omega \in Z,\ \xi \in E} \frac{\|(I - C_\omega)\xi\|}{\|\xi\|} \leq \frac{\|(I - C_\alpha)\eta\|}{\|\eta\|} \leq \|\eta - P_n C_\alpha \eta\| + \|(P_n C_\alpha P_n - C_\alpha)\eta\| < \epsilon,$$

which proves Eq. (2). Let $F(\omega) \equiv \inf_E [\|(I - C_\omega)\xi\| / \|\xi\|]$ for $\omega \in Z$. Since C_ω is continuous in ω on Z, $F(\omega)$ is a real-valued, nonnegative, continuous function of ω on Z and therefore assumes its minimum for some $\Omega \in Z$. By Eq. (2), this minimum is zero, i.e., $\inf_E [\|(I - C_\Omega)\xi\|^2 / \|\xi\|^2] = 0$. Now $\|(I - C_\Omega)\xi\|^2 = (\xi, \xi) - (\xi, H_\Omega \xi)$, where $H_\Omega = C_\Omega^\dagger + C_\Omega - C_\Omega^\dagger C_\Omega$ and $C_\Omega^\dagger$ is the adjoint of C_Ω. The operator H_Ω is completely continuous and Hermitian, so that

$$0 = \inf_E \frac{\|(I - C_\Omega)\xi\|^2}{\|\xi\|^2} = \inf_E \left(1 - \frac{(\xi, H_\Omega \xi)}{(\xi, \xi)}\right) = 1 - \sup_E \frac{(\xi, H_\Omega \xi)}{(\xi, \xi)}$$

implies the existence of a $\zeta \in E$, $\|\zeta\| = 1$, such that $H_\Omega \zeta = \zeta$. Therefore $\|(I - C_\Omega)\zeta\|^2 = (\zeta, (I - C_\Omega^\dagger)(I - C_\Omega)\zeta) = (\zeta, [I - H_\Omega]\zeta) = 0$, so that $\zeta = C_\Omega \zeta$, and the proof is complete.

A few definitions will be convenient in the sequel. A linear operator L with domain D_L and range R_L in the separable Hilbert space E will be called "simple" provided the following conditions are satisfied: $(L1)$ $\overline{D}_L = E$ ($\overline{\ }$ denotes closure); $(L2)$ $\overline{R}_L = E$; $(L3)$ $(\eta, L\zeta) = (L\eta, \zeta)$ for all η and $\zeta \in D_L$; $(L4)$ L has a completely continuous inverse L^{-1} on and into E, such that $L^{-1}L\eta = \eta$ for all $\eta \in D_L$ (which implies that $LL^{-1}\zeta = \zeta$ for all $\zeta \in R_L$). Properties $(L2)$ and $(L3)$ imply that L^{-1} is Hermitian, so that L^{-1} and L admit of a complete orthonormal set of eigenvectors $\{\varphi_l\}_1^\infty$ on $\overline{R}_{L^{-1}} = E$, and we have $L\varphi_l = \lambda_l \varphi_l$, $L^{-1}\varphi_l = (\lambda_l)^{-1}\varphi_l$, where $\{\lambda_l\}_1^\infty$ is a set of real numbers, $|\lambda_1| \leq |\lambda_2| \leq \cdots \leq |\lambda_l| \leq |\lambda_{l+1}| \leq \cdots$, and $|\lambda_l| \to \infty$ as $l \to \infty$. Finally, suppose that L is simple and Z is a subset of the complex plane. A bounded linear operator Q_ω (on and into E for each $\omega \in Z$) with continuous dependence on ω for $\omega \in Z$ and such that the range of $Q_\omega (L^{-1}Q_\omega)^m$ is a subset of R_L for some positive integer $m(\omega)$ will be called "L smooth" on Z.

Theorem 2: Let Z be a compact subset of the complex plane, L be a simple operator in the separable Hilbert space E, and Q_ω be L smooth on Z. Let E_n be the subspace spanned by the first n members of the complete set $\{\varphi_l\}_1^\infty$ of orthonormal eigenvectors of L. Suppose that for any given positive number $N > 0$, there exists an integer $n > N$, an $\alpha(n) \in Z$, and a nonzero $\eta(n) \in E_n$ such that

$$(P_n Q_\alpha P_n + L)\eta = 0, \tag{3}$$

where P_n denotes the projector onto E_n. Then there exists an $\Omega \in Z$ and a nonzero $\zeta \in D_L$ satisfying the equation

$$(Q_\Omega + L)\zeta = 0. \tag{4}$$

Proof: Let $C_\omega \equiv -L^{-1}Q_\omega$. Then C_ω is completely continuous and is a continuous function of ω on Z. The projector P_n commutes with L^{-1}, so that multiplication of Eq. (3) on the left-hand side with L^{-1} yields $(I - P_n C_\alpha)\eta = 0$. By Theorem 1, there exists an $\Omega \in Z$ and a nonzero $\zeta \in E$ satisfying the equation $\zeta = C_\Omega \zeta$. Therefore $\zeta = (C_\Omega)^l \zeta$ for all positive integers l. Since Q_ω is L smooth on Z, $Q_\Omega \zeta = Q_\Omega (C_\Omega)^m \zeta = (-1)^m Q_\Omega (L^{-1}Q_\Omega)^m \zeta \in R_L$, so that $LL^{-1}Q_\Omega \zeta = Q_\Omega \zeta$, i.e., $\zeta = C_\Omega \zeta \in D_L$ and $(Q_\Omega + L)\zeta = 0$.

The next result is our infinite-dimensional generalization (for $Q_\omega = \omega^2 P + \omega A$) of Theorem IV of Ref. 1.

Theorem 3: Suppose that L is a simple operator in the separable Hilbert space E, that L is bounded below on D_L, and that L possesses an odd number of negative eigenvalues. Let Q_ω be L smooth on the real half-line $[0,\infty)$ and be of the form $Q_\omega = \omega^x P + B_\omega$, where x is a positive real number, P is a positive operator on and into E, $\inf_E[(\xi, P\xi)/(\xi,\xi)] > 0, B_0 = 0$, and $\omega^{-x}\|B_\omega\| \to 0$ as $\omega \to \infty$. Suppose that $(\varphi_i, Q_\omega\varphi_j)$ is real for all $\omega \in [0,\infty)$ and all $i,j = 1, 2, \cdots$, where $\{\varphi_l\}_1^\infty$ is a complete orthonormal set of eigenvectors of L. Then there exists an $\Omega \in (0,\infty)$ and a nonzero $\zeta \in D_L$ such that $(Q_\Omega + L)\zeta = 0$.

Proof: Without loss of generality, we may assume that the eigenvalues λ_i of L are arranged in increasing order, i.e., $\lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots \le \lambda_N < 0 < \lambda_{N+1} \le \lambda_{N+2} \le \cdots$, where N is odd. Since $\omega^{-x}\|B_\omega\| \to 0$ as $\omega \to \infty$, there exists $\Delta > 0$ such that $\omega^{-x}\|B_\omega\| < \frac{1}{2}\delta$ for all $\omega \ge \Delta$, where $\delta = \inf_E[(\xi, P\xi)/(\xi,\xi)]$. Let $\omega_1 \equiv \max\{\Delta, [2|\lambda_1|/\delta]^{1/x}\}$ and $Z \equiv [0,\omega_1]$. We show that for each $n \ge N$, Eq. (3) holds for some $\alpha(n) \in Z$ and a nonzero $\eta(n) \in E_n$; the conclusion then follows immediately from Theorem 2 and the fact that 0 is not an eigenvalue of L. Now Eq. (3) is satisfied for nontrivial $\eta \in E_n$ if and only if $F_n(\omega) \equiv \det(a_{ij}) = 0$ for $\omega = \alpha$, where

$$a_{ij} \equiv (\varphi_i, Q_\omega\varphi_j) + (\varphi_i, L\varphi_j)$$
$$= \omega^x(\varphi_i, P\varphi_j) + (\varphi_i, B_\omega\varphi_j) + \lambda_i\delta_{ij},$$

$i,j = 1,2,\ldots,n$ and δ_{ij} is the Kronecker δ. The function $F_n(\omega)$ is real valued and continuous on $[0,\infty)$,

$$F_n(0) = \prod_{i=1}^n \lambda_i < 0$$

for $n \ge N$, $F_n(\omega) \to \infty$ as $\omega \to \infty$, so that if $n \ge N$, $F_n(\omega)$ has a root $\alpha \in (0,\infty)$. For this α, Eq. (3) holds for a nonzero $\eta \in E_n$, and we show that this implies that $\alpha \in Z$. Suppose $\alpha \notin Z$, i.e., suppose $\alpha > \omega_1$. It follows from Eq. (3) that $(\eta, Q_\alpha\eta) + (\eta, L\eta) = 0$, or

$$\alpha^x\left(\frac{(\eta,P\eta)}{(\eta,\eta)} + \alpha^{-x}\frac{(\eta,B_\alpha\eta)}{(\eta,\eta)}\right) = -\frac{(\eta,L\eta)}{(\eta,\eta)} \le |\lambda_1|.$$

Since

$$\alpha > \omega_1 \ge \Delta,\ \alpha^{-x}\left|\frac{(\eta,B_\alpha\eta)}{(\eta,\eta)}\right| \le \alpha^{-x}\|B_\alpha\| < \frac{\delta}{2},$$

then

$$\alpha^x\left(\delta - \frac{\delta}{2}\right) < \alpha^x\left(\frac{(\eta,P\eta)}{(\eta,\eta)} - \alpha^{-x}\left|\frac{(\eta,B_\alpha\eta)}{(\eta,\eta)}\right|\right)$$
$$\le \alpha^x\left(\frac{(\eta,P\eta)}{(\eta,\eta)} + \alpha^{-x}\frac{(\eta,B_\alpha\eta)}{(\eta,\eta)}\right) \le |\lambda_1|.$$

Thus $\alpha^x < 2|\lambda_1|/\delta$, which contradicts $\alpha > \omega_1 \ge (2|\lambda_1|/\delta)^{1/x}$. Hence $\alpha \in Z$, and the proof is complete.

The following theorem, while a finite-dimensional result, is a sharper version of Theorem III of Ref. 1, and serves as the basis for the infinite-dimensional generalization given in Theorem 5.

Theorem 4: Let H and iA be linear Hermitian operators on and into E_n, $\lambda \equiv -\inf_{E_n}[\zeta, H\zeta)/(\zeta,\zeta)] > 0$, $Q \equiv \{\zeta \mid \zeta \in E_n,\ (\zeta, H\zeta) < 0\}$, and suppose that

$$\Delta \equiv \inf_Q\left(-\frac{\|H\zeta\|^2}{4(\zeta,H\zeta)} - \frac{3(\zeta,H\zeta)}{4\|\zeta\|^2} - \frac{\|A\zeta\|^2}{\|\zeta\|^2}\right) > 0.$$

Then there exist $\alpha \in Z \equiv \{\omega \mid \mathrm{Re}\omega \ge \Delta^{1/2}, |\omega|^2 \le \lambda\}$ and a nonzero $\eta \in E_n$ such that

$$(\alpha^2 I + 2\alpha A + H)\eta = 0.$$

Proof: Since we are in E_n, there exists a complex-valued function $\omega(\epsilon)$ and $\xi(\epsilon) \in E_n$ with $\|\xi\| \equiv 1$ defined for all $\epsilon \in [0,1]$ such that $\omega(\epsilon)$ is continuous on $[0,1]$ $\omega(0) = -i\lambda^{1/2}$, and $(\omega^2 I - 2\omega\epsilon iA - H)\xi = 0$ holds for all $\epsilon \in [0,1]$. Define $x(\epsilon) \equiv [\mathrm{Im}\omega(\epsilon)]^2$ and $y(\epsilon) \equiv [\mathrm{Re}\omega(\epsilon)]^2$. Then $x(\epsilon)$ is continuous on $[0,1]$, $x(0) = \lambda > 0$, so that $x(\epsilon)$ is positive for all sufficiently small ϵ. For all ϵ such that $x(\epsilon) > 0$, Eqs. (5) and (11) of Ref. 1 give, respectively,

$$0 < x + y = -(\xi, H\xi) \le \lambda,$$

$$(x+y)(x - 3y + 4\epsilon^2\|A\xi\|^2) = \|H\xi\|^2.$$

These equations imply

$$x = -\|H\xi\|^2/4(\xi,H\xi) - \tfrac{3}{4}(\xi,H\xi) - \epsilon^2\|A\xi\|^2$$
$$\ge -\|H\xi\|^2/4(\xi,H\xi) - \tfrac{3}{4}(\xi,H\xi) - \|A\xi\|^2 \ge \Delta > 0,$$

and therefore the continuity of $x(\epsilon)$ on $[0,1]$ yields $x(\epsilon) \ge \Delta > 0$ for all $\epsilon \in [0,1]$. Since $\omega(\epsilon)$ is continuous on $[0,1]$ and $\omega(0) = -i\lambda^{1/2}$, $\mathrm{Im}\omega(\epsilon) \le -\Delta^{1/2}$ for all $\epsilon \in [0,1]$; in particular, $\mathrm{Im}\omega(1) \le -\Delta^{1/2}$. The choice $\alpha = i\omega(1)$, $\eta = \xi(1)$ completes the proof.

Theorem 5: Let L be a simple operator in the separable Hilbert space E such that $R_{L^{-1}} \subset R_L$, $\mathfrak{L} \equiv L - bI$, b a real number, and A be a bounded linear anti-Hermitian operator on and into E such that $R_{AL^{-1}} \subset R_L$. Suppose that $\lambda_1 \equiv \inf_{D_L}[(\xi,\mathfrak{L}\xi)/(\xi,\xi)] < 0$ and

$$\Delta \equiv \inf_Q\left(-\frac{\|\mathfrak{L}\xi\|^2}{4(\xi,\mathfrak{L}\xi)} - \frac{3(\xi,\mathfrak{L}\xi)}{4\|\xi\|^2} - \frac{\|A\xi\|^2}{\|\xi\|^2}\right) > 0, \qquad (5)$$

where $Q \equiv \{\xi \mid \xi\epsilon D_L, (\xi,\mathfrak{L}\xi) < 0\}$. Then there exists $\Omega \in Z \equiv \{\omega \mid \mathrm{Re}\omega \ge \Delta^{1/2}, |\omega|^2 \le -\lambda_1\}$ and a nonzero $\zeta \in D_L$ such that $(\Omega^2 I + 2\Omega A + \mathfrak{L})\zeta = 0$.

Proof: The facts that A is bounded, $R_{AL}- \subset R_L$, and $R_{L^{-1}} \subset R_L$ imply that $Q_\omega \equiv \omega^2 I + 2\omega A - bI$ is L smooth on the compact set Z. Let $\{\varphi_k\}_1^\infty$ denote a complete orthonormal set of eigenvectors of L (and $\mathfrak{L}$), enumerated so that $\mathfrak{L}\varphi_k = \lambda_k\varphi_k$ and $\lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots$. Now on

$$E_n \equiv \{\xi \mid \xi = \textstyle\sum_1^n \alpha_k \varphi_k\} \subset D_L,$$

$$P_n Q_\omega P_n + L = \omega^2 I + 2\omega P_n A P_n + \mathfrak{L},$$

$$\inf_{E_n} [(\xi, \mathfrak{L}\xi)/(\xi, \xi)] = \lambda_1 < 0,$$

so that for $Q_n \equiv \{\xi \mid \xi \in E_n, (\xi, \mathfrak{L}\xi) < 0\} \subset Q$, we have

$$\Delta_n \equiv \inf_{Q_n}\left(-\frac{\|\mathfrak{L}\xi\|^2}{4(\xi, \mathfrak{L}\xi)} - \frac{3(\xi, \mathfrak{L}\xi)}{4\|\xi\|^2} - \frac{\|P_n A\xi\|^2}{\|\xi\|^2}\right) \ge \Delta,$$

and therefore $Z_n \equiv \{\omega \mid \mathrm{Re}\omega \ge \Delta_n^{1/2}, |\omega|^2 \le -\lambda_1\} \subset Z$. Thus by Theorem 4, for each positive integer n there exists $\alpha(n) \in Z$ and a nonzero $\eta(n) \in E_n$ such that $(\alpha^2 I + 2\alpha P_n A P_n + \mathfrak{L})\eta = 0$, i.e., $(P_n Q_\alpha P_n + L)\eta = 0$. The theorem is now an immediate consequence of Theorem 2.

A simple estimate for the quantity Δ can be easily obtained in terms of $\|A\|$, $\lambda \equiv$ the greatest negative eigenvalue of $\mathfrak{L}$, and $\mu \equiv \inf_{D_L}(\|\mathfrak{L}\xi\|^2/\|\xi\|^2)$. For $\xi \in Q$, $x \equiv \|\xi\|^2/-(\xi, \mathfrak{L}\xi) > 0$, and $0 \le \beta \le 1$, we have

$$\begin{aligned} &-\frac{\|\mathfrak{L}\xi\|^2}{(\xi, \mathfrak{L}\xi)} - 3\frac{(\xi, \mathfrak{L}\xi)}{\|\xi\|^2} \\ &\quad = -(1-\beta)\frac{\|\mathfrak{L}\xi\|^2}{(\xi, \mathfrak{L}\xi)} + \beta\frac{\|\mathfrak{L}\xi\|^2}{\|\xi\|^2}x + 3x^{-1} \\ &\quad \ge (1-\beta)|\lambda| + \beta\mu x + 3x^{-1} \\ &\quad \ge (1-\beta)|\lambda| + 2(3\mu\beta)^{1/2} \\ &\quad \ge \Gamma, \end{aligned}$$

where $\Gamma = |\lambda| + 3\mu|\lambda|^{-1}$ if $3\mu \le \lambda^2$, while $\Gamma = 2(3\mu)^{1/2}$ if $3\mu > \lambda^2$. Therefore $\Delta \ge \frac{1}{4}\Gamma - \|A\|^2$.

A simple but useful special case of Eq. (1), which is not of the type we have considered thus far, is given by

$$p\ddot{\eta} + \left(q\frac{\partial}{\partial x} + \frac{q'}{2}\right)\dot{\eta} + \left(-\frac{\partial}{\partial x}s\frac{\partial}{\partial x} + u\right)\eta(x,t) = 0,$$

$$\dot{\eta} = \frac{\partial \eta}{\partial t}, \quad q' = \frac{dq}{dx}, \tag{6}$$

where $(x, t) \in [a, b] \times [0, \infty)$, and p, q, s, and u are real-valued functions of x defined on $[a, b]$ with the following properties: $p > 0$ on $[a, b]$, $p \in C[a, b]$, $q \in C^1[a, b]$, $|s| > 0$ on $[a, b]$, $s \in C^2[a, b]$, $|q^2 + 4ps| > 0$ on $[a, b]$, and $u \in C[a, b]$. We consider the class Γ of real-valued solutions $\eta(x, t)$ defined on $[a, b] \times [0, \infty)$ such that: (i) $\eta(x, t)$, $\dot{\eta}(x, t)$, $(\partial\eta/\partial x)(x, t)$, and $(\partial^2\eta/\partial t \partial x)$ are continuous on $[a, b] \times [0, \infty)$; (ii) For each fixed $t \in [0, \infty)$, $\eta(x, t) \in \Sigma_0 \equiv \{\varphi \mid \varphi \in C^2[a, b], \varphi(a) = \varphi(b) = 0\}$ and $\dot{\eta}(x, t) \in \Sigma_1 \equiv \{\varphi \mid \varphi \in C^1[a, b], \varphi(a) = \varphi(b) = 0\}$; (iii) η satisfies Eq. (6) for all $(x, t) \in [a, b] \times [0, \infty)$. It follows immediately that $\eta \in \Gamma$ implies that $\ddot{\eta}$ is continuous on $[a, b] \times [0, \infty)$ and that for each fixed $t \ge 0$, $\ddot{\eta} \in \Sigma_2 \equiv \{\varphi \mid \varphi \in C[a, b], \varphi(a) = \varphi(b) = 0\}$.

Theorem 6: Let

$$\Delta = \inf_{\Sigma_0} \frac{\int_a^b [s|\varphi'|^2 + u|\varphi|^2]dx}{\int_a^b [(q^2 + 4ps)/4s]|\varphi|^2 dx}.$$

(a) Suppose $\Delta \ge 0$. Then Eq. (6) admits of no exponential growing modes, i.e., there exist no solutions of Eq. (6) of the form $\eta(x, t) = \mathrm{Re}\xi(x)\, e^{\omega t}$ with $\mathrm{Re}\omega > 0$ and $\xi \in \Sigma_0$.
(b) Suppose $s > 0$ and $\Delta > 0$. Then given any $\eta(x, t) \in \Gamma$, there exists a constant B such that $|\eta(x, t)| < B$ for all $(x, t) \in [a, b] \times [0, \infty)$.
(c) Suppose $s > 0$ and $\Delta = 0$. Then given any $\eta(x, t) \in \Gamma$, there exist constants A, B, and C such that $\eta^2(x, t) \le At^2 + Bt + C$ for all $(x, t) \in [a, b] \times [0, \infty)$.
(d) Suppose $\Delta < 0$. If Δ is finite, then Eq. (6) admits of an exponential growing mode $\eta(x, t) = \xi(x)\, e^{\omega t}$, with $\xi \in \Sigma_0$, $\omega > 0$, and $\omega^2 = -\Delta$. If $\Delta = -\infty$ (this will occur if $s < 0$ and $q^2 + 4ps < 0$; in this case the problem is elliptic and is not well posed, then Eq. (6) admits of exponential-growing modes with arbitrarily large growth rates.

Proof: For each $\eta \in \Gamma$, we have

$$\frac{d}{dt}\int_a^b [p(\dot{\eta})^2 + s(\eta')^2 + \mu\eta^2]dx \equiv 0,$$

so that

$$\int_a^b [p(\dot{\eta})^2 + s(\eta')^2 + \mu\eta^2]dx = M = \text{const}, \quad t \ge 0. \tag{7}$$

If $s > 0$ and $\Delta \ge 0$, then $\hat{p}\int_a^b (\dot{\eta})^2 dx \le M$, $t \ge 0$, where $\hat{p} \equiv \min_{[a,b]} p(x)$. Now

$$\left|\frac{d}{dt}\int_a^b \eta^2 dx\right|^2 = \left|2\int_a^b \eta\dot{\eta}dx\right|^2$$

$$\le 4\int_a^b \eta^2 dx \int_a^b (\dot{\eta})^2 dx \le \frac{4M}{\hat{p}}\int_a^b \eta^2 dx,$$

which implies

$$\int_a^b \eta^2 dx \le \left[t(M/\hat{p})^{1/2} + \left(\int_a^b \eta^2(x, 0)dx\right)^{1/2}\right]^2. \tag{8}$$

Set $\hat{s} \equiv \min_{[a,b]} s(x)$, $\hat{u} \equiv \min_{[a,b]} u(x)$. Then since

$$\eta^2 = \left|\int_a^b \eta'(y, t)dy\right|^2 \le \int_a^x (\eta')^2 dy \int_a^x dy$$

$$\le (x - a)\int_a^b (\eta')^2 dx,$$

Eq. (7) yields

$$\hat{s}\eta^2 \le (x - a)\left(M - \hat{u}\int_a^b \eta^2 dx\right). \tag{9}$$

For the case $s > 0$ and $\Delta > 0$, Eq. (7) implies

$$\Delta r \int_a^b \eta^2 dx \leq M, \tag{10}$$

where

$$r \equiv \min_{[a,b]} \frac{q^2 + 4ps}{s} > 0.$$

Statements (b) and (c) are immediate consequences of Eqs. (8)–(10). Now suppose there exist solutions of Eq. (6) of the form $\eta(x,t) = \mathrm{Re}\,\xi(x)\, e^{\omega t}$, with ω a complex constant. Let $\zeta(x) \equiv |s|^{1/2}\xi(x) \exp[-\frac{1}{2}\omega \int_a^x (q/s)dy]$. Then $\eta(x,t) \in \Gamma$ if and only if $\zeta \in \Sigma_0$ and ζ satisfies the Sturm–Liouville equation

$$\omega^2\left(\frac{q^2 + 4ps}{4s^2}\right)\zeta + \left(-\frac{d^2}{dx^2} + \frac{2ss'' - (s')^2 + 4us}{4s^2}\right)\zeta = 0, \tag{11}$$

For $\zeta \in \Sigma_0$, we have

$$\frac{\int_a^b \bar{\zeta}\,(-\zeta'' + \{[2ss'' - (s')^2 + 4us]/4s^2\}\zeta)dx}{\int_a^b [(q^2 + 4ps)/4s^2]\,|\zeta|^2 dx} = \frac{\int_a^b [s|\varphi'|^2 + u|\varphi|^2]dx}{\int_a^b [(q^2 + 4ps)/4s]\,|\varphi|^2 dx}, \tag{12}$$

where $\varphi \equiv |s|^{-1/2}\zeta$. Statements (a) and (d) follow at once from well-known results for the Sturm–Liouville equation (11).

III. THE STABILITY OF A THIN, ROTATING ANNULAR DISK

We consider the planar oscillations of a thin annular disk (inner radius $a > 0$, outer radius b) rotating about its center with the angular velocity Ω, and restrict our attention to rotationally symmetric modes (those depending only on the distance r from the center of the disk). We adopt the model of Ref. 2. The pertinent equations for the perturbed radial displacement $u(r,t) = bx^{-1/2}\xi(x)e^{\omega\Omega t}$, and the perturbed tangential displacement $v(r,t) = bx^{-1/2}\zeta(x)e^{\omega\Omega t}$, where $x \equiv r/b$, follow at once from Eqs. (11) and (12) of Ref. 2:

$$\left[\omega^2 I + \omega 2\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} \mathfrak{L}_1 & 0 \\ 0 & \mathfrak{L}_2 \end{pmatrix}\right]\begin{pmatrix} \xi(x) \\ \zeta(x) \end{pmatrix} = 0, \tag{13}$$

$\Delta = a/b \leq x \leq 1$, where

$$\mathfrak{L}_1 \equiv \frac{\alpha}{b^2\Omega^2}\,\mathfrak{L} - 1, \qquad \mathfrak{L}_2 \equiv \frac{\beta}{b^2\Omega^2}\,\mathfrak{L} - 1,$$

$$\mathfrak{L} \equiv -\frac{d^2}{dx^2} + \tfrac{3}{4}x^{-2},$$

and α and β are positive constants determined by the elastic properties of the disk and its mass density, with $4\beta > \alpha > 2\beta$. The reader is referred to Ref. 2 for further discussion of these equations. We assume that the disk is clamped along its inner boundary at $r = a$ and that $r = b$ is free; the boundary conditions are accordingly given by[2]

$$\xi(\Delta) = \zeta(\Delta) = 0,$$
$$\xi'(1) - \tfrac{1}{2}(4\beta\alpha^{-1} - 1)\xi(1) = 0 = \zeta'(1) - \tfrac{3}{2}\zeta(1).$$

The domains of definition of $\mathfrak{L}_1$ and $\mathfrak{L}_2$ are taken to be

$$D_1 = \{f(x)\,|\,f \in C^2[\Delta,1], f(\Delta) = 0 = f'(1) - \tfrac{1}{2}(4\beta\alpha^{-1} - 1)f(1)\}$$

and

$$D_2 = \{f(x)\,|\,f \in C^2[\Delta,1], f(\Delta) = 0 = f'(1) - \tfrac{3}{2}f(1)\},$$

respectively.

In the context of the Hilbert space $L_2[\Delta,1]$, the operator $\mathfrak{L}$ with the domain of definition

$$D(\Delta,\gamma) = \{f(x)\,|\,f \in C^2[\Delta,1], f(\Delta) = 0 = f'(1) - \gamma f(1)\}$$

is a strictly positive simple operator, provided $0 < \Delta < 1$ and $\gamma \leq \frac{3}{2}$. Thus $\mathfrak{L}$ is positive on D_2, and since $0 < \frac{1}{2}(4\beta\alpha^{-1} - 1) < \frac{1}{2}$, $\mathfrak{L}$ is also positive on D_1. Let λ_1 denote the least eigenvalue and λ_2 the next greater eigenvalue of $\mathfrak{L}$ on D_2, and let Λ_1 be the least eigenvalue of $\mathfrak{L}$ on D_1. While the eigenvalues of $\mathfrak{L}$ on $D(\Delta,\gamma)$ can be computed from the tables of Bessel functions in Ref. 3, we need only note that the least eigenvalue of $\mathfrak{L}$ on $D(\Delta,\gamma)$ is, for each fixed Δ, a strictly decreasing function of γ; this follows immediately from the minimum principle for the least eigenvalue. Hence $\lambda_1 < \Lambda_1$. Since $\alpha > 2\beta$, it follows at once from the definition of $\mathfrak{L}_1$ and $\mathfrak{L}_2$ that for $|\Omega| < \Omega_c \equiv (\beta\lambda_1)^{1/2}/b$, $\mathfrak{L}_1$ and $\mathfrak{L}_2$ are both strictly positive, while for

$$\Omega_c < |\Omega| < \Omega' \equiv \min\left(\frac{(\beta\lambda_2)^{1/2}}{b}, \frac{(\alpha\Lambda_1)^{1/2}}{b}\right),$$

$\mathfrak{L}_2$ will have precisely one negative eigenvalue and no zero eigenvalue, while $\mathfrak{L}_1$ will be strictly positive. Hence for $|\Omega| < \Omega_c$ or $\Omega_c < |\Omega| < \Omega'$, $\mathfrak{L}_1$ and $\mathfrak{L}_2$ are simple operators in $L_2[\Delta,1]$ with completely continuous Hermitian inverses $\mathfrak{L}_1^{-1}$ and $\mathfrak{L}_2^{-1}$, respectively, so that the operator

$$L \equiv \begin{pmatrix} \mathfrak{L}_1 & 0 \\ 0 & \mathfrak{L}_2 \end{pmatrix}$$

is a simple operator in the Hilbert space $E \equiv L_2[\Delta,1] \times L_2[\Delta,1]$ with the completely continuous Hermitian inverse

$$L^{-1} = \begin{pmatrix} \mathfrak{L}_1^{-1} & 0 \\ 0 & \mathfrak{L}_2^{-1} \end{pmatrix}.$$

Since

$$R_{\mathfrak{L}_1^{-1}} \subset C[\Delta, 1]$$

and

$$R_{\mathfrak{L}_2^{-1}} \subset C[\Delta, 1],$$

we have

$$R_{L^{-1}} \subset C[\Delta, 1] \times C[\Delta, 1] = R_L,$$

and therefore

$$Q_\omega = \omega^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \omega 2 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

is L smooth for $\omega \in [0, \infty)$. If $|\Omega| < \Omega_c$, L and L^{-1} are positive; it follows from Theorem II of Ref. 4 that Eq. (13) admits of a complete set of eigenfunctions (complete in the sense that arbitrary smooth initial data can be expanded in series of the eigenfunctions) with pure imaginary eigenvalues ω_n, so that the system has a complete set of purely oscillatory modes. In this case, one can also show directly from the energy integral for the time-dependent version of Eq. (13) that the system is stable. On the other hand, if $\Omega_c < |\Omega| < \Omega'$, it follows from Theorem 3 that the system is exponentially unstable. Indeed, if we denote the complete orthonormal sets of real eigenvectors of $\mathfrak{L}_1$ and $\mathfrak{L}_2$ by $\{\varphi_n\}_1^\infty$ and $\{\psi_n\}_1^\infty$, respectively, with $\mathfrak{L}_1\varphi_n = \mu_n\varphi_n$, $\mathfrak{L}_2\psi_n = \gamma_n\varphi_n$, $0 < \mu_1 < \mu_2 < \mu_3 < \cdots, \gamma_1 < 0 < \gamma_2 < \gamma_3 < \cdots$, then a complete orthonormal system of eigenvectors of L is given by

$$\begin{pmatrix} 0 \\ \psi_{(n+1)/2} \end{pmatrix}$$

for n odd, and

$$\begin{pmatrix} \varphi_{n/2} \\ 0 \end{pmatrix}$$

for n even; thus L has precisely one negative eigenvalue and exponential instability follows at once from Theorem 3. Thus $\Omega_c = (\beta\lambda_1)^{1/2}/b$ is the critical angular velocity for instability.

IV. STABILITY OF STEADY FLOW OF A ONE-DIMENSIONAL WARM ELECTRON PLASMA

We consider a warm electron plasma, confined in the interval $0 \le x \le b$, satisfying the following set of equations:

$$\frac{\partial n}{\partial t} + \frac{\partial (nv)}{\partial x} = s(x), \tag{14}$$

$$mn\left(\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x}\right) = -kT\frac{\partial n}{\partial x} - en\,E, \tag{15}$$

$$\frac{\partial E}{\partial x} = \frac{e}{\epsilon_0}[n_i(x) - n]. \tag{16}$$

The equations are written in MKS units; ϵ_0 is the permittivity of free space. The quantity $n(x, t)$ is the electron number density, $v(x, t)$ is the macroscopic electron velocity, $s(x)$ is an electron source term, m is the electron mass, k is the Boltzmann constant, T the electron temperature, $-e$ the electron charge, $E(x, t)$ the electric field, and $en_i(x)$ is a fixed background charge density. A state of steady flow, characterized by a 0 subscript on the variables n, v, and E, will exist provided

$$s(x) = \frac{d}{dx}[n_0(x)v_0(x)], \tag{17}$$

$$eE_0(x) = -\frac{d}{dx}\left(kT\ln\frac{n_0(x)}{n_0(0)} + \frac{m}{2}v_0^2(x)\right), \tag{18}$$

$$n_i(x) = \frac{\epsilon_0}{e}\frac{dE_0}{dx} + n_0(x). \tag{19}$$

We now assume small perturbations in n, v, and E about such a state of steady flow, with $n_0(x) > 0$ on $[o, b]$. We restrict our attention to the class of perturbations that are charge neutral, so that the perturbed electric field $\eta(x, t)$ vanishes at o and b, and for which the sum of the perturbed electron current density and the vacuum displacement current vanishes at o and b. The linearization of Eqs. (14)–(16) then gives an equation for η of the form of Eq. (6), with $p = n_0^{-1}$, $q = 2v_0n_0^{-1}$, $s = [(kT/m) - v_0^2]n_0^{-1}$, and $u = e^2/(\epsilon_0 m)$. Thus, if we assume $n_0, v_0 \in C^2[o, b]$, Theorem 6 gives the following stability results:

(i) If $v_0^2 < kT/m$ on $[o, b]$, the system is stable;

(ii) If $v_0^2 > kT/m$ on $[o, b]$, and $\Delta \ge 0$ (which will be the case provided

$$\min_{[o,b]} \frac{v_0^2(x) - kT/m}{b^2\omega_p^2(x)} > \pi^{-2},$$

where $\omega_p^2 = n_0u$ is the local electron plasma frequency), then there are no exponentially growing modes;

(iii) If $v_0^2 > kT/m$, but $\Delta < 0$ (this will occur for

$$\sup_{[o,b]} \frac{v_0^2 - kT/m}{b^2\omega_p^2} < \pi^{-2}),$$

then the system is exponentially unstable.

ACKNOWLEDGMENT

The author would like to thank Professor H. Weitzner for reading the manuscript. The work presented here was sponsored by the US Atomic Energy Commission, under Contract No. AT (30-1)-1480.

[1] E. M. Barston, J. Math. Phys. 8, 523 (1967).
[2] R. Doby, J. Franklin Inst. 288, 203 (1969).
[3] E. Jahnke and F. Emde, *Tables of Functions* (Dover, New York, 1945), pp. 204–205.
[4] E. M. Barston, J. Math. Phys. 9, 2069 (1968).

L-Wave Inverse Scattering Problem

Oscar D. Corbella
Instituto de Matemática, Astronomía, y Física, Universidad Nacional de Córdoba, Argentina
(Received 26 February 1971)

The inverse scattering problem for the Schrödinger equation is considered. Under certain restrictions on some of the odd derivatives of the potential, we obtain expressions for the values of the potential and its derivatives at the origin, as functions of the phase shift and bound state data for any fixed partial wave. Closed expressions for the first coefficients of the expansion of the potential are obtained.

1. INTRODUCTION

We study the inverse problem of the nonrelativistic scattering theory following the approach to obtain exact and explicit relationships between the values of the potential and its derivatives at the origin, and the phase shift (as a function of the linear momentum k) and bound state parameters.

Relationships of this type were first obtained by Newton, [1] and simultaneously by Faddeev, [2] who gave a formula for the value of the potential at the origin as an integral over a function of the phase shift and a sum over the bound state energies, for each partial wave. Later on, Buslaev and Faddeev, [3] Percival, [4] and Roberts[5] found an expression for the value of the second derivative at the origin, as a function of the phase shift and bound state data on S wave. Afterwards, Calogero and Degasperis[6] succeeded in obtaining expressions for the values of the potential and all the derivatives in terms of the S-wave phase shift and bound state parameters. In the case of relativistic equations, the same type of results have been obtain by Degasperis[7] and by the author[8] for the Klein–Gordon and Dirac equations, respectively.

In this paper we intend to solve the problem of higher partial waves ($l \neq 0$) for a Schrödinger equation. We develop a method that allows us, with certain restrictions on some odd derivatives of the potential (see Sec. 4) to calculate the values of the potential and all its derivatives at the origin, in terms of the scattering data, i.e., the phase shift $\delta_l(k)$ as a function of the linear momentum k, the bound state energies, and the normalization constants, for a given partial wave.

The method is based on a theorem allowing us to go from an l-wave Schrödinger equation to an $(l-1)$-wave Schrödinger equation with a modified potential. By iteration of this procedure, an l-wave equation can be related to an S-wave one. In this way we can use the expressions obtained by Calogero and Degasperis in their paper. The method allows us, in principle, to calculate the value of the potential and all its derivatives, and we get closed formulas for the value of the potential and its first five derivatives at the origin. The whole potential, which was considered a holomorphic function of r, can be reconstructed, at least in principle, in this manner.

In obtaining these closed expressions we have been able to sum, with very simple results, certain products of sums which at first look very complicated. These expressions are given in the Appendix.

The units used in this paper are $\hbar = 2m = 1$.

2. THE METHOD OF CALCULATION

Theorem[9]: Let $y(k^2, r)$ be a solution of the differential equation

$$y''(k^2, r) + [k^2 - W(r)]y(k^2, r) = 0 \tag{2.1}$$

and $f(r)$ a function of r, a solution of the nonlinear equation

$$f'(r) = f^2(r) - W(r). \tag{2.2}$$

Let $z(k^2, r)$ be a function defined as

$$z(k^2, r) = f(r)y(k^2, r) + y'(k^2, r). \tag{2.3}$$

Therefore, this function satisfies the equation

$$z''(k^2, r) + [k^2 - V(r)]z(k^2, r) = 0, \tag{2.4}$$

with the modified potential

$$V(r) = W(r) + 2f'(r). \tag{2.5}$$

The theorem is proved by direct substitution.

In particular, if we assume that

$$W(r) = U(r) + l(l+1)/r^2, \tag{2.6}$$

where $U(r)$ is a nonsingular potential[10] and $y_l(k^2, r)$ the solution of Eq. (2.1), we have

$$y_l''(k^2, r) + [k^2 - U(r) - l(l+1)/r^2]\, y_l(k^2, r) = 0, \tag{2.7}$$

which is an l-wave Schrödinger equation. If, as before [Eq. (2.3)], we define

$$y_{l-1}(k^2, r) = f_l(r)y_l(k^2, r) + y_l'(k^2, r), \tag{2.8}$$

where

$$f_l'(r) = f_l'(r) - W(r), \tag{2.9}$$

then $y_{l-1}(k^2, r)$ satisfies the equation

$$y_{l-1}''(k^2, r) + [k^2 - U(r) - l(l+1)/r^2 - 2f_l'(r)] \times y_{l-1}(k^2, r) = 0. \tag{2.10}$$

If we now define $f_l(r)$ as

$$f_l(r) = l/r + g_l(r), \tag{2.11}$$

we get

$$y''_{l-1}(k^2,r) + [k^2 - U(r) - 2g'_l(r) - l(l-1)/r^2] \times y_{l-1}(k^2,r) = 0, \quad (2.12)$$

and, if $g'_l(r)$ is a potential as well behaved as $U(r)$, the function $y_{l-1}(k^2,r)$ satisfies an $(l-1)$-wave Schrödinger equation.

The equation for $g_l(r)$ is

$$g'_l(r) = g_l{}^2(r) + (2l/r)g_l(r) - U(r), \quad (2.13)$$

and under certain conditions on $U(r)$ the function $g'_l(r)$ will be considered as a good potential.

Repeating the same procedure, i.e., in the first step, we define

$$y_{l-2}(k^2,r) = f_{l-1}(r)y_{l-1}(k^2,r) + y'_{l-1}(k^2,r), \quad (2.14)$$

where $f_{l-1}(r)$ is the solution of

$$f'_{l-1}(r) = f^2_{l-1}(r) - U(r) - 2g'_l(r) - (l-1)l/r^2, \quad (2.15)$$

and so on; after l steps we arrive at the equation

$$y''_0(k^2,r) + \left(k^2 - U(r) - 2\sum_{n=1}^{l} g'_n(r)\right) y_0(k^2,r) = 0, \quad (2.16)$$

where the equations satisfied by the l functions $g_n(r)$ are

$$\begin{aligned}
&g'_l(r) = g^2_l(r) + 2lr^{-1}g_l(r) - U(r),\\
&g'_{l-1}(r) = g^2_{l-1}(r) + 2(l-1)r^{-1}g_{l-1}(r) - U(r) - 2g'_l(r),\\
&\vdots\\
&g'_n(r) = g^2_n(r) + 2nr^{-1}g_n(r) - U(r) - 2\sum_{i=n+1}^{l} g'_i(r), \quad 1 \leq n \leq l, \quad (2.17)\\
&\vdots\\
&g'_1(r) = g^2_1(r) + 2r^{-1}g_1(r) - U(r) - 2\sum_{i=2}^{l} g'_i(r).
\end{aligned}$$

Therefore, if we can manage to calculate the potential

$$V(r) = U(r) + 2\sum_{n=1}^{l} g'_n(r) \quad (2.18)$$

of the S-wave Schrödinger equation (2.16), making the following expansions at the origin:

$$\begin{aligned}
&V(r) = \sum V_n r^n, \qquad V_n = \frac{V^{(n)}(0)}{n!} = \frac{1}{n!}\frac{d^n}{dn^n}V(r)\Big|_{r=0},\\
&U(r) = \sum U_n r^n, \qquad U_n = \frac{U^{(n)}(0)}{n!} = \frac{1}{n!}\frac{d^n}{dr^n}U(r)\Big|_{r=0},\\
&g_i(r) = \sum g_{i,n} r^n, \quad (2.19)
\end{aligned}$$

we can reconstruct U_n by

$$V_n = U_n + 2(n+1)\sum_{i=1}^{l} g_{i,n+1}, \quad (2.20)$$

that is, we need to know all the coefficients V_n and $g_{i,n}$.

Then we have reduced an l-wave problem to an S-wave one [in the next section we discuss the condition to be imposed on the coefficients of $U(r)$].

In general we have

$$f'_n(r) = f^2_n(r) - U(r) - \frac{n(n+1)}{r^2} - 2\sum_{i=n+1}^{l} g'_i(r) \quad (2.21)$$

and

$$y_{n-1}(k^2,r) = f_n(r)y_n(k^2,r) + y'_n(k^2,r). \quad (2.22)$$

If all functions $f_n(r)$ vanish at infinity, the l-wave phase shift $\delta_l(k)$ of the $U(r)$ problem will be equal to the S-wave phase shift $\eta_0(k)$ of the $V(r)$ problem; then we shall be able to use the well-known results for the S wave. This point, and that of the bound states, will be discussed in Sec. 6.

3. DETERMINATION OF THE COEFFICIENTS $g_{n,m}$

Let us assume that the functions $g(r)$ and $U(r)$ have the expansions at the origin given by Eqs. (2.19). Replacing in the first of Eqs. (2.17), we get

$$(n+1-2l)g_{l,n+1} - \sum_{s=1}^{n-1} g_{l,s}g_{l,n-s} + U_n = 0, \quad n \geq 2, \quad (3.1)$$

with the initial conditions

$$g_{l,1} = [1/(2l-1)]\,U_0, \quad (3.2)$$

$$g_{l,2} = [1/(2l-2)]U_1, \quad l \neq 1, \quad (3.3)$$

from which we obtain

$$g_{l,n+1} = \frac{1}{2l-(n+1)}\left(U_n - \sum_{s=1}^{n-1} g_{l,s}g_{l,n-s}\right), \quad n \geq 2. \quad (3.4)$$

In this manner we can determine all $g_{l,n}$ as a function of U_n, except the coefficient $g_{l,2l}$. It remains indeterminate but finite if we constrain the potential to satisfy

$$U_{2l-1} = \sum_{s=1}^{2l-2} g_{l,s}g_{l,2l-1-s}. \quad (3.5)$$

To determine $g_{l,2l}$, we use Eq. (2.20) for $n = 2l-1$, from which we get

$$g_{l,2l} = \frac{1}{4l}\left(V_{2l-1} - \sum_{s=1}^{2l-2} g_{l,s}g_{l,2l-1-s} - 4l\sum_{i=1}^{l-1} g_{i,2l}\right). \quad (3.6)$$

Note that this equation only formally determines $g_{l,2l}$ because this coefficient is a function of, for example, $g_{l-1,2l}$, which is a function of $g_{l-1,2l-2}$, which is also undetermined. Later on, we will come back to this problem.

Going down, in the jth step $(l-1 \geq j \geq 2)$ of Eqs. (2.17), we obtain, using the same procedure,

$$g_{j,1} = \frac{1}{2j-1}\left(U_0 + 2\sum_{i=j+1}^{l} g_{i,1}\right), \tag{3.7}$$

$$g_{j,2} = \frac{1}{2j-2}\left(U_1 + 4\sum_{i=j+1}^{l} g_{i,2}\right), \tag{3.8}$$

and

$$g_{j,n+1} = \frac{1}{2j-(n+1)}\left(U_n + 2(n+1)\sum_{i=j+1}^{l} g_{i,n+1} - \sum_{s=1}^{n-1} g_{j,s}g_{j,n-s}\right), \quad n \geq 2, \; l-1 \geq j \geq 2. \tag{3.9}$$

The coefficient $g_{j,2j}$ is indeterminate but finite if

$$U_{2j-1} = \sum_{s=1}^{2j-2} g_{j,s}g_{j,2j-1-s} - 4j\sum_{i=j+1}^{l} g_{i,2j}, \quad l-1 \geq j \geq 2. \tag{3.10}$$

Then we determine it with

$$g_{j,2j} = \frac{1}{4j}\left(V_{2j-1} - \sum_{s=1}^{2j-1} g_{j,s}g_{j,2j-1-s}\right) - \sum_{i=1}^{j-1} g_{i,2j}. \tag{3.11}$$

Finally, after l steps we obtain

$$g_{1,1} = U_0 + 2\sum_{i=2}^{l} g_{i,1}. \tag{3.12}$$

To assume $g_{1,2}$ to be finite, we impose

$$U_1 = -4\sum_{i=2}^{l} g_{i,2}. \tag{3.13}$$

In general we have

$$g_{1,n+1} = \frac{1}{2-(n+1)}\left(U_n + 2(n+1)\sum_{i=2}^{l} g_{i,n+1} - \sum_{s=1}^{n-1} g_{1,s}g_{1,n-s}\right), \quad n \geq 2. \tag{3.14}$$

We can now determine $g_{1,2}$, using Eq. (2.20) with $n = 1$,

$$g_{1,2} = \tfrac{1}{4}V_1. \tag{3.15}$$

4. CONDITIONS ON THE POTENTIAL

Let us postpone the determination of the even coefficients to the next section, and concentrate on the calculation of the odd coefficients that give us certain conditions on the potential. For the sake of clearness, we are using now some results to be derived in the next section.

Equation (3.13) implies $U_1 = 0$. This can be shown by using Eqs. (2.20) and (3.2),

$$U_1 = -\frac{4}{2l-2}U_1 - 4\sum_{i=2}^{l-1}\frac{1}{2i-2}\left(U_1 + 4\sum_{j=i+1}^{l} g_{j,2}\right) = -4U_1\left(\sum_{i=2}^{l}\frac{1}{2i-2} + 4\sum_{i=2}^{l-1}\frac{1}{2i-2}\times\sum_{j=i+1}^{l}\frac{1}{2j-2} + \cdots\right), \tag{4.1}$$

from which [see Eq. (A2)] we obtain

$$\tfrac{1}{2}l(l+1)U_1 = 0,$$

i.e.,

$$l \neq 0, \quad U_1 = 0. \tag{4.2}$$

But this last equation implies

$$\sum_{i=2}^{l} g_{i,2} = 0, \tag{4.3}$$

and from Eq. (3.2) we get

$$g_{l,2} = 0, \quad \text{for} \quad l \geq 2, \tag{4.4}$$

and from Eq. (3.8),

$$g_{l-1,2} = 0, \quad \text{for} \quad l \geq 3, \tag{4.5}$$

and so on; for fixed l we obtain then

$$g_{i,2} = 0, \quad \text{for} \quad 2 \leq i \leq l. \tag{4.6}$$

We calculate now the third coefficient. Equation (2.20) for $n = 3$ and $l = 1$ reads

$$V_3 = U_3 + 8g_{1,4}, \tag{4.7}$$

and from Eqs. (3.4), (3.3), and the result (5.3) of the next section (for U_0 as a function of V_0) we get

$$U_3 = -\tfrac{1}{3}\left(V_3 - \tfrac{2}{3}V_0V_1\right), \quad l = 1. \tag{4.8}$$

For $l = 2$, U_3 must satisfy the condition (3.5), which, recalling Eq. (4.6), we can write as

$$U_3 = 2g_{2,1}g_{2,2} = 0. \tag{4.9}$$

For $l > 2$, using Eqs. (3.10) and (4.6), we get

$$U_3 = -8\sum_{i=3}^{l} g_{i,4} = -8\sum_{i=3}^{l-1}\frac{1}{2i-4}\left(U_3 + 8\sum_{j=i+1}^{l} g_{j,4}\right); \tag{4.10}$$

by iteration we have

$$U_3\left(1 + 8\sum_{i=3}^{l}\frac{1}{2i-4} + 8^2\sum_{i=3}^{l-1}\frac{1}{2i-4}\times\sum_{j=i+1}^{l}\frac{1}{2j-4} + \ldots\right) = 0 \tag{4.11}$$

or, in other words (see the Appendix),

$$U_3(l-1)l(l+1)(l+2)/4! = 0,$$

i.e.,

$$U_3 = 0 \quad \text{for} \quad l \geq 2. \tag{4.12}$$

Furthermore,

$$\sum_{i=3}^{l} g_{i,4} = 0, \tag{4.13}$$

and by using Eq. (3.4) we obtain

$$g_{l,4} = [1/(2l-4)]\, U_3 = 0, \quad l > 2 \quad (\text{if } l = 2, g_{2,4} \neq 0), \tag{4.14}$$

and from Eq. (4.13),

$$g_{l-1,4} = [1/(2l-6)]\, U_3 = 0, \quad l > 3, \tag{4.14'}$$

and so on; finally

$$g_{i,4} = 0, \quad \text{for} \quad 3 \leqslant i \leqslant l. \tag{4.15}$$

Conditions on the fifth coefficient are obtained by using again Eq. (2.20), now for $n = 5$, i.e.,

$$V_5 = U_5 + 12 \sum_{i=1}^{l} g_{i,6}. \tag{4.16}$$

Putting $l = 1$, using Eqs. (3.2), (3.4), (3.14), (4.8), and the results of the next section, Eqs. (5.3) and (5.9) for U_0 and U_2, we get

$$U_5 = -\tfrac{1}{2}\,(V_5 - \tfrac{1}{3} V_0 V_3 - \tfrac{3}{10} V_1 V_2 + \tfrac{4}{45} V_0^2 V_1), \quad l = 1. \tag{4.17}$$

In the same manner we obtain, for $l = 2$,

$$U_5 = \tfrac{1}{10}\,(V_5 - \tfrac{2}{5} V_0 V_3 - \tfrac{3}{10} V_1 V_2 + \tfrac{2}{15} V_0^2 V_1), \quad l = 2. \tag{4.18}$$

For $l = 3$, U_5 must verify Eq. (3.5), i.e.,

$$U_5 = 2 g_{3,1} g_{3,4} + 2 g_{3,2} g_{3,3} = 0, \tag{4.19}$$

where we have used Eqs. (4.6) and (4.15). For $l > 3$, U_5 must verify Eq. (3.10); taking into account Eqs. (4.6) and (4.15), we write

$$U_5 = -12 \sum_{j=4}^{l} g_{j,6}. \tag{4.20}$$

Replacing the values of the coefficients, by iteration we obtain

$$U_5 \left(1 + 12 \sum_{j=4}^{l} \frac{1}{2j-6} + 12^2 \sum_{j=4}^{l} \frac{1}{2j-6} \times \sum_{i=j+1}^{l} \frac{1}{2i-6} + \cdots\right) = 0, \tag{4.21}$$

that is (see the Appendix),

$$U_5\,(l-2)(l-1)l(l+1)(l+2)(l+3)/6! = 0,$$

i.e.,

$$U_5 = 0, \quad \text{for} \quad l \geqslant 3. \tag{4.22}$$

Furthermore, as before, we obtain

$$g_{j,6} = 0, \quad \text{for} \quad 4 \leqslant j \leqslant l. \tag{4.23}$$

We are now ready to determine the general conditions on the potential. We have proved that, for $l > 3$,

$$U_1 = U_3 = U_5 = 0 \tag{4.24}$$

and also that, for $2 \leqslant i \leqslant l$,

$$\begin{aligned} g_{i,2} = 0 &\Rightarrow U_1 = 0, \\ g_{i,4} = 0 &\Rightarrow U_3 = 0, \\ g_{i,6} = 0 &\Rightarrow U_5 = 0. \end{aligned} \tag{4.25}$$

Therefore, to make the general proof by induction, we postulate that

$$g_{i,2n-2} = 0, \quad \text{for} \quad 2 \leqslant n \leqslant i \leqslant l, \tag{4.26}$$

and, given that

$$g_{i,2n-2} = \frac{1}{2i-2n+2}\left(U_{2n-3} + 4(n-1) \sum_{j=i+1}^{l} g_{j,2n-2} - \sum_{s=1}^{2n-4} g_{i,s}\, g_{i,2n-3-s}\right), \tag{4.27}$$

it follows that

$$U_{2n-3} = 0, \quad \text{for} \quad 2 \leqslant n \leqslant l. \tag{4.28}$$

We want to prove now that this postulate implies

$$g_{i,2n} = 0, \quad \text{for} \quad 2 \leqslant n+1 \leqslant i \leqslant l, \tag{4.29}$$

and consequently

$$U_{2n-1} = 0, \quad \text{for} \quad 2 \leqslant n \leqslant l. \tag{4.30}$$

From Eqs. (3.4) and (4.26) we have

$$g_{l,2n} = [1/(2l-2n)]\, U_{2n-1}, \quad l \geqslant n+1, \tag{4.31}$$

and, from Eq. (3.9),

$$g_{i,2n} = \frac{1}{2i-2n}\left(U_{2n-1} + 4n \sum_{j=i+1}^{l} g_{j,2n}\right). \tag{4.32}$$

The condition on U_{2n-1} will be given by Eq. (3.10), but the first sum vanishes because of the postulate; therefore, we get (see the Appendix)

$$U_{2n-1}\left(1 + 4n \sum_{i=n+1}^{l} \frac{1}{2i-2n} + (4n)^2 \sum_{i=n+1}^{l-1} \frac{1}{2i-2n} \times \sum_{j=i+1}^{l} \frac{1}{2j-2n} + \cdots\right) = U_{2n-1}\, \frac{(l-n+1)(l-n+2)\cdots(l+n)}{(2n)!} = 0. \tag{4.33}$$

Then,

$$U_{2n-1} = 0, \quad \text{for} \quad l \geq n+1. \tag{4.34}$$

But this equation implies

$$\sum_{i=n+1}^{l} g_{i,2n} = 0, \tag{4.35}$$

and, as before, we obtain

$$g_{i,2n} = 0 \quad \text{for} \quad 2 \leq n+1 \leq i \leq l. \tag{4.36}$$

QED

These results imply [see Eq. (3.5)]

$$U_{2l-1} = 0. \tag{4.37}$$

Summarizing, in order to solve the problem for fixed l, we must require that

$$U_1 = U_3 = \cdots = U_{2l-3} = U_{2l-1} = 0, \tag{4.38}$$

i.e., all odd derivatives up to $2l-1$ should vanish at the origin.

5. DETERMINATION OF THE COEFFICIENTS OF THE POTENTIAL

From Eqs. (2.20) and (3.8), we have

$$V_0 = U_0 + 2\sum_{i=1}^{l} \frac{1}{2i-1}\left(U_0 + 2\sum_{j=i+1}^{l} g_{j,1}\right), \tag{5.1}$$

from which we obtain by iteration

$$V_0 = U_0\left(1 + 2\sum_{i=1}^{l}\frac{1}{2i-1} + 2^2\sum_{i=1}^{l-1}\frac{1}{2i-1}\sum_{j=i+1}^{l}\frac{1}{2j-1} + \cdots\right), \tag{5.2}$$

i.e. (see the Appendix),

$$U_0 = [1/(2l+1)]\, V_0, \tag{5.3}$$

which is a well-known result of Newton[1] and Faddeev[2] [see Eqs. (2.19)].

By using Eq. (3.9), Eq. (2.20) for n = 2 reads

$$V_2 = U_2 + 6\sum_{i=1}^{l}\frac{1}{2i-3}\left(U_2 + 6\sum_{j=i+1}^{l} g_{j,3} - g_{i,1}^2\right). \tag{5.4}$$

From Eq. (3.8),

$$g_{j,1} = \frac{1}{2j-1}\left(U_0 + 2\sum_{i=j+1}^{l} g_{i,1}\right). \tag{5.5}$$

By iteration (see the Appendix) we obtain

$$g_{j,1} = [(2l+1)/(2j-1)(2j+1)]\, U_0. \tag{5.6}$$

Introducing these results in Eq. (5.4), by iteration we get

$$V_2 = U_2\left(1 + 6\sum_{i=1}^{l}\frac{1}{2i-3} + 6^2\sum_{i=1}^{l-1}\frac{1}{2i-3}\sum_{j=i+1}^{l}\frac{1}{2j-1} + \cdots\right) - U_0^2(2l+1)^2\left(6\sum_{i=1}^{l}\frac{1}{(2i-3)(2i-1)^2(2i+1)^2}\right.$$
$$\left. + 6^2\sum_{i=1}^{l-1}\frac{1}{2i-3}\sum_{j=i+1}^{l}\frac{1}{(2j-3)(2j-1)^2(2j+1)^2} + \cdots\right), \tag{5.7}$$

which, as is proven in the Appendix, is

$$V_2 = -\tfrac{1}{3}(2l-1)(2l+1)(2l+3)\, U_2 + 2l(2l+1)\, U_0^2. \tag{5.8}$$

Recalling Eq. (5.3), we get

$$U_2 = \frac{-3}{(2l-1)(2l+1)(2l+3)}\left(V_2 - \frac{2l}{2l+1}V_0^2\right). \tag{5.9}$$

To obtain U_4, we again use Eq. (2.20) now for n = 4, and, taking into account Eqs. (3.9) and (3.13), we have

$$V_4 = U_4 + 10\sum_{i=1}^{l}\frac{1}{2i-5}\left(U_4 + 10\sum_{j=i+1}^{l} g_{j,5} - 2g_{i,1}g_{i,3}\right) + \tfrac{5}{24}V_1^2. \tag{5.10}$$

From Eq. (3.9), by iteration and using Eq. (5.6), we obtain

$$g_{j,3} = \frac{U_2}{2j-3}\left(1 + 6\sum_{i=j+1}^{l}\frac{1}{2i-3} + 6^2\sum_{i=j+1}^{l-1}\frac{1}{2i-3}\sum_{k=i+1}^{l}\frac{1}{2k-3} + \cdots\right) - \frac{(2l+1)^2}{2j-3}U_0^2\left(\frac{1}{(2j-1)^2(2j+1)^2}\right.$$
$$\left. + 6\sum_{i=j+1}^{l}\frac{1}{(2i-3)(2i-1)^2(2i+1)^2} + 6^2\sum_{i=j+1}^{l-1}\frac{1}{2i-3}\sum_{k=i+1}^{l}\frac{1}{(2k-3)(2k-1)^2(2k+1)^2} + \cdots\right)$$
$$= \frac{(2l-1)(2l+1)(2l+3)}{(2j-3)(2j-1)(2j+1)(2j+3)}U_2 + \frac{(2l+1)}{(2j-3)(2j-1)(2j+1)(2j+3)}\left(3 - \frac{8j(2l+1)}{(2j-1)(2j+1)}\right)U_0^2 \tag{5.11}$$

(results of the sums are given in the Appendix). By iteration in Eq. (5.9), using Eq. (5.6), we have

$$V_4 = U_4\left(1 + 10\sum_{j=1}^{l}\frac{1}{2j-5} + 10^2\sum_{j=1}^{l-1}\frac{1}{2j-5}\sum_{i=j+1}^{l}\frac{1}{2i-5} + \cdots\right) - 2(2l+1)^2\,U_0\,[U_2(2l-1)(2l+3) + 3U_0^2]$$

$$\times\left(10\sum_{j=1}^{l}\frac{1}{(2j-5)(2j-3)(2j-1)^2\,(2j+1)^2\,(2j+3)} + 10^2\sum_{j=1}^{l-1}\frac{1}{2j-5}\sum_{i=j+1}^{l}\right.$$

$$\left.\frac{1}{(2i-5)(2i-3)(2i-1)^2\,(2i+1)^2\,(2i+3)} + \cdots\right) + 16\,(2l+1)^3\,U_0^3\left(10\sum_{j=1}^{l}\right.$$

$$\frac{1}{(2j-5)(2j-3)(2j-1)^3\,(2j+1)^3\,(2j+3)} + 10^2\sum_{j=1}^{l-1}\frac{1}{2j-5}\sum_{i=j+1}^{l}$$

$$\left.\frac{1}{(2i-5)(2i-3)(2i-1)^3\,(2i+1)^3\,(2i+3)} + \cdots\right) + \tfrac{5}{24}\,V_1^2 \qquad (5.12)$$

or (see the Appendix)

$$V_4 = U_4\,[(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)/5.9] - \tfrac{4}{9}\,l(2l+1)\,[(2l-1)(2l+3)\,U_0U_2 - (4l+1)\,U_0^3] + \tfrac{5}{24}\,V_1^2, \qquad (5.13)$$

and from Eqs. (5.3) and (5.9) we finally obtain

$$U_4 = \frac{45}{(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)}\left(V_4 - \frac{4l}{3(2l+1)}\,V_0V_2 + \frac{4l(2l-1)}{9(2l+1)^2}\,V_0^3 - \tfrac{5}{24}\,V_1^2\right). \qquad (5.14)$$

For the even coefficients of higher indices, the calculations are very complicated, and it is too troublesome to derive general formulas. But, in principle, it is possible to obtain all coefficients for any fixed l using the method developed in Secs. 2 and 3 (see, for example, the determination of U_3 for $l = 1$ or U_5 for $l = 1$ and $l = 2$ in Sec. 4). The same is true for the nonvanishing odd coefficients ($U_{2n+1}, n \geq l$).

We emphasize that if the potential is an even function (since only the values of the odd derivatives are restricted), we have formulas to determine it for all partial waves.

Furthermore, notice that the expressions obtained supply relationships between the phase shifts of different partial waves produced by the same potential. They are generalizations of the well-known expression of Newton–Faddeev, i.e., Eq. (5.3),

$$U_0 = \frac{1}{2l+1}\,V_0 = \frac{-8}{\pi(2l+1)}\int_0^\infty dk\,k\,\frac{d}{dk}\,[k\,\delta_l(k)] - \frac{4}{2l+1}\sum_n E_n^l\,. \qquad (5.3')$$

6. DATA AND THE CALCULATION OF THE POTENTIAL

In this section we analyze the relationship between the phase shift, the bound states, and the normalization constants for the different partial waves.

For the phase shifts we approach the problem in the following manner: The phase shift produced by the potential $U(r)$ in P wave is defined by the asymptotic behavior of the regular solution of the equation

$$y_1''(k^2,r) + [k^2 - U(r) - 2/r^2]\,y_1(k^2,r) = 0, \qquad (6.1)$$

i.e.,

$$y_1(k^2,r) \underset{r\to\infty}{\sim} \sin[kr - \pi/2 + \delta_1(k)]. \qquad (6.2)$$

For the S-wave equation deduced from Eq. (6.1),

$$y_0''(k^2,r) + [k^2 - U(r) - 2g_1'(r)]\,y_0(k^2,r) = 0, \qquad (6.3)$$

the phase shift is defined by

$$y_0(k^2,r) \underset{r\to\infty}{\sim} \sin[kr + \bar{\delta}_0(k)], \qquad (6.4)$$

the relationship between the two solutions being

$$y_0(k^2,r) = f_1(r)\,y_1(k^2,r) + y_1'(k^2,r). \qquad (6.5)$$

The function $f_1(r)$ satisfies the equation

$$f_1'(r) = f_1^2(r) - U(r) - 2/r^2 \qquad (6.6)$$

and asymptotically behaves like

$$f_1(r) \underset{r\to\infty}{\sim} 1/r \qquad (6.7)$$

[if we suppose that $U(r)$ is of finite range]. Then,

$$y_0(k^2,r) \underset{r\to\infty}{\sim} \cos[kr - \tfrac{1}{2}\pi + \delta_1(k)] = \sin[kr + \delta_1(k)]; \tag{6.8}$$

therefore, we can identify

$$\delta_1(k) = \bar{\delta}_0(k). \tag{6.9}$$

Notice that the slow vanishing of $g_1'(r) \underset{r\to\infty}{\sim} 3r^{-2}$ produces a behavior of $\bar{\delta}_0(k)$ at low energy similar to a P-wave phase shift

$$\delta_1(k) = \bar{\delta}_0(k) \sim k^3. \tag{6.10}$$

The same scheme is used to go from an l wave to an $l-1$ wave. In other words, the l- and $(l-1)$-wave phase shifts are defined by the asymptotic behavior of the regular solutions of the Eqs. (2.7) and (2.12), respectively, i.e.,

$$y_l(k^2,r) \underset{r\to\infty}{\sim} \sin[kr - \tfrac{1}{2}l\pi + \delta_l(k)], \tag{6.11}$$

$$y_{l-1}(k^2,r) \underset{r\to\infty}{\sim} \sin[kr - \tfrac{1}{2}(l-1)\pi + \bar{\delta}_{l-1}(k)]. \tag{6.12}$$

Given that

$$f_l(r) \underset{r\to\infty}{\sim} lr^{-1}, \tag{6.13}$$

since the relationship between the two solutions is given by Eq. (2.8), we have

$$y_{l-1}(k^2,r) \sim \cos[kr - \tfrac{1}{2}l\pi + \delta_l(k)]$$
$$= \sin[kr - \tfrac{1}{2}(l-1)\pi + \delta_l(k)]; \tag{6.14}$$

therefore, we can identify

$$\delta_l(k) = \bar{\delta}_{l-1}(k). \tag{6.15}$$

The behavior at low energy is

$$\delta_l(k) = \bar{\delta}_{l-1}(k) \sim \text{const}k^{2l+1} \tag{6.16}$$

because $g_l'(r) \sim (2l+1)r^{-2}$.

Repeating the same arguments l times, we get

$$\delta_l(k) = \bar{\delta}_{l-1}(k) = \bar{\bar{\delta}}_{l-2}(k) = \cdots = \eta_0(k), \tag{6.17}$$

where

$\delta_l(k)$ is the l-wave phase shift produced by the potential $U(r)$,

$\bar{\delta}_{l-1}(k)$ is the l-1-wave phase shift produced by the potential $U(r) + 2g_l'(r)$,

$\eta_0(k)$ is the S-wave phase shift produced by the potential

$$U(r) + 2\sum_{i=1}^{l} g_i'(r) = V(r).$$

Then, given the l-wave phase shift $\delta_l(k)$, we can use the formulas of Calogero and Degasperis[6] to determine

$$V_n = V_{(0)}^{(n)}/n!. \tag{6.18}$$

For the bound states we first analyze the relationship between the problems in P and S waves. We start from Eq. (6.1); the Jost solution of this problem is defined by the asymptotic behavior

$$h_1(k,r) \underset{r\to\infty}{\sim} ie^{-ikr}, \tag{6.19}$$

and the Jost function is

$$h_1(k) = \lim_{r\to 0} kr\, h_1(k,r). \tag{6.20}$$

The regular solution can be written as

$$y_1(k^2,r) = (i/2k^2)\,[h_1(-k)\,h_1(k,r) + h_1(k)\,h_1(-k,r)]. \tag{6.21}$$

If for the value $k = -ip$ we have $h_1(k=-ip) = 0$, there exists a bound state in the P wave of energy $-p^2$.

Now we turn to the S-wave problem, using Eq. (6.5); the Jost solution is defined by

$$h_0(k,r) \underset{r\to\infty}{\sim} e^{-ikr}, \tag{6.22}$$

the Jost function is

$$h_0(k) = \lim_{r\to 0} h_0(k,r), \tag{6.23}$$

and the regular solution can be written as

$$y_0(k^2,r) = (i/2k)[h_0(-k)h_0(k,r) - h_0(k)h_0(-k,r)]$$
$$= f_1(r)(i/2k^2)[h_1(-k)h_1(k,r) + h_1(k)h_1(-k,r)]$$
$$+ (i/2k^2)[h_1(-k)h_1'(k,r) + h_1(k)h_1'(-k,r)]. \tag{6.24}$$

If there is a bound state in P wave at energy $-p^2$ for the potential $U(r)$, we have

$$(i/2p)\,[h_0(ip)\,h_0(-ip,r) - h_0(-ip)\,h_0(ip,r)]$$
$$= -[f_1(r)/2p^2]\,h_1(ip)\,h_1(-ip,r)$$
$$-(1/2p^2)\,h_1(ip)\,h_1'(-ip,r). \tag{6.25}$$

Since the rhs vanishes for $r\to\infty$, we should have $h_0(-ip) = 0$ [otherwise $h_0(ip,r)$ diverges]; but this implies a bound state because

$$y_0(-p^2,r) \underset{r\to\infty}{\longrightarrow} 0 \quad \text{and} \quad y_0(-p^2,r) \underset{r\to 0}{\longrightarrow} 0$$

(we assume the potential is not a singular one).

Therefore, if we have a bound state in P wave for the potential $U(r)$ at energy E, there exists a bound state in S wave for the potential $V(r) = U(r) + 2g'(r)$ at the same energy E. This can be expressed as

$$E_n^P[U(r)] = E_n^S[U(r) + 2g'(r)]. \tag{6.26}$$

The converse is also true. This can be shown in the following way: If $V(r)$ produces an S-wave

bound state at $E=-p^2$, we have $h_0(-ip)=0$. By substitution in Eq. (6.24) and taking the limit $r\to\infty$, we obtain

$$0=(1/2p^2)\lim_{r\to\infty}[(r^{-1}-p)\,h_1(ip)\,e^{-pr}+(r^{-1}+p)\,h_1(-ip)\,e^{pr}],$$

but this equation implies $h_1(-ip)=0$, i.e., a P-wave bound state at $E=-p^2$ produced by the potential $U(r)$.

The same scheme can be reproduced without any difficulties for every partial wave; therefore, we can write

$$E_n^l[U(r)]=E_n^s\left(U(r)+2\sum_{i=1}^{l}g_i'(r)\right)=E_n^s[V(r)]. \tag{6.27}$$

For the normalization constants of the bound states, we realize that from Eqs. (2.7)–(2.9) we get

$$C_l^{-1}[U(r)]=\int_0^\infty dr\,y_l^2(-ip,r)=(-p^2)^{-1}\int_0^\infty dr\times y_{l-1}^2(-ip,r). \tag{6.28}$$

Here $y_l(-ip,r)$ is the bound state wavefunction (of energy $E_n^l=-p^2$) normalized with the convention

$$\lim_{r\to 0}[(2l+1)!!r^{-l-1}y_l(E_n^l r)]=1.$$

By iteration we can demonstrate in general that if there exist bound states at $k=-ip_n$, then

$$C_n^l[U(r)]=(-p_n^2)^l\,C_n^s[V(r)], \tag{6.29}$$

i.e.,

$$\frac{4i\,(-p_n^2)^{l+1}}{h_l(ip_n)\,\dot{h}_l(-ip_n)}=\frac{4i\,(-p_n^2)^{l+1}}{F_0(ip_n)\,\dot{F}_0(-ip_n)}, \tag{6.30}$$

where $h_l(k)$ is the Jost function for l wave of the Schrödinger problem with a potential $U(r)$, $F_0(k)$ is the Jost function for S wave of the Schrödinger problem with a potential $V(r)$, and the overhead dot indicates the derivative with respect to k.

Summarizing, if we have as data $\delta_l(k)$, E_n^l, and C_n^l, in order to calculate V_n by Eq. (6.18), we can use the expressions given by Calogero and Degasperis [Eqs. (2.29), (4.20), (4.21), and (4.19) of Ref. 6], being careful to replace

$$\begin{aligned}&\delta_l(k)\text{ where it reads }\eta(k),\\ &E_n^l\text{ where it reads }E_n,\\ &(-E_n^l)^{-l}C_n^l\text{ where it reads }C_n.\end{aligned} \tag{6.31}$$

In conclusion, we are ready now to construct the coefficients U_n using the formulas of Secs. 3 and 4 and to calculate, in principle, the entire potential

$$U(r)=\sum_{n=0}^{\infty}U_n r^n. \tag{6.32}$$

ACKNOWLEDGMENT

The author wishes to thank Professor F. Calogero for his very useful help and for his encouraging comments and suggestions while reading the manuscript.

APPENDIX:

The following formulas were proven by induction[11]:

$$1+2\sum_{j=1}^{l}\frac{1}{2j-1}+2^2\sum_{j=1}^{l-1}\frac{1}{2j-1}\sum_{i=j+1}^{l}\frac{1}{2i-1}+2^3\sum_{j=1}^{l-2}\frac{1}{2j-1}\sum_{i=j+1}^{l-1}\frac{1}{2i-1}\sum_{k=i+1}^{l}\frac{1}{2k-1}+\cdots=2l+1, \tag{A1}$$

$$1+4\sum_{j=2}^{l}\frac{1}{2j-2}+4^2\sum_{j=2}^{l-1}\frac{1}{2j-2}\sum_{i=j+1}^{l}\frac{1}{2i-2}+4^3\sum_{j=2}^{l-2}\frac{1}{2j-2}\sum_{i=j+1}^{l-1}\frac{1}{2i-2}\sum_{k=i+1}^{l}\frac{1}{2k-2}+\cdots=\frac{l(l+1)}{2}. \tag{A2}$$

Similar formulas can be expressed in a more general way as follows: If $n=2p+1$, $l\geq 1$, and $p\geq 0$,

$$1+2n\sum_{j=1}^{l}\frac{1}{2j-n}+(2n)^2\sum_{j=1}^{l-1}\frac{1}{2j-n}\sum_{i=j+1}^{l}\frac{1}{2i-n}+\cdots=\frac{(2l-n+2)(2l-n+4)\cdots(2l+n)}{(2-n)(4-n)\cdots n}; \tag{A3}$$

if $n=2p$, $l\geq p$, and $p\geq 1$,

$$1+2n\sum_{j=p+1}^{l}\frac{1}{2j-n}+(2n)^2\sum_{j=p+1}^{l-1}\frac{1}{2j-n}\sum_{i=j+1}^{l}\frac{1}{2i-n}+\cdots=\frac{(l-p+1)(l-p+2)\ldots(l+p)}{n!}. \tag{A4}$$

In all these expressions we have established the convention

$$\sum_{i=n}^{m}=0\text{ if }m<n.$$

Furthermore, we can prove the following results:

$$1 + 2 \sum_{i=j+1}^{l} \frac{1}{2i-1} + 2^2 \sum_{i=j+1}^{l-1} \frac{1}{2i-1} \sum_{k=i+1}^{l} \frac{1}{2k-1} + \cdots = \frac{2l+1}{2j+1}, \tag{A5}$$

$$1 + 4 \sum_{i=j+1}^{l} \frac{1}{2i-2} + 4^2 \sum_{i=j+1}^{l-1} \frac{1}{2i-2} \sum_{k=i+1}^{l} \frac{1}{2k-2} + \cdots = \frac{l(l+1)}{j(j+1)}. \tag{A6}$$

We note that Eq. (A5), combined with Eq. (A1), and (A6), with (A2), give us

$$\sum_{j=1}^{l} \frac{1}{4j^2-1} = \frac{l}{2l+1}, \tag{A7}$$

$$\sum_{j=2}^{l} \frac{1}{j(j^2-1)} = \tfrac{1}{4}\left(1 - \frac{2}{l(l+1)}\right), \tag{A8}$$

from which, interchanging indices, we get several relationships; for example,

$$\sum_{j=1}^{l} \frac{1}{(2j-1)(2j-3)} = \frac{-l}{2l-1}, \tag{A9}$$

$$\sum_{j=1}^{l} \frac{1}{j(j+1)(j+2)} = \frac{l(l+3)}{4(l+1)(l+2)}. \tag{A10}$$

The generalizations of Eqs. (A5) and (A6) are, for $n = 2p + 1, l \geq 1$, and $p \geq 0$,

$$1 + 2n \sum_{i=j+1}^{l} \frac{1}{2i-n} + (2n)^2 \sum_{i=j+1}^{l-1} \frac{1}{2i-n} \sum_{k=i+1}^{l} \frac{1}{2k-n} + \cdots = \frac{(2l-n+2)(2l-n+4)\cdots(2l+n)}{(2j-n+2)(2j-n+4)\cdots(2j+n)} \tag{A11}$$

and, for $n = 2p, l \geq p$, and $p \geq 1$,

$$1 + 2n \sum_{i=j+1}^{l} \frac{1}{2i-n} + (2n)^2 \sum_{i=j+1}^{l-1} \frac{1}{2i-n} \sum_{k=i+1}^{l} \frac{1}{2k-n} + \cdots = \frac{(l-p+1)(l-p+2)\cdots(l+p)}{(j-p+1)(j-p+2)\cdots(j+p)}, \tag{A12}$$

from which we can get relationships similar to Eqs. (A9) and (A10).

The following relationships (also proved by induction) were used in Sec. 4:

$$\frac{1}{(4j^2-1)^2} + 6 \sum_{i=j+1}^{l} \frac{1}{(2i-3)(4i^2-1)^2} + 6^2 \sum_{i=j+1}^{l-1} \frac{1}{2i-3} \sum_{k=i+1}^{l} \frac{1}{(2k-3)(4k^2-1)^2} + \cdots$$
$$= \frac{1}{(2j+3)(4j^2-1)^2}\left(8j - \frac{3}{2l+1}\right), \tag{A13}$$

$$1 + 6 \sum_{j=1}^{l} \frac{1}{(2j-3)(4j^2-1)^2} + 6^2 \sum_{j=1}^{l-1} \frac{1}{(2j-3)} \sum_{i=j+1}^{l} \frac{1}{(2i-1)(4i^2-1)^2} + \cdots = \frac{1}{2l+1}, \tag{A14}$$

$$10 \sum_{j=1}^{l} \frac{1}{(2j-5)(4j^2-1)^2(4j^2-9)} + 10^2 \sum_{j=1}^{l-1} \frac{1}{2j-5} \sum_{i=j+1}^{l} \frac{1}{(2i-5)(4i^2-1)^2(4i^2-9)} + \cdots = \frac{2l}{9(2l+1)}, \tag{A15}$$

$$10 \sum_{j=1}^{l} \frac{1}{(2j-5)(4j^2-1)^3(4j^2-9)} + 10^2 \sum_{j=1}^{l-1} \frac{1}{2j-5} \sum_{i=j+1}^{l} \frac{1}{(2i-5)(4i^2-1)^3(4i^2-9)} + \cdots = \frac{l(l+1)}{9(2l+1)^2}. \tag{A16}$$

[1] R. G. Newton, Phys. Rev. **101**, 1588 (1956); see also J. Math. Phys. **1**, 319 (1960).
[2] L. D. Faddeev, Dokl. Akad. Nauk SSSR **115**, 878 (1957).
[3] V. S. Buslaev and L. D. Faddeev, Dokl. Akad. Nauk SSSR **132**, 13 (1960) [Sov. Math. Doklady **1**, 451 (1960)].
[4] I. C. Percival, Proc. Phys. Soc. (London) **80**, 1290 (1960).
[5] M. J. Roberts, Proc. Phys. Soc. (London) **84**, 825 (1964).
[6] F. Calogero and A. Degasperis, J. Math. Phys. **9**, 90 (1968).
[7] A. Degasperis, J. Math. Phys. **11**, 551 (1970).
[8] O. D. Corbella, J. Math. Phys. **11**, 1695 (1970).
[9] This is a generalization of F. Calogero's (private communication) basic proof, i.e., the transformation of a problem in P wave to another in S wave. Another transformation of this type was studied by the author (IMAF Report, 1969) (using a method suggested in a previous paper[8]), which, however, leads to a Schrödinger equation with an energy-dependent potential; furthermore, the calculations are very complicated and the results less elegant and complete than those we are giving now.
[10] We restrict the potential $\dot{U}(r)$ to the case where it does not have a bound state (or resonance) of zero energy.
[11] After the author proved these relationships by induction, A. Grunbaun (private communication) gave a more concise and elegant proof: "Let us consider the numbers $c_1, c_2, \ldots, c_l$. Let us form the sums of all their products without repetition; it is easy to prove that

$$1 + c_1 + c_2 + \cdots + c_l + c_1c_2 + c_1c_3 + \cdots + c_{l-1}c_l + \cdots + c_1c_2 \cdots c_l = 1 + \sum_i c_i + \sum_{i<j} c_ic_j + \cdots + c_1c_2 \cdots c_l = (1 + c_1)(1 + c_2) \cdots (1 + c_l).$$

Then, to prove, for example, the relationship (A1) we put $c_i = 2/(2i - 1)$. Therefore,

$$(A1) = \prod_{i=1}^{l} \left(1 + \frac{2}{2i-1}\right) = \prod_{i=1}^{l} \left(\frac{2i+1}{2i-1}\right) = 2l + 1."$$

Most of the other expressions can be proved similarly.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

The Boson Calculus for the Orthogonal and Symplectic Groups

M. A. Lohe and C. A. Hurst
University of Adelaide, Adelaide, South Australia 5001
(Received 16 February, 1971)

The boson calculus as used for $U(n)$ cannot be applied directly to $O(n)$ and $Sp(n)$. Modifications are made to boson operators, in order to obtain new operators which enable explicit states of irreducible representations of $O(n)$ and $Sp(n)$ to be constructed. Calculations for $O(3)$ and $O(4)$ show how these operators permit a greater simplicity, and reveal more fully the group structure than has previously been the case.

1. INTRODUCTION

The importance of bosons in connection with the unitary groups is well known.[1] Using bosons, we can construct explicit states of irreducible representations of the unitary groups.

Let the carrier space of the defining representation of $U(n)$ be the n-dimensional vector space A. Then the carrier spaces of all irreducible representations of $U(n)$ can be projected out of $B = A^{(1)} \times A^{(2)} \times \cdots \times A^{(\lambda)}$, the direct product of λ vector spaces A. The transformation induced by the operations of $U(n)$ commute with transformations permuting the vector spaces among themselves. These latter transformations are completely described by the Young symmetry patterns defined by partitions $[m]$ of λ. Each Young tableau defines a Young symmetrizer which projects B into the invariant subspace defined by the Young tableau. In this way B is decomposed into invariant subspaces.

In order to obtain explicit stages, the space B can be realized with boson operators, i.e.,

$$A_i^{(\sigma)} \leftrightarrow a_i^{\sigma\dagger} \quad i = 1 \cdots n, \quad \sigma = 1 \cdots \lambda,$$

where the bosons satisfy

$$[a_i^{\sigma}, a_j^{\tau\dagger}] = \delta_{ij}\delta^{\sigma\tau}, \quad [a_i^{\sigma}, a_j^{\tau}] = 0 = [a_i^{\sigma\dagger}, a_j^{\tau\dagger}]. \tag{1.1}$$

Application of the Young symmetrizer produces the antisymmetrized combinations

$$a^{\dagger}_{i_1 i_2 \ldots i_k} = \Sigma\epsilon(i_1 i_2 \cdots i_k)\, a_{i_1}^{1\dagger} a_{i_2}^{2\dagger} \cdots a_{i_k}^{k\dagger} \tag{1.2}$$

representing columns of the Young tableau. States of an irreducible representation of $U(n)$ become explicit boson (and multiple boson) operators acting on the vacuum $|0\rangle$.

For the orthogonal and symplectic groups, B must be decomposed further. The operation of contraction (taking the trace) of tensors belonging to B commutes with the orthogonal and symplectic transformations.[2,3] Hence, we must now project out the traceless part of tensors belonging to B, and then apply the Young symmetrizer, so as to decompose B.

If we realize B with boson operators as before, then we must project out the traceless part of products of boson operators. This method is not suitable for use in general, although it has been attempted by Holman[4] for $Sp(4)$. However his space is not completely traceless. A simpler method is to realize B with symmetric operators $a_i^{\sigma\dagger}$, chosen so that B is immediately traceless. If B is to consist of traceless tensors, then our operators $a_i^{\sigma\dagger}$ must satisfy the traceless conditions

$$\begin{aligned} &a_p^{\sigma\dagger} a_p^{\tau\dagger} = 0 \text{ for } O(n) \\ \text{or} \quad &\epsilon_{pq} a_p^{\sigma\dagger} a_q^{\tau\dagger} = 0 \text{ for } Sp(n) \end{aligned} \tag{1.3}$$

where ϵ_{pq}, the symplectic metric, satisfies

$$\epsilon_{pq}\epsilon_{rq} = \delta_{pr}, \quad \epsilon_{pq} = -\epsilon_{qp},$$

repeated $p, q \cdots$ summed from $1 \cdots n$.

One cannot use boson operators for this purpose,

[1] R. G. Newton, Phys. Rev. **101**, 1588 (1956); see also J. Math. Phys. **1**, 319 (1960).
[2] L. D. Faddeev, Dokl. Akad. Nauk SSSR **115**, 878 (1957).
[3] V. S. Buslaev and L. D. Faddeev, Dokl. Akad. Nauk SSSR **132**, 13 (1960) [Sov. Math. Doklady **1**, 451 (1960)].
[4] I. C. Percival, Proc. Phys. Soc. (London) **80**, 1290 (1960).
[5] M. J. Roberts, Proc. Phys. Soc. (London) **84**, 825 (1964).
[6] F. Calogero and A. Degasperis, J. Math. Phys. **9**, 90 (1968).
[7] A. Degasperis, J. Math. Phys. **11**, 551 (1970).
[8] O. D. Corbella, J. Math. Phys. **11**, 1695 (1970).
[9] This is a generalization of F. Calogero's (private communication) basic proof, i.e., the transformation of a problem in P wave to another in S wave. Another transformation of this type was studied by the author (IMAF Report, 1969) (using a method suggested in a previous paper[8]), which, however, leads to a Schrödinger equation with an energy-dependent potential; furthermore, the calculations are very complicated and the results less elegant and complete than those we are giving now.
[10] We restrict the potential $\dot{U}(r)$ to the case where it does not have a bound state (or resonance) of zero energy.
[11] After the author proved these relationships by induction, A. Grunbaun (private communication) gave a more concise and elegant proof: "Let us consider the numbers $c_1, c_2, \ldots, c_l$. Let us form the sums of all their products without repetition; it is easy to prove that

$$1 + c_1 + c_2 + \cdots + c_l + c_1c_2 + c_1c_3 + \cdots + c_{l-1}c_l + \cdots + c_1c_2 \cdots c_l = 1 + \sum_i c_i + \sum_{i<j} c_ic_j + \cdots + c_1c_2 \cdots c_l = (1 + c_1)(1 + c_2) \cdots (1 + c_l).$$

Then, to prove, for example, the relationship (A1) we put $c_i = 2/(2i - 1)$. Therefore,

$$(A1) = \prod_{i=1}^{l} \left(1 + \frac{2}{2i-1}\right) = \prod_{i=1}^{l} \left(\frac{2i+1}{2i-1}\right) = 2l + 1."$$

Most of the other expressions can be proved similarly.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

The Boson Calculus for the Orthogonal and Symplectic Groups

M. A. Lohe and C. A. Hurst
University of Adelaide, Adelaide, South Australia 5001
(Received 16 February, 1971)

The boson calculus as used for $U(n)$ cannot be applied directly to $O(n)$ and $Sp(n)$. Modifications are made to boson operators, in order to obtain new operators which enable explicit states of irreducible representations of $O(n)$ and $Sp(n)$ to be constructed. Calculations for $O(3)$ and $O(4)$ show how these operators permit a greater simplicity, and reveal more fully the group structure than has previously been the case.

1. INTRODUCTION

The importance of bosons in connection with the unitary groups is well known.[1] Using bosons, we can construct explicit states of irreducible representations of the unitary groups.

Let the carrier space of the defining representation of $U(n)$ be the n-dimensional vector space A. Then the carrier spaces of all irreducible representations of $U(n)$ can be projected out of $B = A^{(1)} \times A^{(2)} \times \cdots \times A^{(\lambda)}$, the direct product of λ vector spaces A. The transformation induced by the operations of $U(n)$ commute with transformations permuting the vector spaces among themselves. These latter transformations are completely described by the Young symmetry patterns defined by partitions $[m]$ of λ. Each Young tableau defines a Young symmetrizer which projects B into the invariant subspace defined by the Young tableau. In this way B is decomposed into invariant subspaces.

In order to obtain explicit stages, the space B can be realized with boson operators, i.e.,

$$A_i^{(\sigma)} \leftrightarrow a_i^{\sigma\dagger} \quad i = 1 \cdots n, \quad \sigma = 1 \cdots \lambda,$$

where the bosons satisfy

$$[a_i^{\sigma}, a_j^{\tau\dagger}] = \delta_{ij}\delta^{\sigma\tau}, \quad [a_i^{\sigma}, a_j^{\tau}] = 0 = [a_i^{\sigma\dagger}, a_j^{\tau\dagger}]. \tag{1.1}$$

Application of the Young symmetrizer produces the antisymmetrized combinations

$$a^{\dagger}_{i_1 i_2 \ldots i_k} = \Sigma\epsilon(i_1 i_2 \cdots i_k)\, a_{i_1}^{1\dagger} a_{i_2}^{2\dagger} \cdots a_{i_k}^{k\dagger} \tag{1.2}$$

representing columns of the Young tableau. States of an irreducible representation of $U(n)$ become explicit boson (and multiple boson) operators acting on the vacuum $|0\rangle$.

For the orthogonal and symplectic groups, B must be decomposed further. The operation of contraction (taking the trace) of tensors belonging to B commutes with the orthogonal and symplectic transformations.[2,3] Hence, we must now project out the traceless part of tensors belonging to B, and then apply the Young symmetrizer, so as to decompose B.

If we realize B with boson operators as before, then we must project out the traceless part of products of boson operators. This method is not suitable for use in general, although it has been attempted by Holman[4] for $Sp(4)$. However his space is not completely traceless. A simpler method is to realize B with symmetric operators $a_i^{\sigma\dagger}$, chosen so that B is immediately traceless. If B is to consist of traceless tensors, then our operators $a_i^{\sigma\dagger}$ must satisfy the traceless conditions

$$\begin{aligned} &a_p^{\sigma\dagger} a_p^{\tau\dagger} = 0 \text{ for } O(n) \\ \text{or} \quad &\epsilon_{pq} a_p^{\sigma\dagger} a_q^{\tau\dagger} = 0 \text{ for } Sp(n) \end{aligned} \tag{1.3}$$

where ϵ_{pq}, the symplectic metric, satisfies

$$\epsilon_{pq}\epsilon_{rq} = \delta_{pr}, \quad \epsilon_{pq} = -\epsilon_{qp},$$

repeated $p, q \cdots$ summed from $1 \cdots n$.

One cannot use boson operators for this purpose,

because they cannot be made to satisfy either of Eqs. (1.3).

2. MODIFIED BOSONS

In order to know what operators are to be used, let us see how boson operators are introduced for the unitary groups. We can then see what modifications are necessary.

We can define a representation T of $U(n)$ in a function space R^{nl} by

$$T(U)f(x) = f(U^{-1}x)$$

where

$U \in U(n)$ and $x \in E_n$, the n-dimensional Euclidean space, and $f(x) \in R^{nl}$. This representation will be irreducible if the representation space R^{nl} consists of homogeneous polynomials of degree l. If we wish to raise the degree of $f^l \in R^{nl}$, we simply multiply by x_i because $x_i f^l \in R^{nl+1}$ if $f^l \in R^{nl}$. But raising the degree of f^l corresponds to adding a particle, i.e., applying the creation operator. Similarly, to lower the degree we differentiate:

$$\frac{\partial}{\partial x_j} f^l \in R^{nl-1}.$$

Therefore we make the associations

$$a_i^\dagger \leftrightarrow x_i, \qquad a_j \leftrightarrow \frac{\partial}{\partial x_j} \tag{2.1}$$

and so we have bosons.

Under orthogonal transformations, R^{nl} becomes reducible. $r^2 = x_p^2$ is invariant, so that the subspace $r^2 R^{nl-2}$ is invariant and must be factored out. We may write[5]

$$R^{nl} = H^l \oplus r^2 R^{nl-2}, \tag{2.2}$$

where H^l is the invariant representation space. Now if $h^l \in H^l$, then h^l is orthogonal to $r^2 R^{nl-2}$, i.e.,

$$(h^l, r^2 f^{l-2}) = 0 \text{ for all } f^{l-2} \in R^{nl-2},$$

and therefore

$$(\nabla^2 h^l, f^{l-2}) = 0 \text{ for all } f^{l-2} \in R^{nl-2},$$

since the adjoint of x_i in R^{nl} is $\frac{\partial}{\partial x_i}$, by (2.1).

Hence

$$\nabla^2 h^l = 0, \tag{2.3}$$

i.e., H^l is the space of all harmonic homogeneous polynomials of degree l.

The annihilation operator is unchanged since

$$\frac{\partial}{\partial x_j} h^l \in H^{l-1} \text{ if } h^l \in H^l.$$

However $x_i h^l \notin H^{l+1}$ because $\nabla^2 x_i h^l \neq 0$. In fact

$$(x_i - r^2[\nabla^2, r^2]^{-1}[\nabla^2, x_i])h^l \in H^{l+1} \tag{2.4}$$

(note that ∇^2 commutes with $[\nabla^2, r^2]$ within the harmonic space). We see that the creation operator has been modified, and we now have

$$a_i^\dagger \leftrightarrow (1 - r^2[\nabla^2, r^2]^{-1}\nabla^2)x_i \tag{2.5}$$

$$= x_i - 2r^2[\nabla^2, r^2]^{-1}\frac{\partial}{\partial x_i} \tag{2.6}$$

and

$$a_j \leftrightarrow \frac{\partial}{\partial x_j}. \tag{2.7}$$

These operators, "modified boson operators," satisfy

$$[a_i, a_j] = 0$$

and, hence,

$$[a_i^\dagger, a_j^\dagger] = 0 \tag{2.8}$$

and

$$[a_i, a_j^\dagger] = \delta_{ij} - a_i^\dagger(n/2 + N)^{-1}a_j \tag{2.9}$$

where $N = a_p^\dagger a_p = x_p \frac{\partial}{\partial x_p}$ within the harmonic space.

Now if we define the unique vacuum by $a_i | 0\rangle = 0$ for all $i = 1, \cdots, n$, then it follows from (2.8) and (2.9) that $a_i a_j^\dagger | 0\rangle = \delta_{ij} | 0\rangle$ and then, also

$$a_i a_p^{\dagger 2} | 0\rangle = 0. \tag{2.10}$$

From the uniqueness of the vacuum we have $a_p^{\dagger 2} | 0\rangle = K | 0\rangle$ for some constant K. An arbitrary state $| l\rangle$ can be written as the sum of products of l creation operators, and therefore we have $a_p^{\dagger 2} | l\rangle = K | l\rangle$, i.e., $a_p^{\dagger 2} = K$.

Hence $a_p^2 = \overline{K}$ and then $a_p^2 | 0\rangle = \overline{K} | 0\rangle = 0$ so that we must have $K = 0$, i.e.,

$$a_p^{\dagger 2} = 0. \tag{2.11}$$

This is the traceless condition (1.3) required for our operators. The adjoint relation $a_p^2 = 0$ is the harmonic condition on our space.

We can show from (2.8) and (2.9) that N is the number operator, i.e., $[N, a_i^\dagger] = a_i^\dagger$ and that

$$J_{ij} = -i(a_i^\dagger a_j - a_j^\dagger a_i) \tag{2.12}$$

are the generators of $O(n)$:

$$[J_{ij}, J_{kl}] = i(\delta_{jl}J_{ik} + \delta_{ik}J_{jl} - \delta_{il}J_{jk} - \delta_{jk}J_{il}). \tag{2.13}$$

Also, the $a_i^\dagger$ behave as vectors under orthogonal transformations:

$$[J_{ij}, a_k^\dagger] = i(\delta_{ik}a_j^\dagger - \delta_{jk}a_i^\dagger). \tag{2.14}$$

We notice that often the $a_i^\dagger$ defined by (2.8) and (2.9) may be regarded as ordinary bosons.

For symmetric representations (one row in the Young pattern) we use the operators defined by (2.8) and (2.9) to obtain states of irreducible representations of $O(n)$. In order to include extra rows, we must introduce more variables: x_i^σ $i = 1, \cdots, n$, $\sigma = 1, \cdots, \lambda$ (for λ rows). We then multiply λ spaces like R^{nl}, and factor out the invariant subspaces:

$$R^{nl_1} \times R^{nl_2} \cdots \times R^{nl_\lambda} = H^{(l_\lambda)} \tag{2.15}$$

$$\oplus \bigcup_{\alpha,\beta=1}^{\lambda} (x^\alpha, x^\beta) R^{nl_1} \times \cdots R^{nl_\alpha - 1} \cdots \times R^{nl_\beta - 1} \cdots R^{nl_\lambda}$$

where

$$(l_\lambda) = (l_1, l_2, \cdots, l_\lambda).$$

l_α is the degree of homogeneity of $f^{l\alpha} \in R^{nl\alpha}$, and $(x^\alpha, x^\beta) = x_p^\alpha x_p^\beta$. We see that $h^{(l\lambda)} \in H^{(l\lambda)}$ is orthogonal to polynomials containing the factor (x^α, x^β), $\alpha, \beta = 1 \cdots \lambda$. Hence $h^{(l\lambda)}$ satisfies

$$\nabla_{\alpha\beta} h^{(l_\lambda)} = 0, \qquad \alpha, \beta = 1, \cdots, \lambda, \tag{2.16}$$

where

$$\nabla_{\alpha\beta} = \frac{\partial^2}{\partial x_p^\alpha \, \partial x_p^\beta},$$

and so our invariant carrier space $H^{(l_\lambda)}$ is harmonic in all variables.

The annihilation operator is $\partial/\partial x_i^\sigma$, since

$$\frac{\partial}{\partial x_i^\sigma} h^{(l_\lambda)} \in H^{(l_1 \cdots l_\sigma - 1, \cdots l_\lambda)} \tag{2.17}$$

if $h^{(l\lambda)} \in H^{(l\lambda)}$. The creation operator must have the form

The creation operator must have the form

$$x_i^\sigma - (x^\alpha, x^\beta) A_{\alpha\beta}(\sigma),$$

(repeated $\alpha, \beta, \cdots$ summed from $1, \cdots, \lambda$), where $A_{\alpha\beta}(\sigma)$ is an operator to be determined. We require

$$\nabla_{\gamma\epsilon} (x_i^\sigma - (x^\alpha, x^\beta) A_{\alpha\beta}(\sigma)) h^{(l\lambda)} = 0,$$

$$[\nabla_{\gamma\epsilon}, x_i^\sigma] = [\nabla_{\gamma\epsilon}, (x^\alpha, x^\beta)] A_{\alpha\beta}(\sigma) \tag{2.18}$$

provided

$$[\nabla_{\gamma\epsilon}, A_{\alpha\beta}(\sigma)] = 0. \tag{2.19}$$

Let

$$\Delta(\lambda)_{(\gamma\epsilon)(\alpha\beta)} = [\nabla_{\gamma\epsilon}, (x^\alpha, x^\beta)] \tag{2.20}$$

be a $\lambda^2 \times \lambda^2$ matrix (symmetric within each pair of indices). Then

$$A_{\alpha\beta}(\sigma) = \Delta^{-1}(\lambda)_{(\alpha\beta)(\gamma\epsilon)} [\nabla_{\gamma\epsilon}, x_i^\sigma]$$
$$= 2\Delta^{-1}(\lambda)_{(\alpha\beta)(\gamma\sigma)} \frac{\partial}{\partial x_i^\gamma},$$

where

$$\Delta^{-1}(\lambda)_{(\mu\nu)(\alpha\beta)} \Delta(\lambda)_{(\alpha\beta)(\sigma\tau)} = \delta_{(\mu\nu)(\sigma\tau)}$$
$$= \tfrac{1}{2}(\delta_{\mu\sigma}\delta_{\nu\tau} + \delta_{\mu\tau}\delta_{\nu\sigma}). \tag{2.21}$$

The Δ^{-1} matrix will be handled only through this formal definition, but, for explicit calculations in the carrier space, (2.21) requires more consideration.

Now

$$\Delta(\lambda)_{(\mu\nu)(\sigma\tau)} = 2[n\delta_{(\mu\nu)(\sigma\tau)} + P^{\alpha\mu}\delta_{(\alpha\nu)(\sigma\tau)} + P^{\alpha\nu}\delta_{(\alpha\mu)(\sigma\tau)}], \tag{2.22}$$

where

$$P^{\mu\nu} = x_p^\mu \frac{\partial}{\partial x_p^\nu} \tag{2.23}$$

is a polarization operator and satisfies $[\nabla_{\sigma\tau}, P^{\mu\nu}] = 0$ within $H^{(l\lambda)}$. Hence, the condition (2.19 is satisfied.

We now have for our operators, which depend on the number of rows λ,

$$a_i^{\sigma\dagger}(\lambda) \leftrightarrow [1 - (x^\alpha, x^\beta)\Delta^{-1}(\lambda)_{(\alpha\beta)(\gamma\epsilon)}\nabla_{\gamma\epsilon}] x_i^\sigma$$
$$= x_i^\sigma - 2(x^\alpha, x^\beta)\Delta^{-1}(\lambda)_{(\alpha\beta)(\sigma\gamma)} \frac{\partial}{\partial x_i^\gamma}, \tag{2.24}$$

$$a_i^\sigma \leftrightarrow \frac{\partial}{\partial x_i^\sigma}. \tag{2.25}$$

We see immediately that these operators satisfy

$$[a_i^\sigma, a_j^\tau] = 0$$

and therefore

$$[a_i^{\sigma\dagger}, a_j^{\tau\dagger}] = 0. \tag{2.26}$$

We also have

$$[a_i^\sigma, a_j^{\tau\dagger}] = \delta_{ij}\delta^{\sigma\tau} - 4a_i^{\alpha\dagger}\Delta^{-1}_{(\alpha\sigma)(\tau\beta)} a_j^\beta, \tag{2.27}$$

where Δ^{-1} is expressed implicitly in terms of the a's according to (2.21) and (2.22) (note that $P^{\mu\nu} = a_p^{\mu\dagger} a_p^\nu$). The commutator

$$\left[\frac{\partial}{\partial x_i^\sigma}, \Delta^{-1}_{(\alpha\beta)(\tau\gamma)}\right],$$

which we need in order to obtain this form, is calculated using

$$\left[\frac{\partial}{\partial x_i^\sigma}, \Delta^{-1}\right] \Delta = -\Delta^{-1}\left[\frac{\partial}{\partial x_i^\sigma}, \Delta\right].$$

The relations (2.26) and (2.27) are the defining relations for our operators, when considering λ rows. We rarely need to know Δ^{-1} explicitly, which is fortunate since this inverse matrix quickly becomes complicated. For example, if $\lambda = 2$ we have

$$[a_i, a_j^\dagger] = \delta_{ij} - a_i^\dagger (n/2 + N)^{-1} a_j - (b_i^\dagger - a_i^\dagger (n/2 + N)^{-1} P^\dagger)\Omega^{-1}(b_j - P(n/2 + N)^{-1} a_j)$$

$$[b_i, a_j^\dagger] = -(a_i^\dagger - b_i^\dagger (n/2 + M)^{-1} P)\Omega^{-1}(b_j - P(n/2 + N)^{-1} a_j), \tag{2.28}$$

where

$$a_i^\dagger = a_i^{1\dagger}, b_i^\dagger = a_i^{2\dagger}$$

and

$$\Omega = n + N + M - P^\dagger (n/2 + M)^{-1} P - P(n/2 + N)^{-1} P^\dagger,$$

where

$$N = P^{11}, \quad M = P^{22}, \quad P = P^{12}.$$

We define the unique vacuum state by $a_i^\sigma |0\rangle = 0$ for all $\sigma = 1, \cdots \lambda$ and $i = 1, \cdots n$. We have immediately $a_i^\sigma a_j^{\tau\dagger} |0\rangle = \delta_{ij} \delta^{\sigma\tau} |0\rangle$. One can show from (2.26) and (2.27) that

$$a_i^\mu a_p^{\sigma\dagger} a_p^{\tau\dagger} |0\rangle = 0. \tag{2.29}$$

For this we need to know

$$\Delta^{-1}_{(\mu\nu)(\sigma\tau)} |0\rangle = (1/2n)\, \delta_{(\mu\nu)(\sigma\tau)} |0\rangle \tag{2.30}$$

calculated from $\Delta^{-1} \Delta |0\rangle = I |0\rangle$.

In the same way as before, for one row, we obtain the result that our operators obey the traceless condition $a_p^{\sigma\dagger} a_p^{\tau\dagger} = 0$.

Other details are quickly obtained from (2.27).

$$[P^{\mu\nu}, a_k^{\sigma\dagger}] = a_k^{\mu\dagger} \delta^{\nu\sigma} \tag{2.31}$$

so that $N^\sigma = P^{\sigma\sigma}$ is a number operator and

$$N = \sum_{\sigma=1}^{\lambda} P^{\sigma\sigma}$$

is the total number operator.

The generators can be written as

$$J_{ij} = -i \sum_{\alpha=1}^{\lambda} (a_i^{\alpha\dagger} a_j^\alpha - a_j^{\alpha\dagger} a_i^\alpha). \tag{2.32}$$

The $a_k^{\sigma\dagger}$ behave as vectors under rotations:

$$[J_{ij}, a_k^{\sigma\dagger}] = i(\delta_{ik} a_j^{\sigma\dagger} - \delta_{jk} a_i^{\sigma\dagger}). \tag{2.33}$$

We can also write the generators as

$$J^{\sigma\tau} = -i \sum_{p=1}^{n} (a_p^{\sigma\dagger} a_p^\tau - a_p^{\tau\dagger} a_p^\sigma) \tag{2.34}$$

$$= -i(P^{\sigma\tau} - P^{\tau\sigma})$$

provided $\lambda = n$.

The $J^{\sigma\tau}$ carry out transformations on the upper indices:

$$[J^{\sigma\tau}, a_i^{\mu\dagger}] = i[\delta^{\sigma\mu} a_i^{\tau\dagger} - \delta^{\tau\mu} a_i^{\sigma\dagger}]. \tag{2.35}$$

The analysis for the symplectic groups follows closely that of the orthogonal groups, with only changes in sign, and $\delta_{ij} \to \epsilon_{ij}$.

For one row bosons are sufficient since $\epsilon_{pq} a_p^\dagger a_q^\dagger = 0$. [This is as expected, since $Sp(2)$ is globally isomorphic to $SU(2)$.] For λ rows we have

$$a_i^{\sigma\dagger}(\lambda) \leftrightarrow x_i^\sigma - 2\epsilon(x^\alpha, x^\beta)[\Delta_\epsilon^{-1}(\lambda)]_{(\alpha\beta)(\sigma\gamma)} \epsilon_{ip} \frac{\partial}{\partial x_p^\gamma},$$

$$a_i^\sigma \leftrightarrow \frac{\partial}{\partial x_i^\sigma}, \tag{2.36}$$

where

$$\epsilon(x^\alpha, x^\beta) = \epsilon_{pq} x_p^\alpha x_q^\beta$$

and

$$\Delta^{-1}_{\epsilon_{(\mu\nu)(\alpha\beta)}} \Delta_{\epsilon_{(\alpha\beta)(\sigma\tau)}} = \tfrac{1}{2}(\delta_{\mu\sigma}\delta_{\nu\tau} - \delta_{\nu\sigma}\delta_{\mu\tau}), \tag{2.37}$$

where

$$[\Delta_\epsilon(\lambda)]_{(\alpha\beta)(\sigma\gamma)} = \left[\epsilon_{pq} \frac{\partial^2}{\partial x_p^\alpha \partial x_q^\beta}, \epsilon(x^\sigma, x^\gamma)\right] \tag{2.38}$$

and is antisymmetric within each pair of indices. These operators satisfy

$$[a_i^\sigma, a_j^{\tau\dagger}] = \delta_{ij}\delta^{\sigma\tau} + 4\epsilon_{ip}\epsilon_{jq} a_p^{\alpha\dagger} \Delta^{-1}_{\epsilon_{(\alpha\sigma)(\tau\beta)}} a_q^\beta \tag{2.39}$$

and

$$[a_i^\sigma, a_j^\tau] = 0 = [a_i^{\sigma\dagger}, a_j^{\tau\dagger}],$$

from which one can obtain the required traceless condition

$$\epsilon_{pq} a_p^{\sigma\dagger} a_q^{\tau\dagger} = 0.$$

For two rows [$Sp(4)$] we have

$$[a_i^\sigma, a_j^{\tau\dagger}] = \delta^{\sigma\tau}\delta_{ij} + \epsilon_{ip}\epsilon_{jq}(\delta^{\alpha\tau}\delta^{\beta\sigma} - \delta^{\alpha\beta}\delta^{\sigma\tau}) \times a_p^{\alpha\dagger}(n + N)^{-1} a_q^\beta, \sigma, \tau = 1, 2. \tag{2.40}$$

The generators are

$$S_{ij} = \sum_{\alpha=1}^{\lambda} (\epsilon_{ip} a_p^{\alpha\dagger} a_j^\alpha + \epsilon_{jp} a_p^{\alpha\dagger} a_i^\alpha) \tag{2.41}$$

satisfying

$$[S_{ij}, S_{kl}] = \epsilon_{kj} S_{il} + \epsilon_{li} S_{jk} + \epsilon_{ki} S_{jl} + \epsilon_{lj} S_{ki}. \tag{2.42}$$

Also

$$[S_{ij}, a_k^{\sigma\dagger}] = \delta_{jk}\epsilon_{ip} a_p^{\sigma\dagger} + \delta_{ik}\epsilon_{jp} a_p^{\sigma\dagger}. \tag{2.43}$$

One can also write the generators as $S^{\sigma\tau} = \epsilon^{\sigma\gamma} P^{\gamma\tau} + \epsilon^{\tau\gamma} P^{\gamma\sigma}$, transforming the top index μ of $a_k^{\mu\dagger}$.

It is possible to carry out an analysis similar to that for $O(n)$ and $Sp(n)$ for metrics g which obey certain conditions, such as $g^t g = 1$, so that one

may also have modified bosons for the noncompact groups.

3. BASIS STATES FOR IRREDUCIBLE REPRESENTATIONS OF $O(n)$

In this section we use the modified bosons to obtain the states of highest weight for $O(n)$, from which we will obtain the general state, in the Gel' fand basis, for $O(3)$ and $O(4)$. An arbitrary basis state is obtained from that of highest weight by application of the lowering operators. The raising and lowering operators for $O(n)$ have been obtained by Pang and Hecht[6] and Wong.[7] Wong[8] has indicated how one can obtain the general Gel' fand state using bosons, but it will be seen that our modified bosons permit a much greater simplicity, and reveal the group structure more fully.

The Gel' fand state has been explained by Pang and Hecht.[6] The state of highest weight is

$$|\max\rangle = \left| \begin{array}{l} m_{2k,1}\, m_{2k,2} \cdots m_{2k,k-1} m_{2k,k} \\ m_{2k,1}\, m_{2k,2} \cdots m_{2k,k-1} \\ \quad \vdots \\ m_{2k,1} \\ m_{2k,1} \end{array} \right\rangle \tag{3.1}$$

with

$$m_{2k,1} \geq m_{2k,2} \cdots \geq |m_{2k,k}| \text{ for } O(2k) \tag{3.2}$$

and

$$|\max\rangle = \left| \begin{array}{ll} m_{2k+1,1} m_{2k+1,2} \cdots & m_{2k+1,k} \\ \quad \vdots & \quad m_{2k+1,k} \\ m_{2k+1,1} & \end{array} \right\rangle \tag{3.3}$$

with

$$m_{2k+1,1} \geq m_{2k+1,2} \cdots \geq m_{2k+1,k} \text{ for } O(2k+1). \tag{3.4}$$

Let

$$A_i^{\sigma\dagger} = a_{2i-1}^{\sigma\dagger} - i a_{2i}^{\sigma\dagger} \quad i = 1, \cdots k, \tag{3.5}$$

where the a's are our modified bosons. We will also use

$$\bar{A}_i^{\sigma\dagger} = a_{2i-1}^{\sigma\dagger} + i a_{2i}^{\sigma\dagger}, \quad i = 1, \cdots k. \tag{3.6}$$

Then

$$|\max\rangle = M^{-1/2} (A_1^\dagger)^{m_{n,1}-m_{n,2}} (A_{12}^\dagger)^{m_{n,2}-m_{n,3}} \times \cdots \times (A_{12\ldots k-1}^\dagger)^{m_{n,k-1}-m_{n,k}} (A_{12\ldots k}^\dagger)^{m_{n,k}}, \tag{3.7}$$

where M is the normalization factor, and the antisymmetric combination $A_{12\ldots p}^\dagger$ is defined as in (1.2).

We see that for this expression to be meaningful, all the $m_{n,i}, i = 1, \cdots, k$, must be nonnegative integers satisfying (3.2) and (3.4). Because of our global treatment of $O(n)$, only the tensor representations appear, and the $m_{n,i}$ cannot be half integers. However we can include the case, for $O(2k)$, when $m_{2k,k}$ becomes negative:

$$|\max\rangle = M^{-1/2} (A_1^\dagger)^{m_{2k,1}-m_{2k,2}} \cdots \times (A_{12\ldots k-1}^\dagger)^{m_{2k,k-1}+m_{2k,k}} (\tilde{A}_{12\ldots k}^\dagger)^{-m_{2k,k}}, \tag{3.8}$$

if $m_{2k,k} \leq 0$,

where

$$\tilde{A}_{i_1 i_2 \cdots i_k}^\dagger = \sum \epsilon(i_1 \cdots i_k) A_1^{i_1\dagger} \cdots A_{k-1}^{i_{k-1}\dagger} \bar{A}_k^{i_k\dagger}.$$

To show that $|\max\rangle$ given by (3.7) or (3.8) is the state of highest weight, we use Cartan's theorem which states that the highest-weight polynomial, in a basis for an irreducible representation of a semisimple Lie group, is unique. From the considerations of Sec. 1, we see that (3.7) and (3.8) are states in a basis for an irreducible representation of $O(n)$, since they are linear combinations of traceless tensors, each with a definite symmetry.

The weight of these states is given by

$$J_{2\alpha,2\alpha-1} |\max\rangle = m_{n,\alpha} |\max\rangle \; \alpha = 1, \cdots k. \tag{3.9}$$

We have

$$[J_{2\alpha,2\alpha-1}, A_i^{\sigma\dagger}] = \delta_{i\alpha} A_i^{\sigma\dagger}$$

and

$$[J_{2\alpha,2\alpha-1}, \bar{A}_k^{\sigma\dagger}] = -\delta_{k\alpha} \bar{A}_k^{\sigma\dagger}$$

so that

$$[J_{2\alpha,2\alpha-1}, A_{12\ldots q}^\dagger] = \begin{cases} A_{12\ldots q}^\dagger, q \geq \alpha \\ 0, \quad q < \alpha \end{cases},$$

and

$$[J_{2\alpha,2\alpha-1}, \tilde{A}_{12\ldots k}^\dagger] = \begin{cases} -\tilde{A}_{12\ldots k}^\dagger, \alpha = k \\ \tilde{A}_{12\ldots k}^\dagger, \alpha < k \end{cases}.$$

Hence (3.9) follows.

The states (3.7) and (3.8) are of highest weight because

$$D_{p+1}^p |\max\rangle = 0, p = 1, \cdots k-1,$$
$$A_k^{k-1} |\max\rangle = 0 \text{ for } O(2k) \tag{3.10}$$

and

$$D_{p+1}^p |\max\rangle = 0, p = 1, \cdots k-1,$$
$$E_{2k+1}^k |\max\rangle = 0 \text{ for } O(2k+1), \tag{3.11}$$

where $D_{p+1}^p, A_k^{k-1}, E_{2k+1}^k$ are raising generators of $O(2k)$ and $O(2k+1)$ corresponding to the simple roots, as defined by Wong.[7]

We have

$$[D_{p+1}^p, A_i^{\sigma\dagger}] = \delta_{i-1,p} A_{i-1}^{\sigma\dagger}$$

with

$$[D_{p+1}^p, A_1^{\sigma\dagger}] = 0, p = 1, \cdots k-1$$

and
$$[D^p_{p+1}, \bar{A}^{\sigma\dagger}_k] = 0,$$
so that
$$[D^p_{p+1}, A^\dagger_{12\cdots q}] = 0, q = 1, \cdots k$$
and
$$[D^p_{p+1}, \tilde{A}^\dagger_{12\ldots k}] = 0.$$
Also
$$[A^{k-1}_k, A^{\sigma\dagger}_i] = 0$$
so that
$$[A^{k-1}_k, A^\dagger_{12\ldots q}] = 0, q = 1, \cdots k,$$
and
$$[A^{k-1}_k, \bar{A}^{\sigma\dagger}_k] = -A^{\sigma\dagger}_{k-1}$$
so that
$$[A^{k-1}_k, \tilde{A}^\dagger_{12\ldots k}] = 0.$$
Hence (3.10) follows.

We have also
$$[E^k_{2k+1}, A^{\sigma\dagger}_i] = 0$$
so that (3.11) follows.

Hence (3.7) and (3.8) are solutions of (3.10) and (3.11) with weights given by (3.9) and by Cartan's theorem they are the only solutions. These are then the required states of highest weight.

The task of calculating the normalization M is greatly simplified by the fact that $A^{\sigma\dagger}_i, \bar{A}^{\sigma\dagger}_i$ behave as ordinary bosons, i.e.,
$$[A^\sigma_i, A^{\tau\dagger}_j]\,|L\rangle = 2\delta_{ij}\delta^{\sigma\tau}\,|L\rangle, \tag{3.12}$$
where $|L\rangle$ is a state consisting of A's only. (3.12) can be proved from the commutation relations (2.26) and (2.27), but is most easily seen from the realization (2.24) of $a^{\sigma\dagger}_i$. We have
$$\begin{aligned} A^{\sigma\dagger}_i A^{\tau\dagger}_j\,|0\rangle &= \left[(x^\sigma_{2i-1} - ix^\sigma_{2i}) - 2(x^\alpha, x^\beta)\Delta^{-1}_{(\alpha\beta)(\sigma\gamma)} \right. \\ &\left. \times \left(\frac{\partial}{\partial x^\gamma_{2i-1}} - i\frac{\partial}{\partial x^\gamma_{2i}}\right)\right](x^\tau_{2j-1} - ix^\tau_{2j}) \\ &= (x^\sigma_{2i-1} - ix^\sigma_{2i})(x^\tau_{2j-1} - ix^\tau_{2j}). \end{aligned} \tag{3.13}$$
We see that, in the state of highest weight (3.7), only the boson part of the modified bosons give a contribution.

With the state of highest weight we associate the Young tableau with $m_{n,i}$ i's in the ith row, for $i = 1, \cdots, k$. From this tableau we can write down immediately the normalization in terms of hook lengths.[9] Under an analysis similar to that for this section, $Sp(n)$ reveals many of the same features.

4. STATES FOR $O(3)$ AND $O(4)$

Let us first mention $O(2)$. The general state is
$$|m\rangle = \frac{(a^\dagger_1 - ia^\dagger_2)^m}{(2^m m!)^{1/2}}\,|0\rangle, m \geq 0, \tag{4.1}$$
$$= \frac{(a^\dagger_1 + ia^\dagger_2)^{-m}}{(2^{-m}(-m)!)^{1/2}}\,|0\rangle, m \leq 0, \tag{4.2}$$
and $J_{21}\,|m\rangle = m\,|m\rangle$ (m is any integer). For $O(3)$ the state of highest weight is
$$\left|\begin{matrix} l \\ l \end{matrix}\right\rangle = M(l)^{-1/2}(a^\dagger_1 - ia^\dagger_2)^l\,|0\rangle, M(l) = 2^l l!. \tag{4.3}$$
Let
$$J_\pm = J_{32} \pm iJ_{31}. \tag{4.4}$$
Then the lowering operator is J_- and
$$J_-\left|\begin{matrix} l \\ m \end{matrix}\right\rangle = -i[(l - m + 1)(l + m)]^{1/2}\left|\begin{matrix} l \\ m-1 \end{matrix}\right\rangle. \tag{4.5}$$
We obtain for the general state
$$\left|\begin{matrix} l \\ m \end{matrix}\right\rangle = [M(m)]^{-1/2}(i)^{m-l}(a^\dagger_1 - ia^\dagger_2)^m a^{\dagger l-m}_3\,|0\rangle, \tag{4.6}$$
where
$$M(m) = 2^l l!(l - m)!(l + m)!/2l! \tag{4.7}$$
To obtain this result, we use the traceless condition in the form
$$(a^\dagger_1 - ia^\dagger_2)(a^\dagger_1 + ia^\dagger_2) = -a^{\dagger 2}_3. \tag{4.8}$$
We also interpret negative powers of $a^\dagger_1 - ia^\dagger_2$ with this relation, i.e.,
$$(a^\dagger_1 + ia^\dagger_2) = -(a^\dagger_1 - ia^\dagger_2)^{-1}a^{\dagger 2}_3. \tag{4.9}$$
Hence,
$$\left|\begin{matrix} l \\ -l \end{matrix}\right\rangle = \frac{(a^\dagger_1 + ia^\dagger_2)^l}{(2^l l!)^{1/2}}\,|0\rangle \tag{4.10}$$
is the minimal state.

We could treat the state of highest weight as consisting of bosons, but we could not then use (4.8), and the general state (4.6) would lose its simplicity. One would obtain (4.6) with
$$a^{\dagger l-m}_3 = \left(x_3 - r^2(3 + 2N)^{-1}\frac{\partial}{\partial x_3}\right)^{l-m}$$
in expanded form. The general state (4.6) is the operator form of spherical harmonics.

If we wish to add extra rows to the Young symmetry pattern, then we know[2,3] that tensors for

which the sum of the lengths of the first two columns is greater than three are zero. This is shown in the following relations, which follow from the traceless conditions (1.3).

$$a_{ij}^{\dagger}a_{jk}^{\dagger} = 0, i, j, k = 1, 2, 3 \text{ (no summation)} \quad (4.11)$$

and

$$a_{123}^{\dagger 2} = 0, a_i^{\dagger}a_{123}^{\dagger} = 0, a_{ij}^{\dagger}a_{123}^{\dagger} = 0, i, j = 1, 2, 3. \quad (4.12)$$

For two rows, the state of highest weight is

$$\left| \begin{matrix} l \\ l \end{matrix} \right\rangle \propto (a_1^{\dagger} - ia_2^{\dagger})^{l-1}(a_{32}^{\dagger} - ia_{13}^{\dagger})|0\rangle \quad (4.13)$$

and

$$\left| \begin{matrix} l \\ m \end{matrix} \right\rangle = M(m)^{-1/2}\left[\frac{l}{l+1}\right]^{1/2}(-i)^{l-m}(a_1^{\dagger} - ia_2^{\dagger})^m \times a_3^{\dagger l-m-1}a_{21}^{\dagger}|0\rangle \quad (4.14)$$

to obtain which, we use

$$a_3^{\dagger}(a_{32}^{\dagger} - ia_{13}^{\dagger}) = (a_1^{\dagger} - ia_2^{\dagger})a_{21}^{\dagger}. \quad (4.15)$$

Here l is any positive integer. The $l = 0$ state is

$$(a_{123}^{\dagger}/\sqrt{3!})|0\rangle \text{ (the triple scalar product).} \quad (4.16)$$

For $O(4)$ the state of highest weight is

$$\left| \begin{matrix} m_1 & m_2 \\ m_1 & \\ m_1 & \end{matrix} \right\rangle = M\binom{m_1}{m_1}^{-1/2} A_1^{\dagger m_1-m_2}A_{12}^{\dagger m_2}|0\rangle, \quad (4.17)$$

where

$$M\binom{m_1}{m_1} = \frac{2^{m_2+m_1}(m_1+1)!\, m_2!(m_1-m_2)!}{(m_1-m_2+1)!}, \quad (4.18)$$

provided $m_2 \geq 0$.

The lowering operator, obtained from Wong,[7] is

$$L_- = (iK_-J_{21} - J_-J_{43})(2J_{21} + 1) + \tfrac{1}{2}iJ_-^2K_+, \quad (4.19)$$

where

$$K_{\pm} = J_{42} \pm iJ_{41}. \quad (4.20)$$

Now

$$L_- \left| \begin{matrix} m_1 & m_2 \\ l & \\ l & \end{matrix} \right\rangle = N^{1/2} \left| \begin{matrix} m_1 & m_2 \\ l-1 & \\ l-1 & \end{matrix} \right\rangle, \quad (4.21)$$

where

$$N = 2l(2l+1)(m_1 - l + 1)(m_1 + l + 1)(l + m_2) \times (l - m_2).$$

The action of L_- is remarkably simple, $A_1^{\dagger}$ being changed to $a_4^{\dagger}$:

$$\left| \begin{matrix} m_1 & m_2 \\ l & \\ l & \end{matrix} \right\rangle = i^{l-m_1}M\binom{l}{l}^{-1/2} a_4^{\dagger m_1-l}A_1^{\dagger l-m_2}A_{12}^{\dagger m_2}|0\rangle, \quad (4.22)$$

where

$$M\binom{l}{l} = 2^{2l+m_2-m_1}\frac{(m_1+1)!m_2!(m_1-l)!(l-m_2)!(l+m_2)!(l+m_1+1)!}{(2l+1)!(m_1+m_2)!(m_1-m_2+1)!}. \quad (4.23)$$

In order to obtain (4.22), we must use, in particular,

$$A_{12}^{\dagger}(a_{12}^{\dagger} + a_{34}^{\dagger}) = iA_1^{\dagger}(a_3^{\dagger} - ia_4^{\dagger}). \quad (4.24)$$

The general state of the Gel' fand basis is now obtained by lowering m from its highest value l to a general value m, using $J_-(l-m)$ times on (4.22). One obtains Jacobi polynomials:

$$\left| \begin{matrix} m_1 & m_2 \\ l & \\ m & \end{matrix} \right\rangle = i^{l-m_1}M\binom{l}{m}^{-1/2} P_{l-m}^{(m+m_2,m-m_2)}\left(\frac{a_3^{\dagger}}{ia_4^{\dagger}}\right) \times a_4^{\dagger m_1-m}A_1^{\dagger m-m_2}A_{12}^{\dagger m_2}|0\rangle, \quad (4.25)$$

where

$$M\binom{l}{m} = \frac{2^{2m+m_2-m_1}(m_1+1)!m_2!(m_1-l)!(l-m_2)!(l+m_2)!(l+m_1+1)!}{(2l+1)(m_1+m_2)!(m_1-m_2+1)!(l+m)!(l-m)!}. \quad (4.26)$$

To show this, one uses the formula

$$\frac{d}{dx}P_n^{(\alpha,\beta)}(x) = \tfrac{1}{2}(\alpha+\beta+n+1)P_{n-1}^{(\alpha+1,\beta+1)}(x) \quad (4.27)$$

for positive and negative α and β.

If the top indices of the Jacobi polynomial become negative we use the formula

$$\binom{n}{\alpha}P_n^{(-\alpha,\beta)}(x) = \binom{n+\beta}{\alpha}\left(\frac{x-1}{2}\right)^{\alpha}P_{n-\alpha}^{(\alpha,\beta)}(x). \quad (4.28)$$

The negative exponents of $A_1^{\dagger}$, which may appear,

are interpreted with the relation (4.24) and

$$iA_2^\dagger(a_{12}^\dagger + a_{34}^\dagger) = A_{12}^\dagger \bar{A}_1^\dagger, A_{12}^\dagger \bar{A}_{12}^\dagger = -(a_{12}^\dagger + a_{34}^\dagger)^2. \tag{4.29}$$

Hence, for example, if $m \leq -m_2$,

$$\left| \begin{matrix} m_1 & m_2 \\ l & \\ m & \end{matrix} \right\rangle = i^{l-m_1}(-)^{m_2} 2^{2m} M \binom{l}{m}^{-1/2} \times P_{l+m}^{(-m-m_2, m_2-m)}\left(\frac{a_3^\dagger}{ia_4^\dagger}\right) \times a_4^{\dagger m_1+m} \bar{A}_1^{\dagger -m_2-m} \bar{A}_{12}^{\dagger m_2} \mid 0\rangle. \tag{4.30}$$

If $m_2 = 0$ (i.e., only one row in the Young pattern) the general state (4.25) is expressed in terms of Gegenbauer polynomials.[5]

From the general state, one can find the matrix elements of J_{43}:

$$J_{43} \left| \begin{matrix} m_1 & m_2 \\ l & \\ m & \end{matrix} \right\rangle = i\left[\frac{(l+m+1)(l-m+1)(m_1-l)(m_1+l+2)(l-m_2+1)}{(2l+1)(2l+3)(l+1)^2} \times \cdots \right.$$
$$\left. \times (l+m_2+1)\right]^{1/2} \left| \begin{matrix} m_1 & m_2 \\ l+1 & \\ m & \end{matrix} \right\rangle + \frac{m(m_1+1)m_2}{l(l+1)} \left| \begin{matrix} m_1 & m_2 \\ l & \\ m & \end{matrix} \right\rangle$$
$$- i\left[\frac{(l+m)(l-m)(m_1-l+1)(m_1+l+1)(l-m_2)(l+m_2)}{(2l+1)(2l-1)l^2}\right]^{1/2} \left| \begin{matrix} m_1 & m_2 \\ l-1 & \\ m & \end{matrix} \right\rangle \tag{4.31}$$

which is as required.[10]

This result is obtained by means of the standard differentiation formulae, and recurrence relations for Jacobi polynomials.[11]

One can also carry out a similar analysis when $m_2 \leq 0$. The state of highest weight is

$$\left| \begin{matrix} m_1 & m_2 \\ m_1 & \\ m_1 & \end{matrix} \right\rangle = M^{-1/2} A_1^{\dagger m_1+m_2} \bar{A}_{12}^{\dagger -m_2} \mid 0\rangle, \tag{4.32}$$

where

$$M = \frac{2^{m_1-m_2}(-m_2)!(m_1+1)!}{(m_1+m_2+1)}. \tag{4.33}$$

Formulas similar to (4.29) hold, e.g.,

$$A_1^\dagger(a_{12}^\dagger - a_{34}^\dagger) = i\bar{A}_{12}^\dagger A_2^\dagger, \tag{4.34}$$

and the analysis proceeds in the same way.

1 G. Baird and L. C. Biedenharn, J. Math. Phys. 4, 1449 (1963).
2 H. Weyl, *Classical Groups* (Princeton. U. P., Princeton, N.J., 1946).
3 M. Hamermesh, *Group Theory* (Addison-Wesley, Reading, Mass., 1962).
4 W. J. Holman, III, J. Math. Phys. 10, 1710 (1969).
5 N. Y. Vilenkin, *Special Functions and Theory of Group Representations* (A.M.S. Transl., Providence, Rhode Island, 1968), Chap. IX.
6 S. C. Pang and K. T. Hecht, J. Math. Phys. 8, 1233 (1967).
7 M. K. F. Wong, J. Math. Phys. 8, 1899 (1967).
8 M. K. F. Wong, J. Math. Phys. 10, 1065 (1969).
9 M. Ciftan and L. C. Biedenharn, J. Math. Phys. 10, 221 (1969).
10 I. M. Gel'fand, R. A. Minlos, and Z. Ya. Shapiro, *Representations of the Rotation and Lorentz Groups and their Applications*, (MacMillan, New York), 1963.
11 A. Erdélyi, W. Magnus, F. Oberhettinger, F. Tricomi, *Higher Transcendental Functions* (Bateman Manuscript Project, (McGraw-Hill, New York, 1953) Vol. II.

The Jahn–Teller Theorem

E. I. Blount
Bell Telephone Laboratories Inc. Murray Hill, New Jersey
(Received 24 January 1968; Revised Manuscript Received 30 November 1970)

A compact proof of the Jahn–Teller theorem is given. The method distinguishes between two cases: (1) If the irreducible representation Γ to which the wavefunction belongs is reducible under one of the subgroups G_s which leave one atom invariant; the proof is trivial and would apply in space of any number of dimensions. (2) If Γ remains irreducible under all G_s, more detailed attention is necessary. In two or three dimensions, however, it is straightforward to establish the theorem for this case. It is further shown that in composite-dimensional spaces, some violations of the theorem would be found under (2).

1. INTRODUCTION

In 1937, Jahn and Teller[1] proved the following theorem: If a molecule has a degenerate electronic wavefunction, it is unstable with respect to displacements of the atoms, unless all the atoms lie on a line. The proof was restricted to the case of spinless electrons or a molecule with an even number of electrons. This restriction was soon removed by Jahn,[2] who showed that it is true for an odd number of electrons, except that the Kramers degeneracy does not produce instability. In both cases the kinetic energy of the nuclei was neglected, so that the statements refer to the equilibrium positions of the nuclei in the Born–Oppenheimer approximation. The theorem was proved by exhaustion; that is, for each of a sufficiently large number of structures (in general, several for each point group) and the corresponding possible symmetries of electronic wavefunctions, the theorem was verified as a special case. The result is so simple that a more direct approach seems desirable. Such a proof is the main purpose of this paper

One reason for wanting a more deductive proof is that the proof by exhaustion gives no feeling whether the theorem is "accidental" or whether it reflects a much more general result. With this in mind, we shall proceed as far as possible without restricting ourselves to three dimensions. It will indeed turn out that the theorem is not true in a composite (as opposed to prime) number of dimensions. Unfortunately, the extent of its truth in prime-dimensional spaces will not be fully answered.

As shown by Jahn and Teller, the proof of the theorem is equivalent to the following group-theoretical problem.

Let Γ_D be that representation of the point group G whose basis functions are all the possible linearly independent displacements of the atoms of the molecule under discussion. This will include Γ_V, the possibly reducible representation according to which a vector transforms and Γ_A, the representation of an axial vector—the latter corresponding to rigid rotations of the molecule, the former to rigid translations. We want to consider the representation $\overline{\Gamma}_D = \Gamma_D - \Gamma_V - \Gamma_A$. Now, if Γ is the representation according to which the electronic wave function transforms the products $\psi_\alpha^*\psi_\beta$ belong to the representation $\Gamma^*\Gamma$. The imposition of time-reversal symmetry, however, requires that Γ be a real representation, which may possibly be decomposable into two absolutely irreducible representations. Following Lyubarskii,[3] I shall call such representations, which are irreducible under the restriction that all matrix elements are real, physically irreducible. Time reversal further requires that we consider not Γ^2, but $[\Gamma^2]$, which designates the appropriately symmetrized or antisymmetrized product of Γ with itself. If $\chi(R)$ is the character of Γ, the character of $[\Gamma^2]$ is $[\chi^2] = \frac{1}{2}[\chi^2(R) + K^2\chi(R^2)]$, where $K^2 = 1$ for single group representations and $K^2 = -1$ for double group representations. Now the number of independent matrix elements of a perturbation which transforms according to $\overline{\Gamma}_D$ with states of Γ is

$$N = g^{-1}\sum_R \overline{\chi}_D[\chi^2],$$

the sum being extended over all g elements of the group; $\overline{\chi}_D$ is the character of $\overline{\Gamma}_D$.

Now Γ_D will, in general, contain N_0 displacements, such as expansion of the whole molecule, which belong to the identity representation Γ_0. Such displacements cannot change the symmetry, so we are not interested in them and, finally, we want to consider not $\overline{\Gamma}_D$ but $\Gamma_D' = \Gamma_D - N_0\Gamma_0 - \Gamma_V' - \Gamma_A'$, where $\Gamma_V'(\Gamma_A')$ is $\Gamma_V(\Gamma_A)$ with any identity representations removed to avoid oversubtracting. Finally, then, the essential question is is $N' > 0$?

$$\begin{aligned} N' &\equiv N_D - N_0 - N_V' - N_A', \\ N_D &\equiv \frac{1}{g}\Sigma[\chi^2]\chi_D, \\ N_V' &\equiv \frac{1}{g}\Sigma[\chi^2]\chi_V', \\ N_A' &\equiv \frac{1}{g}\Sigma[\chi^2]\chi_A', \\ N_0 &\equiv \frac{1}{g}\Sigma\chi_D. \end{aligned} \tag{1.1}$$

This is the question Jahn and Teller answered by exhaustion.

It is worthwhile to emphasize that (1.1) has three simple interpretations. The one most frequently encountered is that if (1.1) is satisfied, a displacement of Γ_D' will lower the energy of the electronic state Γ; for since Γ_D' does not contain Γ_0, all matrix elements must lead to a breaking of the degeneracy, with a consequent lowering of the lowest eigenvalue. Alternatively, one can say that the charge density in a particular state ψ_α cannot

have the full symmetry of G, but will in general have components belonging to all other representations which occur in $[\Gamma^2]$. If there are displacements with any of these symmetries, they will feel a force and the molecule will distort. Finally, when we view the molecule as having vibrational degrees of freedom, (1.1) expresses the condition that there be matrix elements between the states of ψ of Γ, and the states formed by exciting a vibrational degree of freedom to its first excited state while leaving the electronic state at the same energy. These matrix elements will then lead to strong correlations between the electronic charge distribution and the nuclear configuration, without charging the over-all symmetry of the state.

2. THE PROOF

We start with an outline of the proof. The first step is to show that the calculation of N_D or N_0 can be reduced to a calculation in the subgroups G_s under which individual atoms are invariant.

The first use to which we put this result is to demonstrate that we can forget about N_V' in (1.1).

We then show that if Γ is reducible under some G_s, the Jahn–Teller instability follows immediately.

The case that Γ is irreducible under all the subgroups of the atoms is then treated in two and three dimensions, where it is easily shown to lead to no difficulties. The consideration of higher dimensions is deferred to the next section.

A. Introduction of Subgroups G_s

We start with the well-known and obvious fact that $\Gamma_D = \Gamma_P \Gamma_V$, where Γ_P is the representation of the group as a group of permutations of the nuclei. If the operation R of G takes nucleus α into the site of nucleus β, we have $D^P_{\beta\alpha}(R) = 1$, if not, it is zero. In general, $D^P_{\beta\alpha}(R) = \delta(\beta, R\alpha)$. Thus

$$\chi_P(R) = \sum_\alpha \delta(\alpha, R\alpha) \text{ and } \chi_D(R) = \chi_V(R) \sum_\alpha \delta(\alpha, R\alpha).$$

Now, in general, a given nucleus is not taken into the positions of all the other nuclei by the operations of G: Γ_P, in general, is intransitive. We can divide the nuclei into transitive sets Γ_s, such that, in each set, each nucleus is carried to the position of any other member of the set by some operation of G.

If, for any representation Γ, we want to know $g^{-1}\sum_G \chi_P(R)\chi(R)$, we can now write

$$g^{-1}\sum_G \chi_P(R)\chi(R) = g^{-1}\sum_{\alpha,R} \delta(\alpha, R\alpha)\chi(R)$$

$$= g^{-1}\sum_s \sum_{\alpha\subset\Gamma_s} \sum_R \delta(\alpha, R\alpha)\chi(R). \qquad (2.1a)$$

If we pick a particular nucleus α, $\delta(\alpha, R\alpha) = 0$ unless R belongs to the subgroup which leaves α invariant. For any other member of the same Γ_s, a similar situation holds and the subgroup will be conjugate and therefore isomorphic to the subgroup for α. Thus the sum of the characters $\chi(R)$ will be the same for the subgroup of each α in one Γ_s, and we can call the subgroup G_s. The order g_s of G_s is clearly g divided by the number of nuclei in Γ_s. Thus we have

$$g^{-1}\sum_G \chi_P(R)\chi(R) = \sum_s g_s^{-1} \sum_{G_s} \chi(R). \qquad (2.1b)$$

In particular, from (1.1)

$$N_D = \sum_s g_s^{-1} \sum_{G_s} [\chi^2]\chi_V,$$

$$N_0 = \sum_s g_s^{-1} \sum_{G_s} \chi_V. \qquad (2.2)$$

B. Elimination of N_v'

The first thing we want to do with this result is to show that we need not worry about N_V' in (1.1). To do this, we shall prove that if any irreducible representation can occur in $[\Gamma^2]$ for some Γ, and if it is contained in Γ_v, it is contained more times in Γ_D. The proof applies in space of arbitrary dimensionality.

Let us then consider a physically irreducible representation Γ_i which occurs l_i times in the reduction of Γ_V'. It is contained n_i times in Γ_D, where, from (2.1a) and (2.2),

$$n_i = \sum_s g_s^{-1} \sum_{G_s} \chi_V' \chi_i = \sum_s g_s^{-1} \sum_{G_{s'j}} \chi_i \chi_j l_j$$

so that

$$n_i \geq l_i N_s \geq l_i,$$

N_s being the number of different transitive sets Γ_s. The equality $n_i = l_i$ holds if and only if the following conditions are fulfilled:

(1) $N_s = 1$. That is, all atoms are the same and are related to each other by symmetry operations of G.
(2) Γ_i is irreducible under G_s.
(3) No other Γ_j in Γ_V is equivalent to Γ_i under G_s.

Now, condition (2) requires that the molecule have zero extension in all l_i subspaces of Γ_V' belonging to Γ_i. (If not, the nonvanishing projection of the radius vector of an atom in Γ_i would be an invariant under G_s and thus belong to Γ_0 under G_s.) From this it follows that G must contain the entire orthogonal group $O(d_i)$ for the subspaces Γ_i. In particular, G would contain the operation J_i, the inversion operator in the subspace. For any Γ, $[\Gamma^2]$ is even under J_i, while Γ_i is odd. Thus, such a Γ_i could not occur in any $[\Gamma^2]$.

Therefore, if Γ_i can occur in $[\Gamma^2]$ and does occur l_i times in Γ_V', it occurs more times in $\Gamma_D (n_i > l_i)$. We can indeed forget about N_V' in (1.1).

We return to consider (2.2). Under any G_s, Γ_V

certainly contains Γ_0 at least once, since G_s is defined as the group under which a vector from the center to a nucleus remains invariant.

C. Γ reducible under some G_s

If, under some G_s, Γ is not physically irreducible, $[\Gamma^2]$ must contain Γ_0 more than once. Thus $N_D - N_0$ will be positive.

This result also has the meaning that in the subrepresentation of Γ_D consisting of motions of the nuclei along their radius vectors (which belong to Γ_0 under G_s), there is at least one set of displacements which transform according to a representation Γ_i which also occurs in $[\Gamma^2]$ and which is not Γ_0. Furthermore, none of these displacements can be a rotation of the molecule as a whole, since rotations are compounded of motions of each atom perpendicular to its radius vector. We need not worry about N_A' in this case, then.

This subsection demonstrates that a molecule is unstable unless Γ is physically irreducible under all G_s.

D. Γ irreducible under all G_s

We must finally consider the case that Γ remains irreducible under all G_s. When Γ_V is completely reduced under G_s, it contains $\Gamma_0 l_0$ times with $l_0 \geq 1$. The remaining part we call Γ_V'. If Γ is physically irreducible under all G_s, we have from 2.2 that

$$N_D - N_0 = \sum_s g_s^{-1} \sum_{G_s} [\chi^2] \chi_V' \text{ (if } \Gamma \text{ is irreducible under all } G_s\text{)} \tag{2.3}$$

In two or three dimensions this problem is quite simple though a bit tedious, at least in comparison with the previous section. The simplicity is due to the fact that the G_s of an atom not at the center of the molecule is one of the following groups:

(1) C_n, one n-fold axis of symmetry.
(2) C_{nv}, C_n supplemented by mirrors containing the axis,
(3) C_s, one mirror plane.

These groups have only one- and two-dimensional physically irreducible representations. Therefore, being degenerate by hypothesis, Γ can only be two-dimensional. The following cases must be considered:

(a) If Γ is a double group representation, it has only the Kramers degeneracy, which cannot be split while time-reversal symmetry is preserved. Hereafter, only single group representations will be considered.

(b) If all atoms are on a line, the physically irreducible representations are characterized by an angular momentum $l, l \geq 0$. $[\Gamma_l^2]$ contains Γ_0 and Γ_{2l} under G_s as under G. Since Γ_V contains only Γ_0 and Γ_1, $N_D = N_0$ and no instability occurs. These are the two exceptions noted by Jahn and Teller.

(c) If, under G, Γ_V has no three-dimensional irreducible component, but the molecule is not linear, there must be atoms whose G_s is a subgroup, not necessarily proper, of C_{2v}. These G_s have only one-dimensional irreducible representations, so Γ could not remain irreducible under it. In other words, this case does not arise.

(d) This leaves the case that Γ_V, and also Γ_A, are three-dimensional irreducible under G, while Γ is two-dimensional under G and all G_s. Evidently, $[\Gamma^2]$ cannot contain Γ_V or Γ_A.

The groups involved are the tetrahedral groups T, T_d, and T_h, the octahedral groups O, O_h, and the icosahedral groups I and I_h. A glance at the character tables shows that the last two have no two-dimensional physically irreducible representations, while the other groups do have some (in the case of T, one pair of absolutely irreducible representations). For all these representations, $[\Gamma^2]$ contains a two-dimensional representation which also occurs in the reduction of the representation corresponding to uniform strains. Since any molecule belonging to one of these groups must have finite extension in all directions, it must have, in its Γ_D, displacements corresponding to all possible strains. Thus this two-dimensional representation contained in $[\Gamma^2]$ is also in Γ_D, which establishes the theorem for this case.

I will briefly sketch the main points of a more deductive proof. One easily shows that if some G_s is C_3 or C_{3v}, its only degenerate representation is contained in both $[\Gamma^2]$ and Γ_V' under G_s, which establishes the instability for such cases. For axes with $n \geq 4$, this argument does not work and we have to show instead that such cases do not arise. We note that Γ^2 must contain a one-dimensional representation other than the identity (and even under inversion if it is in G). Since I is simple, neither it nor I_h have such a representation, and they cannot have a two-dimensional Γ according to this argument. This leaves only the need to show that one cannot have Γ remain irreducible under fourfold axes. This is easy to do using the intermediate group D_4, but to save space we leave the details to the reader if he be interested.

The net result is that the situation posed at the beginning of part (d) can occur only in the groups T, T_d, T_h, O, O_h, and then only if all atoms lie on threefold axes, so that the molecules must consist of a set of cubes or tetrahedra—the atoms being at the apices. Furthermore, the usual assumption of point or spherical nuclei eliminates some of the possibilities, forcing the symmetry to be O_h if the nuclei are arranged on cubes or T_d if some are on tetrahedra. In the former there are two possible Γ's, in the latter, one. Thus the total number of cases under subsection D, aside from the exceptions (a) and (b), is very small,

especially if one considers the number of molecules in the shape of cubes.

E. Two- and Three-Dimensional Results

We conclude this section with two simple results valid in two or three dimensions. They can be proved by general but messy arguments, and I shall merely quote them with the remark that they can be established readily by reference to character tables.

(1) In two or three dimensions, no irreducible component of Γ_A can be contained in any $[\Gamma^2]$ unless it also occurs in $[\Gamma_V^2]$.

(2) For the crystallographic point groups and the icosahedral groups, $[\Gamma^2]$ always contains a symmetry-breaking component of $[\Gamma_V'^2]$ if Γ has more than Kramers degeneracy, where Γ_V' is the degenerate physically irreducible component of Γ_V.

From (2) the validity of the Jahn-Teller theorem for molecules with these symmetries follows from the fact that any such molecule has a distortion with the symmetry of each physically irreducible component of $[\Gamma_V'^2]$, namely those arising from a uniform strain of the molecule in the subspace Γ_V'.

Similarly, (1) shows that N_A' can be neglected in (1.1) for two or three dimensions.

Statement (2) also means that, in crystals, the Jahn-Teller splitting of defect levels can always be accomplished by motions of atoms in the nearest-neighbor shell, provided the shell does not consist of two atoms in a line with the defect, or one atom.

3. EXCEPTIONS IN MORE DIMENSIONS

It will be seen that the last step of the proof gives no confidence in the generality of the theorem. Therefore in this section we shall consider a larger class of groups in all dimensions. I have not been able to treat the general situation of molecules in n dimensions, but the consideration of single-valued groups for regular polytopes[4] in n dimensions yields some interesting results. First we review the types of such polytopes.

It is clear that in any number of dimensions n, there must be an analog to the regular tetrahedron. This is most easily constructed in $n+1$ dimensions and consists of the points $(1, 0, 0, \cdots, 0)$ and all other points on the positive axes at one unit from the origin. Projected into the hyperplane $\Sigma x_i = 1$, this yields α_n, the simplex polytope in n dimensions. Its group is clearly S_{n+1}, the symmetric group on $(n+1)$ objects.

Similarly, in n dimensions, we can consider the $2n$ points $(\pm 1, 0, \cdots, 0)$, etc., which form β_n the cross polytope, the analog of the octahedron. We shall call its group $\mathfrak{O}_n$. It may be characterized as follows. An invariant subgroup Σ_n consists of all diagonal matrices with diagonal elements ± 1; the factor group $\mathfrak{O}_n/\Sigma_n$ is S_n. Thus the order of Σ_n is 2^n, and the order of $\mathfrak{O}_n$ is $2^n n!$ The same group characterizes the measure polytope, the analog of the cube, consisting of the point $(1, 1, \cdots, 1)$ and all points produced from it by Σ_n.

For $n > 4$, this exhausts the regular polytopes. For $n = 4$, there are three others, two belonging to one group, while for $n = 3$ there are, of course, the icosahedron and dodecahedron, and, for $n = 2$, all regular polygons with five sides or more.

We shall proceed with a discussion of $\mathfrak{O}_n$. Σ_n is generated by the groups $\sigma_i, i = 1, \cdots, n$, σ_i being a reflection in the hyperplane $x_i = 0$.

Its 2^n irreducible representations are one dimensional and can be characterized by an array $(1, -1, \cdots)$ indicating which σ_i's are represented by 1 and which by -1. They fall in sets, each member of a set having the same number t, of -1's. Under the full group, the members of a set are associated,[5] and when an irreducible representation of $\mathfrak{O}_n$ is decomposed under Σ_n, it contains members of just one set, and all the members of this set will be contained an equal number of times.

Now consider the group G_s of an atom in a molecule with this symmetry. We can, without loss of generality, write its position as $(a_1, a_2, a_3, \cdots)$, with $a_1 \geq a_2 \geq a_3 \geq \cdots \geq a_n \geq 0$. Then we can call the number of zeros n_0, the number of the smallest positive a, n_1, etc. The group G_s will then be $\mathfrak{O}_{n_0} \times S_{n_1} \cdots$. Σ_{n_0} will be the largest subgroup of Σ_n contained in G_s, and the irreducible representations of G_s will be characterized, among other ways, by t', defined with respect to Σ_{n_0} as t was with respect to Σ_n.

A. The Case $0 < t < n$

(1) If $n_0 \neq 0$, the reduction of Γ under Σ_{n_0} will contain representations with more than one value of t' and will be reducible.

(2) If $n_0 = 0$ but $n_1 \neq n$, we can consider the intermediate group $\mathfrak{O}_{n_1} \times S_{n_2} \times \cdots$; by the argument just made, Γ is reducible under this group, and, *a fortiori*, under $G_s = S_{n_1} \times S_{n_2} \times \cdots$.

(3) If $n_0 = 0$ and $n_1 = n$, we want to know if Γ, irreducible under $\mathfrak{O}_n$, can be irreducible under $G_s = S_n$. This question is answered in the negative in Appendix A for $0 < t < n$.

Thus, for all cases with $0 < t < n$, Γ cannot be irreducible under G_s.

B. The Case $t = n$ or 0

If $t = n$, multiplication by $\Pi^n x_i$ changes it to one with $t = 0$. The squares of the representations are identical so far as symmetry is concerned, so we need only consider the case $t = 0$ explicitly. We note first that $[\Gamma^2]$ cannot contain Γ_V or Γ_A since all powers of Γ contain only components

with $t = 0$, while Γ_V and Γ_A have $t = 1$ and 2, respectively. Thus we need only consider whether $N_D > N_0$.

(1) If $n_0 = 0$ and $n_1 = n$, any representation of $\mathcal{O}_n$ with $t = 0$ is irreducible under $G_s = S_n$. The remaining question in this case is whether $[\Gamma^2]$ contains Γ'_V, the $(n-1)$-dimensional subrepresentation of Γ_V which remains after the component invariant under G_s has been taken out. Here, with $G_s = S_n$, Γ'_V is the representation designated by the partition $(n-1, 1)$. It is shown in Appendix B that, for a very special class of degenerate representations, $[\Gamma^2]$ does not contain $(n-1, 1)$ under S_n. This class contains those representations with rectangular Young patterns and no others. This requires that n be a composite number, not a prime.

If n is composite, a molecule in the form of the measure polytope admits wavefunctions which do not exhibit the Jahn–Teller instability.

(2) For any other set of n_i's, the question is whether a representation Γ of S_n can remain irreducible under $S_{n_0} \times S_{n_1} \times \cdots$. In Appendix B we find that the answer is no unless one n_i is $n-1$ so that G_s is S_{n-1} (or $\mathcal{O}_{n-1}$, which amounts to the same thing for $t = 0, n$). Even then, only Γ's with rectangular Young patterns remain irreducible. As just discussed, $[\Gamma^2]$ does not contain $(n-1, 1)$ under S_n, but under S_{n-1} the pattern is no longer rectangular, so $[\Gamma^2]$ does contain $\Gamma'_V = (n-2, 1)$, and $N_D > N_0$ by (2.2).

Thus, case (1) of Sec. 3B contains the only exceptions to the theorem for groups $\mathcal{O}_n$.

The case for groups S_n is readily seen to be exactly equivalent to case (2) of Sec. 3B. For the group S_n of the simplex polytope in $(n-1)$ dimensions, the only G_s for which a Γ can remain irreducible is S_{n-1} and, just as above, we find that $N_D > N_0$. Thus these groups produce no exceptions.

We conclude this section by checking to see if any further exceptions can be found in a few simple subgroups of $\mathcal{O}_n$ for n prime.

First we consider P_n, the proper subgroup. The three-dimensional example is O. $\mathcal{O}_n$ is the direct product of P_n and J, the inversion group, and its irreducible representations are irreducible representations of P_n with the additional property of being odd or even under inversion. Now let us take a molecule with symmetry P_n (we can assume that, except possibly for an atom at the center, none of its atoms has an inversion image—otherwise it would be unstable under $\mathcal{O}_n$ and, *a fortiori*, under P_n) and combine it with the molecule obtained from it by inversion. This molecule has symmetry $\mathcal{O}_n$ and is unstable, but its Γ_D consists of pairs of representation, identical under P_n, but opposite under J. In fact, it consists of Γ_D for the original molecule, with each Γ_i in Γ_D replaced by $\Gamma_i^+ + \Gamma_i^-$. $[\Gamma^2]$ cannot contain any Γ^-. Thus some Γ_i in Γ_D must be contained in $[\Gamma^2]$, and any molecule with P_n symmetry is unstable if Γ is degenerate.

The group T_n generated by Σ_n^e and S_n, where Σ_n^e is the subgroup of Σ containing an even number of reflections. The full tetrahedral group T_d is an example. This group again does not contain J which commutes with all its members, so $\mathcal{O}_n$ is also the direct product of $\mathcal{O}_n$ and J, and the argument proceeds as before.

Next let us consider Q_n, generated by Σ_n and A_n, the alternating group on n objects. The three-dimensional example is T_h. The analysis of this group proceeds almost step for step like that of $\mathcal{O}_n$, the only different result being that, if $n = l^2 + 1$, the representations with $t = 1$, induced from the representations of A_{n-1} belonging to the partition (l^l), are irreducible under $G_s = A_n$; furthermore, $[\Gamma^2]$ does not contain Γ_V under A_n. However, this does not lead to violation of the Jahn–Teller effect in any prime-dimensional spaces, because, if a molecule contained only atoms with $G_s = A_n$ [that is, atoms at $(1111\cdots)$ and all points obtained from it by sign reversal], it would actually have the full $\mathcal{O}_n$ symmetry.

Finally, we can consider the group R_n, the common subgroup of the other three, generated by Σ_n^e and A_n, exemplified by T. Again, Q_n is the direct product of R_n and J. Thus the argument used for P_n and T_n works, provided we note that a molecule with atoms only at $(111\cdots)$ and points obtained from it by changing an even number of 1's to -1's would have the group T_n.

4. DISCUSSION

We see that it is possible to give a reasonably compact and deductive proof of the Jahn–Teller theorem in two and three dimensions, though final cutting off of the retreat of the special case in the cubic groups is not particularly satisfying. In this sense, it is, perhaps, gratifying that exceptions were found in higher dimensions, since it is now clear that no really general arguments would be expected to work.

It would have been nice to be able to clean up the remaining question: Can there be molecules in prime-dimensional spaces which violate the theorem? I have wasted considerable effort in this direction, with no fruitful result. It is, of course, clear that exceptions, in any case, must be quite rare, but this was obvious before the present investigation.

After the completion of this work, I learned that Ruch and Schönhofer had already published a proof of the theorem which eliminated the detailed examination of special cases.[6] There is a close connection between the two proofs but I feel that the present method uses the basic ideas in a more direct fashion and reveals more clearly the distinction between general and special features.

The result of Sec. 2A above is a more direct and powerful form of the basic argument of Ruch and Schönhofer as contained in their conditions 1 and 2 and their Appendix. As a consequence, they are not led to make the basic distinction between Γ's which are reducible under all G_s and those which remain irreducible under all G_s. It is just this distinction, it seems to me, which is responsible for the peculiar combination of obviousness and difficulty of proof which characterizes the Jahn–Teller theorem. We found that practically all cases fall into the former category, Sec. 2C, for which the proof was remarkably simple. While the proof of the other part was considerably less appealing, it serves to emphasize the rather "lucky" nature of at least this part of the theorem, and to indicate a closer connection with the actual exceptions noted by Jahn and Teller and the imaginary exceptions we found in Sec. 3.

APPENDIX A

We consider whether a representation of $\mathfrak{O}_n$ can be irreducible under S_n. A little contemplation suggests that we try to construct representations of $\mathfrak{O}_n$ as follows. For given t, consider the subgroup $\mathfrak{O}_t \times \mathfrak{O}_{n-t}$. For $\mathfrak{O}_t$ take the product $x_1 x_2^3 x_3^5 \cdots x_t^{2\tau+1}$ and all these obtained from it by permuting the indices. These form a basis for the regular representation of S_t, which can be reduced by choosing linear combinations $A^{\alpha\rho\mu}(x_1 \cdots x_t)$. Proceed similarly for $\mathfrak{O}_{n-t}$, using the first $(n-t)$ positive even integers as exponents, obtaining basis functions $B^{\beta\sigma\nu}(x_{t+1} \cdots x_n)$. Here α and β designate an irreducible representation which will occur, in general, more than once, the occurrences being labeled by ρ and σ, while μ and ν label the rows and columns of the matrices. Now for fixed α, β, ρ, and σ, construct similar functions for all other combinations of t and $(n-t)$ indices. This set of functions for fixed α, β, ρ, and σ, obviously forms the basis for a representation of $\mathfrak{O}_n$, which will be shown to be irreducible. Let us label these functions $\psi(\alpha, \rho, \mu; \beta, \sigma, \nu; S)$, where S stands for the set of indices whose x's have odd exponents. The character of the group element $\Pi(\sigma_i^{n_i})P$ is then

$$\chi(t, \alpha, \beta; n_i, P) = \sum_S \delta(S, PS)\chi_\alpha(P)\chi_\beta(P) \exp(\Sigma n_i s_i)\pi i, \tag{A1}$$

where $\delta(S, PS) = 1$ if P takes the set S itself and zero otherwise. $\chi_\alpha\chi_\beta$ is the character of P in the subgroup of type $S_t \times S_{n-t}$ associated with S, and s_i is 1 or 0, according as i belongs to S or not. Rather than evaluate χ, we shall directly square it and sum over the group:

$$\Sigma\chi^2 = \sum_{n_i, P, S\, S'} \delta(S, PS)\delta(S', PS')\chi_\alpha^2(P)\chi_\beta^2(P) \times \prod_i (-1)^{n_i(s_i - s_i')}. \tag{A2}$$

Now the sum over $n_i = 0, 1$ vanishes if $s_i - s_i' \neq 0$. This must occur for some i if $S \neq S'$. Thus we can restrict the sum to terms $S = S'$, and obtain

$$\Sigma\chi^2 = \sum_{n_t} \sum_{S, P} \delta(S, PS)\chi_\alpha^2(P)\chi_\beta^2(P) = 2^n[n!/t!(n-t)!]\, t!(n-t!) = 2^n n! = g, \tag{A3}$$

where 2^n comes from the sum over n_i, the next factor from the number of S's for given t, and the last two from the sum of $\chi_\alpha^2(P)$ over S_t and the sum of $\chi_\rho^2(P)$ over S_{n-t}, using the irreducibility postulated earlier. Had we used different α's and β's with S and S' we should have found in identical fashion that the characters were orthogonal.

Thus we have a set of irreducible representations of $\mathfrak{O}_n$, characterized by t, α, β. To see if they are complete we need only calculate the sum of the squares of their dimensions.

$$d(t, \alpha, \beta) = d_\alpha d_\beta \frac{n!}{t!(n-t)!}$$

$$\Sigma d^2 = \sum d_\alpha^2 d_\beta^2 \left(\frac{n!}{t!(n-t)!}\right)^2 = \sum_t t!(n-t)! \left(\frac{n!}{t!(n-t)!}\right)^2 = 2^n n!. \tag{A4}$$

Thus, we have a complete set of irreducible representations, each of which is an induced representation of a subgroup $\mathfrak{O}_t \times \mathfrak{O}_{n-t}$.

Now, in respect of S_n, these are induced representations of subgroups $S_t \times S_{n-t}$. We shall use a theorem of Shoda[7] to demonstrate that these representations cannot be irreducible if $0 < t < n$. We write the subgroups more explicitly as $H = S(1, \cdots, t) \times S(t+1, \cdots, n)$ and form the conjugate group XHX^{-1} for $X = (t, t+1)$: $XHX^{-1} = S(1 \cdots t-1, t+1)\, XS(t, t+2, \cdots, n)$. Now H and XHX^{-1} contain the common subgroup $h = S(1 \cdots t-1) \times S(t+2, \cdots, n)$. Now consider a representation Γ of H and the representation Γ_X of XHX^{-1}, where the matrix of the element R of XHX^{-1} in Γ_X is equal to the matrix of the element $X^{-1}RX$ in Γ_X.

If we now restrict Γ and Γ_x to h, each element of h commutes with X. Consequently under h the two representations are identical. Shoda's theorem then states that the induced representation of Γ in S_n is reducible. This procedure breaks down if t is 0 or n.

This demonstrates that, for $0 < t < n$, the irreducible representations of $\mathfrak{O}_n$ are reducible under S_n.

APPENDIX B

We now turn to the question of whether a representation Γ, irreducible under S_n, can be irreducible under $S_{n_1} \times S_{n_2} \times \cdots$. We proceed by supposing that it is.

It follows that Γ is irreducible under the intermediate group $S_m \times S_{n-m}$, where m is the largest of the numbers $n_1 \cdots$. Since this is a direct product, each of its irreducible representations is the product of irreducible representations Γ_m and Γ_{n-m} of the two smaller groups. Upon reduction under the group S_{n-l}, where l is the smaller of m and $n-m$, it must contain only copies of Γ_{n-l}. Finally, then, if we reduce Γ under S_{n-l}, it can contain only Γ_{n-l}.

One finds the representations of S_{n-l} subduced by Γ of S_n by removing regularly[8] l dots, one at a time, from the Young pattern for Γ. For each pattern thus obtained, the corresponding representation occurs if Γ is reduced under S_{n-l}. We therefore want to know if it is possible to have a pattern from which l dots can be removed regularly one at a time in only one way.

Now, one way to remove dots regularly is to start with the bottom of the column farthest to the right, move up it to the top, then to the bottom of the adjacent column and on up, etc., removing each dot encountered until l dots have been removed. Another way is to start at the right end of the bottom row, proceed left to the beginning, then to the right end of the next row, etc. It is clear that these two ways give different final patterns unless one of the following conditions is true:

(1) $l = n-1$ or n. Since we chose l so that $2l \geq n$, this could happen only for $n \leq 2$, when all representations are one-dimensional anyway.

(2) $l = 1$ and the pattern is rectangular — that is, it consists of s rows with t dots each, with $st = n$. This requires that n be composite, not prime, if Γ is to be degenerate.

To sum up, a representation Γ, irreducible under S_n, can be irreducible under $S_{n_1} \times S_{n_2} \times \cdots$ only if the latter group is S_{n-1} and then only if n is composite, and the Young pattern rectangular.

We now turn to the question whether $[\Gamma^2]$ contains Γ'_V, which in all cases of interest is the question whether under S_n, $[\Gamma^2]$ contains $(n-1, 1)$. From Hamermesh[9] we find that Γ^2 contains $(n-1, 1)$ unless Γ has a rectangular pattern. We proceed to show that $\{\Gamma^2\} \equiv \Gamma^2 - [\Gamma^2]$ never contains $(n-1, 1)$.

The representation of S_n as a permutation group on n objects — the representation Γ_P for the simplex polytope in $(n-1)$ dimensions — reduces to Γ_0 and $(n-1, 1)$. Thus for an arbitrary Γ', with character χ', we have according to Eq. (2.1a)

$$\frac{1}{n!}\sum_{S_n} \chi'\chi_P = \frac{1}{(n-1)!}\sum_{S_{n-1}} \chi' = N(n-1),$$

where $N(n-1)$ is the number of times Γ' contains Γ_0 under S_{n-1}.

Now, suppose Γ' is $\{\Gamma^2\}$ for some Γ irreducible under S_n. Under S_{n-1}, Γ reduces to the sum of the representations associated with the Young patterns obtained by regularly removing one dot from the pattern for Γ. Each of these representations occurs just once. Consequently, $\{\Gamma^2\}$ does not contain Γ_P, Γ_0, or $(n-1, 1)$. This holds for any Γ. Therefore, under S_n, $[\Gamma^2]$ contains $(n-1, 1)$ unless it has a rectangular Young pattern.

---

1 H. A. Jahn and E. Teller, Proc. Roy. Soc. (London) A161, 220 (1937).
2 H. A. Jahn, Proc. Roy. Soc. (London) A164, 117 (1938).
3 G. Lyubarskii, *The Application of Group Theory in Physics* (Pergamon, London, 1960).
4 H. S. M. Coxeter, *Regular Polytopes* (MacMillan, New York, 1963), 2nd ed. It appears that the word "polytope" is preferred over "polyhedron" in more than three dimensions.
5 J. S. Lomont, *Applications of Finite Groups* (Academic, New York, 1959), p. 221.
6 E. Ruch and A. Schönhofer, Theoret. Chim. Acta 3, 291 (1965).
7 K. Shoda, Proc. Phys. Math. Soc. Japan (3), 15, 249 (1933). (The theorem is also given by Lomont, p. 225.)
8 M. Hamermesh, *Group Theory and Its Application to Physical Problems* (Addison-Wesley, Reading, Mass., 1962), Chap. 7.
9 Reference 8, pp. 257-8.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Asymptotic Form of the Three-Particle Scattering Wavefunction for Free Incident Particles*

J. Nuttall
Department of Physics, Texas A & M University, College Station, Texas 77843
(Received 18 March 1971)

It is shown that second-order multiple scattering terms lead, in some directions, to an anomalous term in the asymptotic form of the wavefunction for three free incident particles, which falls off as the inverse second power of distance. The boundary of the region in which this occurs is given, together with the form of the wavefunction near this boundary.

INTRODUCTION

A knowledge of the asymptotic form of the coordinate-space wavefunction of a three-body system for the case when three free particles are incident may have several applications. The leading terms in the asymptotic form are related to the T matrix for the process under consideration. Since the T matrix for the case $(3 \to 3)$ has singularities in addition to those present for the T matrix to be used when one particle is incident on a bound state of the other two, we expect to find new terms

It follows that Γ is irreducible under the intermediate group $S_m \times S_{n-m}$, where m is the largest of the numbers $n_1 \cdots$. Since this is a direct product, each of its irreducible representations is the product of irreducible representations Γ_m and Γ_{n-m} of the two smaller groups. Upon reduction under the group S_{n-l}, where l is the smaller of m and $n-m$, it must contain only copies of Γ_{n-l}. Finally, then, if we reduce Γ under S_{n-l}, it can contain only Γ_{n-l}.

One finds the representations of S_{n-l} subduced by Γ of S_n by removing regularly[8] l dots, one at a time, from the Young pattern for Γ. For each pattern thus obtained, the corresponding representation occurs if Γ is reduced under S_{n-l}. We therefore want to know if it is possible to have a pattern from which l dots can be removed regularly one at a time in only one way.

Now, one way to remove dots regularly is to start with the bottom of the column farthest to the right, move up it to the top, then to the bottom of the adjacent column and on up, etc., removing each dot encountered until l dots have been removed. Another way is to start at the right end of the bottom row, proceed left to the beginning, then to the right end of the next row, etc. It is clear that these two ways give different final patterns unless one of the following conditions is true:

(1) $l = n-1$ or n. Since we chose l so that $2l \geq n$, this could happen only for $n \leq 2$, when all representations are one-dimensional anyway.

(2) $l = 1$ and the pattern is rectangular — that is, it consists of s rows with t dots each, with $st = n$. This requires that n be composite, not prime, if Γ is to be degenerate.

To sum up, a representation Γ, irreducible under S_n, can be irreducible under $S_{n_1} \times S_{n_2} \times \cdots$ only if the latter group is S_{n-1} and then only if n is composite, and the Young pattern rectangular.

We now turn to the question whether $[\Gamma^2]$ contains Γ'_V, which in all cases of interest is the question whether under S_n, $[\Gamma^2]$ contains $(n-1, 1)$. From Hamermesh[9] we find that Γ^2 contains $(n-1, 1)$ unless Γ has a rectangular pattern. We proceed to show that $\{\Gamma^2\} \equiv \Gamma^2 - [\Gamma^2]$ never contains $(n-1, 1)$.

The representation of S_n as a permutation group on n objects — the representation Γ_P for the simplex polytope in $(n-1)$ dimensions — reduces to Γ_0 and $(n-1, 1)$. Thus for an arbitrary Γ', with character χ', we have according to Eq. (2.1a)

$$\frac{1}{n!}\sum_{S_n} \chi'\chi_P = \frac{1}{(n-1)!}\sum_{S_{n-1}} \chi' = N(n-1),$$

where $N(n-1)$ is the number of times Γ' contains Γ_0 under S_{n-1}.

Now, suppose Γ' is $\{\Gamma^2\}$ for some Γ irreducible under S_n. Under S_{n-1}, Γ reduces to the sum of the representations associated with the Young patterns obtained by regularly removing one dot from the pattern for Γ. Each of these representations occurs just once. Consequently, $\{\Gamma^2\}$ does not contain Γ_P, Γ_0, or $(n-1, 1)$. This holds for any Γ. Therefore, under S_n, $[\Gamma^2]$ contains $(n-1, 1)$ unless it has a rectangular Young pattern.

---

1 H. A. Jahn and E. Teller, Proc. Roy. Soc. (London) A161, 220 (1937).
2 H. A. Jahn, Proc. Roy. Soc. (London) A164, 117 (1938).
3 G. Lyubarskii, *The Application of Group Theory in Physics* (Pergamon, London, 1960).
4 H. S. M. Coxeter, *Regular Polytopes* (MacMillan, New York, 1963), 2nd ed. It appears that the word "polytope" is preferred over "polyhedron" in more than three dimensions.
5 J. S. Lomont, *Applications of Finite Groups* (Academic, New York, 1959), p. 221.
6 E. Ruch and A. Schönhofer, Theoret. Chim. Acta 3, 291 (1965).
7 K. Shoda, Proc. Phys. Math. Soc. Japan (3), 15, 249 (1933). (The theorem is also given by Lomont, p. 225.)
8 M. Hamermesh, *Group Theory and Its Application to Physical Problems* (Addison-Wesley, Reading, Mass., 1962), Chap. 7.
9 Reference 8, pp. 257-8.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Asymptotic Form of the Three-Particle Scattering Wavefunction for Free Incident Particles*

J. Nuttall
Department of Physics, Texas A & M University, College Station, Texas 77843
(Received 18 March 1971)

It is shown that second-order multiple scattering terms lead, in some directions, to an anomalous term in the asymptotic form of the wavefunction for three free incident particles, which falls off as the inverse second power of distance. The boundary of the region in which this occurs is given, together with the form of the wavefunction near this boundary.

INTRODUCTION

A knowledge of the asymptotic form of the coordinate-space wavefunction of a three-body system for the case when three free particles are incident may have several applications. The leading terms in the asymptotic form are related to the T matrix for the process under consideration. Since the T matrix for the case $(3 \to 3)$ has singularities in addition to those present for the T matrix to be used when one particle is incident on a bound state of the other two, we expect to find new terms

in the asymptotic form. The strongest singularities in T are the δ functions in the disconnected parts, which will give rise to the leading term in the asymptotic form, which is easily written down. The connected part of T, T_c contains rescattering singularities, of which the strongest, poles, correspond to two binary collisions. The purpose of this paper is to discuss the contribution to the asymptotic form coming from these rescattering terms in T_c. For simplicity, we assume that there are three different particles of equal mass ($m = \frac{1}{2}$), interacting through short-range two-body potentials.

It is shown, in the notation of Ref. 1, that in some but not all asymptotic directions there is a contribution of order ρ^{-2} in addition to the usual one that behaves like $\rho^{-5/2}$. We derive an expression for this rescattering contribution and give a formula for the boundary of the region within which it is present. We also indicate what happens near this boundary and in addition show that the anomalous term falls off no faster that ρ^{-1} in the special case when two particles remain close together. The analysis does not hold for two exceptional values of the momentum of any incident particle.

ASYMPTOTIC FORM

We work in the center-of-mass frame and use the notation of Ref. 1, where the momentum of a three-particle state is given by the 6-vector $\hat{K} = (\mathbf{P}_i, \mathbf{Q}_i)$, $i = 1, 2,$ or 3. In terms of the 3-3 T matrix $\langle \hat{K} | T(E) | \hat{K}' \rangle$, the wavefunction corresponding to an initial three-body state of momentum $\hat{K}'$ is, with $E = \hat{K}'^2$

$$\Phi(\hat{\rho}) = (2\pi)^{-3} e^{i\hat{K}'\cdot\hat{\rho}} + (2\pi)^{-9/2} 3^{-3/2} \int d\hat{K} e^{i\hat{\rho}\cdot\hat{K}} \times (E - \hat{K}^2 + i\epsilon)^{-1} \langle \hat{K} | T(E) | \hat{K}' \rangle, \quad (1)$$

where the limit $\epsilon \to 0$ must be taken after performing the integral.

Now the amplitude $\langle \hat{K} | T(E) | \hat{K}' \rangle$ contains disconnected terms of the form

$$T_d = (\tfrac{3}{2})^{3/2} \sum_{i=1}^{3} \delta(\mathbf{P}_i' - \mathbf{P}_i) \langle \mathbf{Q}_i' | t_i(Q_i^2 + i\epsilon) | \mathbf{Q}_i \rangle, \quad (2)$$

which give rise to contributions to Φ of the form

$$\Phi_d(\hat{\rho}) = (2\pi)^{-3} 2^{-3/2} \sum_{i=1}^{3} \chi_{\mathbf{Q}_i}(\mathbf{Y}_i)\, e^{i\mathbf{P}_i\cdot\mathbf{X}_i}. \quad (3)$$

Here $\chi_{\mathbf{Q}}(\mathbf{Y})$ is the scattering part of a two-body wavefunction corresponding to an incident momentum $\mathbf{Q}$. Thus we have

$$\chi_{\mathbf{Q}_i}(\mathbf{Y}_i) = (2\pi)^{-3/2} \int d\mathbf{Q}_i' e^{i\mathbf{Q}_i'\cdot\mathbf{Y}_i} (\mathbf{Q}_i^2 - \mathbf{Q}_i'^2 + i\epsilon)^{-1} \times \langle \mathbf{Q}_i' | T(\mathbf{Q}_i^2 + i\epsilon) | \mathbf{Q}_i \rangle. \quad (4)$$

For large Y, $\chi_{\mathbf{Q}}(\mathbf{Y})$ falls off as Y^{-1}, and so, in general, $\Phi_d(\hat{\rho})$ has leading terms of order ρ^{-1} as $\rho \to \infty$.

The second-order terms in the multiple scattering expansion of T contribute to the connected part of T six terms that each contains a pole for certain values of the external momenta. Typical of these terms is T_c^{13} given by

$$T_c^{13}(\hat{K}) = \langle \mathbf{Q} | t_1(E - \mathbf{P}^2) | -3^{-1/2}(2\mathbf{P}' + \mathbf{P}) \rangle \times \langle 3^{-1/2}(2\mathbf{P} + \mathbf{P}') | t_3(E - \mathbf{P}'^2) | \mathbf{Q}' \rangle \times [D(\mathbf{P}) + i\epsilon]^{-1}, \quad (5)$$

where

$$D(\mathbf{P}) = \tfrac{4}{3}[\tfrac{3}{4}(E - \mathbf{P}'^2) - (\mathbf{P} + \tfrac{1}{2}\mathbf{P}')^2]. \quad (6)$$

We have written $\mathbf{P}, \mathbf{Q}$ for $\mathbf{P}_1, \mathbf{Q}_1$, the final momenta and $\mathbf{P}', \mathbf{Q}'$ for $\mathbf{P}_3', \mathbf{Q}_3'$, the initial momenta. The contribution of this term to Φ is

$$\Phi_c^{13}(\hat{\rho}) = (2\pi)^{-9/2} 3^{-3/2} \int d\mathbf{P} d\mathbf{Q} e^{i(\mathbf{P}\cdot\mathbf{X} + \mathbf{Q}\cdot\mathbf{Y})} \times (E - \mathbf{P}^2 - \mathbf{Q}^2 + i\epsilon)^{-1} T_c^{13}, \quad (7)$$

where $\mathbf{X} = \mathbf{X}_1$ is proportional to the distance between particle 1 and the 23 c.m., and $\mathbf{Y} = \mathbf{Y}_1$ is proportional to the distance between particles 2 and 3.

Now let us assume that $\rho \to \infty$ in such a direction that Y also becomes large, and leave the discussion of the special case when this is not so until later. We may approximate the integral over $\mathbf{Q}$ in (7) by a familiar technique to obtain

$$\Phi_c^{13}(\hat{\rho}) \sim -2^{-7/2}\pi^{-5/2} 3^{-3/2} Y^{-1} \int d\mathbf{P}\; e^{i\mathcal{J}(\mathbf{P})}\, I(\mathbf{P}) / [D(\mathbf{P}) + i\epsilon] \quad \text{as} \quad Y \to \infty, \quad (8)$$

where

$$I(\mathbf{P}) = \langle \mathbf{Y}(E - \mathbf{P}^2)^{1/2}/Y | t_1(E - \mathbf{P}^2) | -3^{-1/2} \times (2\mathbf{P}' + \mathbf{P}) \rangle \langle 3^{-1/2}(2\mathbf{P} + \mathbf{P}') | t_3(\mathbf{Q}'^2) | \mathbf{Q}' \rangle \quad (9)$$

and

$$\mathcal{J}(\mathbf{P}) = \mathbf{P}\cdot\mathbf{X} + Y(E - \mathbf{P}^2)^{1/2}. \quad (10)$$

The asymptotic form of $\Phi_c^{13}(\hat{\rho})$ may be further simplified by considering a complex distortion of the integration manifold $\mathbf{P} \to \mathbf{P} + i\delta\mathbf{P}(\mathbf{P})$, and searching for a choice of $\delta\mathbf{P}(\mathbf{P})$ that leads to a large, negative real part of the exponent in (8) without crossing the singularity at $D(\mathbf{P}) + i\epsilon = 0$. This requires at each $\mathbf{P}$ we be able to find $\delta\mathbf{P}$ satisfying

$$\delta\mathbf{P}\cdot\nabla_{\mathbf{P}}\mathcal{J} > 0$$

and

$$\delta\mathbf{P}\cdot\nabla_{\mathbf{P}} D > 0 \quad \text{if} \quad D = 0.$$

Such a $\delta\mathbf{P}$ will exist except at points satisfying either of the conditions

$$\text{(i)} \quad \nabla_{\mathbf{P}}\mathcal{J} = 0$$
$$\text{(ii)} \quad D = 0 \quad \text{and} \quad \nabla_{\mathbf{P}}\mathcal{J} = -\alpha\nabla_{\mathbf{P}} D \quad \text{with} \quad \alpha > 0. \quad (11)$$

We expect to find a non-exponential-decreasing contribution coming from the integral in the neighborhood of any point satisfying either condition.

There is always just one point satisfying condition (i), and it is given by $\mathbf{P}_0 = \mathbf{X}E^{1/2}/\rho$. If $D(\mathbf{P}_0) \neq 0$, the integral (8) may be evaluated by the method of stationary phase to give the result

$$\Phi_c^{13}(\hat{\rho}) \sim e^{i\pi/4}E^{3/4}3^{-3/2}(4\pi)^{-1}\rho^{-5/2} \times \exp(iE^{1/2}\rho)\, T_c^{13}(E^{1/2}\hat{\rho}/\rho). \tag{12}$$

This $\rho^{-5/2}$ dependence is completely analogous to the result found in the case of a particle incident on a bound pair.

The second condition leads to the equations, with $\mathbf{R} = \mathbf{X}/Y$,

$$(E - \mathbf{P}^2)^{1/2}\mathbf{R} = \mathbf{P} + \beta(\mathbf{P} + \tfrac{1}{2}\mathbf{P}'), \quad \beta > 0 \tag{13}$$

and

$$D(\mathbf{P}) = 0.$$

They may be stated geometrically in terms of Fig. 1 by requiring $C = D$, where $AC = (E - \mathbf{P}^2)^{1/2}\mathbf{R}$ and the point B lies on a circle of radius $[\frac{3}{4}(E - \mathbf{P}'^2)]^{1/2}$.

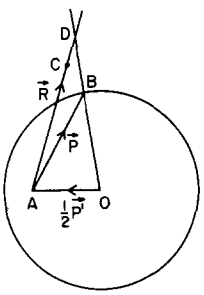

FIG. 1. Geometrical description of Eq. (13), whose solution requires $C = D$. The radius of the circle is $[\frac{3}{4}(E - \mathbf{P}'^2)]^{1/2}$, and AC is $(E - \mathbf{P}^2)^{1/2}\mathbf{R}$.

The point D must lie outside the circle. For the case drawn in Fig. 1, AD increases but AC decreases as AB increases, so that there is never more than one solution to (13), and this is true of all configurations. The limiting case arises when $C = D = B$, so that $\mathbf{P} = (E - \mathbf{P}^2)^{1/2}\mathbf{R}$ or $\mathbf{P} = \mathbf{P}_0$, and $D(\mathbf{P}_0) = 0$. For $D(\mathbf{P}_0) < 0$ there is one solution $\mathbf{P} = \overline{\mathbf{P}}$, and for $D(\mathbf{P}_0) > 0$ there is no solution with positive α, although the point $\overline{\mathbf{P}}$ may still be defined. The curve $D(\mathbf{P}_0) = 0$ in $\hat{\rho}/\rho$ space forms the boundary referred to above.

To evaluate the contribution to (8) from the region near $\mathbf{P} = \overline{\mathbf{P}}$, we choose a distortion of the contour so that $\delta\mathbf{P}\cdot\nabla_{\mathbf{P}}\mathcal{J} > 0$. This will cause the contour to cross the pole at $D(\mathbf{P}) + i\epsilon = 0$; what we require is the residue at that pole. We may calculate this and at the same time investigate what happens if $\mathbf{R}$ is near to satisfying $D(\mathbf{P}_0) = 0$, by changing the variables of integration in (8). Let us choose axes so that the first axis is along $\mathbf{Q}_0 = \overline{\mathbf{P}} + \frac{1}{2}\mathbf{P}'$, the second is perpendicular to $\mathbf{Q}_0$ in the $\mathbf{P}'\mathbf{Q}_0$ plane, and the third perpendicular to both. Thus we have $\mathbf{Q}_0 = (Q_0, 0, 0)$ and $\overline{\mathbf{P}} = (P_1, P_2, 0)$, and we set $\mathbf{P} = \overline{\mathbf{P}} + \mathbf{p}$ with $\mathbf{p} = (p_1, p_2, p_3)$. We now replace the variable p_3 by q given by

$$q = p_2^2 + p_3^2 + (Q_0 + p_1)^2 - Q_0^2.$$

If the phase $\mathcal{J}(\mathbf{P})$ is expanded about the point $\overline{\mathbf{P}}$, we find in terms of the new variables that

$$\mathcal{J}(\mathbf{P}) = -Fp_3^2 - A(p_2 + Bq)^2 - Cq^2 + q\beta Y/2d + \mathcal{J}(\overline{\mathbf{P}}), \tag{14}$$

where

$$\begin{aligned} A &= (Y/2d^3)[d^2(1+\beta) + P_2^2], \\ B &= YP_1P_2/4d^3Q_0A, \\ C &= Y(1+\beta)(\beta d^2 + E)/8dQ_0^2[d^2(1+\beta) + P_2^2], \\ F &= Y(1+\beta)/2d, \end{aligned} \tag{15}$$

and

$$D = -\tfrac{4}{3}q,$$

with

$$d^2 = E - \overline{\mathbf{P}}^2.$$

The volume element in (8), $d\mathbf{P}$, becomes

$$d\mathbf{P} = d\mathbf{p} \approx dp_2dp_3(dq/2Q_0).$$

With these substitutions, the integrals over p_2 and p_3 may be done immediately by the saddle-point technique to give

$$\Phi_c^{13}(\hat{\rho}) \sim i\pi^{-3/2}2^{-9/2}3^{-3/2}Q_0^{-1}I(\overline{\mathbf{P}})(AF)^{-1/2}Y^{-1}e^{i\mathcal{J}(\overline{\mathbf{P}})} \times \int_{-\infty}^{\infty} dq\, \frac{\exp[-i(Cq^2 - q\beta Y/2d)]}{-\frac{4}{3}q + i\epsilon}. \tag{16}$$

If $\beta > 0$, a positive imaginary distortion of the integration contour near $q = 0$ is required to give the exponent in (16) a negative real part, so that we must include the residue at the pole $q = \frac{3}{4}i\epsilon$, which gives a contribution

$$\Phi_c^{13}(\hat{\rho}) \sim 2^{-11/2}\pi^{-1/2}3^{-1/2}Q_0^{-1}I(\overline{\mathbf{P}})(AF)^{-1/2} \times Y^{-1}e^{i\mathcal{J}(\mathbf{P})}\theta(\beta). \tag{17}$$

This contribution to the asymptotic form of Φ_c^{13} falls off as ρ^{-2}, and, if present, is the dominant term. The next term, of order $\rho^{-5/2}$, is given by (12).

When $\mathbf{R}$ is such that $D(\mathbf{P}_0)$ is near to zero, it is not correct to treat the two points satisfying conditions (i) and (ii) of Eq. (11) separately. To obtain a formula which shows how the asymptotic form changes from the region of $\mathbf{R}$ with $\beta > 0$ to the region with $\beta < 0$, we evaluate (16) exactly to give

$$\Phi_c^{13}(\hat{\rho}) \sim 2^{-13/2}\pi^{-1/2}3^{-1/2}Q_0^{-1}I(\overline{\mathbf{P}})(AF)^{-1/2} \times Y^{-1}e^{i\mathcal{J}(\overline{\mathbf{P}})}\operatorname{erfc}\left(\frac{-e^{i\pi/4}\beta Y}{4dC^{1/2}}\right). \tag{18}$$

If $|\beta| Y^{1/2} \gg E^{1/4}$, the argument of the function erfc is large and (18) becomes

$$\Phi_c^{13}(\hat{\rho}) \sim 2^{-13/2}\pi^{-1/2}3^{-1/2}Q_0^{-1}I(\overline{\mathbf{P}})\,(AF)^{-1/2}Y^{-1}e^{i\beta(\overline{\mathbf{P}})} \times \left[2\theta(\beta) + \frac{4C^{1/2}d}{\beta Y}\exp\left(\frac{i\beta^2Y^2}{16d^2C}\right)\right]. \tag{19}$$

The first term in (19) is (17), and it may be shown that, provided $E^{-1/6}Y^{-1/3} \gg |\beta| \gg E^{-1/4}Y^{-1/2}$, the second term is equal to (12) apart from corrections which decrease faster than $\rho^{-5/2}$. Thus we use (19) for β in the range, say, $|\beta| \leq E^{-5/24}Y^{-5/12}$ and the sum of (12) and (17) for other β.

To treat the situation when $\mathbf{X} \to \infty$, with $\mathbf{Y}$ remaining fixed, we go back to (1), which may be written

$$\Phi_c^{13}(\hat{\rho}) = (2\pi)^{-9/2}3^{-3/2}\int d\mathbf{P}\; e^{i\mathbf{P}\cdot\mathbf{X}}H(\mathbf{P},\mathbf{Y})/[D(\mathbf{P}) + i\epsilon], \tag{20}$$

where

$$H(\mathbf{P},\mathbf{Y}) = \int d\mathbf{Q}e^{i\mathbf{Q}\cdot\mathbf{Y}}[E - \mathbf{P}^2 - \mathbf{Q}^2 + i\epsilon]^{-1} \times [D(\mathbf{P}) + i\epsilon]^{-1}T_c^{13}(\hat{K}). \tag{21}$$

An important contribution to (20) will come from the neighborhood of the value of $\mathbf{P}$ for which $D = 0$ and $\mathbf{X} = -\alpha\nabla_{\mathbf{P}}D$, $\alpha > 0$. There is always just one such value, and in fact it is given by the momentum $\overline{\mathbf{P}}$ defined earlier, worked out for the special case in which $\mathbf{R} = \mathbf{X}/Y \to \infty$. The leading term in the expansion of $\Phi_c^{13}(\hat{\rho})$ coming from the neighborhood of $\mathbf{P} = \overline{\mathbf{P}}$ is

$$\Phi_c^{13}(\hat{\rho}) \sim -2^{-11/2}\pi^{-5/2}3^{-1/2}X^{-1}H(\overline{\mathbf{P}},\mathbf{Y}) \times \exp\{-i(\tfrac{1}{2}\mathbf{P}'\cdot\mathbf{X}) - X[\tfrac{3}{4}(E - \mathbf{P}'^2)]^{1/2}\} \quad \text{as} \quad X \to \infty. \tag{22}$$

In view of (4) we may write $H(\overline{\mathbf{P}},\mathbf{Y})$ as

$$H(\overline{\mathbf{P}},\mathbf{Y}) = (2\pi)^{3/2}\chi_{\mathbf{q}}(\mathbf{Y})\langle 3^{-1/2}(2\overline{\mathbf{P}} + \mathbf{P}')|t_3(Q'^2)|\mathbf{Q}'\rangle, \tag{23}$$

with

$$\mathbf{q} = -3^{-3/2}(2\mathbf{P}' + \overline{\mathbf{P}}).$$

It may be seen that as $Y \to \infty$ (22) merges into our previous result (17) obtained for Y large.

For several reasons, such as the singularity of $H(\mathbf{P},\mathbf{Y})$ at $\mathbf{P} = \overline{\mathbf{P}}$, the above analysis may break down if $E = \mathbf{P}'^2$ or $E = 4\mathbf{P}'^2$.

DISCUSSION

It is not hard to understand the physical basis for the dominant contribution to Φ_c given by (17). After their collision, particles 1 and 2 propagate on the energy shell, particle 1 having momentum $(\frac{2}{3})^{1/2}\overline{\mathbf{P}}$, and then particles 2 and 3 scatter. Both between the two collisions and from the collision to the observation point, the wavefunction decreases by a factor proportional to ρ^{-1}, leading to the final ρ^{-2} dependence. In the special case described by (22), there is only one factor ρ^{-1}, since particles 2 and 3 have not traveled far since their collision.

To interpret Eq. (13), we rewrite it as

$$\mathbf{X} - Y\overline{\mathbf{P}}/(E - \overline{\mathbf{P}}^2)^{1/2} = \gamma(\mathbf{P} + \tfrac{1}{2}\mathbf{P}'). \tag{24}$$

Since $(E - \overline{\mathbf{P}}^2)^{1/2}$ is proportional to the relative momentum of particles 2 and 3 after their collision, $Y(E - \overline{\mathbf{P}}^2)^{1/2}$ is proportional to the time since they were together, and $Y(E - \overline{\mathbf{P}}^2)^{-1/2}\overline{\mathbf{P}}$ to the distance particle 1 traveled since then. Thus the left-hand side of (24) is the position of particle 1 relative to the 23 c.m. at that time, and (24) requires that this vector be proportional to the corresponding momentum after the 12 collision.

It should be noted that Gerjuoy[2] previously obtained the ρ^{-2} dependence of Φ_c by a different argument, without going into the detailed behavior that is presented here.

---

* Work supported in part by the Air Force Office of Scientific Research, Office of Aerospace Research, U.S. Air Force, under Grant No. 71-1979.

1 J. Nuttall, Phys. Rev. Letters 19, 473 (1967). Note that the factor $(\frac{2}{3})^{1/2}$ in Eq. (3) of this paper should be $(\frac{3}{2})^{1/2}$.

2 E. Gerjuoy, J. Phys. B 3, 192 (1970); "Configuration Space Three-Body Scattering Theory" (unpublished).

Nearly Symmetric Kinematic and Hydromagnetic Dynamos

A. M. Soward*
Courant Institute of Mathematical Sciences, New York University, New York
(Received 27 January 1971)

Certain aspects of the hydromagnetic and kinematic dynamo theory related to the Earth's magnetic field are considered. The work of Tough and Roberts [J. G. Tough and P. H. Roberts, *Physics of the Earth and Planetary Interiors* (North-Holland, Amsterdam, 1968), Vol. 1, p. 288] on the hydromagnetic dynamo is extended in two respects. First, the most general form of the prescribed body force which is consistent with the model is considered. Secondly, the mean quantity $\langle S_\varphi \rangle$ [see Eqs. (18)] is determined up to order $R^{-1/2}$, where R is the magnetic Reynolds number. It is shown that the remarkable effective variables first introduced by Braginskii {S. I. Braginskii, Zh. Eksp. Teor. Fiz. 47, 1084 (1964) [Sov. Phys. JETP 20, 726 (1965)]} are relevant in the hydromagnetic dynamo in the second approximation. It is also shown by considering a related problem concerning the heat conduction equation that effective variables are unlikely to have any relevance in the kinematic dynamo theory in the third approximation.

I. INTRODUCTION

It is now generally accepted that the Earth's magnetic field is maintained by dynamo action. Specifically it is supposed that magnetohydrodynamic motions of the order of 1 mm sec^{-1}, occurring in the Earth's core, cause a self-excitation of the magnetic field which sustains the field against Ohmic decay.

Several models illustrating the kinematic dynamo have been formulated (see Runcorn[1]). Though these models show conclusively the possibility of dynamo action, it is beyond the scope of kinematic dynamo theory to explain how a body such as the Earth maintains the motions required for dynamo action. Hence, for a full understanding of the problem, the hydromagnetics must be considered. Recently Tough and Roberts[2] extended the Braginskii[3] formulation of the kinematic problem to include the equation of motion. A set of equations [see (21)–(28)] and boundary conditions, which describe the hydromagnetic dynamo, were obtained. A numerical procedure was outlined for solving the equations, but the calculation was not attempted. However, Tough and Roberts[2] found that the remarkable simplifications which Braginskii[3] discovered for the kinematic equations occur also for hydromagnetic dynamos. In this paper the most general body force which is consistent with the model is considered, and the simplifications are extended. No attempt is made to solve the equations.

It is supposed that the fluid in the Earth's core is incompressible:

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

and that the flow is governed by the equation of motion:

$$\mathbf{i}_z \times \mathbf{u} = -\nabla P + \mathbf{j} \times \mathbf{b} + E\nabla^2 \mathbf{u} + \mathbf{F}. \tag{2}$$

The magnetic induction equation is

$$\frac{\partial \mathbf{b}}{\partial t} = R\nabla \times (\mathbf{u} \times \mathbf{b}) + \nabla^2 \mathbf{b}, \tag{3}$$

and

$$\nabla \cdot \mathbf{b} = 0, \quad \mathbf{j} = \nabla \times \mathbf{b}. \tag{4}$$

The only dimensionless numbers characterizing the flow are

$$E = \nu/2\Omega L^2, \quad R = U^* L/\eta, \tag{5}$$

where E is the Ekman number and R is the magnetic Reynolds number. Neglect of the inertia terms in (2) is justified provided both R_d and RR_d are small, where

$$R_d = \eta/2\Omega L^2. \tag{6}$$

In Eqs. (1)–(6), $U^*\mathbf{u}$ is the velocity, $B^*\mathbf{b}$ is the magnetic field, $F^*\mathbf{F}$ is the body force per unit mass, P is the dimensionless pressure, $L\mathbf{r}$ is the position vector, $\Omega \mathbf{i}_z$ is the rotation vector ($|\mathbf{i}_z| = 1$), ν is the kinematic viscosity, η is the magnetic diffusivity, $(L^2/\eta)t$ is the time, and $(B^*/\mu L)\mathbf{j}$ is the electric current (μ is the magnetic permeability). The typical velocity U^* and magnetic field B^* are taken to be

$$U^* = F^*/2\Omega, \quad B^* = (\mu\bar{\rho}L)^{1/2}F^{*1/2}, \tag{7}$$

where $\bar{\rho}$ is the density. The scaling of U^* and B^* is different from that adopted by Tough and Roberts[2] since it is supposed that the body force F appears as an order 1 quantity in the equation of motion. It is assumed that

$$R \gg 1 \quad \text{and} \quad E \ll 1. \tag{8}$$

Since the Ekman number is small, it is likely that viscous effects are confined to boundary layers of thickness order $E^{1/2}$. Therefore it is natural to seek a solution of Eqs. (1)–(4) in two parts. First, an interior solution is sought away from the boundary where diffusive effects are small. Secondly, this solution must be matched with the solution valid close to the boundaries where diffusive effects are important. Tough and Roberts[2] conclude that the viscous boundary layer is to first approximation an axisymmetric Ekman layer, so that the velocity normal to the surface of this layer is related to the tangential velocity by the well-known Ekman layer condition (see Greenspan[4]). This consideration leads Tough and Roberts[2] to assume that

$$R = O(E^{-1/2}). \tag{9}$$

This assumption is also made here.

A solution is sought in the interior of the form

$$\mathbf{F} = \mathbf{F}_p(R,\rho,z,t) + R^{-1/2}\mathbf{F}'(\rho,\varphi,z,t) + R^{-1}F_\varphi(R,\rho,z,t)\mathbf{i}_\varphi, \tag{10a}$$

$$\mathbf{u} = U(R,\rho,z,t)\mathbf{i}_\varphi + R^{-1/2}\mathbf{u}'(R,\rho,\varphi,z,t) + R^{-1}\mathbf{u}_p(R,\rho,z,t), \tag{10b}$$

$$\mathbf{b} = B(R,\rho,z,t)\mathbf{i}_\varphi + R^{-1/2}\mathbf{b}'(R,\rho,\varphi,z,t) + R^{-1}\mathbf{b}_p(R,\rho,z,t), \tag{10c}$$

where ρ is the distance from the axis of rotation, z is the distance along the axis of rotation, φ is the azimuthal angle, and the suffix p denotes meridional components. It is assumed throughout that primed quantities have zero φ average:

$$\langle \mathbf{F}' \rangle = 0, \tag{11}$$

where

$$\langle \mathbf{F}' \rangle = \langle F'_\rho \rangle \mathbf{i}_\rho + \langle F'_\varphi \rangle \mathbf{i}_\varphi + \langle F'_z \rangle \mathbf{i}_z, \qquad \langle f \rangle = \frac{1}{2\pi}\int_0^{2\pi} f\,d\varphi. \tag{12}$$

The meridional components of the velocity and magnetic field are also defined as

$$\mathbf{u}_p = \nabla \times (\psi \mathbf{i}_\varphi), \qquad \mathbf{b}_p = \nabla \times (A\mathbf{i}_\varphi). \tag{13}$$

The body force is assumed to be given, and the problem is to solve for $\mathbf{u}$ and $\mathbf{b}$ subject to suitable boundary conditions.

The nature of the driving force $\mathbf{F}$ is uncertain. It is possible that buoyancy forces resulting from heating caused by radioactive decay are the dominant forces. In this case the predominant part of the force is likely to be axisymmetric, e.g., as a result of a temperature gradient between the equator and the poles. Hence $R^{-1}F_\varphi$ would vanish and $\mathbf{F}_p$ would be large compared to the asymmetric forces. Braginskii[5] proposes an $\mathbf{F}_p$ of precisely this form, which leads him to an equation corresponding to (23a). The possibility of a φ component of $\mathbf{F}$ is naturally associated with the loss of gravitational energy. If, for example, iron particles are sedimenting in the core, there would be a tendency for the particles to drift towards the east through the action of the Coriolis force, thus contributing to a φ component of $\mathbf{F}$. The mechanism of stirring by sedimentation is favored by Braginskii.[5,6] A consistent model may be formulated in the absence of the axisymmetric body force (see Tough and Roberts[2]), but not in the absence of the nonaxisymmetric body force. This suggests that the scaling depends crucially on $R^{-1/2}F'$ and that the values for $\langle \mathbf{F} \rangle$ are the largest consistent with the model. For this reason the characteristic value, F^*, of the force is determined by the requirement that the fluctuating part, $R^{-1/2}\mathbf{F}'$, of the force should be an order $R^{-1/2}$ quantity. Hence, if the fluctuating force is characterized by F'^*, it is equal to $R^{-1/2}F^*$, so that the characteristic force F^* is given by

$$F^* = (L/2\Omega\eta)(F'^*)^2. \tag{14}$$

The implied dependence of $\mathbf{F}_p$ and F_φ on R in (10a) indicates that these quantities may be smaller than order 1.

Some notation is introduced. The operator $\partial_1/\partial\varphi$ is defined to avoid the differentiation of unit vectors,

$$\frac{\partial_1}{\partial\varphi}(f_\rho \mathbf{i}_\rho + f_\varphi \mathbf{i}_\varphi + f_z \mathbf{i}_z) = \frac{\partial f_\rho}{\partial\varphi}\mathbf{i}_\rho + \frac{\partial f_\varphi}{\partial\varphi}\mathbf{i}_\varphi + \frac{\partial f_z}{\partial\varphi}\mathbf{i}_z. \tag{15}$$

The operator $\hat{}$ is defined by

$$\frac{\partial_1}{\partial\varphi}\hat{f}' = f', \tag{16}$$

where $\langle \hat{f}' \rangle = 0$, and results in the useful identity

$$\sum_{j=1}^{N} \langle \hat{f}'_1 \ldots \hat{f}'_{j-1} f'_j \hat{f}'_{j+1} \ldots \hat{f}'_N \rangle = 0. \tag{17}$$

The following variables are introduced:

$$\mathbf{v}' = (1/U)\mathbf{u}'_p, \quad w = \tfrac{1}{2}\rho\langle \mathbf{v}' \times \hat{\mathbf{v}}' \rangle_\varphi, \quad \mathbf{W} = \tfrac{1}{3}\rho^2\langle \hat{\mathbf{v}}'(\mathbf{v}' \times \hat{\mathbf{v}}')_\varphi \rangle, \quad \mathbf{G} = \mathbf{u}' \times \mathbf{b}', \quad \mathbf{S} = \mathbf{j}' \times \mathbf{b}', \tag{18}$$

where

$$\mathbf{j}' = \nabla \times \mathbf{b}'. \tag{19}$$

Since $\mathbf{G}$ and $\mathbf{S}$ have a symmetric part, the bar operator

$$\bar{\mathbf{G}} = \overbrace{[\mathbf{G} - \langle \mathbf{G} \rangle]} \tag{20}$$

is introduced, which has similar properties to the $\hat{}$ operator. It is assumed that all quantities have expansions in powers of $R^{-1/2}$. A departure is made from previous accounts in the scaling of quantities. As in the definitions (10), quantities are scaled so that they are order 1 where possible.

After considerable reductions of Eqs. (1)–(4), some equations can be determined for, the axisymmetric quantities in terms of the new effective variables:

$$A_e = A + wB + R^{-1/2}[(B/U^2)\nabla\cdot(U^2\mathbf{W}) - U\mathbf{W}\cdot\nabla(B/U)],$$

$$\psi_e = \psi + wU + R^{-1/2}(1/U)\nabla\cdot(U^2\mathbf{W}), \tag{21}$$

$$F_{e\varphi} = F_\varphi - w(\nabla \times \mathbf{F}_p)_\varphi + (\rho/B)\langle \mathbf{b}' \times (\nabla \times \hat{\mathbf{F}}') \rangle_\varphi - R^{-1/2}\{(\nabla \times \mathbf{F}_p)_\varphi (1/U^2)\nabla\cdot(U^2\mathbf{W}) + (1/U)\nabla\cdot[U(\nabla \times \mathbf{F}_p)_\varphi \mathbf{W}]\}.$$

In terms of these new variables, the axisymmetric quantities are governed by the equations

$$\rho \frac{D_e}{Dt}\frac{B}{\rho} = \Delta_1 B + \left(\nabla \frac{U}{\rho} \times \nabla \rho A_e\right)_\varphi, \tag{22a}$$

$$\frac{1}{\rho}\frac{D_e}{Dt}(\rho A_e) = \Delta_1 A_e + \Gamma B, \tag{22b}$$

$$U = \frac{B^2}{\rho} + \rho g(\rho, t) - \tfrac{1}{2}\left(\int_{-(r_0^2-\rho^2)^{1/2}}^{z} (\nabla \times \mathbf{F}_p)_\varphi dz - \int_z^{(r_0^2-\rho^2)^{1/2}} (\nabla \times \mathbf{F}_p)_\varphi dz\right), \tag{23a}$$

$$u_{ep} = (1/\rho)(\mathbf{b}_{ep}\cdot\nabla)\rho B + F_{e\phi}, \tag{23b}$$

where

$$\frac{D_e}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}_{ep}\cdot\nabla, \quad \Delta_1 = \nabla^2 - 1/\rho^2, \quad \mathbf{u}_{ep} = \nabla \times (\psi_e \mathbf{i}_\varphi), \quad \mathbf{b}_{ep} = \nabla \times (A_e \mathbf{i}_\varphi), \tag{24}$$

and[7]

$$\Gamma = \rho^{-1}\left\langle (\mathbf{v}' \times \hat{\mathbf{v}}')_\varphi + \left(\mathbf{v}' \times \frac{\partial_1}{\partial \varphi}\mathbf{v}'\right)_\varphi \right\rangle + 2\langle \nabla_p (\mathbf{r}\cdot\mathbf{v}')\cdot\nabla_p \hat{v}_z' \rangle + O(R^{-1/2}). \tag{25}$$

For simplicity the bounding surface is assumed spherical of radius r_0. Moreover, (22) and (23) are correct to order $R^{-1/2}$. Equations (22) and (23) are remarkable in as much as they are identical in form to the equations that result in the absence of asymmetries except for the term ΓB in (22b).

Most of the above equations are well known. Braginskii[3] determined (22) to lowest order, while Tough[8] extended the definitions of effective variables so that the same equations remained valid to order $R^{-1/2}$. Tough and Roberts[2] showed how effective variables were still relevant in the equations governing the motion and obtained (23) partially to lowest order. The new results are obtained with the introduction of $\mathbf{F}_p + R^{-1}F_\varphi \mathbf{i}_\varphi$. By defining an effective azimuthal force $R^{-1}F_{e\varphi}$, it is shown in the next section that (23) is correct to order $R^{-1/2}$. This contrasts with the Tough–Roberts[2] introduction of the term

$$\lambda = \rho\langle \mathbf{v}' \times (\nabla \times \hat{\mathbf{F}}')\rangle_\varphi, \tag{26}$$

which is $F_{e\varphi}$ to lowest order when $\mathbf{F}_p = F_\varphi = 0$. Tough[8] and Tough and Gibson[9] suggest that effective variables may be relevant to kinematic dynamo theory to higher orders; i.e., with a suitable extension of the definitions of the effective quantities to higher orders, Eqs. (22) remain valid. In the last section the heat conduction equation is considered and it is shown that in the third approximation the present simplifications are in no sense possible. It follows that it is unlikely that simplifications can be made to the magnetic induction equation either.

Finally to close the system of equations, the non-axisymmetric parts of the magnetic induction equation

$$\frac{\partial \mathbf{b}'}{\partial t} = R\nabla \times [\mathbf{u}' \times (B\mathbf{i}_\varphi + R^{-1}\mathbf{b}_p) + (U\mathbf{i}_\varphi + R^{-1}\mathbf{u}_p) \times \mathbf{b}'] + R^{1/2}\nabla \times [G - \langle \mathbf{G}\rangle] + \nabla^2 \mathbf{b}' \tag{27}$$

and the equation of motion

$$\mathbf{i}_z \times \mathbf{u}' = -\nabla P' + (\nabla \times \mathbf{b}') \times (B\mathbf{i}_\varphi + R^{-1}\mathbf{b}_p) + [\nabla \times (B\mathbf{i}_\varphi + R^{-1}\mathbf{b}_p)] \times \mathbf{b}' + R^{-1/2}[\mathbf{S} - \langle \mathbf{S}\rangle] + \mathbf{F}' \tag{28}$$

must also be considered. The boundary conditions are the same as those proposed by Tough and Roberts,[2] with one exception: To order $R^{-1/2}$, ψ and ψ_e are no longer equal on the boundary. It is not the purpose of this paper to discuss how Eqs. (22)–(28) may be solved. The reader is referred to Tough and Roberts[2] for a detailed discussion.

II. THE MEAN PART OF THE EQUATION OF MOTION

The principal difficulty in obtaining Eq. (23) is the determination of a suitable representation of the mean quantity $\langle S_\varphi \rangle$ correct to order $R^{-1/2}$. In order that the method should not be obscured by the algebra, many of the routine algebraic manipulations are omitted. Two representations of the meridional magnetic field and meridional electric current provide the key to determining $\langle S_\varphi \rangle$:

$$\frac{U}{\rho}\mathbf{b}_p' = \frac{B}{\rho}\mathbf{u}_p' + R^{-1/2}[\nabla \times \bar{\mathbf{G}}]_p + O(R^{-1}) \tag{29}$$

and

$$\frac{B}{\rho}\mathbf{j}_p' = -\frac{\partial \hat{\mathbf{u}}_p'}{\partial z} + \hat{\mathbf{b}}_p'\cdot\nabla\left(\mathbf{i}_\varphi \times \frac{\nabla \rho B}{\rho}\right) - \left(\mathbf{i}_\varphi \times \frac{\nabla \rho B}{\rho}\right)\cdot\nabla \hat{\mathbf{b}}_p' - R^{-1/2}[\nabla \times \bar{\mathbf{S}}]_p - [\nabla \times \hat{\mathbf{F}}']_p + O(R^{-1}), \tag{30}$$

which are obtained from (27) and (28), respectively. The latter representation appears to be new and is obtained by taking the curl of (28), taking the meridional components, and integrating with respect to φ. Another relation that is useful is

$$\frac{\partial}{\partial z}\left(U - \frac{B^2}{\rho}\right) = -(\nabla \times \mathbf{F}_p)_\varphi + O(R^{-1}), \tag{31}$$

which is obtained by taking the φ component of the curl of the mean part of the equation of motion. Incidently (23a) is an immediate consequence of (31).

Using (30) $\langle S_\varphi \rangle$ is given correct to order $R^{-1/2}$ by

$$\frac{B}{\rho}\langle S_\varphi \rangle = -\left\langle \frac{\partial \hat{\mathbf{u}}_p'}{\partial z} \times \mathbf{b}_p' \right\rangle_\varphi + \left\langle \hat{\mathbf{b}}_p'\cdot\nabla\left(\mathbf{i}_\varphi \times \frac{\nabla \rho B}{\rho}\right) \times \mathbf{b}_p' \right\rangle_\varphi - \left\langle \left(\mathbf{i}_\varphi \times \frac{\nabla \rho B}{\rho}\right)\cdot\nabla \hat{\mathbf{b}}_p' \times \mathbf{b}_p' \right\rangle_\varphi - R^{-1/2}\langle (\nabla \times \bar{\mathbf{S}})_p \times \mathbf{b}_p' \rangle_\varphi - \langle (\nabla \times \hat{\mathbf{F}}')_p \times \mathbf{b}_p' \rangle_\varphi. \tag{32}$$

In the first term $\mathbf{b}'_p$ is replaced by the value given by (29). The second and third terms are simplified by use of relation (17). These alterations lead to

$$\frac{B}{\rho}\langle S_\varphi\rangle = \frac{B}{\rho U}\frac{\partial}{\partial z}(U^2 w) - \frac{1}{2B}\langle \mathbf{b}'_p \times \hat{\mathbf{b}}'_p\rangle_\varphi \frac{\partial}{\partial z}\left(\frac{B^2}{\rho}\right) + \frac{B}{\rho^2}\left(\mathbf{i}_\varphi \times \frac{\nabla\rho B}{\rho}\right)\cdot\nabla\left(\frac{\rho^2}{2B}\langle \mathbf{b}'_p \times \hat{\mathbf{b}}'_p\rangle_\varphi\right) + R^{-1/2}\frac{\rho}{U}\left\langle (\nabla\times\bar{\mathbf{G}})_p \times \frac{\partial \hat{\mathbf{u}}'_p}{\partial z}\right\rangle_\varphi - R^{-1/2}\langle(\nabla\times\bar{\mathbf{S}})_p \times \mathbf{b}'_p\rangle_\varphi - \langle(\nabla\times\hat{\mathbf{F}}')\times\mathbf{b}'_p\rangle_\varphi. \tag{33}$$

Evidently (29) leads to the identity

$$(\rho/2B^2)\langle \mathbf{b}'_p \times \hat{\mathbf{b}}'_p\rangle_\varphi = w + R^{-1/2}(\rho^2/BU^2) \times \langle(\nabla\times\bar{\mathbf{G}})_p \times \hat{\mathbf{u}}'_p\rangle_\varphi, \tag{34}$$

correct to order $R^{-1/2}$. Substituting (34) into (33) and making use of (31) gives

$$\langle S_\varphi\rangle = \frac{\partial}{\partial z}(Uw) - \frac{1}{\rho}\left(\mathbf{i}_\varphi \times \frac{\nabla\rho B w}{\rho}\right)\cdot\nabla\rho B - w(\nabla\times\mathbf{F}_p)_\varphi - \frac{\rho}{B}\langle(\nabla\times\hat{\mathbf{F}}')_p\times\mathbf{b}'_p\rangle_\varphi + R^{-1/2} \times\left[\frac{\rho^2}{BU}\left\langle(\nabla\times\bar{\mathbf{G}})_p\times\frac{\partial\hat{\mathbf{u}}'_p}{\partial z}\right\rangle_\varphi + \frac{1}{B}\left(\mathbf{i}_\varphi\times\frac{\nabla\rho B}{\rho}\right)\cdot\nabla\left(\frac{\rho^2 B}{U^2}\langle(\nabla\times\bar{\mathbf{G}})_p\times\hat{\mathbf{u}}'_p\rangle_\varphi\right) - \frac{\rho}{B}\langle(\nabla\times\bar{\mathbf{S}})_p\times\mathbf{b}'_p\rangle_\varphi\right] + O(R^{-1}). \tag{35}$$

At this point (23b) may be obtained correct to lowest order.

In order to determine $\langle S_\varphi\rangle$ to order $R^{-1/2}$ the last three terms in (35) must be considered. However, for these terms only the lowest-order approximations for $\mathbf{b}'$ and $\mathbf{j}'$ need be considered. Consequently, to this order of accuracy, $\mathbf{b}'$ and $\mathbf{u}'$ are related simply by $\mathbf{b}'_p/B = \mathbf{u}'_p/U = \mathbf{v}'$. In evaluating these terms the identity

$$\mathbf{i}_\varphi\times(\nabla\times\hat{\mathbf{f}}') = (1/\rho)\nabla(\rho\hat{\mathbf{f}}'_\varphi) - (1/\rho)\mathbf{f}' \tag{36}$$

is useful. Now it is clear that

$$\mathbf{G} = \rho U^2(\mathbf{i}_\varphi\times\mathbf{v}')\mathbf{v}')\hat{\mathbf{v}}'\cdot B/U), \tag{37}$$

to the required order of accuracy. Hence, by use of (36) and (37) it can be shown that

$$\frac{\rho^2}{BU}\left\langle(\nabla\times\bar{\mathbf{G}})_p\times\frac{\partial\hat{\mathbf{u}}'_p}{\partial z}\right\rangle_\varphi = -\frac{\rho}{BU}\left\langle\frac{\partial\hat{\mathbf{u}}'_p}{\partial z}\cdot\mathbf{G}_p\right\rangle = -\frac{1}{BU}\frac{\partial}{\partial z}(U^3\mathbf{W})\cdot\nabla\frac{B}{U} \tag{38}$$

and

$$\frac{\rho^2 B}{U^2}\langle(\nabla\times\bar{\mathbf{G}})_p\times\hat{\mathbf{u}}'_p\rangle_\varphi = -\frac{\rho B}{U^2}\langle\hat{\mathbf{u}}'_p\cdot\mathbf{G}_p\rangle = -3UB(\mathbf{W}\cdot\nabla)\frac{B}{U}. \tag{39}$$

Repeated use of relation (17) is required to obtain (38). The last term in (35) becomes

$$-(\rho/B)\langle(\nabla\times\bar{\mathbf{S}})_p\times\mathbf{b}'_p\rangle_\varphi = (1/B)\nabla\cdot\langle\rho S_\varphi\hat{\mathbf{b}}'_p\rangle = (1/B)\nabla\cdot(\mathbf{J}_1+\mathbf{J}_2+\mathbf{J}_3), \tag{40}$$

where

$$\mathbf{J}_1 = -\frac{\rho^2}{B}\left\langle\left(\frac{\partial\hat{\mathbf{u}}'_p}{\partial z}\times\mathbf{b}'_p\right)_\varphi\hat{\mathbf{b}}'_p\right\rangle,$$
$$\mathbf{J}_2 = \frac{\rho^2}{B}\left\langle\left[\hat{\mathbf{b}}'_p\cdot\nabla\left(\mathbf{i}_\varphi\times\frac{\nabla\rho B}{\rho}\right)\times\mathbf{b}'_p\right]_\varphi\hat{\mathbf{b}}'_p\right\rangle, \tag{41}$$
$$\mathbf{J}_3 = -\frac{\rho^2}{B}\left\langle\left[\left(\mathbf{i}_\varphi\times\frac{\nabla\rho B}{\rho}\right)\cdot\nabla\hat{\mathbf{b}}'_p\times\mathbf{b}'_p\right]_\varphi\hat{\mathbf{b}}'_p\right\rangle.$$

In obtaining (40) the value of $\mathbf{j}'_p$ given by (30) is substituted into S_φ. Evaluation of $\mathbf{J}_2$ is a little awkward, although the values of $\mathbf{J}_1$ and $\mathbf{J}_3$ are obtained in a way similar to (38). After some manipulation, $\mathbf{J}_1, \mathbf{J}_2$, and $\mathbf{J}_3$ may be conveniently expressed as

$$\mathbf{J}_1 = \frac{B}{U^2}\frac{\partial}{\partial z}(U^3\mathbf{W}),$$
$$\mathbf{J}_2 = -(B^2\mathbf{W}\cdot\nabla)\left(\mathbf{i}_\varphi\times\frac{\nabla\rho B}{\rho}\right) + \frac{B^2}{\rho}\frac{\partial B}{\partial z}\mathbf{W}, \tag{42}$$
$$\mathbf{J}_3 = \left(\mathbf{i}_\varphi\times\frac{\nabla\rho B}{\rho}\right)\cdot\nabla(B^2\mathbf{W}) - \frac{3B^2}{\rho}\frac{\partial B}{\partial z}\mathbf{W}.$$

Collecting together Eqs. (35)–(42) gives an expression for $\langle S_\varphi\rangle$ in which all the means of products of fluctuating quantities are given in terms of w and $\mathbf{W}$. However, some considerable simplifications to (35) can still be made. In particular Eqs. (38)–(42) lead to the identity

$$-\frac{1}{BU}\frac{\partial}{\partial z}(U^3\mathbf{W})\cdot\nabla\frac{B}{U} - \frac{1}{B}\left(\mathbf{i}_\varphi\times\frac{\nabla\rho B}{\rho}\right)\cdot\nabla\left(3UB\mathbf{W}\cdot\nabla\frac{B}{U}\right) + \frac{1}{B}\nabla\cdot(\mathbf{J}_1+\mathbf{J}_2+\mathbf{J}_3) = \frac{\partial}{\partial z}\left(\frac{1}{U}\nabla\cdot(U^2\mathbf{W})\right) + \frac{1}{\rho}\left(\mathbf{i}_\varphi\times\frac{\nabla\rho B}{\rho}\right)\cdot\nabla\left[\rho\left(\frac{B}{U^2}\nabla\cdot(U^2\mathbf{W}) - U\mathbf{W}\cdot\nabla\frac{B}{U}\right)\right] + \frac{1}{U}\nabla\cdot\left[\frac{\partial}{\partial z}\left(U-\frac{B^2}{\rho}\right)U\mathbf{W}\right] + \frac{1}{U^2}\frac{\partial}{\partial z}\left(U-\frac{B^2}{\rho}\right)\nabla\cdot(U^2\mathbf{W}), \tag{43}$$

which is an expression for the last three terms of (35). Hence, after substituting the result into (35) and making use of (31), $\langle S_\varphi\rangle$ becomes

$$\langle S_\varphi\rangle = \frac{\partial}{\partial z}(\psi_e - \psi) - (1/\rho^2)[\mathbf{i}_\varphi\times\nabla\rho(A_e - A)]\cdot\nabla\rho B + (F_{e\varphi} - F_\varphi) + O(R^{-1}), \tag{44}$$

where the effective variables (21) have been introduced. Together with the φ component of the

mean part of the equation of motion (2), namely

$$u_\rho = (1/\rho)(\mathbf{b}_p \cdot \nabla)\rho B + F_\varphi + \langle S_\varphi \rangle, \tag{45}$$

this result establishes (23b).

III. EFFECTIVE VARIABLES

A preliminary investigation is made to see whether effective variables may be found which reduce the mean part of the magnetic induction equation to the form (22) correct to order R^{-1}. Though it will be shown that this possibility is unlikely, a certain structure is beginning to appear [see (63)]. This structure will be fully exploited in a subsequent paper, and will indicate why effective variables occur in the low-order approximations.

The amount of algegra involved in determining the order R^{-1} terms that must be included in (22) is immense, and the calculation has not been attempted. Instead the related problem concerning the heat conduction equation:

$$\frac{\partial \theta^*}{\partial t} + R\,\mathbf{u}\cdot\nabla\theta^* = \nabla^2\theta^*, \tag{46}$$

where θ^* is a scalar quantity, is considered. A solution is sought of the form

$$\theta^* = \Theta(R,\rho,z,t) + R^{-1/2}\theta'(R,\rho,\varphi,z,t), \tag{47}$$

where $\mathbf{u}$ is given by (10b). As in the case of the magnetic induction equation, it can be shown that the mean part of (46) is given by

$$(D_e/Dt)\Theta = \nabla^2\Theta, \tag{48}$$

correct to order $R^{-1/2}$, where (D_e/Dt) is the effective material derivative (24). Evidently if effective variables cannot be found that reduce the mean part of (46)–(48), it is most unlikely that the required simplifications can be made to the magnetic induction equation either, which is more complicated and exhibits most of the features of (46).

The equation for the mean part of (46) is

$$D\Theta/Dt + \langle Q \rangle = \nabla^2\Theta, \tag{49}$$

where

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}_p\cdot\nabla, \qquad Q = \mathbf{u}'\cdot\nabla\theta'. \tag{50}$$

The equation for the fluctuating part leads to

$$\frac{U}{\rho}\theta' = -\hat{\mathbf{u}}'\cdot\nabla\Theta - R^{-1/2}\overline{Q} - R^{-1}\left(\frac{D\hat{\theta}'}{Dt} - \nabla^2\hat{\theta}'\right). \tag{51}$$

Repeated use of (51) gives

$$\langle Q \rangle = I_1 + R^{-1/2}I_2 + R^{-1}(I_3 + I_4), \tag{52}$$

where

$$I_1 = -\langle \mathbf{u}'\cdot\nabla[(\rho/U)\hat{\mathbf{u}}\cdot\nabla\Theta]\rangle = -(1/\rho)[\nabla(\rho U w)\times\nabla\Theta]_\varphi,$$

$$I_2 = \langle \mathbf{u}'\cdot\nabla\overline{\{(\rho/U)\mathbf{u}'\cdot\nabla[(\rho/U)\hat{\mathbf{u}}'\cdot\nabla\Theta]\}}\rangle$$

$$= -(1/\rho)[\nabla\{(\rho/U)\nabla\cdot(U^2\mathbf{W})\}\times\nabla\Theta]_\varphi, \tag{53}$$

$$I_3 = -\langle \mathbf{u}'\cdot\nabla((\rho/U)\mathbf{u}'\cdot\nabla\overline{\{(\rho/U)\mathbf{u}'\cdot\nabla[(\rho/U)\hat{\mathbf{u}}'\cdot\nabla\Theta]\}})\rangle$$

$$I_4 = -\left\langle \hat{\mathbf{u}}'\cdot\nabla\left\{\frac{\rho}{U}\left[\frac{D}{Dt}\left(\frac{\rho}{U}\hat{\mathbf{u}}'\cdot\nabla\Theta\right) - \nabla^2\left(\frac{\rho}{U}\hat{\mathbf{u}}'\cdot\nabla\Theta\right)\right]\right\}\right\rangle .$$

The expressions for I_1 and I_2 together with (49) give (48).

In order to show that effective variables do not exist at the next approximation, it is sufficient to consider a planar model[10]. In place of the coordinates ρ, φ, z the coordinates x^*, y^*, z^* are introduced, where $x^* = z$, $y^* = \rho - \rho_0$, and $z^* = \rho_0\varphi$. The limit $\rho_0 \to \infty$ is taken, and the asterisk is subsequently dropped. The simplification, though unnecessary, does make the subsequent analysis clearer.

Tensorial notation[11] is adopted to facilitate the evaluation of I_3. Relation (17) gives the identity

$$0 = \left\langle u_i'\frac{1}{U}\hat{u}_j'\frac{1}{U}\hat{u}_k'\frac{1}{U}\hat{u}_l'\Theta\right\rangle_{,ijkl}. \tag{54}$$

Differentiation with respect to the i suffix is carried out and use of (17) leads to

$$0 = -6\left\langle\overline{\left(\frac{1}{U}\mathbf{u}'\cdot\nabla\frac{1}{U}\hat{u}_k'\right)}u_j'\frac{1}{U}\hat{u}_l'\Theta\right\rangle_{,jkl}$$

$$-3\left\langle u_j'\frac{1}{U}\hat{u}_k'\frac{1}{U}\hat{u}_l'\left(\frac{1}{U}\hat{\mathbf{u}}'\cdot\nabla\Theta\right)\right\rangle_{,jkl} + 3\alpha \tag{55}$$

where

$$\alpha = \left(\left\langle \mathbf{u}'\cdot\nabla\frac{1}{U}\hat{u}_j'\right\rangle\left\langle\frac{1}{U}\hat{u}_k'\frac{1}{U}\hat{u}_l'\right\rangle\Theta\right)_{,jkl}. \tag{56}$$

The above procedure is repeated (differentiation with respect to the j suffix) and leads to

$$0 = 6\left\langle u_k'\left[\frac{1}{U}\mathbf{u}'\cdot\nabla\overline{\left(\frac{1}{U}\mathbf{u}'\cdot\nabla\frac{1}{U}\hat{u}_l'\right)}\right]\Theta\right\rangle_{,kl}$$

$$+6\left\langle u_k'\left(\overline{\frac{1}{U}\mathbf{u}'\cdot\nabla\frac{1}{U}\hat{u}_l'}\right)\frac{1}{U}\hat{u}'\cdot\nabla\Theta\right\rangle_{,kl}$$

$$+6\left\langle u_k'\frac{1}{U}\hat{u}_l'\overline{\left[\frac{1}{U}\mathbf{u}'\cdot\nabla\left(\frac{1}{U}\hat{\mathbf{u}}'\cdot\nabla\Theta\right)\right]}\right\rangle_{,kl}$$

$$+3\alpha - 6\beta - 3\gamma, \tag{57}$$

where

$$\beta = \left(\left\langle \mathbf{u}'\cdot\nabla\frac{1}{U}\hat{u}_k'\right\rangle\left\langle\frac{1}{U}\hat{u}_l'\frac{1}{U}\hat{\mathbf{u}}'\cdot\nabla\Theta\right\rangle\right)_{,kl},$$

$$\gamma = \left[\left\langle\frac{1}{U}\hat{u}_k'\frac{1}{U}\hat{u}_l'\right\rangle\left\langle\mathbf{u}'\cdot\nabla\left(\frac{1}{U}\hat{\mathbf{u}}'\cdot\nabla\Theta\right)\right\rangle\right]_{,kl}. \tag{58}$$

The procedure is followed for a third time (differentiation with respect to the k suffix) and leads

to the identity

$$0 = -\nabla\cdot(\mathbf{V}\Theta) + I_3 + \left\langle \hat{\mathbf{u}}'\cdot\nabla\left[\frac{1}{U}\left(\mathbf{u}_e^{(0)} - \mathbf{u}_p\right)\cdot\nabla\left(\frac{1}{U}\hat{\mathbf{u}}'\cdot\nabla\Theta\right)\right]\right\rangle, \quad (59)$$

where

$$\mathbf{V} = -\left\langle \mathbf{u}'\cdot\nabla\left[\frac{1}{U}\mathbf{u}'\cdot\nabla\left(\frac{1}{U}\mathbf{u}'\cdot\nabla\frac{1}{U}\hat{\mathbf{u}}'\right)\right]\right\rangle_p + \left\langle \hat{\mathbf{u}}'\cdot\nabla\left(\frac{1}{U}(\mathbf{u}_e^{(0)} - \mathbf{u}_p)\cdot\nabla\frac{1}{U}\hat{\mathbf{u}}'\right)\right\rangle_p, \quad (60)$$

and $\mathbf{u}_e^{(0)}$ is given by

$$\mathbf{u}_e^{(0)} = \mathbf{u}_p - \left\langle \mathbf{u}'\cdot\nabla\left(\frac{1}{U}\hat{\mathbf{u}}'\right)\right\rangle. \quad (61)$$

The above definition of $\mathbf{u}_e^{(0)}$ differs from the lowest-order approximation $\mathbf{u}_{ep}$ only in the z component.

Setting $\Theta = 1$ in (59) leads to the identity

$$\nabla\cdot\mathbf{V} = 0. \quad (62)$$

From the definitions (53) and the identity (59) it follows that (49) is

$$\left(\frac{\partial}{\partial t} + (\mathbf{u}_{ep} + R^{-1}\mathbf{V})\cdot\nabla - \nabla^2\right)\Theta = R^{-1}\left\langle \hat{\mathbf{u}}'\cdot\nabla\left[\frac{1}{U}\left(\frac{\partial}{\partial t} + \mathbf{u}_e^{(0)}\cdot\nabla - \nabla^2\right)\left(\frac{1}{U}\hat{\mathbf{u}}'\cdot\nabla\Theta\right)\right]\right\rangle. \quad (63)$$

There appears to be no representation of the right-hand side of (63) which is simpler than that given, and it seems unlikely that effective variables exist to this order. Before ruling out effective variables completely, a precise definition is given of effective variables for the heat conduction equation. Effective variables are said to exist if a quantity $\Theta_e(R, \mathbf{u}; \Theta)$ can be constructed which satisfies the heat conduction equation

$$\frac{\partial}{\partial t}\Theta_e + \mathbf{u}_{ep}\cdot\nabla\Theta_e = \nabla\cdot(\lambda_e\nabla\Theta_e), \quad (64)$$

where Θ_e is convected with a velocity $\mathbf{u}_{ep}(R, \mathbf{u})$ in a medium whose diffusivity is $\lambda_e(R, \mathbf{u})$. The quantities $\lambda_e, \mathbf{u}_{ep}, \Theta_e$ are effective variables. The point of view taken in constructing this definition is that a function Θ_e may be chosen which will satisfy an equation whose character is similar to (46) in the case of planar (or axial) symmetry. This is essentially the Braginskii[3] formulation. Finally it is supposed that λ_e and $\mathbf{u}_{ep}$ have unique expansions in powers of $R^{-1/2}$, so that

$$\lambda_e = 1 + R^{-1}\lambda_e^{(2)}, \qquad \mathbf{u}_{ep} = \mathbf{u}_{ep}^{(0)} + R^{-1/2}\mathbf{u}_{ep}^{(1)} + R^{-1}\mathbf{u}_{ep}^{(2)}, \quad (65)$$

correct to order R^{-1} where the first two terms in $\mathbf{u}_{ep}$ are given by (21). Since I_3 and I_4 contain only one time derivative and four space derivatives, the most general form Θ_e is

$$\Theta_e = \Theta + R^{-1}(\alpha\Theta + \beta_i\Theta_{,i} + T_{ij}\Theta_{,ij}). \quad (66)$$

Substituting this form of Θ_e into (64) and making a correspondence with (49) to order R^{-1} leads to the identity

$$\left(\frac{\partial}{\partial t} + \mathbf{u}_{ep}^{(0)}\cdot\nabla - \nabla^2\right)(\alpha\Theta + \beta_i\Theta_{,i} + T_{ij}\Theta_{,ij}) + \mathbf{u}_{ep}^{(2)}\cdot\nabla\Theta - \nabla\cdot(\lambda_e^{(2)}\nabla\Theta) \equiv I_3 + I_4, \quad (67)$$

which must be satisfied for all choices of Θ. Equating coefficients of the fourth-order derivatives of Θ gives

$$T_{ij} = -(1/U^2)\langle \hat{u}_i'\hat{u}_j'\rangle, \qquad i,j = 1,2. \quad (68)$$

Then equating the third-order derivatives of Θ gives

$$(\beta_i - T_{il,l})\delta_{jk} = T_{ij,k}, \qquad i,j,k = 1,2, \quad (69)$$

where

$$\delta_{jk} = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases}.$$

In general $T_{ij,k} \neq 0$ when $j \neq k$, in which case (69) has no solution. This establishes conclusively that effective variables do not exist in the heat conduction equation to order R^{-1}.

It does not appear possible to make any direct correspondence between the formulations (46), (47), and (49) for the heat conduction equation and that for the magnetic induction equation. However the expression for $-\langle Q\rangle$ is very similar to the expression for $[\nabla\times\langle \mathbf{G}\rangle_p]_\varphi$, which is

$$[\nabla\times\langle \mathbf{G}\rangle_p]_\varphi = \left\langle \rho\mathbf{u}'\cdot\nabla\left(\hat{\mathbf{u}}'\cdot\nabla\frac{B}{U}\right)\right\rangle - R^{-1/2} \times \left\langle \rho\mathbf{u}'\cdot\nabla\left[u'\cdot\nabla\left(\frac{\rho}{U}\hat{\mathbf{u}}'\cdot\nabla\frac{B}{U}\right)\right]\right\rangle + 0(R^{-1}). \quad (70)$$

The order R^{-1} terms are similar in character to I_3 and I_4. Exactly the same features encountered above will occur in the magnetic induction equation, specifically in (22a). Therefore it is to be expected that effective variables will have no relevance beyond an accuracy of order $R^{-1/2}$.

ACKNOWLEDGMENTS

The author wishes to thank Professor S. Childress for many useful discussions and suggestions during the course of this study. This work was supported by the National Science Foundation, Grant No. NSF-GP-19617.

* Present address: School of Mathematics, University of Newcastle upon Tyne, NE1 7IU, England.

1 *The Application of Modern Physics to the Earth and Planetary Interiors*, edited by S. K. Runcorn (Wiley-Interscience, New York, 1969).

2 J. G. Tough and P. H. Roberts, *Physics of the Earth and Planetary Interiors* (North-Holland, Amsterdam, 1968), Vol. 1, p. 288.

3 S. I. Braginskii, Zh. Eksp. Teor. Fiz. **47**, 1084 (1964) [Sov. Phys. JETP **20**, 726 (1965)].

4 H. P. Greenspan, *The Theory of Rotating Fluids* (Cambridge U.P., New York, 1968).

5 S. I. Braginskii, Geomagnetizm i Aeronomiya Ser. IV, 5, 898 (1964) [Geomagnetism and Aeronomics Ser. IV, 5, 698 (1964)].

6 S. I. Braginskii, Zh. Eksp. Teor. Fiz. **47**, 2178 (1964) [Sov. Phys. JETP **20**, 1462 (1965)].

7 The reader is refered to Tough (Ref. 8) or Tough and Gibson (Ref. 9) for the order $R^{-1/2}$ terms in the expression for Γ.

8 J. G. Tough, Geophys. J. Roy. Astron. Soc. Can. **13**, 393 (1967).

9 J. G. Tough and R. D. Gibson, in Ref. 1, p. 555.

10 This procedure has been adopted before by Braginskii (Ref. 6).

11 Note the equivalence $(i_x, i_y, i_z) = (i_1, i_2, i_3)$ is subsequently assumed for the coordinate axes.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Structure of Neutral Mesonic Atoms Formed in Liquid Helium. III. More Accurate Treatment of the Electron Wavefunction*

L. C. Chen,† J. Guo,‡ and J. E. Russell
Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221

(Received 7 April 1971)

The ground-state energy of a spinless nonrelativistic electron in the field of two fixed spinless nuclei with charges +2 and −1 is computed exactly for a large number of values of the internuclear separation. The calculation is performed using a method devised many years ago by Baber and Hassé. The results of this calculation are then used to estimate values, for a few highly excited states of $\alpha\pi^-e^-$ and αK^-e^- atoms, of a correction to a previous calculation of the binding energy. This energy correction increases, by one unit, a previous estimate of the multipolarity of the most favored Auger transition from a circular orbit of the αK^-e^- atom with $n = 29$; a similar increase is found to be most likely for circular orbits of the $\alpha\pi^-e^-$ atom with $n = 20$ and circular orbits of the $\alpha\bar{p}e^-$ atom with $n = 32$, 35, and 37. For αK^-e^- atoms with $n = 27$ and 29, the energy corrections cause the calculated energy difference between a circular and a nearly circular orbit with the same principal quantum number to be between 15 and 30% smaller than had been estimated previously. Two other corrections are estimated and are found to be probably negligible. One of these corrections is the inaccuracy in the calculated binding energy of a heliumlike mesonic atom, as obtained using the Born–Oppenheimer approximation, which is associated with the angular correlation between the positions of the electron and the meson. The other correction is the change in the computed value of the mean meson orbital radius which occurs when the interactions responsible for the electron–meson angular correlation are taken into account.

1. INTRODUCTION

This paper is concerned with the binding energies and wavefunctions for some highly excited states of heliumlike mesonic atoms. Its purpose is to present a more accurate treatment than has previously been given[1,2] of the effects of the dipole and higher-multipole electrostatic interactions of the electron with the meson in such atoms. References 1 and 2 are referred to in this paper as I and II, respectively.

Two corrections are made to the binding energy. The more important of these corrections is found in Sec. 2 by using the results of an exact calculation of the ground-state energy of an electron in the field of two fixed particles with charges +2 and −1. This exact calculation is performed using a method developed many years ago by Baber and Hassé.[3] The energy correction obtained in Sec. 2 is, in each instance, rather different from an estimate of the same quantity made in I, where some very rough approximations were employed. Furthermore, the difference between the values of this energy correction for two almost degenerate states with the same principal quantum number is not, in any instance, even qualitatively similar to the estimate of this difference obtained in I. Nevertheless, the use of the more accurate energy correction does not appear to change significantly any conclusions reached earlier.

The other energy correction is associated with the Born–Oppenheimer approximation, which was used in I to compute the atomic wavefunctions and binding energies. The accuracy of this approximation has already been investigated, to a certain extent, in II, where it was assumed that only the monopole electron–meson interaction is effective. In Sec. 3 of the present paper, a very rough estimate is made of the extent to which the accuracy of the Born–Oppenheimer approximation is affected by that distortion of the electron wavefunction which is due to the dipole and higher-multipole electron–meson interactions. It is found that this energy correction is likely to be negligibly small.

Finally, in Sec. 4, a very rough estimate is made of the extent to which these dipole and higher-multipole interactions might cause some previous estimates of the mean meson orbital radius to be in error. This correction is also found to be probably negligibly small.

In each instance that is considered, the electron is in a 1*s* orbit, and the meson is in a circular or nearly circular orbit with large principal quantum number n. In a circular orbit, the orbital angular momentum l is given by $l = n - 1$. For the sake of brevity, a state of the mesonic atom in which the meson is in a circular or nearly circular orbit, and in which the electron is in a 1*s* orbit, is frequently referred to in this paper simply as a

* Present address: School of Mathematics, University of Newcastle upon Tyne, NE1 7IU, England.

1 *The Application of Modern Physics to the Earth and Planetary Interiors*, edited by S. K. Runcorn (Wiley-Interscience, New York, 1969).

2 J. G. Tough and P. H. Roberts, *Physics of the Earth and Planetary Interiors* (North-Holland, Amsterdam, 1968), Vol. 1, p. 288.

3 S. I. Braginskii, Zh. Eksp. Teor. Fiz. **47**, 1084 (1964) [Sov. Phys. JETP **20**, 726 (1965)].

4 H. P. Greenspan, *The Theory of Rotating Fluids* (Cambridge U.P., New York, 1968).

5 S. I. Braginskii, Geomagnetizm i Aeronomiya Ser. IV, 5, 898 (1964) [Geomagnetism and Aeronomics Ser. IV, 5, 698 (1964)].

6 S. I. Braginskii, Zh. Eksp. Teor. Fiz. **47**, 2178 (1964) [Sov. Phys. JETP **20**, 1462 (1965)].

7 The reader is refered to Tough (Ref. 8) or Tough and Gibson (Ref. 9) for the order $R^{-1/2}$ terms in the expression for Γ.

8 J. G. Tough, Geophys. J. Roy. Astron. Soc. Can. **13**, 393 (1967).

9 J. G. Tough and R. D. Gibson, in Ref. 1, p. 555.

10 This procedure has been adopted before by Braginskii (Ref. 6).

11 Note the equivalence $(i_x, i_y, i_z) = (i_1, i_2, i_3)$ is subsequently assumed for the coordinate axes.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Structure of Neutral Mesonic Atoms Formed in Liquid Helium. III. More Accurate Treatment of the Electron Wavefunction*

L. C. Chen,† J. Guo,‡ and J. E. Russell
Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221

(Received 7 April 1971)

The ground-state energy of a spinless nonrelativistic electron in the field of two fixed spinless nuclei with charges +2 and −1 is computed exactly for a large number of values of the internuclear separation. The calculation is performed using a method devised many years ago by Baber and Hassé. The results of this calculation are then used to estimate values, for a few highly excited states of $\alpha\pi^-e^-$ and αK^-e^- atoms, of a correction to a previous calculation of the binding energy. This energy correction increases, by one unit, a previous estimate of the multipolarity of the most favored Auger transition from a circular orbit of the αK^-e^- atom with $n = 29$; a similar increase is found to be most likely for circular orbits of the $\alpha\pi^-e^-$ atom with $n = 20$ and circular orbits of the $\alpha\bar{p}e^-$ atom with $n = 32$, 35, and 37. For αK^-e^- atoms with $n = 27$ and 29, the energy corrections cause the calculated energy difference between a circular and a nearly circular orbit with the same principal quantum number to be between 15 and 30% smaller than had been estimated previously. Two other corrections are estimated and are found to be probably negligible. One of these corrections is the inaccuracy in the calculated binding energy of a heliumlike mesonic atom, as obtained using the Born–Oppenheimer approximation, which is associated with the angular correlation between the positions of the electron and the meson. The other correction is the change in the computed value of the mean meson orbital radius which occurs when the interactions responsible for the electron–meson angular correlation are taken into account.

1. INTRODUCTION

This paper is concerned with the binding energies and wavefunctions for some highly excited states of heliumlike mesonic atoms. Its purpose is to present a more accurate treatment than has previously been given[1,2] of the effects of the dipole and higher-multipole electrostatic interactions of the electron with the meson in such atoms. References 1 and 2 are referred to in this paper as I and II, respectively.

Two corrections are made to the binding energy. The more important of these corrections is found in Sec. 2 by using the results of an exact calculation of the ground-state energy of an electron in the field of two fixed particles with charges +2 and −1. This exact calculation is performed using a method developed many years ago by Baber and Hassé.[3] The energy correction obtained in Sec. 2 is, in each instance, rather different from an estimate of the same quantity made in I, where some very rough approximations were employed. Furthermore, the difference between the values of this energy correction for two almost degenerate states with the same principal quantum number is not, in any instance, even qualitatively similar to the estimate of this difference obtained in I. Nevertheless, the use of the more accurate energy correction does not appear to change significantly any conclusions reached earlier.

The other energy correction is associated with the Born–Oppenheimer approximation, which was used in I to compute the atomic wavefunctions and binding energies. The accuracy of this approximation has already been investigated, to a certain extent, in II, where it was assumed that only the monopole electron–meson interaction is effective. In Sec. 3 of the present paper, a very rough estimate is made of the extent to which the accuracy of the Born–Oppenheimer approximation is affected by that distortion of the electron wavefunction which is due to the dipole and higher-multipole electron–meson interactions. It is found that this energy correction is likely to be negligibly small.

Finally, in Sec. 4, a very rough estimate is made of the extent to which these dipole and higher-multipole interactions might cause some previous estimates of the mean meson orbital radius to be in error. This correction is also found to be probably negligibly small.

In each instance that is considered, the electron is in a 1*s* orbit, and the meson is in a circular or nearly circular orbit with large principal quantum number n. In a circular orbit, the orbital angular momentum l is given by $l = n - 1$. For the sake of brevity, a state of the mesonic atom in which the meson is in a circular or nearly circular orbit, and in which the electron is in a 1*s* orbit, is frequently referred to in this paper simply as a

circular or nearly circular orbit. The numerical calculations reported in the present paper are, for the most part, concerned only with a few states of the $\alpha\pi^-e^-$ and αK^-e^- atoms.

The particular notation employed here is chosen to permit a ready comparison with previous work. The unit of energy is the rydberg; the unit of distance is the hydrogen Bohr radius; and the unit of mass is the electron mass.

2. MORE ACCURATE BORN–OPPENHEIMER ENERGIES

A. Introduction

It was shown in I that the wavefunction for a helium-like mesonic atom is given rather accurately by a solution of the equation

$$H_b\Psi_b(\mathbf{r}_e,\mathbf{r}_\mu)=E_b\Psi_b(\mathbf{r}_e,\mathbf{r}_\mu), \tag{2.1a}$$

$$H_b=-\nabla_e^2-\frac{4}{r_e}-\frac{1}{M}\nabla_\mu^2-\frac{4}{r_e}+\frac{2}{|\mathbf{r}_e-\mathbf{r}_\mu|}. \tag{2.1b}$$

The positions of the electron and the meson with respect to the α particle are denoted by $\mathbf{r}_e$ and $\mathbf{r}_\mu$, respectively. The reduced mass of the meson and α particle is denoted by M.

If the Born–Oppenheimer approximation is used to solve Eqs. (2.1), the wavefunction Ψ_b is given approximately by

$$\Psi_b^d(\mathbf{r}_e,\mathbf{r}_\mu)=\phi_b^d(\mathbf{r}_\mu)u_{bde}(\mathbf{r}_e,\mathbf{r}_\mu), \tag{2.2}$$

where the meson wavefunction ϕ_b^d is defined by the equation

$$H_b^d\phi_b^d(\mathbf{r}_\mu)=E_b^d\phi_b^d(\mathbf{r}_\mu), \tag{2.3a}$$

$$H_b^d=-\frac{1}{M}\nabla_\mu^2-\frac{4}{r_\mu}+E_{bde}(r_\mu). \tag{2.3b}$$

The $1s$ electron wavefunction u_{bde} and the energy $E_{bde}(r_\mu)$ are defined by the equation

$$H_{bde}u_{bde}(\mathbf{r}_e,\mathbf{r}_\mu)=E_{bde}(r_\mu)u_{bde}(\mathbf{r}_e,\mathbf{r}_\mu), \tag{2.4a}$$

$$H_{bde}=-\nabla_e^2-\frac{4}{r_e}+\frac{2}{|\mathbf{r}_e-\mathbf{r}_\mu|}. \tag{2.4b}$$

The eigenvalue E_b^d in Eq. (2.3) is an approximate value of E_b. Equations (2.2)–(2.4) do not appear in I because at the time those papers were written it was not realized that Eq. (2.4) can be solved exactly.

Instead, in I, an equation similar to (2.3) was solved. This equation is

$$H_c^{dv}\phi_c^{dv}(\mathbf{r}_\mu)=E_c^{dv}\phi_c^{dv}(\mathbf{r}_\mu), \tag{2.5a}$$

$$H_c^{dv}=-\frac{1}{M}\nabla_\mu^2-\frac{4}{r_\mu}+E_{dev}(r_\mu). \tag{2.5b}$$

The eigenvalue E_c^{dv} is an approximate value of E_b^d. The function $E_{dev}(r_\mu)$ is an approximate value of the ground-state eigenvalue of the equation

$$H_{de}u_{de}(\mathbf{r}_e,r_\mu)=E_{de}(r_\mu)u_{de}(\mathbf{r}_e,r_\mu), \tag{2.6a}$$

$$H_{de}=-\nabla_e^2-\frac{4}{r_e}+\begin{pmatrix}2/r_\mu, & r_e<r_\mu\\ 2/r_e, & r_e>r_\mu\end{pmatrix}. \tag{2.6b}$$

The function $E_{dev}(r_\mu)$, which is a variational estimate of $E_{de}(r_\mu)$, is obtained by approximating u_{de} with a $1s$ hydrogenic function, the variational parameter being the effective nuclear charge. This variational wavefunction is denoted by u_{dev}. The operator H_{de} is similar to H_{bde}, the only difference being that the dipole and higher-multipole interactions between the electron and the meson are neglected. The neglected interactions, which will be denoted by H', are given by

$$H'=\sum_{p=1}^{\infty}H_p, \tag{2.7}$$

where

$$H_p=\frac{8\pi}{2p+1}\begin{pmatrix}r_e^p/r_\mu^{p+1}, & r_e<r_\mu\\ r_\mu^p/r_e^{p+1}, & r_e>r_\mu\end{pmatrix}\times\sum_m Y_{p,m}^*(\hat{r}_\mu)Y_{p,m}(\hat{r}_e). \tag{2.8}$$

B. Correction to Binding Energy

Because of the substantial amount of labor that would be required, it was decided not to perform another Born–Oppenheimer calculation in order to determine E_b^d. Instead, Eq. (2.4) was solved for a large number of values of r_μ, and then the wavefunctions ϕ_c^{dv} obtained in I were used to estimate values of the energy difference $E_b^d-E_c^{dv}$ with first-order perturbation theory. This energy difference is assumed to be given approximately by

$$E_b^d-E_c^{dv}\simeq\delta E_c^{dv}, \tag{2.9}$$

where

$$\delta E_c^{dv}=\int|\phi_c^{dv}(\mathbf{r}_\mu)|^2[E_{bde}(r_\mu)-E_{dev}(r_\mu)]d\tau_\mu. \tag{2.10}$$

Because Baber and Hassé[3] have described their method of solving Eq. (2.4) in considerable detail, only a brief outline of the calculation of $E_{bde}(r_\mu)$ is presented here. Equation (2.4) is separable in prolate spheroidal coordinates. Consequently, u_{bde} may be written as the product of three functions. One of these functions is $e^{im\phi}/(2\pi)^{1/2}$, where m is the azimuthal quantum number. Baber and Hassé represented each of the other two functions, which are both real, by an infinite series of terms of a judiciously chosen form.[4] In each series, the terms have coefficients which satisfy a three-term recurrence relation. It can be shown

that, for solutions with coefficients having acceptable asymptotic forms, both recurrence relations are equivalent to infinite continued fractions. Both of these infinite continued fractions relate r_μ and E_{bde} to m and the other separation constant, which is denoted by A. For a given value of r_μ, the ground-state binding energy is the lowest value of E_{bde} for which both fractions are satisfied by $m = 0$ and the same value of A.

It can be shown that each of the infinite continued fractions is equivalent to a series for A in positive powers of r_μ and E_{bde}. However, as noted by Baber and Hassé, these series converge rather slowly in some instances. A tedious algebraic calculation would be required to derive series for A which are carried to orders high enough to obtain a sufficiently accurate solution to Eq. (2.4) for all necessary values of r_μ. Consequently, in the investigation reported here, each fraction was truncated after a suitably large number of continuations, which is essentially equivalent to employing convergent series. A computer was then used to determine E_{bde} by trial and error.

Figure 1 shows $E_{bde} - E_{dev}$ as a function of r_μ. The energy correction δE_c^{dv} is given in Table I for several circular and nearly circular orbits of the $\alpha\pi^-e^-$ and αK^-e^- atoms. Values of E_c^{dv}, which are taken from I, and the resulting estimates of E_b^d, as obtained using the approximate equality (2.9), are also given in Table I. Although the energy E_c^{dv} was computed to an accuracy of 10^{-4} Ry, the values of δE_c^{dv} and E_b^d are only given to an accuracy of 10^{-3} Ry, because it is believed that the numerical evaluation of the integral in Eq. (2.10) is, in each instance, probably not accurate to much better than a few tenths of a percent.

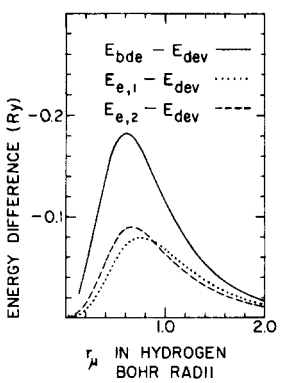

FIG. 1. Energy differences $E_{bde} - E_{dev}$, $E_{e,1} - E_{dev}$, and $E_{e,2} - E_{dev}$ as functions of r_μ.

TABLE I. Approximate binding energy $E_b^d \simeq E_c^{dv} + \delta E_c^{dv}$ for some circular and nearly circular orbits of $\alpha\pi^-e^-$ and αK^-e^- atoms. Orbits with $l = n - 1$ and $l = n - 2$ are grouped separately.

Atom	n	l	E_c^{dv} (Ry)	δE_c^{dv} (Ry)	E_b^d (Ry)
$\alpha\pi^-e^-$	18	17	−4.9238	−0.132	−5.056
	17	16	−5.1491	−0.165	−5.314
	16	15	−5.4865	−0.170	−5.657
	15	14	−5.9541	−0.156	−6.110
	18	16	−4.9873	−0.121	−5.108
	17	15	−5.2235	−0.147	−5.371
	16	14	−5.5534	−0.159	−5.712
	15	13	−6.0087	−0.155	−6.164
αK^-e^-	29	28	−5.4267	−0.175	−5.602
	28	27			
	27	26	−5.9420	−0.157	−6.099
	29	27	−5.4682	−0.166	−5.634
	28	26			
	27	25	−5.9743	−0.156	−6.130

These energy corrections supersede the results of some previous attempts made in I and II. In each instance, the magnitude of δE_c^{dv} is more than five times larger than that of a correction given in II, where a similar estimate was made using the wavefunction ϕ_c^{dv} and first-order perturbation theory, but with the energy difference $E_{de} - E_{dev}$ as the perturbation instead of $E_{bde} - E_{dev}$. Obviously, replacing the electron wavefunction u_{de} with the variational function u_{dev} causes a much smaller error in the estimate of the atomic binding energy than neglecting the interaction H'.

For circular orbits of the αK^-e^- atom with $n = 27$ or 29, the magnitude of δE_c^{dv} is two or three times larger than that of either of two energy corrections calculated in I, where the interaction H' was taken into account and where the resulting distortion of the electron wavefunction was approximated, in a very rough fashion, by one or the other of two functions having fairly simple analytic forms. It is apparent that the use of the distorted wave functions developed in I should generally lead to corrections that are, at best, only qualitatively reliable.

C. Effect on Auger Rates

Auger rates for the mesonic atoms being considered here depend sensitively on the multipole order of the transition.[5-7] Transitions with multipole orders differing by one unit generally proceed with rates that differ by a factor of $\sim 10^3$. The kinetic energy k^2 of an electron ejected in a transition of multipolarity L from a heliumlike mesonic atom in a circular orbit with principal quantum number n and binding energy E_b is given by

$$k^2 = E_b + \frac{4M}{(n - L)^2} \tag{2.11}$$

if, in the final state, the meson is also in a circular orbit. For a circular orbit, the multipole order $L_{\min}$ of the most favored transition is equal to the magnitude of the lowest energetically allowed change in the meson principal quantum number.

The lowest allowed values of L were estimated in I for a large number of circular orbits of $\alpha\pi^-e^-$, αK^-e^-, and $\alpha\bar{p}e^-$ atoms by replacing E_b in Eq. (2.11) with a variational energy E_c^v found by using a simple two-parameter wavefunction. The variational wavefunction, which is denoted by Ψ_c^v, is the product of two hydrogenic functions, one of which describes a $1s$ electron with effective nuclear charge z, and the other, a meson in a cir-

cular orbit with principal quantum number n and effective nuclear charge Z. The variational parameters are z and Z. Estimates of k^2 obtained in this manner are denoted by $(k_c^v)^2$. Because $E_c^v > E_b$, the estimates of $L_{\min}$ obtained in I are lower limits to the actual values.

The results given in Table I and Fig. 1 indicate that, in a few cases, the energy correction δE_c^{dv} is large enough that the lowest energetically allowed value of L is one unit greater than the estimate obtained in I, provided it is assumed that the energy difference $E_b - E_b^d$ is negligibly small. For the particular circular orbits listed in Table I, a revised value of $L_{\min}$ is necessary only in the case of $\alpha K^- e^-$ atoms with $n = 29$, for which $L_{\min} = 5$ instead of 4. Although no detailed calculations have been performed, a comparison of the values of $(k_c^v)^2$ with the values of the energy difference $E_c^{dv} - E_c^v$ given in I and with the behavior of the energy difference $E_{bde} - E_{dev}$ shown in Fig. 1 indicates that the other circular orbits for which $L_{\min}$ is one unit larger than had been estimated in I are $\alpha \bar{p} e^-$ atoms with $n = 32$, 35, and 37 and $\alpha \pi^- e^-$ atoms with $n = 20$. The rough estimates of the energy difference $E_b - E_b^d$ made in II and in Sec. 3 of the present paper are not large enough to alter these conclusions.

D. Energy Difference ϵ_b^d

Table II gives the difference ϵ_b^d between the values of E_b^d for a circular and a nearly circular orbit

TABLE II. Energy differences ϵ_c^{dv}, $\delta\epsilon_c^{dv}$, and ϵ_b^d for some principal levels of $\alpha\pi^- e^-$ and $\alpha K^- e^-$ atoms.

Atom	n	ϵ_c^{dv} (Ry)	$\delta\epsilon_c^{dv}$ (Ry)	ϵ_b^d (Ry)
$\alpha\pi^- e^-$	18	−0.0635	0.012	−0.052
	17	−0.0744	0.017	−0.057
	16	−0.0669	0.012	−0.055
	15	−0.0546	0.001	−0.054
$\alpha K^- e^-$	29	−0.0415	0.010	−0.032
	28			
	27	−0.0323	0.001	−0.031

with the same principal quantum number n. This energy difference is defined by

$$\epsilon_b^d = E_{b,n-2}^d - E_{b,n-1}^d, \tag{2.12}$$

where the dependence on l of the eigenvalue of Eq. (2.3) is indicated by denoting it by $E_{b,l}^d$ rather than by E_b^d. The values of ϵ_b^d given in Table II were found using the estimates of E_b^d given in Table I. For the purpose of comparison, Table II also lists values of ϵ_c^{dv} and $\delta\epsilon_c^{dv}$, which are defined by

$$\epsilon_c^{dv} = E_{c,n-2}^{dv} - E_{c,n-1}^{dv} \tag{2.13}$$

and

$$\delta\epsilon_c^{dv} = \epsilon_b^d - \epsilon_c^{dv}. \tag{2.14}$$

The notation employed in Eq. (2.13) is similar to that of Eq. (2.12).

In both instances, the value of ϵ_b^d given for the $\alpha K^- e^-$ atom in Table II is between 15 and 30% smaller in magnitude than the estimate of this energy difference given in I, where it is denoted by ϵ^{dv}. This surely weakens the arguments presented in I and elsewhere[6,8] to the effect that a Stark transition from a highly excited circular orbit of this atom is not likely to occur during a collision with a He atom in a bubble chamber. Nevertheless, provided the energy difference $E_b - E_e^d$ can be neglected, these arguments are probably not weakened very effectively: The values of ϵ_b^d are still considerably greater in magnitude than the estimates of the Stark matrix element made in Ref. 8, and they are also still large enough so that a very substantial change in the magnitude of the relative linear momentum of the two atoms probably must accompany a Stark transition.

The method by which the correction to ϵ_c^{dv} was obtained in I is unreliable. Unlike the values of δE_c^{dv} given in Table I, the values of the correction $\delta\epsilon_c^{dv}$ given in Table II are not even qualitatively similar to the corresponding estimates given in I, since even the signs are different in each case. The reason for this discrepancy is that while, in a perturbation calculation, approximating the perturbing interaction and replacing the absolute square of a wavefunction with a δ function, which are essentially the approximations that were made in I, may, in some circumstances, lead to an energy correction that is more or less qualitatively accurate, it is much less likely that the difference between the results of two such calculations will be reliable, particularly if this difference is relatively small.

E. Approximate Representation of Distortion of Electron Wavefunction

Because the approximate electron wavefunctions developed in I to take into account the effects of the interaction H' lead to only qualitatively reliable estimates of δE_c^{dv} and to entirely wrong estimates of $\delta\epsilon_c^{dv}$, and because these same wavefunctions, or a generalization of one of them, are employed again in Secs. 3 and 4 of the present paper to make some rough estimates of other corrections, it seems worthwhile to investigate somewhat further the extent to which their use may lead to results which are only poor, rather than totally inadequate. The two approximate solutions developed in I were found by using normalized variational wavefunctions of the form

$$u_e(\mathbf{r}_e, \mathbf{r}_\mu) = u_{dev}(\mathbf{r}_e, r_\mu)[1 + a(r_\mu) g(\mathbf{r}_e, \mathbf{r}_\mu)] \times [1 + \zeta(r_\mu) a^2(r_\mu)]^{-1/2}, \tag{2.15}$$

where, for a given value of $\mathbf{r}_\mu$, g is the product of $\hat{r}_e \cdot \hat{r}_\mu$ and a smoothly varying function of r_e. The

quantity a, which depends on r_μ, is a variational parameter, and ζ is defined by

$$\zeta(r_\mu) = \int [u_{dev}(\mathbf{r}_e, r_\mu) g(\mathbf{r}_e, \mathbf{r}_\mu)]^2 d\tau_e. \quad (2.16)$$

The two choices of g used in I are

$$g_1(\mathbf{r}_e, \mathbf{r}_\mu) = 2\hat{r}_e \cdot \hat{r}_\mu \begin{cases} r_e/r_\mu^2, & r_\mu - r_e > \Delta \\ r_\mu/r_e^2, & r_e - r_\mu > \Delta \end{cases}, \quad (2.17)$$

where Δ is an exceedingly small, positive quantity, and

$$g_2(\mathbf{r}_e, \mathbf{r}_\mu) = 2\hat{r}_e \cdot \hat{r}_\mu \times \begin{cases} (r_e/r_\mu^2)[1 - (3r_e)/(5r_\mu)], & r_e < r_\mu \\ (r_\mu/r_e^2)[1 - (3r_\mu)/(5r_e)], & r_e > r_\mu \end{cases}. \quad (2.18)$$

In addition to the energy difference $E_{bde} - E_{dev}$, Fig. 1 also shows $E_{e,1} - E_{dev}$ and $E_{e,2} - E_{dev}$, where $E_{e,1}$ and $E_{e,2}$ are, respectively, the electron variational binding energies obtained with $g = g_1$ and $g = g_2$. These two energy differences, which are roughly equal, are both substantially smaller than $E_{bde} - E_{dev}$, thus indicating that u_e, with either $g = g_1$ or $g = g_2$, gives a poor, but probably not completely unacceptable, approximation to that distortion of the electron wavefunction which is due to the interaction H'. Although all corrections obtained employing either form of u_e should be interpreted with a certain degree of caution, it seems reasonable to assume that the use of such a function should lead, in most instances, to results which are at least qualitatively reliable.

3. ACCURACY OF BORN–OPPENHEIMER APPROXIMATION

If only the monopole part of the electrostatic interaction between the electron and the meson is effective, as is assumed in Eq. (2.6), the angular motion of one of these particles is not coupled to that of the other, and the wavefunction for the mesonic atom may be written as the product of a correlated radial wavefunction and two spherical harmonics. The argument given in I to justify the use of the Born–Oppenheimer approximation in calculating this radial wavefunction is that the rms radial velocity of the meson is two orders of magnitude smaller than that of the electron in most of the instances considered. The accuracy of this approximation, insofar as it is applied only to the radial motion of the two particles, has been investigated in II and has been found to be rather good. But with the more accurate description of the motion of the electron given by the wavefunction u_{bde}, it seems appropriate also to estimate that inaccuracy in the Born–Oppenheimer energy which is associated with the angular correlation between the electron and the meson, because the rms velocity of the meson, as distinct from its rms radial velocity, is only little more than one order of magnitude smaller than that of the electron in most of the instances investigated.

The method employed here to estimate this energy correction is a straightforward generalization of the one used in II. Therefore, the discussion given here is not overly detailed. Although a formal expression for the energy correction will be given in terms of the function u_{bde}, numerical values will be estimated using the much more tractable, but considerably less accurate, electron wavefunctions developed in I to take into account the effects of the interaction H'.

The energy difference $E_b - E_b^d$ should be given approximately by

$$E_b - E_b^d \simeq \int \Psi_b^{d*}(H_b - H_{bo}^d)\Psi_b^d d\tau_\mu d\tau_e, \quad (3.1)$$

where H_{bo}^d is an operator of which Ψ_b^d is an exact eigenfunction with eigenvalue E_b^d. It is readily verified that the operator

$$H_{bo}^d = H_b + \frac{1}{M}\left(\frac{2}{\Psi_b^d}\nabla_\mu \phi_b^d \cdot \nabla_\mu u_{bde} + \frac{1}{u_{bde}}\nabla_\mu^2 u_{bde}\right) \quad (3.2)$$

satisfies the equation

$$H_{bo}^d \Psi_b^d = E_b^d \Psi_b^d. \quad (3.3)$$

Accordingly, the approximate expression for the energy correction is

$$E_b - E_b^d \simeq -\frac{1}{M}\int (2\Psi_b^{d*}\nabla_\mu \phi_b^d \cdot \nabla_\mu u_{bde} + \Psi_b^{d*}\phi_b^d \nabla_\mu^2 u_{bde}) d\tau_\mu d\tau_e. \quad (3.4)$$

Because the ground-state electron wavefunction u_{bde} is real, and because it is normalized to unity for all $\mathbf{r}_\mu$, it is possible to show, in a manner analogous to that outlined in II, that (3.4) may be put in the form

$$E_b - E_b^d \simeq \frac{1}{M}\int |\phi_b^d \nabla_\mu u_{bde}|^2 d\tau_\mu d\tau_e. \quad (3.5)$$

It is convenient to rewrite the approximate equality (3.5) in the form

$$E_b - E_b^d \simeq \delta E_{b,r}^d + \delta E_{b,\Omega}^d, \quad (3.6)$$

where

$$\delta E_{b,r}^d = \frac{1}{M}\int |\phi_b^d \frac{\partial}{\partial r_\mu} u_{bde}|^2 d\tau_\mu d\tau_e, \quad (3.7)$$

$$\delta E_{b,\Omega}^d = \frac{1}{M}\int |\phi_b^d|^2 \left[\left(\frac{\partial}{r_\mu \partial \theta_\mu} u_{bde}\right)^2 + \left(\frac{\partial}{r_\mu \sin\theta_\mu \partial \phi_\mu} u_{bde}\right)^2\right] d\tau_\mu d\tau_e. \quad (3.8)$$

An approximate expression for $\delta E_{b,r}^d$ may be found by replacing ϕ_b^d and u_{bde} in Eq. (3.7) with ϕ_c^{dv} and u_{dev}, respectively. Values of this approximate

expression were computed in II, where it was denoted by δE_c^{μ}. There appears to be little reason to believe that the use of more accurate wavefunctions would substantially improve this approximation to $\delta E_{b,r}^{d}$.

Unlike $\delta E_{b,r}^{d}$, the term $\delta E_{b,\Omega}^{d}$ vanishes if there is no correlation between $\hat{r}_{\mu}$ and $\hat{r}_e$. Consequently, it is necessary, in this instance, to take into account the angular distortion of the electron wavefunction. It seems unlikely that inserting a doubly infinite series for u_{bde}, as given by Baber and Hassé, into Eq. (3.8) would lead to anything that could be easily evaluated. Therefore, it is assumed that the electron wavefunction may be approximated with a function of the type specified by Eq. (2.15). A straightforward calculation shows that the resulting approximate expression for $\delta E_{b,\Omega}^{d}$ is

$$\delta E_{b,\Omega}^{d} \simeq \frac{2}{M}\int |\phi_b^d(\mathbf{r}_{\mu})|^2 r_{\mu}^{-2} a^2(r_{\mu})\,[u_{dev}(\mathbf{r}_e, r_{\mu}) \times g(\mathbf{r}_e, \mathbf{r}_{\mu})]^2\,[1+\zeta(r_{\mu})a^2(r_{\mu})]^{-1}\,d\tau_{\mu}d\tau_e . \quad (3.9)$$

It will now be shown, by making some further approximations, that $\delta E_{b,\Omega}^{d}$ is surely rather small in each case of any interest, thereby eliminating the need of a more elaborate calculation. For the sake of simplicity, only circular orbits are considered. For the large values of n being considered here, the meson radial wavefunction is sharply peaked in the neighborhood of the mean meson orbital radius $\bar{r}_{\mu}$. Therefore, because the integrand in Eq. (3.9) does not change sign, it seems reasonable to assume that a very large error will not arise from replacing the argument r_{μ} of the functions a, ζ, u_{dev}, and g with $\bar{r}_{\mu}$. It is also assumed that ϕ_b^d may be satisfactorily approximated by a hydrogenic function characterized by the effective nuclear charge Z. The energy correction is then given approximately by

$$\delta E_{b,\Omega}^{d} \simeq \frac{2MZ^2\zeta(\bar{r}_{\mu})\,a^2(\bar{r}_{\mu})}{n^3(n-\frac{1}{2})\,[1+\zeta(\bar{r}_{\mu})\,a^2(\bar{r}_{\mu})]} . \quad (3.10)$$

Values of $a(\bar{r}_{\mu})$ and $\zeta(\bar{r}_{\mu})$ were computed in I, using both $g = g_1$ and $g = g_2$, for the circular orbits of the $\alpha K^- e^-$ atom with $n = 27, 28$, and 29. Table III gives approximate values of $\delta E_{b,\Omega}^{d}$ for these orbits. The corrections are denoted by either $\delta E_{b,\Omega,1}^{d}$ or $\delta E_{b,\Omega,2}^{d}$, depending on the function used for g. The values of Z employed in the calculation are those which were determined in I using the variational wavefunction Ψ_c^v. The estimates of $\delta E_{b,\Omega}^{d}$ are an order of magnitude smaller than the approximate values of $\delta E_{b,r}^{d}$ which were computed in II and which, for the purpose of comparison, are given again in Table III. It is entirely possible that the use of more accurate electron wavefunctions might result in rather larger estimates of $\delta E_{b,\Omega}^{d}$. And it is certain that the difference in the meson masses causes this energy correction to be several times larger for $\alpha\pi^- e^-$ atoms than for $\alpha K^- e^-$ atoms of comparable energy. Nevertheless, it appears most unlikely that a more elaborate calculation would result in estimates of $E_b - E_b^d$ large enough to change significantly the conclusions reached in Sec. 2.

TABLE III. Energy corrections $\delta E_{b,r}^{d}$, $\delta E_{b,\Omega,1}^{d}$, and $\delta E_{b,\Omega,2}^{d}$ for some circular orbits of the $\alpha K^- e^-$ atom.

n	$\delta E_{b,r}^{d}$ (Ry × 10^{-4})	$\delta E_{b,\Omega,1}^{d}$ (Ry × 10^{-5})	$\delta E_{b,\Omega,2}^{d}$ (Ry × 10^{-5})
29	7	3	5
28		3	5
27	9	3	5

4. CORRECTION TO MEAN MESON ORBITAL RADIUS

The distortion due to the interaction H' has been estimated for the electron wavefunction, but not for the meson wavefunction. It was argued in I that the relatively large mass of the meson should prevent its wavefunction from being distorted nearly as much as that of the electron when H' is taken into account. Nevertheless, it seems worthwhile to obtain a rough estimate of the correction to the mean meson orbital radius, because the interaction between the mesonic atom and a He atom, which was estimated in Ref. 8 for a few cases of special interest, depends to some extent on this radius. However, because the dependence is not a very sensitive one, it should suffice to demonstrate that the correction is likely to be quite small. As in Ref. 8, only circular orbits are considered here.

An accurate way of determining the correction would be to solve Eq. (2.3) numerically and then to compare the mean radius obtained using the wavefunction ϕ_b^d with that obtained using ϕ_c^{dv}. However, the determination of E_{bde} requires a not entirely negligible amount of computer time for each value of r_{μ}. For the highly excited circular orbits being considered here, the meson radial wavefunction varies so rapidly with r_{μ} that a very small step length is required for the numerical integration. Consequently, it was decided to estimate the correction by generalizing some relatively simple variational calculations described in I.

A three-parameter variational wavefunction was employed in the calculation described here. This function has the form

$$\Psi_b^v(\mathbf{r}_e, \mathbf{r}_{\mu}) = \Psi_c^v(\mathbf{r}_e, \mathbf{r}_{\mu})\,[1 + aG(\mathbf{r}_e, \bar{r}_{\mu}, \hat{r}_{\mu})]/N^{1/2} . \quad (4.1)$$

In Eq. (4.1), as in previous work, Ψ_c^v denotes the product of two hydrogenic functions, one of which describes an electron in a 1s orbit with effective nuclear charge z, and the other, a meson in a circular orbit with principal quantum number n and effective nuclear charge Z. However, in this instance, in order to be able to construct the function G in such a form that it is obviously a generalization of the function g_1 defined by Eq. (2.17), it is

assumed that the azimuthal quantum number of the meson is zero in the state Ψ_c^v. The function G is given by

$$G(\mathbf{r}_e, \bar{r}_\mu, \hat{r}_\mu) = [2(\tfrac{4}{3}\pi)^{1/2}/C(l', 1, l; 0, 0)] \times \begin{Bmatrix} r_e/\bar{r}_\mu^2, & \bar{r}_\mu - r_e > \Delta \\ \bar{r}_\mu/r_e^2, & r_e - \bar{r}_\mu > \Delta \end{Bmatrix} [Y_{l,0}(\hat{r}_\mu)]^{-1} \times \sum_{m'} C(l', 1, l; m', -m') Y_{l',m'}(\hat{r}_\mu) Y_{1,-m'}(\hat{r}_e), \quad (4.2)$$

where Δ is an exceedingly small, positive quantity and where

$$l = n - 1, \quad (4.3)$$

$$l' = l \pm 1. \quad (4.4)$$

The quantity $\bar{r}_\mu$, which is the mean meson orbital radius for the state Ψ_c^v, is given in terms of Z by

$$\bar{r}_\mu = n(n + \tfrac{1}{2})/(MZ). \quad (4.5)$$

The Clebsch–Gordan coefficients in Eq. (4.2) are expressed in the notation of Rose.[9] If, in Eq. (4.2), $\bar{r}_\mu$ is replaced with r_μ and if $\hat{r}_\mu$ is assumed to be in the direction of the positive z axis, the quantity G becomes identical to $[(2l' + 1)/(2l + 1)]^{1/2} g_1$. The quantity N in Eq. (4.1) is a normalization factor. The variational parameters for the wavefunction Ψ_b^v are z, Z, and a.

The wavefunction Ψ_b^v, which is obviously an eigenfunction of the total orbital angular momentum operator for the two particles, is orthogonal to the wavefunctions for all states with total orbital angular momentum different from l, thereby making possible a variational calculation. The function Ψ_b^v takes into account approximately not only the distortion of the electron wavefunction, but also, by means of the parameter Z, the possibility that the interaction H' may distort the radial meson wavefunction. The wavefunction Ψ_b^v is to be compared with the two-parameter variational function employed in I, which is of the same form as Ψ_c^v and which is also denoted by Ψ_c^v, but which is not necessarily characterized by the same values of z and Z. The difference between the optimum values of Z for these two variational wavefunctions should lead to a rough estimate of the correction to the mean meson orbital radius.

The parameters z, Z, and a are determined by minimizing the value of the integral

$$\int \Psi_b^{v*} H_b \Psi_b^v d\tau_\mu d\tau_e .$$

Because of the particular form chosen for Ψ_b^v, only the monopole, dipole, and quadrupole electron–meson interactions have to be taken into account. In a somewhat similar calculation described in I, where the meson was treated as a classical point charge and where the electron wavefunction was approximated with a function of the type specified by Eq. (2.15), it was shown that the distortion parameter a can be calculated to within an accuracy of a few percent even if the quadrupole interaction is ignored. Since G is really only a generalization of the function g_1 used in the semiclassical calculation described in I, it seems likely that a similar approximation can be made here. Therefore, in order to shorten what would otherwise be an extremely lengthy calculation, it is assumed that, in the three-parameter variational computation, the Hamiltonian H_b may be approximated by

$$H_b \simeq -\nabla_e^2 - \frac{4}{r_e} - \frac{1}{M}\nabla_\mu^2 - \frac{4}{r_\mu} + H_0 + H_1, \quad (4.6)$$

where both H_0 and H_1 are multipole interactions of the type specified by Eq. (2.8). It is probable that the principal source of error in the calculation is not the approximation given by (4.6), but the inadequacy of the function G as an accurate representation of the relative distortion of the electron wavefunction.

The derivation of the approximate expression for the variational energy is straightforward. Because of its considerable length, this expression is not reproduced here. It is found, for both $l' = l + 1$ and $l' = l - 1$, that $\alpha\pi^- e^-$ atoms with $n \leq 18$, $\alpha K^- e^-$ atoms with $n \leq 32$, and $\alpha\bar{p}e^-$ atoms with $n \leq 42$ all have values of Z for the circular orbits which differ by $\lesssim 1\%$ from the corresponding values determined in I using the undistorted variational wavefunction Ψ_c^v. It then follows from Eq. (4.5) that, in each of these instances, the mean meson orbital radii associated with the distorted and the undistorted variational wavefunctions differ by $\lesssim 1\%$. Although it is quite possible that a calculation using more accurate wavefunctions would result in somewhat larger estimates of the difference between the two radii, the differences obtained here are so small that there appears to be little reason to pursue the matter further.

---

* Work supported in part by National Science Foundation under Grant No. GP-20889.

† Present address: Dept. of Physics, University of Wisconsin, Madison, Wisc. 53706.

‡ Present address: Dept. of Electrical Engineering, University of Washington, Seattle, Wash. 98105.

1 J. E. Russell, Phys. Rev. A **1**, 721 (1970); **1**, 735 (1970).

2 J. E. Russell, Phys. Rev. A **2**, 2284 (1970).

3 W. G. Baber and H. R. Hassé, Proc. Cambridge Phil. Soc. **31**, 564 (1935).

4 This statement is a simplification. The contribution of Baber and Hassé was the discovery of a series representation of the function depending on the variable $\eta = (r_e - r_{e\mu})/r_\mu$, where $r_{e\mu} = |\mathbf{r}_e - \mathbf{r}_\mu|$. Series representations of the function depending on the variable $\xi = (r_e + r_{e\mu})/r_\mu$ had been given previously by Hylleraas [E. A. Hylleraas, Z. Physik **71**, 739 (1931)] and also Jaffé [G. Jaffé, Z. Physik **87**, 535 (1934)]. The series given by Hylleraas and Jaffé, though different in form, are equivalent. The numerical computations reported in the present paper were, for the most part, carried out

using the solution obtained by Jaffé. However, as a check on the accuracy of the computer program, the value of E_{bde} was calculated for a few values of r_μ using the solution of Hylleraas.

[5] A. S. Wightman, thesis (Princeton University, 1949)(unpublished).

[6] G. T. Condo, Phys. Letters **9**, 65 (1964).

[7] J. E. Russell, Phys. Rev. A **1**, 742 (1970).

[8] J. E. Russell, Phys. Rev. **188**, 187 (1969).

[9] M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957), pp. 32–7.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Scattering from a Periodic Corrugated Structure: Thin Comb with Soft Boundaries

John A. DeSanto
Naval Research Laboratory, Washington, D.C. 20390
(Received 4 February 1971)

An incident plane wave is scattered from a surface, corrugated in one dimension, and given by an infinite number of periodic, finite-depth, infinitesimally thin parallel plates (thin comb) having soft boundary conditions. The solutions of the Helmholtz equation are assumed to be upgoing plane waves above the plates and standing waves in the plate wells. Both have unknown amplitude coefficients. Continuity of the solutions and their derivatives across the common boundary yields a doubly infinite set of linear equations for the unknown amplitudes. The equations are solved using the modified residue calculus technique due to Mittra. The amplitudes are expressed as values or residues of a certain meromorphic function. The residue calculus and Wiener–Hopf techniques are related; thus, an example of a solvable finite-range Wiener–Hopf-type problem is presented. Numerical evaluations of reflection coefficients are presented as a function of frequency, depth, and incident angle. The Wood P anomaly and the Brewster-angle anomaly are demonstrated. Results for backscatter at near-grazing incidence are also presented, and correspondences between the reflection coefficients and amplitude phases, as a function of depth, are indicated.

1. INTRODUCTION

The problem considered in this paper is the calculation of the scattered field when a plane wave is incident on a (one-dimensional) periodic corrugated surface. The surface is given by an infinite number of periodically spaced, infinitesimally thin parallel plates having a finite depth (thin comb). The surface is thus a grating of thin spikes. The geometry is illustrated in Fig. 1. Both plates and bottom are assumed to satisfy the soft

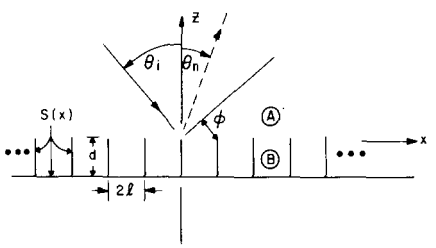

FIG. 1. Plane wave at angle θ_i incident on an infinite number of periodic (period $2l$), finite depth (d), thin parallel plates extending to $\pm\infty$ in y. θ_n are the scattering angles and $S(x)$ the surface. ϕ is the phase lag for a ray reaching $x = 2l$ as opposed to $x = 0$. Region A is $z \geq 0$, and region B, $0 \geq z \geq -d$.

boundary condition. Problems of this type are treated in the books of Weinstein[1] and Beckmann and Spizzichino.[2] Hurd[3] gave an approximate solution to a similar problem with a hard boundary. He used residue calculus methods from complex function theory to solve a set of linear equations which yielded an approximate solution to the problem. The residue calculus method is related to the Wiener–Hopf method.[4] Stewart and Gallaway[5] and Hessel and Oliner[6] described the types of anomalies which arise when treating such surfaces, and Tseng[7] pointed out an additional anomaly by discussing the problem using a scattering matrix technique and calculating the dispersion curves which arise. In this paper we wish to solve the problem exactly using a modification of the residue calculus technique due to Mittra, Lee, and Vanblaricum.[8]

In Sec. 2 the basic formulation of the problem is presented. A single frequency is considered. The harmonic time dependence is separated from the two-dimensional wave equation, and the resulting Helmholtz equation for the wavefunction or velocity potential $\psi(x, z)$ is solved in two regions: region A above the plates $z \geq 0$, and region B between the plates $0 \geq z \geq -d$. ψ in region A is assumed to be the sum of the incident wave and the scattered wave, the latter given by a superposition of plane waves with unknown amplitudes and propagating in directions given by the grating equation. ψ in region B is assumed to be a superposition of standing waves (with unknown amplitudes) in both x and z directions. The soft boundary condition is used. The two solutions and their derivatives are matched across the common domain to yield two infinite sets of equations for the amplitudes.

The equations are solved in Sec. 3. The residue series of certain integrals of a constructed meromorphic function $f(\omega)$ are shown to reproduce the infinite sets of equations. The amplitude coefficients in region A are particular residues of $f(\omega)$ and the coefficients in region B particular values of $f(\omega)$.

The details of constructing $f(\omega)$ are given in Sec. 4. If the plates were semi-infinite in depth, as in

using the solution obtained by Jaffé. However, as a check on the accuracy of the computer program, the value of E_{bde} was calculated for a few values of r_μ using the solution of Hylleraas.

[5] A. S. Wightman, thesis (Princeton University, 1949)(unpublished).

[6] G. T. Condo, Phys. Letters **9**, 65 (1964).

[7] J. E. Russell, Phys. Rev. A **1**, 742 (1970).

[8] J. E. Russell, Phys. Rev. **188**, 187 (1969).

[9] M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957), pp. 32–7.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Scattering from a Periodic Corrugated Structure: Thin Comb with Soft Boundaries

John A. DeSanto
Naval Research Laboratory, Washington, D.C. 20390
(Received 4 February 1971)

An incident plane wave is scattered from a surface, corrugated in one dimension, and given by an infinite number of periodic, finite-depth, infinitesimally thin parallel plates (thin comb) having soft boundary conditions. The solutions of the Helmholtz equation are assumed to be upgoing plane waves above the plates and standing waves in the plate wells. Both have unknown amplitude coefficients. Continuity of the solutions and their derivatives across the common boundary yields a doubly infinite set of linear equations for the unknown amplitudes. The equations are solved using the modified residue calculus technique due to Mittra. The amplitudes are expressed as values or residues of a certain meromorphic function. The residue calculus and Wiener–Hopf techniques are related; thus, an example of a solvable finite-range Wiener–Hopf-type problem is presented. Numerical evaluations of reflection coefficients are presented as a function of frequency, depth, and incident angle. The Wood P anomaly and the Brewster-angle anomaly are demonstrated. Results for backscatter at near-grazing incidence are also presented, and correspondences between the reflection coefficients and amplitude phases, as a function of depth, are indicated.

1. INTRODUCTION

The problem considered in this paper is the calculation of the scattered field when a plane wave is incident on a (one-dimensional) periodic corrugated surface. The surface is given by an infinite number of periodically spaced, infinitesimally thin parallel plates having a finite depth (thin comb). The surface is thus a grating of thin spikes. The geometry is illustrated in Fig. 1. Both plates and bottom are assumed to satisfy the soft

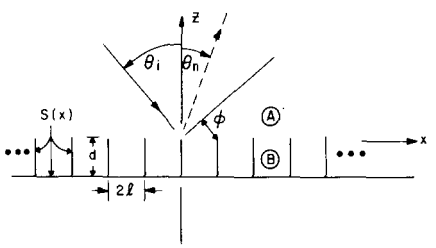

FIG. 1. Plane wave at angle θ_i incident on an infinite number of periodic (period $2l$), finite depth (d), thin parallel plates extending to $\pm\infty$ in y. θ_n are the scattering angles and $S(x)$ the surface. ϕ is the phase lag for a ray reaching $x = 2l$ as opposed to $x = 0$. Region A is $z \geq 0$, and region B, $0 \geq z \geq -d$.

boundary condition. Problems of this type are treated in the books of Weinstein[1] and Beckmann and Spizzichino.[2] Hurd[3] gave an approximate solution to a similar problem with a hard boundary. He used residue calculus methods from complex function theory to solve a set of linear equations which yielded an approximate solution to the problem. The residue calculus method is related to the Wiener–Hopf method.[4] Stewart and Gallaway[5] and Hessel and Oliner[6] described the types of anomalies which arise when treating such surfaces, and Tseng[7] pointed out an additional anomaly by discussing the problem using a scattering matrix technique and calculating the dispersion curves which arise. In this paper we wish to solve the problem exactly using a modification of the residue calculus technique due to Mittra, Lee, and Vanblaricum.[8]

In Sec. 2 the basic formulation of the problem is presented. A single frequency is considered. The harmonic time dependence is separated from the two-dimensional wave equation, and the resulting Helmholtz equation for the wavefunction or velocity potential $\psi(x, z)$ is solved in two regions: region A above the plates $z \geq 0$, and region B between the plates $0 \geq z \geq -d$. ψ in region A is assumed to be the sum of the incident wave and the scattered wave, the latter given by a superposition of plane waves with unknown amplitudes and propagating in directions given by the grating equation. ψ in region B is assumed to be a superposition of standing waves (with unknown amplitudes) in both x and z directions. The soft boundary condition is used. The two solutions and their derivatives are matched across the common domain to yield two infinite sets of equations for the amplitudes.

The equations are solved in Sec. 3. The residue series of certain integrals of a constructed meromorphic function $f(\omega)$ are shown to reproduce the infinite sets of equations. The amplitude coefficients in region A are particular residues of $f(\omega)$ and the coefficients in region B particular values of $f(\omega)$.

The details of constructing $f(\omega)$ are given in Sec. 4. If the plates were semi-infinite in depth, as in

the Carlson–Heins problem,[9,10] the meromorphic functions to be constructed would depend on the z component of the normalized wavenumber q_j in region B. Hence the various amplitude coefficients would also. Here, for finite-depth plates, $f(\omega)$ has zeros at values $\bar{q}_j$ which are shifted from the q_j. The shift is calculated by an iteration procedure outlined in Sec. 4A. The edge condition is shown to hold in Sec. 4B and the intensity relation is derived in Sec. 4C. Since the surface is lossless, the latter yields an explicit expression for the reflection coefficient which is used as a check in the calculations. Finally, the amplitude coefficients in region A are explicitly evaluated in Sec. 4D.

The numerical results are presented in Sec. 5. Reflection coefficients for the various spectral orders are given as a function of incident frequency, incident angle, and depth of the corrugations. The Wood P anomaly and the Brewster-angle anomaly are demonstrated, and results for back scatter at near-grazing incidence are presented. A maximum occurs in the backscatter reflection coefficient when the angle of reflection is the negative of incident angle. Correspondences between the reflection coefficients and amplitude phases, as a function of depth, are also indicated.

Summary and conclusions are presented in Sec. 6.

There are two appendices. Appendix A is concerned with some properties of the infinite products in the paper, and Appendix B, with the algebraic part of the behavior of the residue functions for large arguments.

2. BASIC FORMALISM

The problem is to solve the two-dimensional Helmholtz equation for a plane wave incident at angle θ_i on an infinite number of periodic (period $2l$), infinitesimally thin parallel plates, of finite depth d, and with soft boundaries illustrated in Fig. 1. The Helmholtz equation is ($e^{-i\omega t}$ is assumed throughout)

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}+k^2\right)\psi(x,z)=0, \tag{2.1}$$

where ψ is the scalar wave function or velocity potential.[11] The incident wavenumber is $k=2\pi/\lambda$, where λ is the wavelength. The surface is given by (see Fig. 1)

$$S(x)=\begin{cases}-d, & x\neq 0,\pm 2l,\pm 4l,\cdots,\\ 0, & x=0,\pm 2l,\pm 4l,\cdots\end{cases} \tag{2.2}$$

and the soft boundary condition by

$$\psi[x,S(x)]=0. \tag{2.3}$$

ψ has the following restrictions:

(a) ψ and $\nabla\psi$ are finite in each subregion except at the sharp edges of the plates where $\psi=O(r^{1/2})$ and $|\nabla\psi|=O(r^{-1/2})$ as the edge is approached (r is the radial distance from the edge). This is the usual edge condition.[12]

(b) ψ and $\nabla\psi$ are continuous in each subregion and across the $z=0$ interface.

(c) Apart from the incident wave, ψ represents outgoing waves as $z\to\infty$.

It will be shown that the following wave functions satisfy restrictions (a) and (c) and Eq. (2.3) in regions A and B, respectively. For $z\geq 0$ (region A) ψ is written

$$\psi_A(x,z)=\psi_i(x,z)+\psi_{sc}(x,z), \tag{2.4}$$

with ψ_i the incident plane wave ($\alpha_0=\sin\theta_i$, $\beta_0=\cos\theta_i$)

$$\psi_i(x,z)=e^{ik(\alpha_0 x-\beta_0 z)} \tag{2.5}$$

and ψ_{sc} the scattered wave, written as a superposition of plane waves propagating in the positive z direction:

$$\psi_{sc}(x,z)=\sum_{n=-\infty}^{\infty}A_n e^{ik(\alpha_n x+\beta_n z)}, \tag{2.6}$$

where $\alpha_n=\sin\theta_n$, $\beta_n=\cos\theta_n$, and θ_n is the scattering angle given by the grating equation below. The A_n coefficients are to be determined. The scattering coefficient $R(x,z)$ is defined by

$$R(x,z)=\psi_{sc}(x,z)/\psi_i(x,z). \tag{2.7}$$

Since the surface is periodic, so is R:

$$R(x+2l,z)=R(x,z). \tag{2.8}$$

This implies the grating equation

$$\alpha_n=\alpha_0+n\Lambda, \tag{2.9}$$

where $\Lambda=\lambda/2l$ is the normalized wavelength. For $0\geq z\geq -d$ (region B), ψ is written as a series of standing waves in both x and z directions. It is given, for $0\leq x\leq 2l$, by

$$\psi_B(x,z)=\sum_{j=1}^{\infty}B_j\sin(p_j kx)\sin[q_j k(z+d)], \tag{2.10}$$

with $(p_j)^2+(q_j)^2=1$ and where the boundary condition [Eq. (2.3)] has been satisfied at $x=0$ and $z=-d$. To satisfy Eq. (2.3) at $x=2l$ requires p_j to be given by

$$p_j=j\Lambda/2. \tag{2.11}$$

Now, ψ_B/ψ_i has period $2l$. Thus for other values of x, ψ_B is given by

$$(e^{-ik\alpha_0 x}\psi_B(x,z))_{x=x_1+2ml}=e^{-ik\alpha_0 x_1}\psi_B(x_1,z), \tag{2.12}$$

where $0\leq x_1\leq 2l$. Substituting Eqs. (2.4) and (2.10) into the continuity conditions (b) given by

$$\psi_A(x,0)=\psi_B(x,0), \tag{2.13}$$

$$\frac{\partial \psi_A}{\partial z}(x,0) = \frac{\partial \psi_B}{\partial z}(x,0), \tag{2.14}$$

and projecting out the B_j coefficients by the usual procedure yields the set of equations

$$\sum_{n=-\infty}^{\infty} (A_n + \delta_{no})K_{nj} = \tfrac{1}{2}B_j \sin(q_j kd), \tag{2.15}$$

$$\sum_{n=-\infty}^{\infty} \beta_n(A_n - \delta_{no})K_{nj} = \frac{1}{2i}q_j B_j \cos(q_j kd), \tag{2.16}$$

where δ_{no} is the Kronecker δ:

$$\delta_{no} = \begin{cases} 1, & n = 0 \\ 0, & n \neq 0 \end{cases}$$

and the coefficients K_{nj} are given by

$$K_{nj} = \frac{1}{2l}\int_0^{2l} \sin(p_j kx)e^{ik\alpha_n x}dx$$
$$= (\Lambda/2\pi)p_j(\beta_n^2 - q_j^2)^{-1}[1 - (-)^j e^{2\pi i\alpha_0/\Lambda}]. \tag{2.17}$$

At this point Hurd[3] makes an approximation which consists in neglecting the terms $e^{iq_j kd}$ which occur in the right-hand sides of Eqs. (2.15) and (2.16). The approximation is not necessary, however, and we do not make it. Multiplying Eq. (2.15) by q_j and successively adding and subtracting the result from Eq. (2.16) yields the set of equations

$$\sum_{n=-\infty}^{\infty} [(\beta_n \pm q_j)A_n - (\beta_n \mp q_j)\delta_{no}]K_{nj} = \frac{q_j B_j}{2i}e^{\pm iq_j kd}. \tag{2.18}$$

Multiplying Eq. (2.18) by $e^{\mp iq_j kd}$, respectively, successively adding and subtracting the resulting equations, and using Eq. (2.17) yields, after rearranging, the set of equations

$$\sum_{n=-\infty}^{\infty} A_n\left(\frac{e^{-iq_j kd}}{\beta_n - q_j} \pm \frac{e^{iq_j kd}}{\beta_n + q_j}\right) - \left(\frac{e^{-iq_j kd}}{\beta_0 + q_j} \pm \frac{e^{iq_j kd}}{\beta_0 - q_j}\right)$$
$$= \begin{cases} (2\pi q_j/i\Lambda p_j)B_j[1 - (-)^j e^{2\pi i\alpha_0/\Lambda}]^{-1}. \\ 0 \end{cases} \tag{2.19}$$

Equations (2.19) will be solved in the next section.

3. SOLUTION OF THE EQUATIONS

The solution of Eqs. (2.19) is given in this section. Consider the meromorphic function $f(\omega)$ specified by the following properties:

(a) $f(\omega)$ has simple poles at $\omega = \beta_n, n = 0, \pm 1, \pm 2, \cdots$ and a simple pole at $\omega = -\beta_0$.
(b) $f(\omega)$ has simple zeros at $\omega = \bar{q}_j$, $j = 1, 2, \cdots$. These zeros will be determined from the condition

$$f(q_j) - e^{2iq_j kd}f(-q_j) = 0. \tag{3.1}$$

(c) $f(\omega)$ approaches zero as $|\omega| \to \infty$.
(d) The wavefunction ψ approaches zero as $r^{1/2}$ as the edge of a plate is approached (r is the radial distance from the edge). Equivalently, $\partial\psi/\partial r$ approaches infinity as $r^{-1/2}$ as $r \to 0$.[12] It will also be demonstrated how properties (b)–(d) are interrelated.

Consider integrals of the form

$$\frac{1}{2\pi i}\left(e^{-iq_j kd}\int_{C_s}\frac{f(\omega)d\omega}{\omega - q_j} \pm e^{iq_j kd}\int_{C_s}\frac{f(\omega)d\omega}{\omega + q_j}\right), \tag{3.2}$$

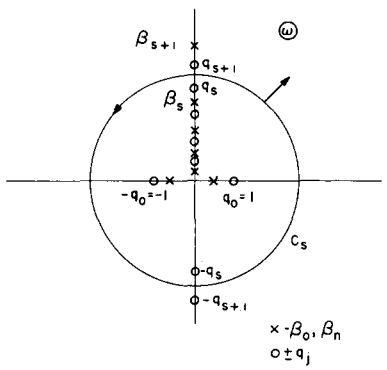

FIG. 2. Contour of integration C_s for the residue calculus technique. A possible configuration of the poles $\beta_n(|n| \leq s)$ and $-\beta_0$, and points $\pm q_j(j \leq s)$ is shown. (β_n poles for n negative are not indicated.)

where the contours C_s enclose the points $\omega = \pm q_j$ for $j \leq s, -\beta_0$, and β_n for $|n| \leq s$ as illustrated in Fig. 2. As s approaches infinity, the contour C_s approaches an infinite contour and Eq. (3.2) approaches zero because of property (c) above. Using the Cauchy residue theorem, the residue series of Eqs. (3.2) are given by

$$\sum_{n=-\infty}^{\infty} r(\beta_n)\left(\frac{e^{-iq_j kd}}{\beta_n - q_j} \pm \frac{e^{iq_j kd}}{\beta_n + q_j}\right)$$
$$+ [e^{-iq_j kd}f(q_j) \pm e^{iq_j kd}f(-q_j)]$$
$$+ r(-\beta_0)\left(\frac{e^{-iq_j kd}}{-\beta_0 - q_j} \pm \frac{e^{iq_j kd}}{-\beta_0 + q_j}\right) = 0, \tag{3.3}$$

where $r(\beta)$ is the residue of $f(\omega)$ at $\omega = \beta$. Using Eq. (3.1), Eq. (3.3) becomes

$$\sum_{n=-\infty}^{\infty} r(\beta_n)\left(\frac{e^{-iq_j kd}}{\beta_n - q_j} \pm \frac{e^{iq_j kd}}{\beta_n + q_j}\right)$$
$$- r(-\beta_0)\left(\frac{e^{-iq_j kd}}{\beta_0 + q_j} \pm \frac{e^{iq_j kd}}{\beta_0 - q_j}\right)$$
$$= \begin{cases} -2e^{-iq_j kd}f(q_j). \\ 0 \end{cases} \tag{3.4}$$

Equation (3.4) is equivalent to Eq. (2.19) if the following identifications are made:

$$r(-\beta_0) = 1, \tag{3.5}$$

$$A_n = r(\beta_n), \tag{3.6}$$

$$B_j = [1 - (-)^j e^{2\pi i\alpha_0/\Lambda}]\Lambda p_j e^{-iq_j kd} f(q_j)/\pi i q_j. \tag{3.7}$$

Thus, knowing the function $f(\omega)$ determines the amplitude coefficients A_n and B_j from Eqs. (3.6) and (3.7), respectively. The function $f(\omega)$ is constructed in the next section.

4. CONSTRUCTION OF $f(\omega)$

The function $f(\omega)$ is defined by properties (a)–(d) in Sec. 3. It is constructed as follows. Define the following infinite products [which are discussed in Appendix A in Eqs. (A10), (A9), and (A8), respectively]:

$$\Pi(\omega, \bar{q}) = \prod_{n=1}^{\infty} \left(1 - \frac{\omega'}{\bar{q}_j}\right) \left(\frac{2\bar{q}_j}{ij\Lambda}\right) e^{2\omega/ij\Lambda},$$

$$\Pi_1(\omega, \beta) = \prod_{n=1}^{\infty} \left(1 - \frac{\omega}{\beta_n}\right) \left(\frac{\beta_n}{in\Lambda}\right) e^{\omega/in\Lambda},$$

$$\Pi_2(\omega, \beta) = \prod_{j=1}^{\infty} \left(1 - \frac{\omega}{\beta_{-n}}\right) \left(\frac{\beta_{-n}}{in\Lambda}\right) e^{\omega/in\Lambda},$$

Equation (A10) is used to satisfy property (b). Equations (A8) and (A9) are used to satisfy (a). Thus $f(\omega)$, satisfying properties (a) and (b), can be written

$$f(\omega) = \frac{g(\omega)}{\omega^2 - \beta_0^2} \frac{\Pi(\omega, \bar{q})}{\Pi_{12}(\omega, \beta)}, \tag{4.1}$$

where $\Pi_{12}(\omega, \beta) \equiv \Pi_1(\omega, \beta)\Pi_2(\omega, \beta)$ and $g(\omega)$ is an entire function which will be determined. Asymptotic properties of these infinite products yield as $|\omega| \to \infty$ $[\arg(\omega) \neq \pi/2]$ (see Appendix A)

$$f(\omega) \sim [g(\omega)/\omega^{3/2}] e^{2\omega(\ln 2)/i\Lambda}, \tag{4.2}$$

where some constant terms have been absorbed in $g(\omega)$. The domain $\arg(\omega) = \pi/2$ can be included as discussed in Appendix A and does not change the following choice of $g(\omega)$ given by

$$g(\omega) = (g_0 + g_1\omega) e^{2i\omega(\ln 2)/\Lambda}, \tag{4.3}$$

where g_0 and g_1 are constants to be determined. This choice of $g(\omega)$ guarantees that $f(\omega) \to 0$ algebraically as $|\omega| \to \infty$. Thus property (c) is satisfied. It will be shown that if $g_1 \neq 0$, $\partial\psi_A/\partial r = O(r^{-3/2})$ as the edge of a plate is approached (r is the radial distance from an edge). This type of behavior is too singular.[12] Thus the edge property (d) implies $g_1 = 0$. Similarly for $g_0 \neq 0$ it will be shown that $\partial\psi_A/\partial r = O(r^{-1/2})$, the correct edge behavior. Using Eqs. (4.1) and (4.3), the above discussion, and evaluating the constant g_0 using Eq. (3.5) yields for $f(\omega)$

$$f(\omega) = \frac{2\beta_0}{\beta_0^2 - \omega^2} \frac{\Pi_{12}(-\beta_0, \beta)}{\Pi_{12}(\omega, \beta)} \times \frac{\Pi(\omega, \bar{q})}{\Pi(-\beta_0, \bar{q})} e^{2i(\ln 2\chi\omega + \beta_0)/\Lambda}. \tag{4.4}$$

A. Edge Condition

In order to check that property (d) hold, it will be shown that, as the edge of a plate is approached (i.e., as the radius r from the $x = z = 0$ plate edge approaches zero), the scattered part of the term $\partial\psi_A/\partial r$ (proportional, e.g., to the velocity on the plate) goes to infinity like $r^{-1/2}$. Proving this derivative condition is simpler than showing that ψ_A approaches zero like $r^{1/2}$, and choosing the solution in region A is more straightforward than working with the solution in region B for this particular problem. Both the function and the derivative relations are equivalent, however. The scattered part of the wavefunction is given by Eq. (2.6):

$$\psi_{sc}(x, z) = \sum_{n=-\infty}^{\infty} A_n e^{ik(\alpha_n x + \beta_n z)}. \tag{2.6}$$

In terms of cylindrical coordinates r and θ given by

$$x = r\sin\theta \equiv r\alpha, \qquad z = r\cos\theta \equiv r\beta$$

Eq. (2.6) can be written as

$$\psi_{sc}(r, \theta) = \sum_{n=-\infty}^{\infty} A_n e^{ikr(\alpha_n\alpha + \beta_n\beta)}. \tag{4.5}$$

Differentiating Eq. (4.5) with respect to r yields

$$\frac{\partial\psi_{sc}}{\partial r}(r, \theta) = ik \sum_{n=-\infty}^{\infty} A_n(\alpha_n\alpha + \beta_n\beta) e^{ikr(\alpha_n\alpha + \beta_n\beta)}. \tag{4.6}$$

Consider part of this sum defined by

$$S_1(r, \theta) \equiv \sum_{n=1}^{\infty} A_n(\alpha_n\alpha + \beta_n\beta) e^{ikr(\alpha_n\alpha + \beta_n\beta)}. \tag{4.7}$$

For large n, $i\alpha_n \sim \beta_n = iO(n)$, and $A_n = O(n^{-3/2})$ (see Appendix B). Thus the sum S_1 is, *up to some bounded function*, equal to the sum defined by

$$\Sigma_1(r) = \sum_{n=1}^{\infty} n^{-1/2} e^{iKrn}, \tag{4.8}$$

where K is complex with positive imaginary part. The sum Σ_1 can be bounded above and below as

$$\int_1^{\infty} n^{-1/2} e^{iKrn} dn \leq \Sigma_1(r) \leq \int_0^{\infty} n^{-1/2} e^{iKrn} dn. \tag{4.9}$$

The integral on the right-hand side of Eq. (4.9) is an elementary integral[13]

$$\int_0^\infty n^{-1/2} e^{iKrn} dn = (\pi/iKr)^{1/2}. \tag{4.10}$$

The integral on the left-hand side of Eq. (4.9) can be written as

$$\int_1^\infty n^{-1/2} e^{iKrn} dn = \int_0^\infty n^{-1/2} e^{iKrn} dn - \int_0^1 n^{-1/2} e^{iKrn} dn. \tag{4.11}$$

The first integral on the right-hand side of Eq. (4.11) is just Eq. (4.10). The second integral can be written by expanding the exponential in powers of r (which is small):

$$\begin{aligned}\int_0^1 n^{-1/2} e^{iKrn} dn &= \int_0^1 n^{-1/2}\{1 + iKrn + \cdots\} dn \\ &= \int_0^1 n^{-1/2} dn + iKr \int_0^1 n^{1/2} dn + \cdots \\ &= 2 + iKr(\tfrac{2}{3}) + \cdots \\ &\to 2 \quad \text{as} \quad r \to 0.\end{aligned} \tag{4.12}$$

Combining these results it is obvious that as $r \to 0$, $\Sigma_1(r) = O(r^{-1/2})$. Similarly, another part of the sum in Eq. (4.6), $S_2(r, \theta)$, running from $n = -\infty$ to -1 can be defined and shown to go like $r^{-1/2}$ as $r \to 0$. Therefore, since the $n = 0$ term in Eq. (4.6) is bounded, the sum Eq. (4.6) can be written as $r \to 0$ as

$$\frac{\partial \psi_{sc}}{\partial r}(r, \theta) = ik\{S_1(r, \theta) + S_2(r, \theta)\} + B(r, \theta), \tag{4.13}$$

where $B(r, \theta)$ is some bounded function, and hence it is obvious that $\partial\psi_{sc}(r, \theta)/\partial r = O(r^{-1/2})$ as $r \to 0$. Since the incident plane wave and its radial derivative are bounded, it has thus also been shown, using Eq. (2.4) that $\partial\psi_A(r, \theta)/\partial r = O(r^{-1/2})$ as $r \to 0$. Thus, property (d) is fulfilled. It can easily be seen that if $g_1 \neq 0$ in Sec. 4, then $\partial\psi_A/\partial r = O(r^{-3/2})$ as $r \to 0$. The latter behavior is also singular.

B. Flux Conservation

In order to derive a relation which expresses the conservation of flux, consider the following integral relation:

$$\oint_c d\mu \psi^*(x, z) \overleftrightarrow{\partial}_n \psi(x, z) = 0, \tag{4.14}$$

which follows from Green's theorem and the fact that ψ and ψ^* are solutions of the Helmholtz equation. ∂_n is the derivative in the direction of the inward normal (n) to the closed contour of integration $C = 12 \cdots 81$ (see Fig. 3). The arc-length is μ, the * is complex conjugation, and the notation $\overleftrightarrow{\partial}$ is defined by $\psi^* \overleftrightarrow{\partial} \psi \equiv \psi^*(\partial\psi) - (\partial\psi^*)\psi$. The integrals along paths $\widehat{45}$ and $\widehat{67}$ vanish since ψ_B is zero on these paths. Integrals along the semicircles $\widehat{34}$ and $\widehat{78}$ vanish as $\epsilon \to 0$. This follows from the edge condition (d). The integrals

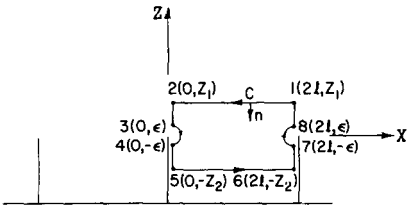

FIG. 3. Contour of integration $C = 12 \cdots 81$ for the flux conservation relation in Sec. 4B. The (x, z) coordinates of the points are shown, as well as the inward normal n.

along the paths $\widehat{23}$ and $\widehat{81}$ cancel each other because of the periodicity of ψ_A. Substituting ψ_B from Eq. (2.10) and performing the integral along the path $\widehat{56}$ shows that this integral also vanishes. Thus Eq. (4.14) becomes

$$\int_0^{2l} dx \psi_A^*(x, z_1) \overleftrightarrow{\partial}_z \psi_A(x, z_1) = 0. \tag{4.15}$$

Substituting ψ_A from Eqs. (2.4)–(2.6) and performing the integrals yields the flux conservation result or, since the surface is lossless, the reflection coefficient R:

$$R \equiv \sum_n (\beta_n/\beta_0)|A_n|^2 = 1, \tag{4.16}$$

where the sum is over all n such that β_n is real, i.e., over real scattering orders. This result is used in Sec. 5 to provide a check on the accuracy of the evaluation of A_n. In addition the individual spectral reflection coefficients R_n defined by

$$R_n = (\beta_n/\beta_0)|A_n|^2 \tag{4.17}$$

are plotted as a function of various parameters.

C. Zero Shifting

In order to calculate the $\bar{q}_j$ it is convenient to define the shift δ_j as the difference between $\bar{q}_j$ and q_j:

$$\delta_j = \bar{q}_j - \bar{q}_j. \tag{4.18}$$

The procedure to calculate the δ_j terms is due to Mittra, Lee, and Vanblaricum.[8] In order to satisfy the edge condition we have chosen (see Appendix A) that for large j, $\bar{q}_j \sim ij\Lambda/2 \sim q_j$. Thus for large j

$$\delta_j \approx 0. \tag{4.19}$$

For general j, the δ_j terms are found from Eq. (3.1):

$$f(q_j) - e^{2iq_j kd} f(-q_j) = 0. \tag{3.1}$$

Substituting Eq. (4.4) into Eq. (3.1) and rearranging terms yields

$$\frac{\Pi(q_j, \bar{q})}{\Pi(-q_j, \bar{q})} = e^{2iq_j(kd - 2\ln 2)/\Lambda} \frac{\Pi_{12}(q_j, \beta)}{\Pi_{12}(-q_j, \beta)}. \tag{4.20}$$

Using Eqs. (A10) and (4.18) the lhs of Eq. (4.20) can

be written

$$\prod_{n=1}^{\infty}\left(\frac{\delta_n + q_n - q_j}{\delta_n + q_n + q_j}\right) e^{-4iq_j/n\Lambda}. \tag{4.21}$$

Factoring the product in Eq. (4.21), substituting the result into Eq. (4.20), and rearranging terms yields

$$\left(\frac{\delta_j^{(m+1)}}{\delta_j^{(m+1)} + 2q_j} e^{-4iq_j/j\Lambda}\right) \times \prod_{n=1}^{j-1} \frac{\delta_n^{(m+1)} + q_n - q_j}{\delta_n^{(m+1)} + q_n + q_j} e^{-4iq_j/n} = \text{rhs} \prod_{n=j+1}^{\infty}\left(\frac{\delta_n^{(m)} + q_n + q_j}{\delta_n^{(m)} + q_n - q_j}\right) e^{4iq_j/n\Lambda}, \tag{4.22}$$

where rhs stands for the right-hand side of Eq. (4.20). Superscripts have been added to the δ_n terms to indicate that Eq. (4.22) is to be used as an iterative equation to calculate the δ_n terms. The procedure is as follows:

(i) For large j, $\delta_j \approx 0$ from Eq. (4.19). This is assumed to be the zeroth interation ($m = 0$) and is substituted in the rhs of Eq. (4.22).

(ii) The first iterations $\delta_1^{(1)}, \delta_2^{(1)}, \cdots, \delta_J^{(1)}$ are then calculated up to a $j = J$ such that $\delta_{J+1}^{(1)}, \delta_{J+2}^{(1)}, \cdots$, are zero to any desired accuracy. In practice we set this accuracy at $\epsilon = 3 \times 10^{-4}$, so that $\delta_1^{(1)}, \cdots, \delta_J^{(1)}$ are greater than ϵ and $\delta_{J+1}^{(1)}, \cdots$ less than ϵ. The terms $\delta_{J+1}^{(1)}, \cdots$ were then set equal to zero throughout the successive iterations.

(iii) The first iterations are then substituted into the rhs of Eq. (4.22) and second iterations are calculated. Iterations are continued until the Nth iteration yields $\max_j |\delta_j^{(N-1)} - \delta_j^{(N)}| < \epsilon$, where the maximum value is over all j such that δ_j is in the iteration set.

(iv) In practice, once the iteration set of δ_j's was found, successive iterations were calculated as either (a) a forward iteration, *viz.* first calcuate $\delta_1^{(2)}$, then $\delta_2^{(2)}$ using $\delta_1^{(2)}$, etc., such that the calculation of $\delta_J^{(2)}$ used the second iterations $\delta_1^{(2)}, \cdots, \delta_{J-1}^{(2)}$ and similarly for higher interations, or (b) a backward iteration, where we first calculate $\delta_J^{(2)}$, then $\delta_{J-1}^{(2)}$ using $\delta_J^{(2)}$, etc., such that the calculation of $\delta_1^{(2)}$ used the second iterations $\delta_J^{(2)}, \cdots, \delta_2^{(2)}$ and similarly for higher iterations.

The backward iteration generally converged faster. The advantages of this scheme are that good starting values are known for all δ_n and asymptotic values are known exactly. Also, matrix inversion is avoided, and each iteration is checked to see how well it satisfies Eq. (3.1). Generally, the iterations converged rapidly (less than 12 iterations). Some examples of δ_j and R are shown in Table I.

TABLE I. Some representative values of $\delta_j^{(n)}$ calculated using Sec. 4C for three different sets of parameters $\alpha_0 = \sin(\theta_i)$, $\Lambda = \lambda/2l$, and kd. The calculated total reflection coefficient R and the number of iterations, N, necessary to satisfy the error criterion, are also shown.

Parameters	j	$\text{Re}(\delta_j^{(N)})$	$\text{Im}(\delta_j^{(N)})$
$\alpha_0 = 0.8$	1	− 0.0686	− 0.0632
$\Lambda = 0.95$	2	− 0.3361	0.0373
(a) $kd = 3.2$	3	− 0.0001	0.0004
$R = 1.0000$			
$N = 5$			
$\alpha_0 = 0.707$	1	− 0.0100	− 0.0172
$\Lambda = 0.63$	2	− 0.0625	0.0010
(b) $kd = 3.2$	3	− 0.3625	0.0788
$R = 1.0001$			
$N = 6$			
$\alpha_0 = 0.1$	1	− 0.0432	− 0.3183
$\Lambda = 0.51$	2	0.0268	− 0.0232
(c) $kd = 2.0$	3	0.0569	− 0.1520
$R = 1.0001$	4	0.0575	0.0795
$N = 17$	5	0.0043	0.0033
	6	0.0003	0.0004
	7	0.0002	0.0002

D. Calculation Of A_n

In order to calculate the coefficient A_n from Eq. (3.6) it is necessary to know the residue of $f(\omega)$ at $\omega = \beta_n$. To find this we first need to calculate

$$\lim_{\omega \to \beta_n}\left(\frac{(\omega - \beta_n)}{\Pi_{12}(\omega, \beta)}\right). \tag{4.23}$$

This can be done as follows. Using the fact that (see Appendix A)

$$\Pi(\omega)\Pi(-\omega) = \prod_{n=1}^{\infty}\left(1 - \frac{\omega^2}{n^2}\right) = \frac{\sin(\pi\omega)}{\pi\omega},$$

it is straightforward to derive from Eqs. (A8) and (A9):

$$\Pi_{12}(\omega, \beta)\Pi_{12}(-\omega, \beta) = \frac{\sin\{\pi[\alpha_0 + (1 - \omega^2)^{1/2}]/\Lambda\}}{\pi[\alpha_0 + (1 - \omega^2)^{1/2}]/\Lambda} \times \frac{\sin\{\pi[\alpha_0 - (1 - \omega^2)^{1/2}]/\Lambda\}}{\pi(\alpha_0 - (1 - \omega^2)^{1/2}]/\Lambda}. \tag{4.24}$$

Solving Eq. (4.24) for $\Pi_{12}(\omega, \beta)$, substituting the result into Eq. (4.23) and performing the resulting calculation yields

$$\lim_{\omega \to \beta_n}\left(\frac{\omega - \beta_n}{\Pi_{12}(\omega, \beta)}\right) = \frac{\pi\alpha_n}{\Lambda\beta_n} \frac{(\alpha_0^2 - \alpha_n^2)\Pi_{12}(-\beta_n, \beta)}{\sin(2\pi\alpha_0/\Lambda)}. \tag{4.25}$$

A further useful relation which can be derived from Eq. (4.24) is

$$\Pi_{12}(-\beta_0, \beta) = \frac{\sin(2\pi\alpha_0/\Lambda)}{(2\pi\alpha_0/\Lambda)\Pi_{12}(\beta_0, \beta)}. \tag{4.26}$$

Substituting Eqs. (4.25) and (4.26) into Eqs. (3.6) and (4.4) yields

$$A_n = \frac{-\beta_0\alpha_n}{\beta_n\alpha_0} \frac{\Pi_{12}(-\beta_n, \beta)}{\Pi_{12}(\beta_0, \beta)} \frac{\Pi(\beta_n, \bar{q})}{\Pi(-\beta_0, \bar{q})} \times e^{2i(\beta_0 + \beta_n)(\ln 2)/\Lambda}. \tag{4.27}$$

This result is used to calculate R_n from Eq. (4.17). The results are presented in the next section.

5. RESULTS AND DISCUSSION

There are two steps in the calculation of the reflection coefficients R_n. The first is to find the δ_j shifts by the procedure outlined in Sec. 4C. The second is to substitute these δ_j terms into Eq. (4.27) and to evaluate numerically the A_n coefficients. The latter requires a note on how to evaluate the infinite products. First, take the sum of the logarithms of the terms in the product. The first hundred terms ($n = 1, \cdots, 100$) are added, and the tail of the product or remainder ρ is approximated by an integral. If the real and imaginary parts of ρ satisfy the (box) norm $\| \rho \| \equiv | \mathrm{Re}\rho | + | \mathrm{Im}\rho | < 0.2$, then ρ is added to the product. If not, then the next hundred terms are taken, etc., either until the norm is less than 0.2 or until a thousand terms are taken. If, for $n = 1000$, the norm is still greater than 0.2, it is just added into the sum. [Note that for the product Π_{12} we must take 200 terms and multiply symmetrically since only in this way does the product converge (see Appendix A).] The error thus introduced into each product is of the order of $\| \rho \|/n$, which for $n = 100$ is less than 0.2%. The error in the amplitude is thus less than 1%. This evaluation in each case was checked by calculating R from Eq. (4.16). A few worst cases of R differed from $R = 1$ in the third decimal place. The majority of cases were one to an accuracy of four or five decimal places. (See Table I.)

The results are presented in Figs. 4–13. In Figs. 4–6, the spectral reflection coefficients R_n and amplitude phases ϕ_n (in radians, $-\pi$ to π) defined by $A_n = |A_n| e^{i\varphi_n} = (R_n \beta_0/\beta_n)^{1/2} e^{i\varphi_n}$ are plotted with respect to the parameter kd for incident angles $\theta_i \approx 5.8°$ ($\alpha_0 = 0.1$, Fig. 4), $\theta_i = 45°$ ($\alpha_0 = 0.707$, Fig. 5) and $\theta_i = 85°$ ($\alpha_0 = 0.99619$, Fig. 6). In each case $\Lambda = 0.63$. Note that the changing parameter kd can be thought of as either variable

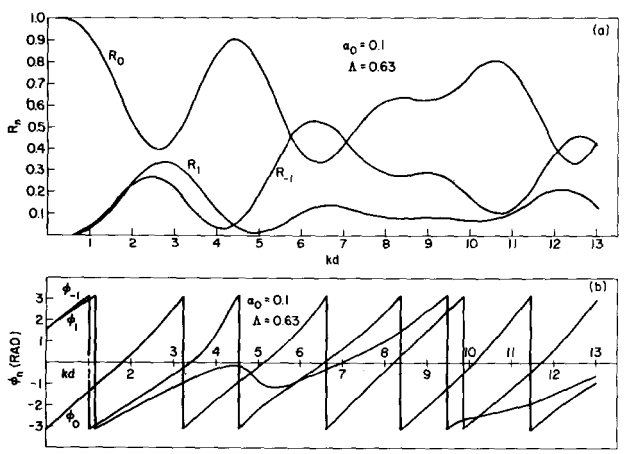

FIG. 4. (a) Reflection coefficients R_n and (b) amplitude phases ϕ_n, plotted as a function of the "depth" parameter kd with $\alpha_0 = 0.1$ (incident angle $\theta_i \approx 5.8°$) and $\Lambda = 0.63$.

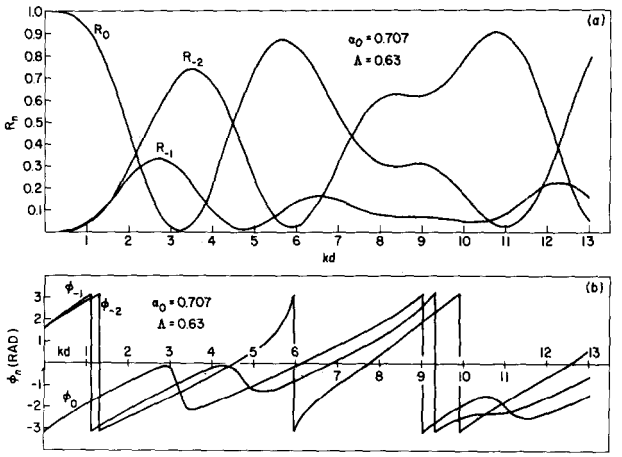

FIG. 5. (a) Reflection coefficients R_n and (b) amplitude phases ϕ_n, plotted as a function of the "depth" parameter kd with $\alpha_0 = 0.707$ (incident angle $\theta_i = 45°$) and $\Lambda = 0.63$.

frequency, fixed depth or fixed frequency, variable depth. The reflection coefficients shown add up to 1. Also at $kd = 0$, $\phi_0 = -\pi$, as is to be expected for a soft surface. It is also found that the minima of the reflection coefficients R_n are correlated with the zeros of $\partial^2\phi_n/\partial(kd)^2$, and the magnitude of R_n at its minima is correlated with the magnitude of $\partial\phi_n/\partial(kd)$. (A discussion of these assertions will be presented in a future paper.) Some examples are the points $kd \cong 4.9$ in Fig. 4, $kd \cong 3.2, 4.8$, and 11 in Fig. 5, and $kd \cong 9$ in Fig. 6. The vanishing of R_0 in Fig. 5(a) is an example of the Brewster-angle anomaly[5–7] where for certain parameter values the specular scattering is extinguished and all the energy goes into the other scattering orders.

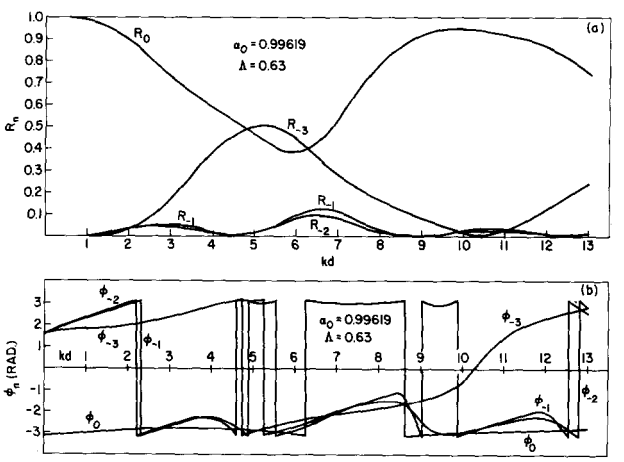

FIG. 6. (a) Reflection coefficients R_n, and (b) amplitude phases ϕ_n, plotted as a function of the "depth" parameter kd with $\alpha_0 = 0.99619$ (incident angle $\theta_i = 85°$) and $\Lambda = 0.63$.

Figure 7(a) is an example of the Wood P anomaly[5–7] i.e., the rapid exchange of energy between specular and backscatter orders as one of the parameters is varied. Again note, in Fig. 7(b), the above-mentioned correspondence between R_n and ϕ_n. Also the large jump in ϕ_{-1} at $kd \approx 4.7$ in Fig. 7(b) corresponds to the zero in R_{-1} (and its slope) at the same point.

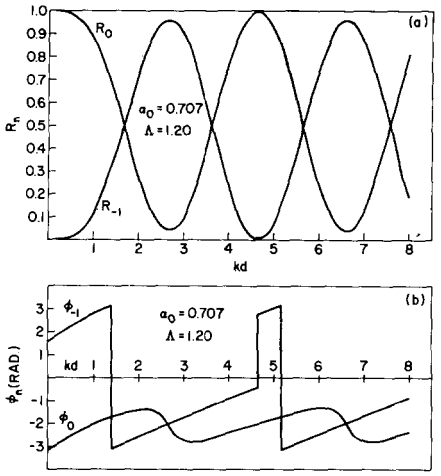

FIG. 7. (a) Reflection coefficients R_n, and (b) amplitude phases ϕ_n, plotted vs kd for $\alpha_0 = 0.707$ ($\theta_i = 45°$) and $\Lambda = 1.20$. The two spectral orders exhibit the Wood P anomaly.

Figures 8–11 present the variations in the reflection coefficients R_n and phases ϕ_n as a function of the incident angle θ_i, where $\alpha_0 = \sin\theta_i$. Figure 8 presents results for $\Lambda = 0.63$ and $kd = 2.0$. Note that for $\alpha_0 = 0, R_1 = R_{-1}$ and the field is symmetrical. At those places where a new spectral order either enters or leaves the set of scattering orders, an anomaly occurs in the behavior of the

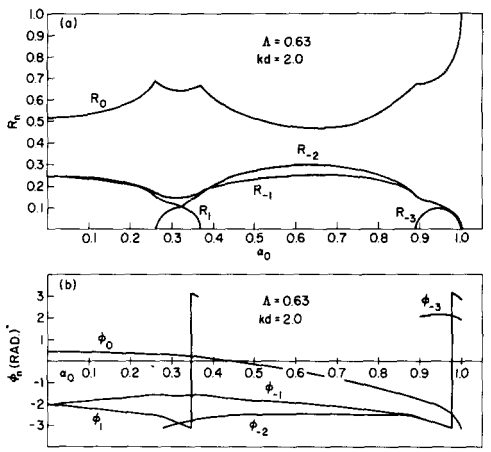

FIG. 8. (a) Reflection coefficients R_n, and (b) phases ϕ_n, plotted as a function of α_0, the sine of the incident angle (θ_i) for $\Lambda = 0.63$ and $kd = 2$. Cusps in the amplitudes are due to Rayleigh anomalies.

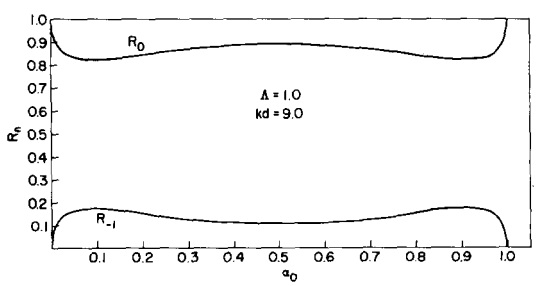

FIG. 9. Reflection coefficients R_n plotted vs $\alpha_0 = \sin\theta_i$, where θ_i = incident angle. The parameters $\Lambda = 1$ and $kd = 9$ give very slowly varying R_n.

remaining spectral orders and is called a Rayleigh anomaly.[5-7] It is illustrated most strongly by the cusp behavior in R_0. Figure 9, with $\Lambda = 1$ and $kd = 9$, is presented as an example of a slowly varying reflection coefficient behavior over the full range of incident angles. In Fig. 10(a) just the opposite is true, and the Wood P anomaly is illustrated as occurring when α_0 varies. Again the field symmetry for $\alpha_0 = 0$ is obvious. Figure 11 shows backscatter reflection coefficients at near-grazing incidence ($80° \leq \theta_i \leq 89°$) for two values of Λ: $\Lambda = 0.99235$ and $\Lambda = 0.49618$, and three values of kd. Note that as kd increases, so do the reflection coefficients. The maxima of the reflection coefficients occur when $\theta_n = -\theta_i$, i.e., when the backscatter angle is just the negative of the incident angle.

Figures 12 and 13 present values of R_n and ϕ_n as a function of Λ. Only the three principal scattering orders are plotted in Fig. 12 for values $\alpha_0 = 0.1$ and $k\theta = 2$. The cusp in R_0 at $\Lambda = 0.9$ is due to the extinction of the $n = 1$ spectral order, and is a Rayleigh anomaly. Bumps on other parts of the R_n curves are due to other Rayleigh anomalies whose spectral orders are not shown. The phase

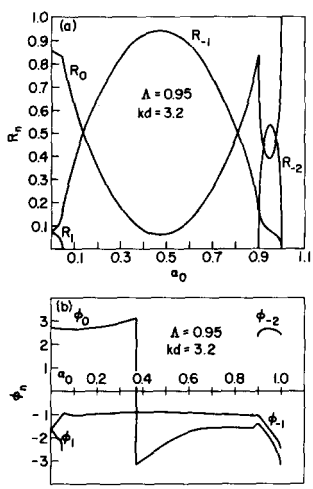

FIG. 10 (a) Reflection coefficients R_n, and (b) amplitude phases ϕ_n, plotted versus $\alpha_0 = \sin\theta_i$ for $\Lambda = 0.95$ and $kd = 3.2$. The Wood P anomaly is illustrated in (a).

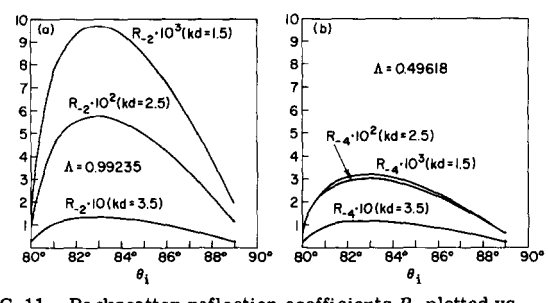

FIG. 11. Backscatter reflection coefficients R_n plotted vs incident (grazing) angle θ_i for (a) $\Lambda = 0.99235$ and (b) $\Lambda = 0.49618$ and $kd = 1.5, 2.5$, and 3.5. The maximum in each R_n occurs when the scattering angle $\theta_n = -\theta_i$ for the given values of Λ.

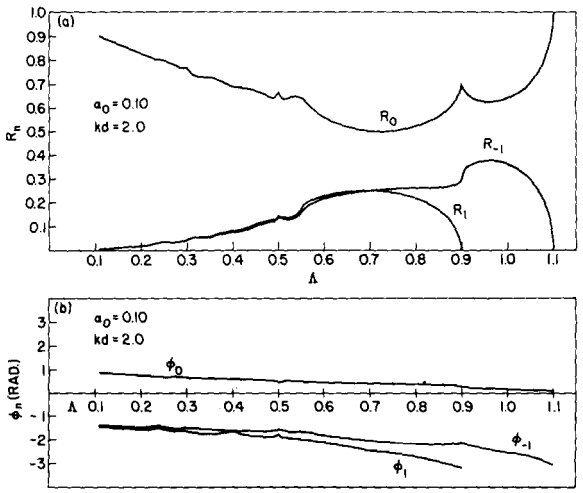

FIG. 12. (a) Three principle reflection coefficients R_n, and (b) amplitude phases ϕ_n, plotted vs $\Lambda = \lambda/2l$ for $\alpha_0 = 0.1$ and $kd = 2$. There is a Rayleigh anomaly at $\Lambda = 0.9$ and several Rayleigh anomalies (for small Λ) whose spectral orders are not shown.

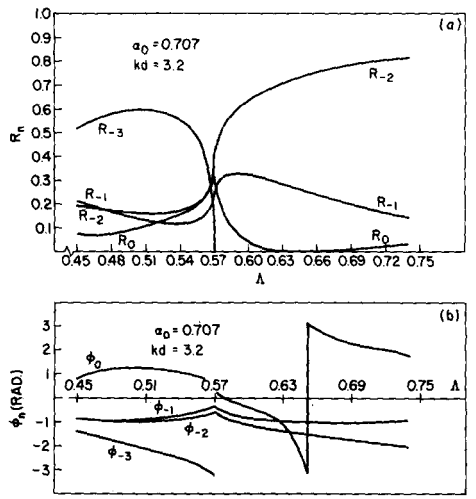

FIG. 13. (a) Reflection coefficients R_n, and (b) amplitude phases ϕ_n, plotted vs $\Lambda = \lambda/2l$ for $\alpha_0 = 0.707$ ($\theta_i = 45°$) and $kd = 3.2$. A sharp Rayleigh anomaly is illustrated by the vanishing of R_{-3} at $\Lambda \approx 0.57$. There is anomalous behavior in the phases at this point also.

behavior in Fig. 12(b) is very stable. Figure 13(a) shows a much sharper Rayleigh anomaly at $\Lambda \approx 0.57$, caused by the vanishing of R_{-3}. At this value of Λ, the phase behavior in Fig. 13(b) also shows some anomalous behavior.

6. SUMMARY AND CONCLUSIONS

It has been shown how to solve for the scattered field when a plane wave is incident on a one-dimensional corrugated surface of infinitesimally thin, periodic, finite-depth parallel plates. The soft boundary condition was used. The solution was given via complex function theory and a rapidly convergent iterative procedure. Matrix inversion was avoided. Numerical evaluations of reflection coefficients R_n and amplitude phases ϕ_n were given for various values of the parameters of the problem, α_0, Λ, and kd. In particular the Rayleigh anomaly, Wood P anomaly, and Brewster-angle anomaly were each illustrated. Also pointed out was a correspondence between R_n minima and zeros of $\partial^2\phi_n/\partial(kd)^2$ and one between the magnitude of R_n at its minima and the magnitude of $\partial\phi_n/\partial(kd)$.

Since we have only been interested in the field in region A we have not evaluated the B_j coefficients, although they could easily be done.

A similar problem with the surface having a hard boundary will be presented in a future publication.

ACKNOWLEDGMENTS

I am grateful to W. Ament for pointing out Mittra's work to me, to B. Hurdle and K. Flowers for several conversations and encouragement, and to N. Wright and G. Frisk for the numerical work. The reviewer has pointed out that many of the mathematical techniques used herein can be found in the recent book by Mittra and Lee.[14]

APPENDIX A: PROPERTIES OF INFINITE PRODUCTS

Weierstrass's definition of the gamma function $\Gamma(\omega)$, where ω is a complex variable given by[13]

$$\{\Gamma(\omega)\}^{-1} = \omega e^{\gamma\omega} \prod_{n=1}^{\infty} \left(1 + \frac{\omega}{n}\right) e^{-\omega/n}, \tag{A1}$$

where γ is the Euler–Mascheroni constant. The factor on the right-hand side of Eq. (A1) is an infinite product and shows that $\Gamma(\omega)$ has simple poles at $\omega = -1, -2, \cdots$. Define the infinite product $\Pi(\omega)$ which vanishes at the positive integers by

$$\Pi(\omega) = \prod_{n=1}^{\infty} \left(1 - \frac{\omega}{n}\right) e^{\omega/n}. \tag{A2}$$

The exponential factor guarantees the absolute and uniform convergence of the product.[15] $\Pi(\omega)$ is obviously related to the gamma function via

$$\Pi(\omega) = -e^{\gamma\omega}/\omega\Gamma(-\omega). \tag{A3}$$

It is necessary to construct asymptotic properties of infinite products which have the form $\Pi(\omega/i\Delta)$, where Δ is a real positive quantity. To do this it is necessary to consider asymptotic properties of $\Gamma(i\omega/\Delta)$ which are given by Stirling's approximation.[15] Using this approximation there results as $|\omega| \to \infty$, $\arg(\omega) \neq \pi/2$:

$$\Pi(\omega/i\Delta) \sim e^{-\pi i/4}(\Delta/2\pi\omega)^{1/2} e^{-i(\omega/\Delta)(\gamma + \ln\omega - \ln\Delta - 1 + \pi i/2)} \tag{A4}$$

and as $|\omega| \to \infty$ for $\arg(\omega) = \pi/2$,

$$\Pi(\omega/i\Delta) \sim e^{\pi i/4} \sin(\pi\omega/i\Delta) e^{-\pi\omega/\Delta} (\Delta/2\pi\omega)^{1/2} \times e^{-i(\omega/\Delta)(\gamma + \ln\omega - \ln\Delta - 1 + \pi/2)}. \tag{A5}$$

Equation (A5) follows by noting that

$$\Pi(\omega/i\Delta)\Pi(-\omega/i\Delta) = (i\Delta/\omega\pi)\sin(\omega\pi/i\Delta)$$

and expanding $\Pi(-\omega/i\Delta)$ using Stirling's approximation which is now valid for $-\pi/2 < \arg(\omega) < 3\pi/2$, and, in particular, for $\arg(\omega) = \pi/2$.

The procedure used in this paper for constructing infinite products with nonintegral zeros is illustrated by the following example: Let the infinite product have zeros at the points D_m for $m = 1, 2, 3, \cdots$. It will thus contain terms like $(1-\omega/D_m)$. If, for large $m, D_m \sim im\Delta$, where Δ is real and positive, the $(1 - \omega/D_m)$ term is to be multiplied by $(D_m/im\Delta)\exp(\omega/i\Delta m)$. The final infinite product is defined by

$$\Pi(\omega, D) = \prod_{m=1}^{\infty} (1 - \omega/D_m)(D_m/im\Delta)e^{\omega/i\Delta m}. \tag{A6}$$

The exponential guarantees that the product is both absolutely and uniformly convergent,[13] provided the product $\Pi(D_m/i\Delta m)$ is. The latter product is included for convenience with regard to asymptotic properties as seen below.

To find the behavior of Eq. (A6) for large ω, divide Eq. (A6) term by term by a modified form of Eq. (A2) given by $\Pi(\omega/i\Delta)$. For large ω, the result is unity. That is, for large ω, there results

$$\Pi(\omega, D) \sim \Pi(\omega/i\Delta) \tag{A7}$$

and the asymptotic value of $\Pi(\omega, D)$ is thus known from Eq. (A4).

Specific infinite products used in this paper are given by

$$\Pi_1(\omega, \beta) = \prod_{n=1}^{\infty}\left(1 - \frac{\omega}{\beta_n}\right)\left(\frac{\beta_n}{in\Lambda}\right)e^{\omega/in\Lambda} \tag{A8}$$

for the product with zeros at $\omega = \beta_n$ $(n = 1, 2, \cdots)$,

$$\Pi_2(\omega, \beta) = \prod_{n=-1}^{\infty}\left(1 - \frac{\omega}{\beta_n}\right)\left(\frac{\beta_n}{i|n|\Lambda}\right)e^{\omega/i|n|\Lambda}$$
$$= \prod_{n=1}^{\infty}\left(1 - \frac{\omega}{\beta_n}\right)\left(\frac{\beta_{-n}}{in\Lambda}\right)e^{\omega/in\Lambda} \tag{A9}$$

for the product with zeros at $\omega = \beta_n$ $(n = -1, -2, \cdots)$ and

$$\Pi(\omega, \bar{q}) = \prod_{m=1}^{\infty}\left(1 - \frac{\omega}{q_m}\right)\left(\frac{2\bar{q}_m}{im\Lambda}\right)e^{2\omega/im\Lambda} \tag{A10}$$

for the product with zeros at $\omega = \bar{q}_m$ $(m = 1, 2, \cdots)$.

Following the above discussion, note that the products $\Pi(\beta_{\pm n}/in\Lambda)$ do not converge because of the α_0 term in $\beta_{\pm n}$. However, the products Π_1 and Π_2 always occur together, and $\Pi_1\Pi_2$ converges since $\Pi(-\beta_n\beta_{-n}/n^2\Lambda^2)$ does. Also in Eq. (A10) we have specified that for large m, $\bar{q}_m \sim im\Lambda/2 \sim q_m$.

For large ω, following Eq. (A6), we have.

$$\Pi_1(\omega, \beta) \sim \Pi_2(\omega, \beta) \sim \Pi(\omega/i\Lambda),$$

$$\Pi(\omega, \bar{q}) \sim \Pi(2\omega/i\Lambda);$$

and hence, using Eq. (A4) as $|\omega| \to \infty$, $\arg(\omega) \neq \pi/2$

$$\Pi_1(\omega, \beta) \sim \Pi_2(\omega, \beta) \sim e^{-\pi i/4}(\Lambda/2\pi\omega)^{1/2}$$
$$\times e^{(\omega/i\Lambda)(\gamma - 1 + \pi i/2 - \ln n\Lambda + 1 n\omega)}, \tag{A11}$$

$$\Pi(\omega, \bar{q}) \sim e^{-\pi i/4}(\Lambda/4\pi\omega)^{1/2}$$
$$\times e^{(2\omega/i\Lambda)(\gamma - 1 + \pi i/2 - \ln(\Lambda/2) + \ln\omega)} \tag{A12}$$

Asymptotic expansions for $\arg(\omega) = \pi/2$ can be found in a manner similar to the discussion following Eq. (A5).

APPENDIX B: ASYMPTOTIC ALGEBRAIC BEHAVIOR OF THE RESIDUE FUNCTION

In Sec. 4A following Eq. (4. 7), it was stated that the asymptotic behavior of A_n (for n large) is $n^{-3/2}$, where A_n is given by Eq. (3. 6). This can be illustrated as follows. From Eqs. (A2) and (A4) it is possible to write, for large ω,

$$\{\Pi(\omega)\}^{-1} = O(\omega^{1/2}), \tag{B1}$$

where exponential factors have been neglected since only the algebraic behavior is of interest. The question we wish to answer is, what is the algebraic behavior of the residue $R(m)$ defined by

$$R(m) = \lim_{\omega \to m}\{\omega - m)/\Pi(\omega)\}, \tag{B2}$$

where m is a large positive integer? It is possible to write

$$\{\Pi(\omega)\}^{-1} = \frac{\pi\omega}{\sin(\pi\omega)}\Pi(-\omega). \tag{B3}$$

This has the effect of exposing the poles of $\{\Pi(\omega)\}^{-1}$ through the $\sin(\pi\omega)$ factor. Hence

$$R(m) = m\pi\Pi(-m)\lim_{\omega \to m}\{(\omega - m)/\sin(\pi\omega)\}$$
$$= m(-)^m\Pi(-m). \tag{B4}$$

For m positive and large the asymptotic expansion of $\Pi(-m)$ has algebraic behavior $m^{-1/2}$. This follows from Eq. (A3) and Stirling's approximation to the gamma function. Thus from Eq. (B4)

$$R(m) = O(m^{1/2}),$$

which is the same algebraic behavior as $\{\Pi(\omega)\}^{-1}$. Hence the residue of the function has the same asymptotic algebraic behavior as the function. Thus, for example, generalizing this result, A_n, given by Eq. (3. 6), behaves like $n^{-3/2}$ for large n because $r(\beta_n) \sim f(\beta_n) \sim n^{-3/2}$ for large n.

[1] L. A. Weinstein (Vaynshteyn), *The Theory of Diffraction and the Factorization Method* (Golem, Boulder, Colo., 1969).
[2] P. Beckmann and A. Spizzichino, *The Scattering of Electromagnetic Waves from Rough Surfaces* (Macmillan, New York, 1963).
[3] R. A. Hurd, Can. J. Phys. **32**, 727 (1954).
[4] B. Noble, *The Wiener-Hopf Technique* (Pergamon, New York, 1958).
[5] J. E. Stewart and W. S. Gallaway, Appl. Opt. **1**, 421 (1962).
[6] A. Hessel and A. A. Oliner, Appl. Opt. **4**, 1275 (1965).
[7] D. Y. Tseng, "Guiding and Scattering of Electromagnetic Fields by Corrugated Structures," Ph.D. Thesis (Polytechnic Institute of Brooklyn, 1967).
[8] R. Mittra, S. W. Lee, and G. F. Vanblaricum, Int. J. Eng. Sci. **6**, 395 (1968).
[9] J. F. Carlson and A. E. Heins, Quart. Appl. Math. **4**, 313 (1947); **5**, 82 (1947).
[10] F. Berz, Proc. IEEE (London) **98**, 47 (1951), Part III.
[11] In the analogous electromagnetic problem, the electric vector **E** is in the y direction, $\mathbf{E} = \hat{j} E_y(x, z)$ and the (x, z) plane is that of the magnetic vector (TE polarization). ψ can then be thought of as the scalar field $\psi(x, z) = E_y(x, z)$ from which the entire electromagnetic field can be derived using Maxwell's equations.
[12] See, e.g., C. J. Bouwkamp, Rept. Progr. Phys. **17**, 35 (1954) or M. Born and E. Wolf, *Principles of Optics* (Pergamon, New York, 1964).
[13] Bateman Manuscript Project, *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill, New York, 1953), Vol. 1, Chap. 1.
[14] R. Mittra and S. W. Lee, *Analytical Techniques in the Theory of Guided Waves* (Macmillan, New York, 1971).
[15] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge U.P., New York 1962).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Multiple Density Correlations in a Many-Particle System*†

F. Y. Wu
Department of Physics, Northeastern University, Boston, Massachusetts 02115
(Received 22 March 1971)

A closed expression similar to the Ursell-Mayer expansion is obtained for the static multiple density correlation function $I_n = \langle \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} \rangle$ of a many-particle system. It is shown that I_n breaks into products of lower ones, if there exist partial momentum conservations among the $\mathbf{k}$'s. Using the convolution approximation for the n-particle correlation function, we evaluate I_n in a closed form. The result is shown to be accurate in the small k region.

I. INTRODUCTION

The static multiple density correlation functions

$$I_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = \langle \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} \rangle \tag{1}$$

play an important role in the study of many-particle systems. The notation $\langle\ \rangle$ denotes the expectation value for a quantum mechanical system or the canonical ensemble average for a classical system; $\rho_{\mathbf{k}}$ is the density fluctuation. In the theory of quantum liquids,[1] for example, I_n's are the overlapping matrix elements of the phonon states. A detailed knowledge of these integrals would then permit the construction of a complete set of orthonormal states. In the configurational space we have

$$\rho_{\mathbf{k}} = \sum_{i=1}^{N} \exp(i\mathbf{k} \cdot \mathbf{r}_i), \tag{2}$$

where $\mathbf{r}_i$ is the coordinate of the ith particle and N the total number of particles. The evaluation of I_n then requires a knowledge of the n-particle distribution function g_n. In order to have a reasonable estimate of these matrix elements, one usually uses the Kirkwood superposition approximation[2] or the convolution approximation[3,4] for g_n. It is quite difficult, however, to assess the accuracy of these estimates. Furthermore, the algebra involved in these evaluations is quite tedious. For example, one has to consider explicitly whether there exist partial momentum conservations among the $\mathbf{k}$'s. Besides a few special cases that have been considered,[5-9] no general expression is known for I_n.

In this paper we shall consider this general problem. We first derive in Sec. II a general expression for I_n. From this expression and the assumed cluster property of the distribution functions, we are able to see that I_n breaks into product of lower ones if there exist partial momentum conservations among the $\mathbf{k}$'s. Consequently, some of the results previously obtained using the superposition approximation are seen to be exact. This general discussion also permits us to assess the accuracy of the estimation obtained by using the convolution approximation. In Sec. III we use the convolution approximation to evaluate I_n. A closed expression is obtained and is shown to be accurate in the small k region. Some applications of our result are given in Sec. IV.

II. GENERAL FORMULATION

The quantity of interest is I_n defined by Eq. (1). Explicitly we write

$$I_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = Q_N^{-1} \int W_N \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} d\mathbf{r}_1 \cdots d\mathbf{r}_N, \tag{3}$$

where

$$Q_N = \int W_N d\mathbf{r}_1 \cdots d\mathbf{r}_N$$

and W_N is symmetric in the particle coordinates $\{\mathbf{r}_1, \cdots, \mathbf{r}_N\}$ and is given by

$$W_N = \exp[-V(\mathbf{r}_1, \cdots, \mathbf{r}_N)/kT] \tag{4a}$$

for a classical system,

[1] L. A. Weinstein (Vaynshteyn), *The Theory of Diffraction and the Factorization Method* (Golem, Boulder, Colo., 1969).
[2] P. Beckmann and A. Spizzichino, *The Scattering of Electromagnetic Waves from Rough Surfaces* (Macmillan, New York, 1963).
[3] R. A. Hurd, Can. J. Phys. **32**, 727 (1954).
[4] B. Noble, *The Wiener-Hopf Technique* (Pergamon, New York, 1958).
[5] J. E. Stewart and W. S. Gallaway, Appl. Opt. **1**, 421 (1962).
[6] A. Hessel and A. A. Oliner, Appl. Opt. **4**, 1275 (1965).
[7] D. Y. Tseng, "Guiding and Scattering of Electromagnetic Fields by Corrugated Structures," Ph.D. Thesis (Polytechnic Institute of Brooklyn, 1967).
[8] R. Mittra, S. W. Lee, and G. F. Vanblaricum, Int. J. Eng. Sci. **6**, 395 (1968).
[9] J. F. Carlson and A. E. Heins, Quart. Appl. Math. **4**, 313 (1947); **5**, 82 (1947).
[10] F. Berz, Proc. IEEE (London) **98**, 47 (1951), Part III.
[11] In the analogous electromagnetic problem, the electric vector **E** is in the y direction, $\mathbf{E} = \hat{j} E_y(x, z)$ and the (x, z) plane is that of the magnetic vector (TE polarization). ψ can then be thought of as the scalar field $\psi(x, z) = E_y(x, z)$ from which the entire electromagnetic field can be derived using Maxwell's equations.
[12] See, e.g., C. J. Bouwkamp, Rept. Progr. Phys. **17**, 35 (1954) or M. Born and E. Wolf, *Principles of Optics* (Pergamon, New York, 1964).
[13] Bateman Manuscript Project, *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill, New York, 1953), Vol. 1, Chap. 1.
[14] R. Mittra and S. W. Lee, *Analytical Techniques in the Theory of Guided Waves* (Macmillan, New York, 1971).
[15] E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge U.P., New York 1962).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Multiple Density Correlations in a Many-Particle System*†

F. Y. Wu
Department of Physics, Northeastern University, Boston, Massachusetts 02115
(Received 22 March 1971)

A closed expression similar to the Ursell-Mayer expansion is obtained for the static multiple density correlation function $I_n = \langle \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} \rangle$ of a many-particle system. It is shown that I_n breaks into products of lower ones, if there exist partial momentum conservations among the $\mathbf{k}$'s. Using the convolution approximation for the n-particle correlation function, we evaluate I_n in a closed form. The result is shown to be accurate in the small k region.

I. INTRODUCTION

The static multiple density correlation functions

$$I_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = \langle \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} \rangle \tag{1}$$

play an important role in the study of many-particle systems. The notation $\langle\ \rangle$ denotes the expectation value for a quantum mechanical system or the canonical ensemble average for a classical system; $\rho_{\mathbf{k}}$ is the density fluctuation. In the theory of quantum liquids,[1] for example, I_n's are the overlapping matrix elements of the phonon states. A detailed knowledge of these integrals would then permit the construction of a complete set of orthonormal states. In the configurational space we have

$$\rho_{\mathbf{k}} = \sum_{i=1}^{N} \exp(i\mathbf{k} \cdot \mathbf{r}_i), \tag{2}$$

where $\mathbf{r}_i$ is the coordinate of the ith particle and N the total number of particles. The evaluation of I_n then requires a knowledge of the n-particle distribution function g_n. In order to have a reasonable estimate of these matrix elements, one usually uses the Kirkwood superposition approximation[2] or the convolution approximation[3,4] for g_n. It is quite difficult, however, to assess the accuracy of these estimates. Furthermore, the algebra involved in these evaluations is quite tedious. For example, one has to consider explicitly whether there exist partial momentum conservations among the $\mathbf{k}$'s. Besides a few special cases that have been considered,[5-9] no general expression is known for I_n.

In this paper we shall consider this general problem. We first derive in Sec. II a general expression for I_n. From this expression and the assumed cluster property of the distribution functions, we are able to see that I_n breaks into product of lower ones if there exist partial momentum conservations among the $\mathbf{k}$'s. Consequently, some of the results previously obtained using the superposition approximation are seen to be exact. This general discussion also permits us to assess the accuracy of the estimation obtained by using the convolution approximation. In Sec. III we use the convolution approximation to evaluate I_n. A closed expression is obtained and is shown to be accurate in the small k region. Some applications of our result are given in Sec. IV.

II. GENERAL FORMULATION

The quantity of interest is I_n defined by Eq. (1). Explicitly we write

$$I_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = Q_N^{-1} \int W_N \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} d\mathbf{r}_1 \cdots d\mathbf{r}_N, \tag{3}$$

where

$$Q_N = \int W_N d\mathbf{r}_1 \cdots d\mathbf{r}_N$$

and W_N is symmetric in the particle coordinates $\{\mathbf{r}_1, \cdots, \mathbf{r}_N\}$ and is given by

$$W_N = \exp[-V(\mathbf{r}_1, \cdots, \mathbf{r}_N)/kT] \tag{4a}$$

for a classical system,

$$W_N = |\psi(\mathbf{r}_1, \cdots, \mathbf{r}_N)|^2 \tag{4b}$$

for a quantum mechanical system.

Here V is the total potential energy and ψ is the wavefunction describing the system.

Let us define as in Ref. 4 the n-particle distribution function

$$g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n) = \frac{N!}{(N-n)!} Q_N^{-1} \rho^{-n} \times \int W_N d\mathbf{r}_{n+1} \cdots d\mathbf{r}_N, \tag{5}$$

where ρ is the particle number density. An immediate consequence of this definition is the sequential relation

$$\rho \int g_{n+1}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1}) d\mathbf{r}_{n+1} = (N-n) g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n). \tag{6}$$

The following cluster condition is also expected to hold for an infinite homogeneous and isotropic system such as a liquid:

$$\lim_{r_{in} \to \infty} g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n) = g_{n-1}(\mathbf{r}_1, \cdots, \mathbf{r}_{n-1}), \quad i = 1, 2, \cdots, n-1. \tag{7}$$

We shall assume (7) in later discussions.

It is convenient to define at this point the cluster functions f_n as follows:

$$\begin{aligned} g_1(\mathbf{r}_1) &= f_1(\mathbf{r}_1) = 1, \\ g_2(\mathbf{r}_1, \mathbf{r}_2) &= f_1(\mathbf{r}_1) f_2(\mathbf{r}_2) + f_2(\mathbf{r}_1, \mathbf{r}_2), \\ g_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) &= f_1(\mathbf{r}_1) f_1(\mathbf{r}_2) f_1(\mathbf{r}_3) + f_1(\mathbf{r}_1) f_2(\mathbf{r}_2, \mathbf{r}_3) \\ &\quad + f_1(\mathbf{r}_2) f_2(\mathbf{r}_3, \mathbf{r}_1) + f_1(\mathbf{r}_3) f_2(\mathbf{r}_1, \mathbf{r}_2) \\ &\quad + f_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), \end{aligned} \tag{8}$$

etc.

The structure of Eq. (8) is identical to that of the Ursell–Mayer expansion in classical statistical mechanics.[10] We shall use the compact notation

$$\mathbf{g} = \alpha \mathbf{f} \quad \text{or} \quad f = \alpha^{-1} \mathbf{g} \tag{8'}$$

to denote the structural relation (8) between any two sets of functions g_n and f_n.

The function f_n is symmetric in its n coordinates. The cluster condition (7) implies the following condition on f:

$$\lim_{r_{ij} \to \infty} f_n(r_1, \cdots, r_n) = 0, \quad 1 \le i < j \le n. \tag{9}$$

Namely, f_n is significant only when the n particles are clustered together. Also it is easy to establish by induction that the sequential relation (6) implies the condition

$$\rho \int f_{n+1}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1}) d\mathbf{r}_{n+1} = -n f_n(\mathbf{r}_1, \cdots, \mathbf{r}_n). \tag{10}$$

We shall also need the Fourier transforms of the g and f functions:

$$\begin{aligned} G_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) &= \rho^n \int g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n) \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \cdots + \mathbf{k}_n \cdot \mathbf{r}_n)] d\mathbf{r}_1 \cdots d\mathbf{r}_n, \\ F_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) &= \rho^n \int f_n(\mathbf{r}_1, \cdots, \mathbf{r}_n) \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \cdots + \mathbf{k}_n \cdot \mathbf{r}_n)] d\mathbf{r}_1 \cdots d\mathbf{r}_n. \end{aligned} \tag{11}$$

With these definitions we now proceed to evaluate I_n. Substituting Eq. (2) into Eq. (3) and making use of the definition Eq. (11), one readily obtains the following:

$$\begin{aligned} I_1(\mathbf{k}_1) &= G_1(\mathbf{k}_1), \\ I_2(\mathbf{k}_1, \mathbf{k}_2) &= G_1(\mathbf{k}_1 + \mathbf{k}_2) + G_2(\mathbf{k}_1, \mathbf{k}_2), \\ I_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) &= G_1(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) + G_2(\mathbf{k}_1, \mathbf{k}_2 + \mathbf{k}_3) \\ &\quad + G_2(\mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_1) + G_2(\mathbf{k}_3, \mathbf{k}_1 + \mathbf{k}_2) \\ &\quad + G_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3), \end{aligned} \tag{12}$$

etc.,

$$I_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = \sum G_l \text{ (all distinct partitions of the } \mathbf{k}'\text{s)}.$$

A typical term of Eq. (12), e.g., $G_l(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4 + \mathbf{k}_5, \cdots)$, comes from the contribution in Eq. (3) when $\mathbf{r}_1 = \mathbf{r}_2$, $\mathbf{r}_3 = \mathbf{r}_4 = \mathbf{r}_5$, etc., where l is the number of distinct $\mathbf{r}$'s. We shall use the compact notation

$$\mathbf{I} = \beta \mathbf{G} \quad \text{or} \quad \mathbf{G} = \beta^{-1} \mathbf{I} \tag{12'}$$

to denote the structural relation (12) between any two sets of functions I_n and G_n.

It is clear from the definitions (11), (8), and (8') that

$$\mathbf{G} = \alpha \mathbf{F}. \tag{13}$$

Hence, from (12'),

$$\mathbf{I} = \beta \alpha \mathbf{F}. \tag{14}$$

We now make use of the identity

$$\beta \alpha = \alpha \beta, \tag{15}$$

which can be proved by observing that every term in $\beta \alpha$ F is in $\alpha \beta$ F and vice versa. We then arrive at

$$\mathbf{I} = \alpha \mathbf{U}, \tag{16}$$

where

$$\mathbf{U} = \beta \mathbf{F}. \tag{17}$$

Equation (16) is our *main result.* Note that the derivation of Eq. (16) involves only the definitions of the g, f, G, and F functions and is therefore exact. The cluster condition of Eq. (7) has not been used in these discussions.

We now discuss properties of the U functions defined by (17) as implied by the sequential and the cluster properties (6) and (7). It is easy to see from Eqs. (10) and (11) that

$$F_{n+1}(\mathbf{k}_1, \cdots, \mathbf{k}_n, 0) = -nF_n(\mathbf{k}_1, \cdots, \mathbf{k}_n). \tag{18}$$

As a consequence of Eq. (18), one can establish the relation

$$U_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = 0 \quad \text{if any } k_i = 0. \tag{19}$$

Equation (19) is, of course, a consequence of the sequential relation Eq. (6) and is therefore exact. For example, Eqs. (17) and (19) recover the identity

$$I_{n+1}(\mathbf{k}_1, \cdots, \mathbf{k}_n, 0) = NI_n(\mathbf{k}_1, \cdots, \mathbf{k}_n), \tag{20}$$

which is implied by the definition (3).

The cluster condition (9) has the important consequence that F_n defined by Eq. (11) is of the order of N. Furthermore, from the translational invariance of f_n we see that F_n vanishes unless $\mathbf{k}_1 + \cdots + \mathbf{k}_n = 0$. Since each U function is a linear combination of single F functions, we conclude that

$$\mathrm{U}_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = \delta_{\mathbf{k}_1+\cdots+\mathbf{k}_n,0} O(N). \tag{21}$$

In particular

$$\mathrm{U}_1(\mathbf{k}) = \delta_{\mathbf{k},0} N. \tag{22}$$

It follows then that the leading contribution in I_n [Eq. (16)] comes from the terms containing the most number of nonvanishing momentum-conserving δ functions. That is, the leading contribution can be broken into product of lower I_n's if there exist partial momentum conservations among the k's (the degenerate case). The degeneracy factor can be easily counted. For example,

$$\langle \prod_i (\rho_{\mathbf{k}_i} \rho_{-\mathbf{k}_i})^{n_i} \rangle = \prod_i n_i! [U_2(\mathbf{k}_i, -\mathbf{k}_i)]^{n_i} [1 + O(N^{-1})]. \tag{23}$$

This result was first derived by Jackson and Feenberg[5,7] in an elaborate analysis using the generalized Kirkwood superposition approximation for g_n. Since only g_2 enters in the expression of U_2, we see that, to the lead order in N, Eq. (23) is exact. Indeed, an alternate derivation[11] of Eq. (23) using the generating function technique does not involve the use of higher distribution functions. The exact result is generated by the superposition approximation because the latter satisfies the cluster condition (7). Another example of application of Eq. (16) is the evaluation of the following matrix element[8] which enters in the theory of dispersion of phonons in liquid He[4]:

$$I_5(\mathbf{k}, 1, -\mathbf{k}-1, \mathbf{h}, -\mathbf{h}) = U_3(\mathbf{k}, 1, -\mathbf{k}-1) U_2(\mathbf{h}, -\mathbf{h}) \times [1 + O(N^{-1})], kl \,|\, \mathbf{k}+1 \,|\, h \neq 0. \tag{24}$$

This integral was first evaluated by Lai, Sim, and Woo[8] using convolution approximations to g_3, g_4, and g_5. It is now clear that only g_3 and g_2 enter on the right-hand side of Eq. (24) consistent to a recent remark by Feenberg.[9] Finally we remark that if $\delta_{\mathbf{k}_1+\cdots+\mathbf{k}_n,0}$ is the only nonvanishing momentum-conserving factor, then

$$I_n(\mathbf{k}_1, \cdots, \mathbf{k}_n) = U_n(\mathbf{k}_1, \cdots, \mathbf{k}_n). \tag{16'}$$

III. EVALUATION OF U_n BY THE CONVOLUTION APPROXIMATION

In this section we evaluate the U functions defined by Eq. (17) using the convolution form $g_n^{(c)}$ for g_n. If we define

$$\mathbf{f}^{(c)} = \alpha^{-1} \mathbf{g}^{(c)} \tag{25}$$

and let $F_n^{(c)}$ be the Fourier transform [Eq. (11)] of $f_n^{(c)}$, our goal is then to compute

$$\mathbf{U}^{(c)} = \beta \mathbf{F}^{(c)}. \tag{26}$$

First, we remark that since $g_n^{(c)}$ satisfies the sequential relation exactly, $U_n^{(c)}$ shall satisfy Eq. (19). In fact, our result, Eq. (34'), yields precisely

$$U_n^{(c)} \propto k_1 k_2 \cdots k_n \text{ for small } k\text{'s and } n \geq 3. \tag{27}$$

In the ensuing discussions it is again convenient $U_n^{(c)}$ is quite accurate, at least in the small k regions. Any correction would be of higher than the nth power in k's.

In the ensuring discussions it is again convenient to introduce a diagrammatic notation for algebraic expressions. Readers are referred to the basic conventions and definitions given in Sec. III of Ref. 4. The principal definitions and a few new additions[12] are now reviewed.

A graph is a collection of points with lines joining certain pairs of points. A *root* (or root point) is a point with a numeral label and is represented by an open circle. Unlabeled points are represented by solid, or black, circles. An *n-rooted* graph has precisely n root points, labeled from 1 to n. A *node* is a point having three or more incident lines. These lines *intersect* at the node point. A *terminal point* has only one line incident. The line incident to a terminal point will be called a *terminal line*. A *Cayley tree* is a connected graph containing no cycles, i.e., one cannot return to a point on a Cayley tree by following a sequence of lines.

To obtain the mathematical expression represented by a graph, one simply writes for each black point a factor $\rho \int d\mathbf{r}_k$, where k is taken to be the label of this black point, and for each line connecting two points labeled i and j writes a factor $f_2(|\mathbf{r}_i - \mathbf{r}_j|)$. Any isolated root point has a factor 1. With these conventions, the convolution form for g_n is[4]

$g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$ = the collection of all distinct n-rooted graphs consisting of *connected* and *disconnected* Cayley trees provided that each black point is a node. (28)

A moment's reflection using (25) and (28) now yields

$f_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$ = the collection of all distinct *connected* n-rooted Cayley trees provided that each black point is a node. (29)

It is now possible to evaluate the Fourier transform $F_n^{(c)}$ of $f_n^{(c)}$. Since every term in $f_n^{(c)}$ is a Cayley tree, the result is quite simple and can be expressed in terms of the Fourier transform of $f_2 = g_2 - 1$,

$$u(k) = S(k) - 1 = \rho \int e^{i\mathbf{k}\cdot\mathbf{r}} [g_2(r) - 1] d\mathbf{r}. \quad (30)$$

In fact, every term in $F_n^{(c)}(\mathbf{k}_1, \cdots, \mathbf{k}_n)$ can also be conveniently represented by a graph related to the graph of $f_n^{(c)}$. The following further graph definitions will be useful.

A *normal* graph is one in which all roots are terminal points. Thus Fig. 1(b) is a normal graph while Fig. 1(a) is not. We speak of the following process which converts a graph into a normal one as the normalization of a graph. The normalization process is simply to remove the label of any nonterminal root point, thus leaving a black point, add a new root point with this label, and connect it to the black point by a *dotted* line. In this way the graph of Fig. 1(a) is normalized into that of Fig. 1(b). We see that a normalized graph will now have two kinds of lines, the solid and the dotted ones. The dotted lines are always terminal lines.

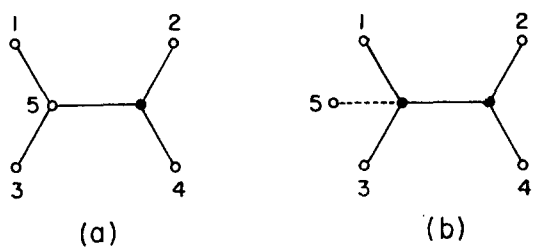

FIG. 1. Normalization of a graph [graph (a) is normalized into graph (b)].

Consider a given graph $\mathcal{G}$ in $f_n^{(c)}$. We leave it for the readers to verify that the Fourier transform [Eq. (11)] of this graph can be obtained by the following rules:

1. Normalize $\mathcal{G}$ if it contains nonterminal root points.
2. In the normalized graph label the terminal line (solid or dotted) connected to the ith root with momentum $\mathbf{k}_i$.
3. If all lines incident to a node are labeled except one, then label this remaining line with a momentum equal to the sum of all the previously labeled momenta surrounding this node.
4. Repeat 3 until all lines are labeled.
5. For each *solid* line labeled by $\mathbf{k}$ write a factor $u(k)$. For each *dotted* line write a factor 1.
6. The Fourier transform of $\mathcal{G}$ is the product of all factors in 5 and the factor $N\delta_{\mathbf{k}_1+\cdots+\mathbf{k}_n,0}$.

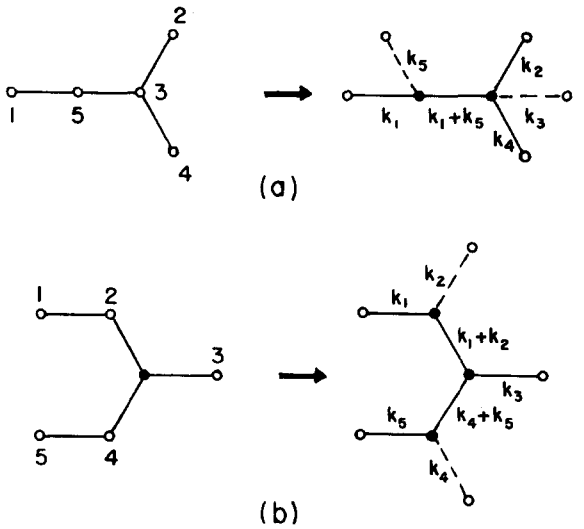

FIG. 2. Fourier transforms of two terms of $f_5^{(c)}$.

We remark that the momentum labelings are unique because the graphs are all Cayley trees and because the total momentum is conserved. Two examples are given in Fig. 2. The graphs on the left are two typical terms of $f_5^{(c)}$, while the graphs on the right are their Fourier transforms. Explicitly Fig. 2 says the following:

$$\text{(a)}\quad \rho^5 \int f_{15} f_{53} f_{23} f_{34} \exp[i(\mathbf{k}_1\cdot\mathbf{r}_1 + \cdots + \mathbf{k}_5\cdot\mathbf{r}_5)] \times d\mathbf{r}_1 \cdots d\mathbf{r}_5 = N u_1 u_{1+5} u_2 u_4 \delta_{1+2+3+4+5},$$

$$\text{(b)}\quad \rho^6 \int f_{12} f_{26} f_{36} f_{46} f_{45} \exp[i(\mathbf{k}_1\cdot\mathbf{r}_1 + \cdots + \mathbf{k}_5\cdot\mathbf{r}_5) \times d\mathbf{r}_1 \cdots d\mathbf{r}_6 = N u_1 u_{1+2} u_3 u_{4+5} u_5 \delta_{1+2+3+4+5},$$

where we have adopted the shorthand notations

$$u_1 = u(\mathbf{k}_1), \quad u_{1+2} = u(|\mathbf{k}_1 + \mathbf{k}_2|), \quad \delta_{1+2} = \delta_{\mathbf{k}_1+\mathbf{k}_2,0}, \quad \text{etc.} \quad (31)$$

Thus we arrive at

$F_n^{(c)}(\mathbf{k}_1, \cdots, \mathbf{k}_n)$ = the collection of all graphs of $f_n^{(c)}$ subject to the rules 1–6. (32)

$F_n^{(c)}$ for $n = 1, 2, 3, 4$ are given explicitly in Fig. 3, where only the topologically distinct graphs are shown and the momentum labels have been deleted.

It is seen from Fig. 3 that in the expression of $F_n^{(c)}$ there exist pairs of graphs which are identical except that in one graph a given terminal line is solid while in the other the same terminal line is dotted. We may then combine these two graphs into a single one so that this terminal line is doubled (solid and dotted lines). The weight of this

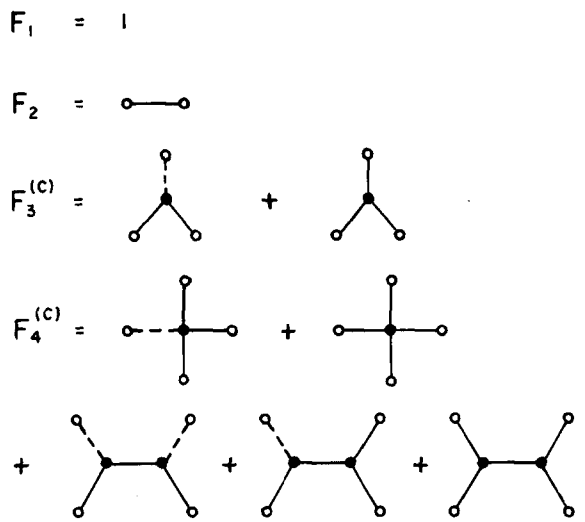

FIG. 3. Diagrammatic representations of $F_n^{(c)}$ for $n = 1, 2, 3, 4$.

double line is now $u(k) + 1 = S(k)$. However, we cannot do this simultaneously for two or more terminal lines intersecting at one node because according to our rules of normalization no graph has intersecting dotted lines. This problem is resolved when we substitute Eq. (32) into Eq. (26) to compute $U_n^{(c)}$. From the definition (12) or (12′) we see that in some graphs of $U_n^{(c)}$ the terminal lines have momenta which are the sums of individual $\mathbf{k}_i$'s. These graphs can be converted to have intersecting dotted lines and give rise to precisely those graphs we need. First a dotted terminal line having a momentum $\Sigma\mathbf{k}_i$ can be split into several terminal lines, each having a label $\mathbf{k}_i$. For a solid terminal line having a momentum $\Sigma\mathbf{k}_i$, one simply adds new terminal points and connects all these new points to the original terminal point by dotted lines. Three examples of such conversion for graphs $U_4^{(c)}$ are shown in Fig. 4. Consider

$$U_4^{(c)}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4) = \cdots + F_2(\mathbf{k}_1,\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4) + \cdots + F_3^{(c)}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4) + \cdots .$$

The graph of $F_2(\mathbf{k}_1,\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4) = Nu_1\delta_{1+2+3+4}$ is the one on the left in Fig. 4(a). By the above process this graph is converted to the one on the right in Fig. 4(a). The latter now has four root points with single momentum labels. Similarly, Fig. 4(b) denotes the same conversion for the term $Nu_2u_{3+4}\delta_{1+2+3+4}$ in $F_3^{(c)}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4)$, etc. Note that this process results in the same algebraic expression because of rule 3 above.

After converting all graphs of $U_n^{(c)}$ in Eq. (26) according to this rule, we see that

$U_n^{(c)}(\mathbf{k}_1,\cdots,\mathbf{k}_n)$ = the collection of all distinct normal n-rooted Cayley trees provided that each black point is a node. The terminal lines can be either solid or dotted, each considered as distinct. (33)

Of course, rules 2-6 must be used in Eq. (33). The identity between Eqs. (33) and (26) can be established by observing that every graph in Eq. (26) is in Eq. (33) and vice versa.

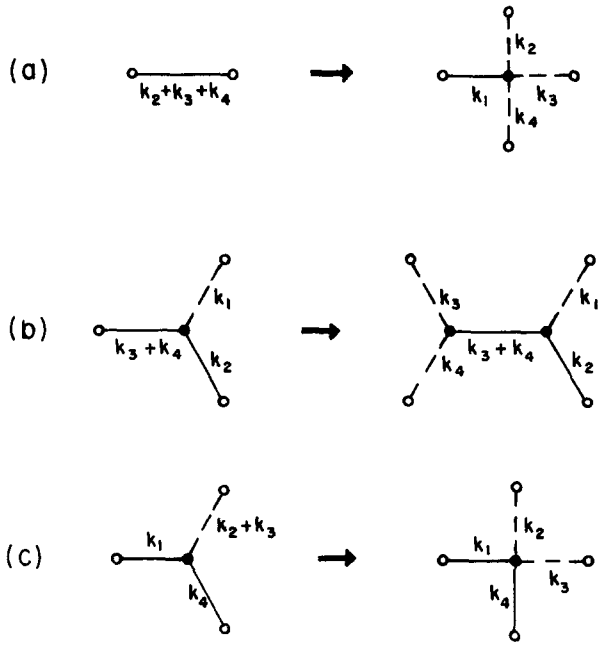

FIG. 4. Reduction of three graphs in $U_4^{(c)}$ to single momentum labels for the terminal lines

It is now possible to combine the solid and dotted lines of all the terminal lines at the same time to form double lines. Thus we arrive at our final result:

$U_n^{(c)}(\mathbf{k}_1,\cdots,\mathbf{k}_n)$ = the collection of all distinct normal n-rooted Cayley trees provided that each black point is a node. All terminal lines are double (solid and dotted) lines. (34)

Graphs for $U_n^{(c)}$ are shown in Fig. 5 for $n = 1, 2, 3, 4, 5$, where all momentum labels are deleted and

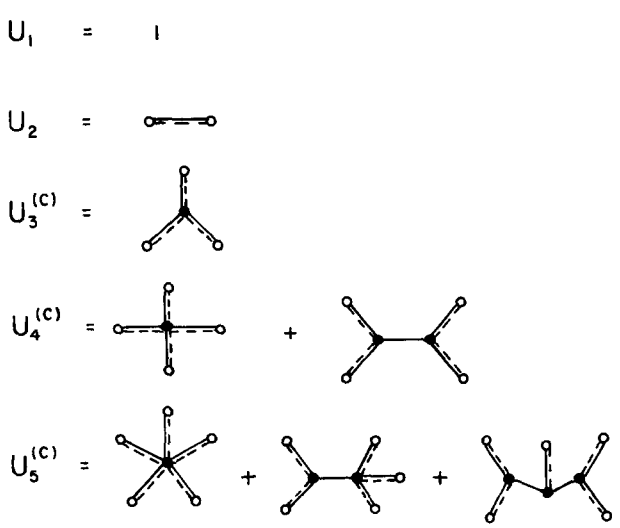

FIG. 5. Diagrammatic representations of $U_n^{(c)}$ for $n = 1, 2, 3, 4, 5$. The double lines have weights $S(k_i)$ while the single lines have weights $u(k)$ (see text).

only the topologically distinct graphs are shown. Again rules 2–6 must be used in Eq. (34) with the following addition to rule 5:

> For each double terminal line with a label k write a factor $S(k)$.

Explicitly, Eq. (34) reads

$$U_2(\mathbf{k}_1,\mathbf{k}_2) = N\delta_{1+2}S_1,$$

$$U_n^{(c)}(\mathbf{k}_1,\cdots,\mathbf{k}_n) = N\delta_{1+2+\cdots+n}S_1\cdots S_n(1+A_n), \quad n\geq 3 \tag{34'}$$

with[13]

$$A_3 = 0,$$

$$A_4 = u_{1+2}+u_{1+3}+u_{1+4}, \tag{34''}$$

$$A_5 = \sum_{1\leq i<j\leq 5} u_{i+j} + \sum_{1\leq i<j<k\leq 5} u_{i+j}u_{i+j+k}.$$

A_4 and A_5 can be read off from Fig. 5. In general, A_n is some linear combination of products of the u's and can be represented by the diagrams in (34) with the terminal lines stripped. We note the factor $S_1\cdots S_n$ in $U_n^{(c)}$ for $n\geq 3$. Since in a liquid $S(k)\propto k$ for small k,[1,14] we arrive at Eq. (27), the result quoted earlier.

IV. ORTHONORMAL BASIS

One possible application of our result is the construction of orthonormal bases in the quantum theory of liquid He^4. Jackson and Feenberg[5] first considered this problem in the paired phonon space. We now briefly outline their result (with somewhat simplified analysis) and indicate the direction of possible extensions.

Consider the normalized ± k phonon states

$$\psi_{l+s,l} = C_{ls}\,\psi_o\rho_k^{l+s}\rho_{-k}^{l}, \quad \text{for fixed integral } s, \tag{35}$$

where ψ_o is the ground state wavefunction and the normalization constant $C_{ls} = [NS(k)]^{-(l+2s)/2}\times$ $[(l+2s)!]^{-1/2}$ can be determined from Eq. (23). We wish to construct the orthonormal set $|p\rangle$ defined by the linear transformation

$$|p\rangle = \sum_{l=0}^{p} a_{pl}\psi_{l+s,l}, \tag{36}$$

where for brevity the dependences of $|p\rangle$ on s and a_{pl} have been deleted.

A convenient set of equations to work with is[5]

$$a_{pp}\langle p|\psi_{h+s,h}\rangle = \delta_{hp}, \quad h\leq p. \tag{37}$$

Via Eq. (35) for $\psi_{h+s,h}$, Eq. (37) becomes

$$\sum_{l=0}^{p} a_{pp}a_{pl}\frac{(l+h+s)!}{[(2l+s)!\,(2h+s)!]^{1/2}} = \delta_{hp}, \quad h\leq p. \tag{38}$$

To solve Eq. (38), we define

$$a_{pp}a_{pl} = \frac{[(2l+s)!\,(2p+s)!]^{1/2}}{(l+s)!\,p!}\,\alpha_l \tag{39}$$

and multiply Eq. (38) by the factor $[(2h+s)!]^{1/2}/h!$. The result is the equation

$$\sum_{l=0}^{p}\binom{l+h+s}{h}\alpha_l = \delta_{hp}, \quad h\leq p. \tag{40}$$

Comparing Eq. (40) with the identity[15]

$$\sum_{l=0}^{p}(-1)^{l+p}\binom{p}{l}\binom{l+h+s}{h} = \delta_{ph}, \quad h\leq p, \tag{41}$$

we find

$$\alpha_l = (-1)^{l+p}\binom{p}{l}; \tag{42}$$

hence

$$a_{pl} = (-1)^{l+p}\left[\binom{p}{l}\binom{2l+s}{l}\binom{p+s}{l+s}\right]^{1/2}. \tag{43}$$

This completes the construction of the orthonormal set $|p\rangle$ in the paired phonon space.

One direction of possible extensions is to construct an orthonormal basis using the n-phonon states

$$\psi_m^{(n)} = C_m\psi_o(\rho_{\mathbf{k}_1}\cdots\rho_{\mathbf{k}_n})^m, \quad m = 0,1,2,\cdots, \tag{44}$$

where $\mathbf{k}_1+\cdots+\mathbf{k}_n = 0$. One can indeed carry out a similar analysis for finding the orthonormal basis

$$|p\rangle = \sum_{l=0}^{p} a_{pl}\psi_l^{(n)}. \tag{45}$$

The resulting equation to solve turns out to be

$$\sum_{l=0}^{p}\binom{h+l}{h}^{n-1}\alpha_l = \delta_{hp}, \quad h\leq p, \tag{46}$$

where

$$\alpha_l = \left[\binom{2l}{l}\binom{2p}{p}\right]^{-(n-1)/2}a_{pp}a_{pl}.$$

Unfortunately, we have been unable to find the solution of this equation for $n\geq 3$. However, since our result shows that the two and higher phonon states are essentially independent in computing the matrix elements, it would be possible to include only a few $\psi_m^{(c)}$ for small values of m and n. This would then constitute an extension of the case $n=3$ and $m=0,1$ considered by Davison and Feenberg.[16]

ACKNOWLEDGMENT

I wish to thank Professor E. Feenberg for suggesting this investigation.

* Work supported by National Science Foundation Grant Nos. GP-9041 and GP-25306.
† Some results of this paper have been reported in Phys. Letters **34A**, 446 (1971).

1 E. Feenberg, *Theory of Quantum Fluids* (Academic, New York, 1969).
2 J. G. Kirkwood, J. Chem. Phys. **3**, 300 (1935).
3 H. W. Jackson and E. Feenberg, Rev. Mod. Phys. **34**, 686 (1962).
4 F. Y. Wu and M. K. Chien, J. Math. Phys. **11**, 1912 (1970).
5 H. W. Jackson and E. Feenberg, Ann. Phys. (N.Y.) **15**, 266 (1961).
6 D. K. Lee, Phys. Rev. **162**, 134 (1967).
7 C. E. Campbell and E. Feenberg, Phys. Rev. **188**, 396 (1969).
8 H. W. Lai, H. K. Sim, and C. W. Woo, Phys. Rev. A **1**, 1536 (1970).
9 E. Feenberg, Phys. Rev. A **2**, 2158 (1970).
10 See, for example, J. de Boer, Rept. Progr. Phys. **12**, 329 (1948).
11 See Sec. 3. 4 of Ref. 1 or E. Feenberg, Am. J. Phys. **38**, 684 (1970).
12 We follow, whenever possible, the definitions of J. W. Essam and M. E. Fisher, Rev. Mod. Phys. **42**, 271 (1970).
13 A_4 was first obtained by Lee in Ref. 6.
14 D. Pines and P. Nozières, *The Theory of Quantum Fluids* (Benjamin, New York, 1966), Chap. 2.
15 The identity (41) can be derived by evaluating at $x = 1$ the hth derivative of the identity

$$(x-1)^p x^{s+h} = \sum_{l=0}^{p} (-1)^{l+p} \binom{p}{l} x^{l+s+h}$$

[see J. Riordan, *Combinatorial Identities* (Wiley, New York, 1968), p. 11]. We also remark that Eq. (41) is a generalization of one of the two binomial coefficient identities obtained by D. M. Rosenbaum, J. Math. Phys. **8**, 1973 (1967), and H. W. Gould, J. Math. Phys. **10**, 49 (1969). Their identity *(B)* corresponds to taking $h = p - 1$ in Eq. (41).
16 T. B. Davison and E. Feenberg, Ann. Phys. (N.Y.) **53**, 559 (1969).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Trapped Surfaces and the Development of Singularities*

David Walter Pajerski
California State College, California, Pennsylvania
and
Ezra T. Newman
University of Pittsburgh, Pittsburgh, Pennsylvania

(Received 22 October 1970; Revised Manuscript Received 19 November 1970)

The study of singularities in general relativity was given a strong impetus by a topological approach due to Penrose and others, and powerful theorems concerning their existence have been developed. In particular a theorem by Penrose states that under certain conditions the existence of a trapped surface in a space-time guarantees that singularities will develop. Using the spin coefficient formalism we generalize from the Schwarzschild solution and prove the existence of a wide class of solutions possessing such trapped surfaces by displaying the solutions to terms linear in a certain null coordinate. Then, using an asymptotic procedure, the method is generalized to include a class of solutions possessing "asymptotically trapped surfaces."

1. INTRODUCTION

In 1965 Penrose presented a remarkable theorem on the existence space-time singularities which must follow from the existence of a trapped surface (a trapped surface being a compact spacelike 2-surface such that both sets of null rays orthogonal to the surface have negative divergence at every point of the surface).[1] From this theorem great interest in trapped surfaces has developed. The theorem requires the existence of a global Cauchy hypersurface (GCH). A GCH in a space-time M is a three-dimensional submanifold S in M such that any timelike curve in M without endpoint has one and only one point in common with S. The notion of a GCH is related to the Laplacian idea of determinism (that the entire future of the universe can be completely determined by knowing the positions and velocities of all particles in the universe at one time, i.e., on one three-dimensional spacelike submanifold) by the fact that the Laplacian idea of determinism requires the existence of a GCH. That is, if a GCH does not exist in M, then for any three-dimensional spacelike submanifold I that we choose as our "initial" hypersurface ("present" state of the universe) we will be able to find an event A to the future of I through which there pass nonspacelike, i.e., either timelike or null, curves which have no event in common with I. In this situation we see that, loosely speaking, such nonspacelike curves can transmit information to A without that information having ever registered on I. Thus, in order to maintain the "classical" notion of determinism we must assume the existence of a GCH. The conclusions in Secs. 4 and 5 assume the existence of a GCH in the space-times discussed.

Previous to the Penrose theorem it was believed by many (for example, see Lifshitz and Khalatnikov[2]) that the necessary collapse to a singularity of spherically symmetric matter within the Schwarzschild radius was simply due to the high symmetry involved. The Penrose theorem, with its lack of symmetry assumptions, denies this simple explanation and, in the consideration of space-time singularities, shifts attention away from the symmetry properties of the situation, focusing instead on the existence of trapped surfaces for $r < 2M$. The Penrose theorem says that this, rather than the symmetry, is the crucial factor guaranteeing the eventual singularity at $r = 0$ for collapsing matter. The Schwarzschild solution presents us with a situation from which to generalize and thereby show the existence of a general class of solutions exhibiting such trapped surfaces and the attendant singularities.

* Work supported by National Science Foundation Grant Nos. GP-9041 and GP-25306.
† Some results of this paper have been reported in Phys. Letters **34A**, 446 (1971).

1 E. Feenberg, *Theory of Quantum Fluids* (Academic, New York, 1969).
2 J. G. Kirkwood, J. Chem. Phys. **3**, 300 (1935).
3 H. W. Jackson and E. Feenberg, Rev. Mod. Phys. **34**, 686 (1962).
4 F. Y. Wu and M. K. Chien, J. Math. Phys. **11**, 1912 (1970).
5 H. W. Jackson and E. Feenberg, Ann. Phys. (N.Y.) **15**, 266 (1961).
6 D. K. Lee, Phys. Rev. **162**, 134 (1967).
7 C. E. Campbell and E. Feenberg, Phys. Rev. **188**, 396 (1969).
8 H. W. Lai, H. K. Sim, and C. W. Woo, Phys. Rev. A **1**, 1536 (1970).
9 E. Feenberg, Phys. Rev. A **2**, 2158 (1970).
10 See, for example, J. de Boer, Rept. Progr. Phys. **12**, 329 (1948).
11 See Sec. 3. 4 of Ref. 1 or E. Feenberg, Am. J. Phys. **38**, 684 (1970).
12 We follow, whenever possible, the definitions of J. W. Essam and M. E. Fisher, Rev. Mod. Phys. **42**, 271 (1970).
13 A_4 was first obtained by Lee in Ref. 6.
14 D. Pines and P. Nozières, *The Theory of Quantum Fluids* (Benjamin, New York, 1966), Chap. 2.
15 The identity (41) can be derived by evaluating at $x = 1$ the hth derivative of the identity

$$(x-1)^p x^{s+h} = \sum_{l=0}^{p} (-1)^{l+p} \binom{p}{l} x^{l+s+h}$$

[see J. Riordan, *Combinatorial Identities* (Wiley, New York, 1968), p. 11]. We also remark that Eq. (41) is a generalization of one of the two binomial coefficient identities obtained by D. M. Rosenbaum, J. Math. Phys. **8**, 1973 (1967), and H. W. Gould, J. Math. Phys. **10**, 49 (1969). Their identity *(B)* corresponds to taking $h = p - 1$ in Eq. (41).
16 T. B. Davison and E. Feenberg, Ann. Phys. (N.Y.) **53**, 559 (1969).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Trapped Surfaces and the Development of Singularities*

David Walter Pajerski
California State College, California, Pennsylvania
and
Ezra T. Newman
University of Pittsburgh, Pittsburgh, Pennsylvania

(Received 22 October 1970; Revised Manuscript Received 19 November 1970)

The study of singularities in general relativity was given a strong impetus by a topological approach due to Penrose and others, and powerful theorems concerning their existence have been developed. In particular a theorem by Penrose states that under certain conditions the existence of a trapped surface in a space-time guarantees that singularities will develop. Using the spin coefficient formalism we generalize from the Schwarzschild solution and prove the existence of a wide class of solutions possessing such trapped surfaces by displaying the solutions to terms linear in a certain null coordinate. Then, using an asymptotic procedure, the method is generalized to include a class of solutions possessing "asymptotically trapped surfaces."

1. INTRODUCTION

In 1965 Penrose presented a remarkable theorem on the existence space-time singularities which must follow from the existence of a trapped surface (a trapped surface being a compact spacelike 2-surface such that both sets of null rays orthogonal to the surface have negative divergence at every point of the surface).[1] From this theorem great interest in trapped surfaces has developed. The theorem requires the existence of a global Cauchy hypersurface (GCH). A GCH in a space-time M is a three-dimensional submanifold S in M such that any timelike curve in M without endpoint has one and only one point in common with S. The notion of a GCH is related to the Laplacian idea of determinism (that the entire future of the universe can be completely determined by knowing the positions and velocities of all particles in the universe at one time, i.e., on one three-dimensional spacelike submanifold) by the fact that the Laplacian idea of determinism requires the existence of a GCH. That is, if a GCH does not exist in M, then for any three-dimensional spacelike submanifold I that we choose as our "initial" hypersurface ("present" state of the universe) we will be able to find an event A to the future of I through which there pass nonspacelike, i.e., either timelike or null, curves which have no event in common with I. In this situation we see that, loosely speaking, such nonspacelike curves can transmit information to A without that information having ever registered on I. Thus, in order to maintain the "classical" notion of determinism we must assume the existence of a GCH. The conclusions in Secs. 4 and 5 assume the existence of a GCH in the space-times discussed.

Previous to the Penrose theorem it was believed by many (for example, see Lifshitz and Khalatnikov[2]) that the necessary collapse to a singularity of spherically symmetric matter within the Schwarzschild radius was simply due to the high symmetry involved. The Penrose theorem, with its lack of symmetry assumptions, denies this simple explanation and, in the consideration of space-time singularities, shifts attention away from the symmetry properties of the situation, focusing instead on the existence of trapped surfaces for $r < 2M$. The Penrose theorem says that this, rather than the symmetry, is the crucial factor guaranteeing the eventual singularity at $r = 0$ for collapsing matter. The Schwarzschild solution presents us with a situation from which to generalize and thereby show the existence of a general class of solutions exhibiting such trapped surfaces and the attendant singularities.

We proceed by discussing and exhibiting a new coordinate system for the Schwarzschild solution which is particularly well suited for describing the trapped surfaces and for the generalization of the Schwarzschild solution. (This new coordinate system for the Schwarzschild line element not only covers the entire Kruskal manifold, but yields for the metric explicit functions of the coordinates, in contrast to the Kruskal form which uses implicit functions.)

We next show, by means of the spin-coefficient formalism, how characteristic initial data can be given, such that a wide class of solutions show the development of a trapped surface. The solutions are determined to linear terms in a variable u, which labels null hyper surfaces. The behavior of two spin coefficients in the neighborhood of the surface $u = 0$ then enables us to accept the existence of trapped surfaces in this neighborhood. In general these solutions possess a radiation field and deviate significantly from spherical symmetry. For special data the Schwarzschild solution can be recovered. Finally, in conclusion, we show how these solutions can be further generalized by suitably relaxing conditions on the $u = 0$ hypersurface and obtaining asymptotic solutions which possess the trapped surface property.

2. SCHWARZSCHILD LINE ELEMENT

The Schwarzschild metric in retarded Eddington–Finkelstein coordinates is given by

$$d_c{}^2 = (1 - 2m/r)du^2 + 2dudr - r^2(d\theta^2 + \sin^2\theta d\phi^2), \tag{2.1}$$

and in advanced coordinates by

$$d_a{}^2 = (1 - 2m/r)dv^2 - 2dvdr - r^2(d\theta^2 + \sin^2\theta d\phi^2). \tag{2.2}$$

In the Kruskal diagram, Fig. 1, metric (2.1) applies in the region AC, while metric (2.2) applies in AB.

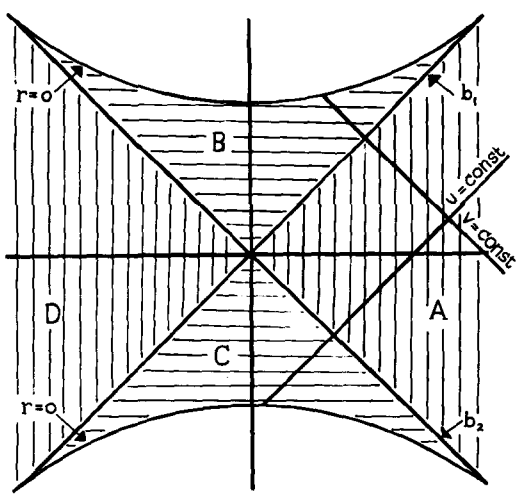

FIG 1. Kruskal diagram.

There is no reason why retarded coordinates cannot be introduced in the AB region, though it is usually reserved for advanced coordinates. Denoting the new retarded light cones by $\bar{u}$ and the affine distance on each cone by s, we see that the coordinate transformation

$$\begin{aligned} \bar{u} &= 8m^2(1 - r/2m)e^{r/2m - v/4m}, \\ s &= e^{v/4m - r/2m}, \\ \theta' &= \theta, \\ \phi' &= \phi, \end{aligned} \tag{2.3}$$

with inverse

$$\begin{aligned} r &= 2m - \bar{u}s/4m, \\ v &= 4m \log s + 4m - \bar{u}s/2m, \\ \theta &= \theta', \\ \phi &= \phi', \end{aligned}$$

takes metric (2.2) into the form[3,4]

$$d_a{}^2 = \left(\frac{-2s^2}{8m^2 - \bar{u}s}\right)d\bar{u}^2 + 2d\bar{u}ds - \left(2m - \frac{\bar{u}s}{4m}\right)^2 \times (d\theta^2 + \sin^2\theta d\phi^2). \tag{2.4}$$

In Fig. 1, b_1 and b_2, the Schwarzschild radius, are given, respectively, by $\bar{u} = 0$ and $s = 0$. The two singular lines $r = 0$ are given by $8m^2 - \bar{u}s = 0$. It is interesting to note that this coordinate system covers the entire Kruskal region $ABCD$, with the following values:

$$\begin{aligned} A &\longleftrightarrow \bar{u} < 0, s > 0, \\ B &\longleftrightarrow \bar{u} > 0, s > 0, \\ C &\longleftrightarrow \bar{u} < 0, s < 0, \\ D &\longleftrightarrow \bar{u} > 0, s < 0. \end{aligned}$$

In the remainder of the paper we shall be concerned with the neighborhood of the surface $\bar{u} = 0$ and the analogous region for more general metrics.

3. THE FORMALISM

We are interested in the solution of a characteristic initial value problem of the empty-space Einstein field equations. The spin-coefficient formalism provides a convenient method for approaching this problem. For complete details of this formalism the reader is referred to Newman and Penrose.[5] We give a summary of the formalism sufficient for our purposes here.

In a four-dimensional Riemannian space of signature -2, a set of vectors $(\mathbf{l}, \mathbf{n}, \mathbf{m}, \bar{\mathbf{m}})$ is chosen, where $\mathbf{l}$ and $\mathbf{n}$ are null and $\mathbf{m}$ is formed from unit spacelike vectors $\mathbf{a}$ and $\mathbf{b}$ by

$$\mathbf{m} = \tfrac{1}{2}\sqrt{2}\,(\mathbf{a} - i\mathbf{b}),$$

with the following orthonormality conditions:[6]

$$\begin{aligned} &l_\mu n^\mu = m_\mu \bar{m}^\mu = 1, \\ &l_\mu l^\mu = n_\mu n^\mu = m_\mu m^\mu = \bar{m}_\mu \bar{m}^\mu = 0, \\ &l_\mu m^\mu = l_\mu \bar{m}^\mu = n_\mu m^\mu = n_\mu \bar{m}^\mu = 0. \end{aligned} \tag{3.1}$$

A set of equations equivalent to the empty-space field equations can be written in terms of the tetrad vectors, the tetrad components of the Weyl tensor $C_{\mu\nu\rho\sigma}$ defined as

$$\begin{aligned} \psi_0 &\equiv -C_{\alpha\beta\gamma\delta} l^\alpha m^\beta l^\gamma m^\delta, \\ \psi_1 &\equiv -C_{\alpha\beta\gamma\delta} l^\alpha n^\beta l^\gamma m^\delta, \\ \psi_2 &\equiv -C_{\alpha\beta\gamma\delta} \bar{m}^\alpha n^\beta l^\gamma m^\delta, \\ \psi_3 &\equiv -C_{\alpha\beta\gamma\delta} \bar{m}^\alpha n^\beta l^\gamma n^\delta, \\ \psi_4 &\equiv -C_{\alpha\beta\gamma\delta} \bar{m}^\alpha n^\beta \bar{m}^\gamma n^\delta, \end{aligned} \tag{3.2}$$

and the spin coefficients defined as follows:[7]

$$\begin{aligned} \kappa &\equiv l_{\mu;\nu} m^\mu l^\nu, & \pi &\equiv -n_{\mu;\nu} \bar{m}^\mu l^\nu, \\ \rho &\equiv l_{\mu;\nu} m^\mu \bar{m}^\nu, & \mu &\equiv -n_{\mu;\nu} \bar{m}^\mu m^\nu, \\ \lambda &\equiv -n_{\mu;\nu} \bar{m}^\mu \bar{m}^\nu, & \nu &\equiv -n_{\mu;\nu} \bar{m}^\mu n^\nu, \\ \sigma &\equiv l_{\mu;\nu} m^\mu m^\nu, & \tau &\equiv l_{\mu;\nu} m^\mu n^\nu, \\ \beta &\equiv \tfrac{1}{2}(l_{\mu;\nu} n^\mu m^\nu - m_{\mu;\nu} \bar{m}^\mu \bar{m}^\nu), \\ \gamma &\equiv \tfrac{1}{2}(l_{\mu;\nu} n^\mu n^\nu - m_{\mu;\nu} \bar{m}^\mu n^\nu), \\ \epsilon &\equiv \tfrac{1}{2}(l_{\mu;\nu} n^\mu l^\nu - m_{\mu;\nu} \bar{m}^\mu l^\nu), \\ \alpha &\equiv \tfrac{1}{2}(l_{\mu;\nu} n^\mu \bar{m}^\nu - m_{\mu;\nu} \bar{m}^\mu \bar{m}^\nu). \end{aligned} \tag{3.3}$$

Before displaying this set of equations, a somewhat specialized coordinate and tetrad system will be introduced. One of the coordinates $x^0 = u$ will label a family of null hypersurfaces, and the vector **l** will be chosen to be tangent to the family of null geodesics lying in the hypersurfaces $u =$ const. Another coordinate $x^1 = s$ is chosen as an affine parameter along these null geodesics. The coordinates (x^2, x^3) are chosen to label the null geodesics on each surface $u =$ const. The tetrad vectors **n** and **m** are required to be parallelly propagated along **l**. In this manner, some of the coordinate and tetrad freedom is eliminated.

With the above coordinate system, the metric tensor takes the form

$$g^{\mu\nu} = l^\mu n^\nu + n^\mu l^\nu - m^\mu \bar{m}^\nu - \bar{m}^\mu m^\nu$$

$$= \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & g^{11} & g^{12} & g^{13} \\ 0 & g^{12} & & \\ & & & g^{ij} \\ 0 & g^{13} & & \end{bmatrix} \tag{3.4}$$

and tetrad vectors become

$$\begin{aligned} l^\mu &= \delta^\mu_1, \; l_\mu = \delta^0_\mu, \\ m^\mu &= \omega \delta^\mu_1 + \xi^k \delta^\mu_k, \\ n^\mu &= \delta^\mu_0 + U\delta^\mu_1 + X^k \delta^\mu_k. \end{aligned} \tag{3.5}$$

The metric can be expressed in terms of the tetrad components ω, ξ^k, U, and X^k as

$$\begin{aligned} g^{11} &= 2(U - \omega\bar{\omega}), \\ g^{1k} &= X^k - (\xi^k \bar{\omega} + \bar{\xi}^k \omega), \\ g^{ij} &= -(\xi^i \bar{\xi}^j + \bar{\xi}^i \xi^j). \end{aligned} \tag{3.6}$$

We also have

$$\kappa = \pi = \epsilon = 0, \quad \rho = \bar{\rho}, \quad \tau = \bar{\alpha} + \beta. \tag{3.7}$$

A set of equations equivalent to the empty-space field equations can now be written as follows:

$$D\xi^i = \rho\xi^i + \sigma\bar{\xi}^i, \tag{3.8a}$$

$$D\omega = \rho\omega + \sigma\bar{\omega} - (\bar{\alpha} + \beta), \tag{3.8b}$$

$$DX^i = (\bar{\alpha} + \beta)\bar{\xi}^i + (\alpha + \bar{\beta})\xi^i, \tag{3.8c}$$

$$DU = (\bar{\alpha} + \beta)\bar{\omega} + (\alpha + \bar{\beta})\omega - (\gamma + \bar{\gamma}), \tag{3.8d}$$

$$D\rho = \rho^2 + \sigma\bar{\sigma}, \tag{3.8e}$$

$$D\sigma = 2\rho\sigma + \psi_0, \tag{3.8f}$$

$$D\tau = \tau\rho + \bar{\tau}\sigma + \psi_1, \tag{3.8g}$$

$$D\alpha = \alpha\rho + \beta\bar{\sigma}, \tag{3.8h}$$

$$D\beta = \beta\rho + \alpha\sigma + \psi_1, \tag{3.8i}$$

$$D\gamma = \tau\alpha + \bar{\tau}\beta + \psi_2, \tag{3.8j}$$

$$D\lambda = \lambda\rho + \mu\bar{\sigma}, \tag{3.8k}$$

$$D\mu = \mu\rho + \lambda\sigma + \psi_2, \tag{3.8l}$$

$$D\nu = \tau\lambda + \bar{\tau}\mu + \psi_3, \tag{3.8m}$$

$$\delta X^i - \Delta\xi^i = (\mu + \bar{\gamma} - \gamma)\xi^i + \bar{\lambda}\bar{\xi}^i, \tag{3.9a}$$

$$\delta\bar{\xi}^i - \bar{\delta}\xi^i = (\bar{\beta} - \alpha)\xi^i + (\bar{\alpha} - \beta)\bar{\xi}^i, \tag{3.9b}$$

$$\delta\bar{\omega} - \bar{\delta}\omega = (\bar{\beta} - \alpha)\omega + (\bar{\alpha} - \beta)\bar{\omega} + (\mu - \bar{\mu}), \tag{3.9c}$$

$$\delta U - \Delta\omega = (\mu + \bar{\gamma} - \gamma)\omega + \bar{\lambda}\bar{\omega} - \bar{\nu}, \tag{3.9d}$$

$$\Delta\lambda - \bar{\delta}\nu = 2\alpha\nu + (\bar{\gamma} - 3\gamma - \mu - \bar{\mu})\lambda - \psi_4, \tag{3.9e}$$

$$\delta\rho - \bar{\delta}\sigma = (\beta + \bar{\alpha})\rho + (\bar{\beta} - 3\alpha)\sigma - \psi_1, \tag{3.9f}$$

$$\delta\alpha - \bar{\delta}\beta = \mu\rho - \lambda\sigma - 2\alpha\beta + \alpha\bar{\alpha} + \beta\bar{\beta} - \psi_2, \tag{3.9g}$$

$$\delta\lambda - \bar{\delta}\mu = (\alpha + \bar{\beta})\mu + (\bar{\alpha} - 3\beta)\lambda - \psi_3, \tag{3.9h}$$

$$\delta\nu - \Delta\mu = \gamma\mu - 2\nu\beta + \bar{\gamma}\mu + \mu^2 + \lambda\bar{\lambda}, \tag{3.9i}$$

$$\delta\gamma - \Delta\beta = \tau\mu - \sigma\nu + (\mu - \gamma + \bar{\gamma})\beta + \bar{\lambda}\alpha, \tag{3.9j}$$

$$\delta\tau - \Delta\sigma = 2\tau\beta + (\bar{\gamma} + \mu - 3\gamma)\sigma + \bar{\lambda}\rho, \tag{3.9k}$$

$$\Delta\rho - \bar{\delta}\tau = (\gamma + \bar{\gamma} - \bar{\mu})\rho - 2\alpha\tau - \lambda\sigma - \psi_2, \tag{3.9l}$$

$$\Delta\alpha - \bar{\delta}\gamma = \rho\nu - \tau\lambda - \lambda\beta + (\bar{\gamma} - \gamma - \bar{\mu})\alpha - \psi_3, \tag{3.9m}$$

where

$$\delta \equiv \omega \frac{\partial}{\partial s} + \xi^k \frac{\partial}{\partial x^k},$$
$$\Delta \equiv U \frac{\partial}{\partial s} + \frac{\partial}{\partial u} + X^k \frac{\partial}{\partial x^k}, D \equiv \frac{\partial}{\partial s}. \quad (3.10)$$

We will also have need of the Bianchi identities written in this formalism:

$$D\psi_1 - \bar{\delta}\psi_0 = 4\rho\psi_1 - 4\alpha\psi_0, \quad (3.11a)$$
$$D\psi_2 - \bar{\delta}\psi_1 = 3\rho\psi_2 - 2\alpha\psi_1 - \lambda\psi_0, \quad (3.11b)$$
$$D\psi_3 - \bar{\delta}\psi_2 = 2\rho\psi_3 - 2\lambda\psi_1, \quad (3.11c)$$
$$D\psi_4 - \bar{\delta}\psi_3 = \rho\psi_4 + 2\alpha\psi_3 - 3\lambda\psi_2, \quad (3.11d)$$
$$\Delta\psi_0 - \delta\psi_1 = (4\gamma - \mu)\psi_0 - (4\tau + 2\beta)\psi_1 + 3\sigma\psi_2, \quad (3.12a)$$
$$\Delta\psi_1 - \delta\psi_2 = \nu\psi_0 + (2\gamma - 2\mu)\psi_1 - 3\tau\psi_2 + 2\sigma\psi_3, \quad (3.12b)$$
$$\Delta\psi_2 - \delta\psi_3 = 2\nu\psi_1 - 3\mu\psi_2 + (-2\tau + 2\beta)\psi_3 + \sigma\psi_4, \quad (3.12c)$$
$$\Delta\psi_3 - \delta\psi_4 = 3\nu\psi_2 - (2\gamma + 4\mu)\psi_3 + (4\beta - \tau)\psi_4. \quad (3.12d)$$

Equations (3.8) and (3.11) are termed the radial equations. The equations containing Δ determine the u behavior of the solution. (The u here and in all that follows is to be considered as the same type of coordinate as the $\bar{u}$ in the previous section.)

The spin coefficients μ and ρ provide a convenient characterization of trapped surfaces. Given a spacelike two-dimensional surface, S, lying in a u = const null surface and whose tangent space (at any point) is spanned by $\mathbf{m}$ and $\bar{\mathbf{m}}$, the vector fields $\mathbf{l}$ and $\mathbf{n}$ are the two null vector fields orthogonal to the surface. Thus if both $\mathbf{l}$ and $\mathbf{n}$ have negative divergence at all points on S and if S is compact, then S is a trapped surface. With the above choice of coordinate system and tetrad we have

$$\rho = -\tfrac{1}{2}\,\mathrm{divl}, \quad (3.13a)$$

and[8]

$$\mu + \bar{\mu} = \mathrm{divn}. \quad (3.13b)$$

Thus S is a trapped surface if it is compact with $\rho > 0$ and $\mu + \bar{\mu} < 0$ everywhere on S.

4. THE GENERALIZATION OF THE SCHWARZSCHILD SOLUTION

The $(\bar{u}, s, \theta, \phi)$ coordinate system used in the expression of the Schwarzschild metric of Eq.(2.4) is a coordinate system suitable for use in the spin-coefficient formalism. That is, $\bar{u}$ is a coordinate labeling null hypersurfaces, s is an affine parameter along null geodesics in each surface $\bar{u}$ = const, and (θ, ϕ) label these null geodesics. The metric variables, Weyl tensor components, and spin coefficients of the Schwarzschild solution when expressed in this coordinate system become (here we drop the bar over the u):

$$\lambda = \sigma = \nu = \kappa = \tau = \pi = \epsilon = 0,$$
$$\mu = \frac{-8m^2 s}{(8m^2 - us)^2}, \quad \rho = \frac{-u}{us - 8m^2},$$
$$\gamma = -s\left(4 - \frac{us}{4m^2}\right) \cdot \frac{1}{8(2m - us/4m)^2},$$
$$\alpha = -\frac{\sqrt{2}}{4} \frac{\cot\theta}{(2m - us/4m)} e^{-i\phi},$$
$$\beta = \frac{\sqrt{2}}{4} \frac{\cot\theta}{(2m - us/4m)} e^{i\phi},$$
$$U = \frac{s^2}{8m^2 - us}, \quad \xi^2 = \frac{\sqrt{2}}{2(2m - us/4m)}, \quad (4.1)$$
$$\xi^3 = \frac{\sqrt{2}i}{2\sin\theta(2m - us/4m)}, \quad X^k = \omega = 0,$$
$$\psi_2 = \frac{-m}{(2m - us/4m)^3}, \quad \psi_0 = \psi_1 = \psi_3 = \psi_4 = 0.$$

As was mentioned in Sec. 2, we shall be concerned with the properties of the solution in the vicinity of the null surface, $u = 0$, and hence we consider the expansion of the metric and other pertinent variables around $u = 0$. In particular we have[9]

$$\rho = \frac{1}{8m^2} u + O'(u^2) \quad (4.2)$$

and

$$\mu = \frac{-s}{8m^2} - \frac{1}{32} \frac{s^2 u}{m^4} + O'(u^3). \quad (4.3)$$

The two-dimensional surfaces S, defined by (u = const, s = const, $s > 0$) change their character as we cross the $u = 0$ surface. On the positive side of $u = 0$, we have $\rho > 0$ and $\mu < 0$. Therefore, here S is a trapped surface. On the other hand, to the negative side of $u = 0$ we have $\rho < 0$ and $\mu < 0$, and here S is not a trapped surface.

This is the situation to be generalized. We shall solve the spin-coefficient form of the field equations in the neighborhood of the $u = 0$ null surface, subject to the condition that $\rho = 0$ at $u = 0$. This solution is expressible in terms of several arbitrary functions (data), whose specification completely determines a particular solution. From this solution, by a certain choice of one of the functions, we prove the existence of a large class of solutions exhibiting trapped surfaces. The method of solution is as follows. Equations (3.8) and (3.11) are integrated subject to $\rho = 0$, and thus the s behavior of all the spin coefficients and field variables is obtained on the initial surface $u = 0$. Each integration introduces a "constant of integration" [actually a function of (x^2, x^3)]. Some of these constants of integration are eliminated by judicious use of the

coordinate and tetrad freedom.[10] The nonradial equations without Δ then yield relations among the remaining constants of integration. Finally the Δ derivative equations give the u behavior, allowing us to propagate the solution off the $u = 0$ surface.

Also, in obtaining the solution we present, one other assumption is made, whose complete meaning is not clear, but which appears to be necessary in order to obtain the class of solutions we wish to discuss. It should be made clear that this assumption is in the form of both a restriction on solutions and a coordinate condition, i.e., some violations of this assumption can be obtained by a coordinate transformation, but the most general violations cannot be so obtained (see Ref. 10). The assumption is that the constant of integration associated with τ, namely, $\tau(0, 0, x^i)$, is zero. From this restriction and using up all coordinate and tetrad freedom to eliminate most arbitrary functions, the procedure outlined above leads to the solution presented in Eq. (4.4). The solution is written with the help of differential operators, $\eth$ and $\bar{\eth}$,[11] defined by

$$\eth\eta \equiv - P^{1-q}\,\nabla(P^q\eta),$$
$$\bar{\eth}\eta \equiv - P^{1+q}\,\bar{\nabla}(P^{-q}\eta),$$

where η is a quantity of spin weight q with ∇ given by $\nabla \equiv \partial/\partial x^2 + i\partial/\partial x^3$, and P is a real-valued function of (x^2, x^3) related to the Gaussian curvature on the two-surfaces $u = 0$, $s = \text{const}$ [see Eq. (4.6)].[12]

In order to use these definitions in Eqs. (4.4), we assign spin weights 2, 0, 0, and -2 respectively to the quantities $\bar{\lambda}^0, \psi_2^0, \log P$, and λ^0.

The covariant form of the metric, accurate to first order in u, is now given by

$$g_{00} = 2\psi_2^0 s^2 - \{[2\psi_2^0\psi_2^0 - \tfrac{1}{3}(\bar{\eth}\eth\psi_2^0)]s^3 + [\tfrac{1}{2}(\eth\eth\lambda^0) + \tfrac{1}{2}(\bar{\eth}\bar{\eth}\bar{\lambda}^0)]s^2\}u \tag{4.4a}$$

$$g_{01} = 1, \tag{4.4b}$$

$$g_{11} = g_{12} = g_{13} = 0, \tag{4.4c}$$

$$g_{02} = (-1/P)\{\tfrac{1}{2}[(\eth\psi_2^0) + (\bar{\eth}\psi_2^0)]s^2 + [(\bar{\eth}\bar{\lambda}^0) + (\eth\lambda^0)]s\}u, \tag{4.4d}$$

$$g_{03} = (i/P)\{\tfrac{1}{2}[(\eth\psi_2^0) - (\bar{\eth}\psi_2^0)]s^2 + [(\bar{\eth}\bar{\lambda}^0) - (\eth\lambda^0)]s\}u, \tag{4.4e}$$

$$g_{22} = -1/P^2 - 1/P^2\{2\psi_2^0 s + (\lambda^0 + \bar{\lambda}^0) - (\lambda^0 - \bar{\lambda}^0)^2\}u, \tag{4.4f}$$

$$g_{23} = (i/P^2)(\lambda^0 - \bar{\lambda}^0)u, \tag{4.4g}$$

$$g_{33} = -1/P^2 - 1/P^2\{2\psi_2^0 s - (\lambda^0 + \bar{\lambda}^0) - (\lambda^0 - \bar{\lambda}^0)^2\}u. \tag{4.4h}$$

We also have spin coefficients ρ and μ given by

$$\rho = -\psi_2^0 u \tag{4.5a}$$

$$\mu = \psi_2^0 s + \{-2\psi_2^0\psi_2^0 s^2 - \lambda^0\bar{\lambda}^0 + \tfrac{1}{4}(\eth\bar{\eth}\psi_2^0)s^2 - \tfrac{1}{2}(\eth\eth\lambda^0)s\}u, \tag{4.5b}$$

with

$$\psi_2^0 = -\tfrac{1}{2}(\eth\bar{\eth}\log P), \tag{4.6}$$

where[13] λ^0 is an arbitrary real function of (x^2, x^3).

We point out here and emphasize that, from Eq. (4.6), $(-2\psi_2^0)$ is the Gaussian curvature of the various 2-surfaces S_b defined by

$$S_b \equiv \{(u, s, x^2, x^3) \mid u = 0,\ s = b,\ (x^2, x^3) \text{ in their ranges}\},$$

which are essentially slices of the null surface $u = 0$. In the Schwarzschild solution these 2-surfaces are spheres, i.e., compact with constant positive Gaussian curvature. In the present case we choose the surfaces S_b to be complete surfaces with Gaussian curvature, K, positive and bounded away from zero ($0 < k \leq K$, where k is some positive constant). These are free data that can be arbitrarily specified, and these choices imply that the S_b are compact.

Note that the metric tensor, up to linear terms in u, depends on the function $P(x^i)$, which determines the two-dimensional metric of the above slices, and on the function $\lambda^0(x^i)$, whose physical meaning is obscure, though it might be interpreted in terms of the radiation running parallel to the surface $u = 0$. The Weyl tensor, up to linear u terms, possesses two further functions of x^i: ψ_4^0 and $\dot{\psi}_4^0$ (Ref. 10); it seems reasonable to interpret them as the radiation field parallel to the $u = 0$ surface and the derivative of this radiation field.

The main results of this section can be obtained from a study of ρ and μ [Eqs. (4.5)] and from the fact, mentioned above, that ψ_2^0 is related to the Gaussian curvature K of the S_b by $\psi_2^0 = -\frac{1}{2}K$. Here, since $\omega|_{u=0} = 0$, the S_b are spatial 2-surfaces spanned (at any point) by $\mathbf{m}$ and $\bar{\mathbf{m}}$ [see Eq. (3.5)] and thus -2ρ and 2μ give (essentially) the divergence of the two sets of null rays orthogonal to the S_b (see Sec. 3). It is easy to show that a coordinate transformation of the form

$$u' = u,$$
$$s' = s + f(s, x^2, x^3)u,$$
$$x^{k'} = x^k$$

can be found such that (to terms linear in u) the vectur $\mathbf{m}$ is a linear combination of the natural basis vectors of x'^2 and x'^3. Therefore the surfaces $S'_{\epsilon b}$ defined by

$$S'_{\epsilon b} \equiv \{(u', s' x^{2'}, x^{3'}) \mid u' = \epsilon, s' = b, (x^{2'}, x^{3'}) \text{in their ranges}\}$$

are spatial 2-surfaces spanned by $\mathbf{m}$ and $\bar{\mathbf{m}}$ and hence -2ρ and 2μ give the divergence of the two sets of null rays orthogonal to the $S'_{\epsilon b}$. Also, since the surfaces $S'_{\epsilon b}$ reduce to S_b at $\epsilon = 0$, the compactness of $S'_{\epsilon b}$ follows from continuity. It is clear from Eqs. (4.5) that a suitable choice of one of the $S'_{\epsilon b}$, i.e., a choice of ϵ small enough, implies that ρ is positive and μ negative on this surface. Thus there exist surfaces such that the conditions discussed in Sec. 3 for the existence of trapped surfaces are satisfied. The Penrose theorem becomes applicable and hence singularities must develop in this space (assuming the existence of a GCH, see the Introduction). We comment finally that, with appropriate choice of data, Eqs. (4.4) could of course represent small perturbations of the Schwarzschild solution (which has a GCH), and for these solutions the existence of trapped surfaces follows essentially from the stability of the initial value problem in general relativity.

5. ASYMPTOTICALLY TRAPPED SURFACES

We can generalize the previous result and obtain asymptotic results. That is, we can obtain a class of asymptotic solutions, linearized in u, which exhibit trapped surfaces. In Sec. 4 we required the assumption that ρ be zero on an initial null hypersurface. What we do now is to relax this condition and require instead that on an initial null hypersurface, ρ approaches zero sufficiently fast as a function of the radial coordinate s. Since we will be doing expansions around $u = 0$, the coefficients in the expansions will be functions only of (s, x^2, x^3). We adopt the notation of letting a carat over a function indicate the function evaluated at $u = 0$. In addition a superscript zero on a function indicates that the function is independent of s. In Ref. 5 asymptotic results of the integration of the spin-coefficient form of the field equations are obtained under the assumption that $\psi_0 = O(s^{-5})$ and[14] $D\psi_0 = O(s^{-6})$ along with certain "uniform smoothness conditions" as

$$\begin{aligned} &d_i\psi_0 = O(s^{-5}), \cdots, d_i d_j d_k d_l \psi_0 = O(s^{-5}), \\ &\qquad i,j,k,l = 2,3 \\ &d_i D\psi_0 = O(s^{-6}), \cdots, d_i d_j d_k D\psi_0 = O(s^{-6}), \end{aligned} \tag{5.1}$$

where

$$d_i = \frac{\partial}{\partial x^i}, \qquad i = 2,3\ .$$

We follow this procedure, but with slightly stronger conditions than those above imposed at an initial null hypersurface labeled $u = 0$. These assumptions are

$$\hat{\psi}_0 = \psi_0^0 s^{-5} + O(s^{-6}), \tag{5.2}$$

$$D\hat{\psi}_0 = -5\psi_0^0 s^{-6} + O(s^{-7}) \tag{5.3}$$

and "smoothness conditions"

$$\begin{aligned} &d_i\hat{\psi}_0 = (d_i\psi_0^0)s^{-5} + O(s^{-6}), \cdots, \\ &d_i d_j d_k d_l \psi_0 = (d_i d_j d_k d_l \psi_0^0)s^{-5} + O(s^{-6}), \\ &d_i D\hat{\psi}_0 = -5(d_i\psi_0^0)s^{-6} + O(s^{-7}), \cdots, \\ &d_i d_j d_k D\hat{\psi}_0 = -5(d_i d_j d_k \psi_0^0)s^{-6} + O(s^{-7}). \end{aligned} \tag{5.4}$$

Also, in order to obtain the class of solutions desired, we shall have need of further assumptions. The specific further assumptions will be explicitly written when need for them arises. Here we merely note that they are not without motivation, being straightforward generalizations of conditions that obtain in the Schwarzschild solution of Eq. (2.4) and the solution of Eqs. (4.4). We now deal with the formal problem of obtaining the asymptotic solution.

As in the case $\hat{\rho} = 0$ the first step in obtaining the asymptotic solution is to do the s integrations on the $u = 0$ surface and again each integration introduces a constant of integration, an arbitrary function of (x^2, x^3). We then use up all coordinate and tetrad freedom (to a certain order in u) and make use of the nonradial equations to eliminate most arbitrary functions.[10] The u-derivative equations then allow the propagation of the solution off the $u = 0$ surface, yielding the solution linearized in u. The decisive step in the above procedure is doing the s integrations at $u = 0$. These are asymptotic integrations, and the procedure employed follows rather closely the corresponding procedure in Ref. 5. We indicate briefly this procedure which leads to expressions for ρ and μ. An analysis of their behavior indicates that the trapped surface property of the solution, Eqs. (4.4), of the previous section can be generalized to an asymptotically trapped surface property.

Concerning ourselves with the asymptotic integrations we note that Eqs. (3.8e) and (3.8f) can be written as

$$DZ = Z^2 + Q, \tag{5.5}$$

where

$$Z = \begin{bmatrix} \hat{\rho} & \hat{\sigma} \\ \hat{\sigma} & \hat{\rho} \end{bmatrix}, \qquad Q = \begin{bmatrix} 0 & \hat{\Psi}_0 \\ \hat{\Psi} & 0 \end{bmatrix}. \tag{5.6}$$

In Ref. 3 it is found that if $\hat{\Psi}_0$ is such that $\int s|\hat{\Psi}_0|ds = O(1)$, which is certainly satisfied in the present case, then the solution to Eq. (5.5) is given by

$$Z = -(DY)Y^{-1}, \tag{5.7}$$

where

$$Y = sF + E + O(s^{-2}), \qquad DY = F + O(s^{-3}),$$

with E and F constant matrices. Thus, if F is nonsingular, Z is given by

$$Z = -s^{-1}I + s^{-2}EF^{-1} + O(s^{-3}),$$

and this is the situation considered in Ref. 5.[15] If F is singular, however, the situation is quite different. In fact if $F = 0$ and E is nonsingular, then $Z = O(s^{-3})$. This is the situation we now consider.[16]

Since it is permissible to integrate the order symbols (but not differentiate them), we can substitute the information $Z = O(s^{-3})$ back into Eq. (3.8f), integrate, and obtain

$$\hat{\sigma} = -\tfrac{1}{4}\overset{0}{\psi}_0 s^{-4} + O(s^{-5}), \tag{5.8}$$

with the lack of precision in the specification of $\hat{\psi}_0$ preventing us from obtaining better results. Substituting Eq. (5.8) [and also using the information $Z = O(s^{-3})$] into Eq. (3.8e) and integrating, we obtain

$$\hat{\rho} = (-\overset{0}{\psi}_0\overset{0}{\bar{\psi}}_0/16\cdot 7)s^{-7} + O(s^{-8}), \tag{5.9}$$

and again the initial assumption on $\hat{\psi}_0$ prevents a better estimate.

At this point the following lemma is indispensible (see Ref. 5).

Lemma. Let the complex $(n \times n)$ matrix B and the complex column n vector b be given functions of s, where

$$B = O(s^{-2}), \quad b = O(s^{-2}). \tag{5.10}$$

Let the $(n \times n)$ matrix A be independent of s and have no eigenvalue with positive real part. Suppose also that any eigenvalue of A with vanishing real part is regular (i.e., its multiplicity is equal to the number of linearly independent eigenvectors corresponding to it). Then all the solutions of

$$Dy = (As^{-1} + B)y + b \tag{5.11}$$

are bounded as $s \to \infty$, y being a complex column vector function of s.

This lemma can be applied to the pair of equations obtained by taking an x^i derivative of Eqs. (3.8e) and (3.8f), i.e., to

$$Dd_i\hat{\rho} = 2\hat{\rho}d_i\hat{\rho} + \hat{\sigma}d_i\hat{\bar{\sigma}} + \hat{\bar{\sigma}}d_i\hat{\sigma}, \tag{5.12a}$$

$$Dd_i\hat{\sigma} = 2\hat{\sigma}d_i\hat{\rho} + 2\hat{\rho}d_i\hat{\sigma} + d_i\hat{\psi}_0. \tag{5.12b}$$

By the lemma, since $A = O, B = O(s^{-2})$, and $b = O(s^{-2})$, we have $d_i\hat{\rho}, d_i\hat{\sigma}, d_i\hat{\bar{\sigma}} = O(1)$. Substituting the information back into Eq. (5.12a), *making the assumption that $d_i\hat{\rho}$ possess a limit at $s = \infty$*, and integrating, we have $\int_\infty^s Dd_i\hat{\rho}ds' = d_i\hat{\rho} - (d_i\hat{\rho})_{s=\infty} = O(s^{-3})$. Now, since $(\hat{\rho})_{s=\infty} = 0$, it can be shown that $(d_i\hat{\rho})_{s=\infty} = 0$, and thus

$$d_i\hat{\rho} = O(s^{-3}). \tag{5.13a}$$

In a similar manner, assuming that $d_i\hat{\sigma}$ possesses a limit at $s = \infty$, we conclude that

$$d_i\hat{\sigma} = O(s^{-3}). \tag{5.13b}$$

For the purposes of the present program we need, in fact, to assume that $d_id_j\hat{\rho}$, $d_id_i\hat{\sigma}$, $d_id_jd_k\hat{\rho}$, $d_id_jd_k\hat{\sigma}$, $d_id_jd_kd_l\hat{\rho}$, and $d_id_jd_kd_l\hat{\sigma}$ all possess limits at $s = \infty$.[17] Arguing as above, we obtain

$$d_id_j\hat{\rho}, d_id_j\hat{\sigma}, \cdots, d_id_jd_kd_l\hat{\rho}, d_id_jd_kd_l\hat{\sigma} = O(s^{-3}). \tag{5.14}$$

At this point, with no further assumptions except the additional requirement that $\tau(0, 0, x^i) = 0$ (the same remarks apply on this requirement as were made in the case $\hat{\rho} = 0$, Sec. 4), it is a fairly straightforward procedure to apply the lemma to the rest of the radial equations to obtain the asymptotic behavior of all variables at $u = 0$. The Δ equations then immediately determine the u behavior off the $u = 0$ surface, enabling us to express the complete asymptotic solution to terms linear in u.[10] For present purposes we need only consider the expressions for ρ and μ:

$$\rho = (-\overset{0}{\psi}_0\overset{0}{\bar{\psi}}_0/7\cdot 16)s^{-7} + O(s^{-8}) - [\overset{0}{\psi}_2 + O(s^{-4})]u, \tag{5.15}$$

$$\begin{aligned}\mu = {} & \overset{0}{\psi}_2 s - (1/4\cdot 12)(\bar{\delta}\bar{\delta}\overset{0}{\psi}_0)s^{-2} + O(s^{-3}) \\ & + \{-2\overset{0}{\psi}_2\overset{0}{\psi}_2 s^2 + \tfrac{1}{4}\delta\bar{\delta}\overset{0}{\psi}_2 s^2 - \tfrac{1}{2}(\delta\bar{\delta}\lambda^0)s - \lambda^0\bar{\lambda}^0 \\ & + [(1/4\cdot 12)(\delta\bar{\delta}\bar{\delta}\bar{\delta}\overset{0}{\psi}_0) + (1/\sqrt{2}\cdot 12)\delta(\overset{0}{\bar{\psi}}_0\delta\overset{0}{\psi}_2) \\ & - (1/\sqrt{2}\cdot 6)\delta(\overset{0}{\psi}_2\delta\overset{0}{\bar{\psi}}_0) + (1/4\cdot 12)(\bar{\delta}\overset{0}{\bar{\psi}}_0)(\bar{\delta}\overset{0}{\psi}_2) \\ & - (1/4\cdot 12)(\delta\overset{0}{\bar{\psi}}_0)(\delta\overset{0}{\psi}_2)]s^{-1} + O(s^{-2})\}u. \end{aligned} \tag{5.16}$$

Here λ^0 is a datum and $\overset{0}{\psi}_2 (= -\tfrac{1}{2}\delta\bar{\delta}\log P)$ is related to the Gaussian curvature of a 2-surface S_∞, whose contravariant metric h^{ij} $(i, j = 2, 3)$, is defined as $h^{ij} \equiv \lim_{s\to\infty} g^{ij}(u = 0, s, x^2, x^3)$. We denote the underlying set of points of this metric space as $S_\infty \equiv \{(0, \infty, x^2, x^3) | (x^2, x^3)$ in their ranges$\}$. This is essentially the slice of the $u = 0$ hypersurface at $s = \infty$. Again, and with the same kind of reasoning as was used in Sec. 4, we make the assumption that S_∞ is compact and has Gaussian curvature that is positive and bounded away from zero. As in Sec 4 we would like to conclude that on some 2-surface in the neighborhood of $u = 0, \rho$ is positive and μ is negative. If this condition obtains, i.e., both null rays converging, we can conclude for the existence of asymptotically trapped surfaces. The term "asymptotically trapped surfaces" is used since the proof is based on an asymptotic solution

Again one can show that it is possible to choose a coordinate transformation of the form

$$u' = u, \tag{5.17}$$

$$s' = s + f(s, x^2, x^3)u, \tag{5.18}$$

$$x^{k'} = x^k, \tag{5.19}$$

such that (to terms linear in u) the vector $\mathbf{m}$ is a linear combination of the natural basis vectors of $x^{k'}$. Thus again the surfaces $S_{\epsilon b}$ defined by

$$S_{\epsilon b} \equiv \{(u', s', x^{2'}, x^{3'}) \mid u = \epsilon, s = b, (x^{2'}, x^{3'}) \text{ in their ranges}\}, \tag{5.20}$$

are spanned by $\mathbf{m}$ and $\bar{\mathbf{m}}$.

As b approaches infinity and ϵ approaches zero the properties of the $S_{\epsilon b}$ approach continuously the properties of S_∞, which implies that there exists a neighborhood of $b = \infty, \epsilon = 0$ in which the surfaces $S_{\epsilon b}$ are compact. From the definition of the $S_{\epsilon b}$, this implies a neighborhood of $s = \infty$ (the asymptotic region) and $u = 0$ such that the $S_{\epsilon b}$ are compact. As in Sec. 4, $\mu + \bar{\mu}$ and $-2p$ give the divergence of the two sets of null rays orthogonal to the $S_{\epsilon b}$. Since $(-\psi_2^0)$ is chosen to be positive and bounded away from zero, it appears from Eqs. (5.19) and (5.20) that, assuming we can neglect all higher orders (in u) of (5.19) and (5.20), there are points in any neighborhood of $u = 0, s = \infty$ at which ρ is positive and $\mu + \bar{\mu}$ is negative. Hence it appears that some of the $S_{\epsilon b}$ are trapped surfaces.

The objection to the argument is, of course, that the higher-order terms (in u) of the expressions for ρ and μ will be functions of s, and it is not immediately apparent that we can ignore their influence. The question needs to be explored. Fortunately it is not difficult to carry out such an investigation. The s dependence of the coefficients of these higher-order terms comes in explicitly through explicit polynomial expressions in s or implicitly through the order symbols. The order symbols cause us no concern since their influence is negligible when compared with the explicit positive powers of s that occur and, in fact, we need only look at the highest positive power of s occurring. To obtain the coefficients of these higher-order terms one takes successive u derivatives of Eqs. (3.9i) and (3.9l) and obtains expressions for the successive u derivatives of μ and ρ which, when evaluated at $u = 0$, are essentially the above-mentioned coefficients. These u derivitives of μ and ρ of order greater than 2 involve u derivatives of order 2 or higher of the other variables and so necessitate going back to Eqs. (3.8), (3.9), (3.11), and (3.12) and taking successive u derivatives to obtain the appropriate expressions. The whole process proceeds forward in the recursive manner of using the second- (and lower-) order information in the third-derivative expressions to get third-derivative information, then substituting this third- (and lower-) order information into the fourth-derivative expressions to get fourth-order information and so forth. Since we need only look at the highest powers of s involved, the process is not difficult and one quickly sees the trend of events. It turns out that in general each successive u derivative contains one higher power of s than the previous u derivative. This comparison between successive u derivatives holds for all successive pairs of u derivatives except for (zero, first) and (first, second) pairs. Here the general rule breaks down mainly because of the way the coordinate and tetrad freedom was used and because of the condition $\tau^0 = 0$, i.e., we were able to eliminate some of the powers of s through the use of coordinate and tetrad freedom (see Ref. 10) and the condition $\tau^0 = 0$ eliminated some others. Thus, neglecting all but the highest power of s in each coefficient, ρ and μ have the forms

$$\rho = A_0 s^{-7} + A_1 u + A_2 s u^2 + \cdots + A_n s^{n-1} u^n + \cdots, \tag{5.21}$$

$$\mu = B_0 s + B_1 s^2 u + B_2 s^4 u^2 + \cdots + B_n s^{n+2} u^n + \cdots, \tag{5.22}$$

where $A_0 = -\psi_0^0 \bar{\psi}_0^0/7 \cdot 16, A_1 = -\psi_2^0, B_0 = \psi_2^0$ and the rest of the A's and B's are functions only of (x^2, x^3). Letting u approach zero (as $s \to \infty$) as $u = a/s^7$, where a is an arbitrary constant, we have $\rho = (A_0 + aA_1)s^{-7}$ + (terms which go to zero faster than s^{-7}), $\mu = B_0 s$ + (terms which go to zero faster than s^{-5}).

Thus by choosing $a > -A_0/A_1$, we can guarantee that, for s sufficiently large, $\rho > 0$. Also, for s large, $\mu < 0$ since $B_0 = \psi_2^0$ and ψ_2^0 is negative by choice (Gaussian curvature of S_∞ is positive and bounded away from zero). We conclude that there exist $S_{\epsilon b}$ which are (asymptotically) trapped surfaces.

Thus the expressions, accurate to first order in u, of which the ρ and μ of Eqs. (5.15) and (5.16) are a part (Ref. 10) constitute a wide class of solutions of the Einstein field equations that admit trapped surfaces. We expect that in asymptotically flat space-times this is the most general situation in which trapped surfaces can develop.

ACKNOWLEDGMENTS

The authors would like to thank Dr. A. Janis for useful suggestions, Dr. W. Hallidy for helpful discussions, and Dr. R. Penrose for originally suggesting the problem.

---

* Work supported in part by the Aerospace Research Laboratories, Office of Aerospace Research, U.S. Air Force.

1 R. Penrose, Phys. Rev. Letters **14**, 57 (1965).

2 E. M. Lifshitz and I. M. Khalatnikov, Advan. Phys. **12**, 185 (1963).

3 If, instead of transforming the metric (2.2) to the metric (2.4), we wish to transform the metric (2.1) to the metric (2.4), we must use the transformation

$$\bar{u} = -e^{-u/4m}, \quad \theta' = \theta,$$
$$s = (4mr - 8m^2)e^{u/4m}, \quad \phi' = \phi.$$

4 It has been pointed out to us that this form of the Schwarzschild metric has previously been discovered by W. Israel, Phys. Rev. **143**, 1016 (1966).

5 E. Newman and R. Penrose, J. Math. Phys. 3, 566 (1962).

6 Greek indices range from 0 to 3. Roman indices have the range (2, 3).

7 A semicolon denotes covariant differentiation and a comma denotes ordinary differentiation.

8 Equation (3.13b) is not strictly true; it is true only if n is tangent to a null geodesic with geodesic normalization. However if a family of null geodesics n′ chosen to coincide with n on S, is used, its divergence will be given by $\mu + \bar{\mu}$.

[9] $f(u, s, \theta, \phi) = O'(g(u))$ means that $|f(u, s, \theta, \phi)| < g(u)\mathbf{F}(s, \theta, \phi)$ for some function F independent of u, and for all sufficiently small u.

[10] D. Pajerski *"Trapped Surfaces and the Development of Singularities,"* Ph.D. Thesis (University of Pittsburgh, 1969) (unpublished).

[11] E. Newman and R. Penrose, J. Math. Phys. 7, 863 (1966).

[12] In Ref. 11 the operator $\eth$ is defined in terms of complex coordinates, $(\zeta, \bar{\zeta})$, related to (x^2, x^3) by $\zeta = -x^2 + ix^3$, $\bar{\zeta} = -x^2 - ix^3$. In this coordinate system the line element has the form $ds^2 = -d\zeta d\bar{\zeta}/P^2$. The definition of $\eth$ is then $\eth\eta \equiv 2P^{1-q}(\partial/\partial\zeta)(P^q\eta)$, where η is a quantity of spin weight q.

[13] Though λ^0 is real, the complex-conjugate notation is used in Eqs. (4.4) and (4.5) in order to give the correct indication of spin weights.

[14] The meaning of the order symbol used here is that $f(u, s, x^i) = O(g(s))$ means $|f(u, s, x^i)| < g(s)F(u, x^i)$ for some function F independent of s and for all sufficiently large s.

[15] In Ref. 5 this is referred to as the asymptotically spherical case.

[16] In Ref. 5 this is referred to as the asymptotically plane case

[17] This circumstance we find rather surprising since in the asymptotically spherical case, i.e., $\rho = -s^{-1} + O(s^{-2})$, one needs no assumptions beyond those on ψ_0 (see Ref. 5).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Unified Treatment of Diatomic Electron Interaction Integrals over Slater-type Atomic Orbitals*

David M. Silver

Applied Physics Laboratory, The Johns Hopkins University, Silver Spring, Maryland 20910

(Received 12 April 1971)

General expressions are developed for the evaluation of both Coulomb and hybrid electron repulsion integrals over basis sets of arbitrary Slater-type atomic orbitals. In each case, a single numerical integration over a product of a one-center and a two-center charge distribution function is required for the recovery of the integrals. The one-center charge distribution functions are shared by both integral types. The two-center charge distributions are different for the two cases, but the constants and special functions required are the same. The results lead to an efficient computer-oriented procedure for the resolution of these integrals. The charge distribution functions can be used to obtain two-center overlap, nuclear attraction, kinetic energy, and, somewhat less efficiently, exchange integrals as well.

INTRODUCTION

The use of Slater-type atomic orbitals as a basis for the expansion of molecular wavefunctions leads to good descriptions of physical systems at the expense of computational difficulties in the evaluation of multicenter electron-repulsion integrals. Among the diatomic integrals that arise, the Coulomb integrals are energetically the most significant while hybrid integrals are the most numerous. Accurate and efficient methods for the evaluation of all diatomic integrals remain important even in the context of many-center molecule calculations.

Recently, analytical expressions have been developed for the evaluation of Coulomb integrals.[1] Since the scheme is amenable to computer usage, programs have been developed and incorporated into a general diatomic integral package for evaluating all two-center Coulomb,[1] hybrid,[2] and exchange[3] integrals. The latter two formulations take advantage of the charge distribution concept,[4] and considerable savings of computer time are achieved in this way. The Coulomb formulation,[1] on the other hand, relies on rapid handling of each integral on a one-by-one basis with very little computational material being carried over from one integral to the next.

The hybrid formulation[2] employs one final numerical integration over simple charge distribution functions. Application of this method to Coulomb integrals allows a further exploitation since certain computed charge distribution quantities can be used by both Coulomb and hybrid integrals in common. The computational efficiencies gained in this respect offset the introduction of a final numerical integration for the Coulomb integrals. The exchange formulation[3] employs one final numerical integration over a rapidly convergent infinite series of charge distribution functions. Application of the hybrid scheme to exchange integrals is less effective since a double numerical integration arises plus an infinite series.

In previous work, explicit expressions have been developed for Coulomb and hybrid integrals.[5-10] Charge distribution procedures involving two final numerical integrations have appeared.[11] Hybrid and exchange integrals have been evaluated using ellipsoidal methods, while a Fourier convolution method has been employed for Coulomb integrals.[12]

In addition, general multicenter methods have been employed for these integrals.[13,14] A review of other pertinent techniques has also appeared.[15] The present treatment for Coulomb integrals offers advantages in that general expressions are given for all combinations of orbitals, only one final numerical integration is needed, charge distribution quantities can be computed and used for more than one type of integral, and the methods are specifically oriented to the two-center nature of these integrals.

In the following, the derivation of formulas is sketched and final expressions are shown. The hybrid integral is handled first to demonstrate the method to be used[2] and to establish the present notations. The final expressions given here are modified from those previously given[2] so as to be able to utilize certain efficiencies in the unified treatment. The Coulomb integral is next resolved

[9] $f(u, s, \theta, \phi) = O'(g(u))$ means that $|f(u, s, \theta, \phi)| < g(u)\mathbf{F}(s, \theta, \phi)$ for some function F independent of u, and for all sufficiently small u.

[10] D. Pajerski *"Trapped Surfaces and the Development of Singularities,"* Ph.D. Thesis (University of Pittsburgh, 1969) (unpublished).

[11] E. Newman and R. Penrose, J. Math. Phys. 7, 863 (1966).

[12] In Ref. 11 the operator $\eth$ is defined in terms of complex coordinates, $(\zeta, \bar{\zeta})$, related to (x^2, x^3) by $\zeta = -x^2 + ix^3$, $\bar{\zeta} = -x^2 - ix^3$. In this coordinate system the line element has the form $ds^2 = -d\zeta d\bar{\zeta}/P^2$. The definition of $\eth$ is then $\eth\eta \equiv 2P^{1-q}(\partial/\partial\zeta)(P^q\eta)$, where η is a quantity of spin weight q.

[13] Though λ^0 is real, the complex-conjugate notation is used in Eqs. (4.4) and (4.5) in order to give the correct indication of spin weights.

[14] The meaning of the order symbol used here is that $f(u, s, x^i) = O(g(s))$ means $|f(u, s, x^i)| < g(s)F(u, x^i)$ for some function F independent of s and for all sufficiently large s.

[15] In Ref. 5 this is referred to as the asymptotically spherical case.

[16] In Ref. 5 this is referred to as the asymptotically plane case

[17] This circumstance we find rather surprising since in the asymptotically spherical case, i.e., $\rho = -s^{-1} + O(s^{-2})$, one needs no assumptions beyond those on ψ_0 (see Ref. 5).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Unified Treatment of Diatomic Electron Interaction Integrals over Slater-type Atomic Orbitals*

David M. Silver

Applied Physics Laboratory, The Johns Hopkins University, Silver Spring, Maryland 20910

(Received 12 April 1971)

General expressions are developed for the evaluation of both Coulomb and hybrid electron repulsion integrals over basis sets of arbitrary Slater-type atomic orbitals. In each case, a single numerical integration over a product of a one-center and a two-center charge distribution function is required for the recovery of the integrals. The one-center charge distribution functions are shared by both integral types. The two-center charge distributions are different for the two cases, but the constants and special functions required are the same. The results lead to an efficient computer-oriented procedure for the resolution of these integrals. The charge distribution functions can be used to obtain two-center overlap, nuclear attraction, kinetic energy, and, somewhat less efficiently, exchange integrals as well.

INTRODUCTION

The use of Slater-type atomic orbitals as a basis for the expansion of molecular wavefunctions leads to good descriptions of physical systems at the expense of computational difficulties in the evaluation of multicenter electron-repulsion integrals. Among the diatomic integrals that arise, the Coulomb integrals are energetically the most significant while hybrid integrals are the most numerous. Accurate and efficient methods for the evaluation of all diatomic integrals remain important even in the context of many-center molecule calculations.

Recently, analytical expressions have been developed for the evaluation of Coulomb integrals.[1] Since the scheme is amenable to computer usage, programs have been developed and incorporated into a general diatomic integral package for evaluating all two-center Coulomb,[1] hybrid,[2] and exchange[3] integrals. The latter two formulations take advantage of the charge distribution concept,[4] and considerable savings of computer time are achieved in this way. The Coulomb formulation,[1] on the other hand, relies on rapid handling of each integral on a one-by-one basis with very little computational material being carried over from one integral to the next.

The hybrid formulation[2] employs one final numerical integration over simple charge distribution functions. Application of this method to Coulomb integrals allows a further exploitation since certain computed charge distribution quantities can be used by both Coulomb and hybrid integrals in common. The computational efficiencies gained in this respect offset the introduction of a final numerical integration for the Coulomb integrals. The exchange formulation[3] employs one final numerical integration over a rapidly convergent infinite series of charge distribution functions. Application of the hybrid scheme to exchange integrals is less effective since a double numerical integration arises plus an infinite series.

In previous work, explicit expressions have been developed for Coulomb and hybrid integrals.[5-10] Charge distribution procedures involving two final numerical integrations have appeared.[11] Hybrid and exchange integrals have been evaluated using ellipsoidal methods, while a Fourier convolution method has been employed for Coulomb integrals.[12]

In addition, general multicenter methods have been employed for these integrals.[13,14] A review of other pertinent techniques has also appeared.[15] The present treatment for Coulomb integrals offers advantages in that general expressions are given for all combinations of orbitals, only one final numerical integration is needed, charge distribution quantities can be computed and used for more than one type of integral, and the methods are specifically oriented to the two-center nature of these integrals.

In the following, the derivation of formulas is sketched and final expressions are shown. The hybrid integral is handled first to demonstrate the method to be used[2] and to establish the present notations. The final expressions given here are modified from those previously given[2] so as to be able to utilize certain efficiencies in the unified treatment. The Coulomb integral is next resolved

along the same lines. The application of this technique to exchange integrals is also considered. Finally a discussion is presented of the various special functions required for this analysis.

I. DEFINITIONS

For computational efficiency, the Slater-type atomic orbital $\chi_i(P,t)$, situated at center P and a function of the electron coordinates t, is defined as follows:

$$\chi_i(P,t) = N_i r_{Pt}^{n_i-1} \exp(-\zeta_i r_{Pt})(2l_i+1)^{-1/2} \times Y_{l_i m_i}(\theta_{Pt}\varphi_{Pt}), \tag{1}$$

where n, l, and m are quantum numbers, ζ is an orbital exponent, N is a normalization constant

$$N_i = (2\zeta_i)^{n_i+1/2}[(2l_i+1)/(2n_i)!]^{1/2}, \tag{2}$$

and Y_{lm} is a real, normalized spherical harmonic. The previously defined[16] coordinate systems are to be used at centers A and B, with R representing the separation distance between them.

The hybrid H and Coulomb C integrals of interest here are written:

$$H = \int dV_2 U_A(2)\chi_3(A,2)\chi_4(B,2), \tag{3}$$

$$C = \int dV_2 U_A(2)\chi_5(B,2)\chi_6(B,2), \tag{4}$$

where the one-electron potential U_A has the form,

$$U_A(2) = \int dV_1 \chi_1(A,1)\chi_2(A,1) r_{12}^{-1}. \tag{5}$$

Thus, both integrals involve integration over the same one-center distribution.

The integrations over the coordinates of a two-center charge distribution are to be performed via the bipolar coordinates[2,17]:

$$\int dV \rightarrow \int_0^\infty dr_A \int_{|R-r_A|}^{R+r_A} dr_B \int_0^{2\pi} d\varphi r_A r_B R^{-1}. \tag{6}$$

The expansion of a product of two spherical harmonics on the same center is given by

$$Y_{l_1 m_1}(\theta\varphi)Y_{l_2 m_2}(\theta\varphi) = \sum_{l=|l_1-l_2|}^{l_1+l_2}{}' \sum_{m}^{(m_1,m_2)} \left(\frac{(2l_1+1)(2l_2+1)(2l+1)}{4\pi}\right)^{1/2} \times q_{lm}(l_1 m_1, l_2 m_2) Y_{lm}(\theta\varphi), \tag{7}$$

where the prime on the summation over l implies $\Delta l = 2$, and the sum over m denotes that m takes the two values, m_+ and m_-, given by

$$m_\pm = \mathrm{sgn}(m_1)\ \mathrm{sgn}(m_2)\,|\,|m_1| \pm |m_2|\,|, \tag{8}$$

and

$$\mathrm{sgn}(x) = x/|x|, \quad \mathrm{sgn}(0) = 1. \tag{9}$$

The functions q_{lm} have been described.[1,8] Expansion of the inverse interparticle distance is given by

$$r_{12}^{-1} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{(2l+1)} \sigma^l \gamma^{-l-1} Y_{lm}(\theta_1\varphi_1) Y_{lm}(\theta_2\varphi_2), \tag{10}$$

where σ and γ denote, respectively, the smaller and greater of r_1 and r_2. The following expansion is used to transfer a solid spherical harmonic from center B to center A:[18-23]

$$r_B^l Y_{lm}(\theta_B\varphi_B) = \sum_{K=|m|}^{l} \left(\frac{2l+1}{2K+1}\right)^{1/2} p_K(lm) r_A^K R^{l-K} \times Y_{Km}(\theta_A\varphi_A), \tag{11}$$

where the constant p_K is defined by

$$p_K(lm) = \frac{(-1)^{K+m}}{(l-K)!}\left(\frac{(l+m)!(l-m)!}{(K+m)!(K-m)!}\right)^{1/2}. \tag{12}$$

The parameter definitions,

$$n_a = n_1 + n_2, \quad \alpha = \zeta_1 + \zeta_2, \tag{13}$$

$$n_b = n_5 + n_6, \quad \beta = \zeta_5 + \zeta_6, \tag{14}$$

are used in the sequel.

II. CHARGE DISTRIBUTION POTENTIAL

The reduction of the potential function U_A of Eq. (5) is straightforward.[2,6,11] Combining Eqs. (7) and (10), using the orthogonality properties of the spherical harmonics and collecting terms gives the result:

$$U_A(2) = \sum_{l=|l_1-l_2|}^{l_1+l_2}{}' \sum_{m}^{(m_1,m_2)} \left(\frac{4\pi}{(2l+1)}\right)^{1/2} \times Y_{lm}(\theta_{A2}\varphi_{A2}) f_{lm}(r_{A2}). \tag{15}$$

The one-center charge distribution function is thereby defined:

$$f_{lm}(r) = N_1 N_2 q_{lm}(l_1 m_1, l_2 m_2) r^{n_a} \times [E_{n_a+l}(\alpha r) + A_{n_a-l-1}(\alpha r)], \tag{16}$$

in which the auxiliary functions E_n and A_n are as follows:

$$E_n(x) = \int_0^1 dt\, t^n \exp(-xt), \tag{17}$$

$$A_n(x) = \int_1^\infty dt\, t^n \exp(-xt). \tag{18}$$

The latter two functions, discussed in a later section, can be quite easily computed[1] through recursion relations and series representation and constitute no difficulty to the calculation of the function f_{lm}. Therefore the one-center charge distribution is an elementary function and has a parametric dependence only on the quantum numbers and orbital exponents of the two orbitals located on nucleus A.

III. HYBRID INTEGRALS

Incorporating the expression for the potential, U_A of Eq. (15), gives the following equation for the hybrid integral of Eq. (3):

$$H = N_3 N_4 \int dV_2 \sum_{lm} \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{lm}(\theta_{A2}\varphi_{A2}) f_{lm}(r_{A2}) \times r_{A2}^{n_3-1} \exp(-\zeta_3 r_{A2}) r_{B_2}^{n_4-1} \exp(-\zeta_4 r_{B2}) \times [(2l_3+1)(2l_4+1)]^{-1/2} Y_{l_3 m_3}(\theta_{A_2}\varphi_{A_2}) Y_{l_4 m_4} \times (\theta_{B_2}\varphi_{B2}). \quad (19)$$

The two functions on center A, $Y_{l_3 m_3}$ and Y_{lm}, can be combined through use of Eq. (7) to give a sum of terms containing Y_{LM}. The harmonic on center B can be transferred to center A with Eq. (11), giving Y_{Km_4}. Finally Eq. (7) can be used to combine the latter with Y_{LM} to yield a series containing $Y_{\Lambda\mu}$:

$$H = N_3 N_4 \sum_{l=|l_1-l_2|}^{l_1+l_2}{}' \sum_{m}^{(m_1,m_2)} \int dV_2 f_{lm}(r_{A2}) \sum_{L=|l-l_3|}^{l+l_3}{}' \sum_{M}^{(m,m_3)} \sum_{K=|m_4|}^{l_4} \sum_{\Lambda=|L-K|}^{L+K}{}' \sum_{\mu}^{(M,m_4)} r_{A2}^{n_3+K-1} \exp(-\zeta_3 r_{A2}) \times r_{B2}^{n_4-l_4-1} \exp(-\zeta_4 r_{B2}) R^{l_4-K}(2L+1) p_K(l_4 m_4) \times q_{LM}(l_3 m_3, lm) q_{\Lambda\mu}(LM, Km_4) \left(\frac{2\Lambda+1}{4\pi}\right)^{1/2} \times Y_{\Lambda\mu}(\theta_{A2}\varphi_{A2}). \quad (20)$$

The integration over the angular variable φ_{A2} can now be performed:

$$\int_0^{2\pi} d\varphi Y_{\Lambda\mu}(\theta\varphi) = \delta_{\mu 0}(4\pi)^{1/2} \mathcal{P}_\Lambda^0(\cos\theta), \quad (21)$$

where $\mathcal{P}$ is a normalized, associated Legendre function. The total integral is nonzero only if $\mu = 0$, which implies $M = m_4$. Specifically, this means that the equation

$$\operatorname{sgn}(m_4)|m_4| = \operatorname{sgn}(m_1)\operatorname{sgn}(m_2) \times \operatorname{sgn}(m_3)|[|(|m_1| \pm |m_2|)| + |m_3|]| \quad (22)$$

must be satisfied with at least one of the four possible choices of ± signs. The particular form of the orthogonality relation in Eq. (22) is a consequence of the order in which the three spherical harmonics have been coupled and is equivalent to the conditions

$$\operatorname{sgn}(m_1)\operatorname{sgn}(m_2)|(|m_1| \pm |m_2|)| = \operatorname{sgn}(m_3)\operatorname{sgn}(m_4)|(|m_3| \pm |m_4|)|. \quad (23)$$

The remaining integrations indicated in Eq. (6) can now be performed to give the final result:

$$H = \sum_{l=|l_1-l_2|}^{l_1+l_2}{}' \sum_{m}^{(m_1 m_2)} \int_0^\infty dr_A f_{lm}(r_A) F_{lm}(r_A), \quad (24)$$

with the second charge distribution function F_{lm} given by

$$F_{lm}(r_A) = N_3 N_4 \sum_{L=|l_3-l|}^{l_3+l}{}' \sum_{M}^{(m,m_3)} \delta_{M,m_4} \sum_{K=|m_4|}^{l_4} \sum_{\Lambda=|L-K|}^{L+K}{}' (2L+1) p_K(l_4 m_4) q_{Lm_4}(l_3 m_3, lm) q_{\Lambda 0}(Lm_4, Km_4) \times R^{l_4-K-1} r_A^{n_3+K} \exp(-\zeta_3 r_A) B_{\Lambda, n_4-l_4}(r_A, R; \zeta_4), \quad (25)$$

where the auxiliary function B is simply related to the previously defined[2] function $\mathfrak{B}$,

$$B_{\Lambda,n}(r, R; \zeta) = (2\Lambda+1)^{1/2} \mathfrak{B}_\Lambda^n(r, R; \zeta). \quad (26)$$

These functions are discussed in detail in a later section.

In passing, it should be noted that the two-center overlap integral

$$S = \int dV_t \chi_3(A, t) \chi_4(B, t) \quad (27)$$

can be evaluated as a special case of the hybrid formulation. The spherical harmonic $Y_{l_4 m_4}$ on center B is transferred to center A via Eq. (11) and expanded with $Y_{l_3 m_3}$ by using Eq. (7). The result, after performing the integrations in Eq. (6), is given by

$$S = \int_0^\infty dr_A F_{00}(r_A). \quad (28)$$

Although this is a particularly simple result, more direct procedures are available[16] which are not encumbered by the final numerical integration. However, once the functions F_{lm} are available, the evaluation of the two-center overlap, nuclear attraction, and kinetic energy integrals can be achieved through a minimal computational effort. In particular, the latter integrals are obtained from the following:

$$V_2 = \int dV_t r_{At}^{-1} \chi_3(A, t) \chi_4(B, t), \quad (29)$$

$$V_2 = \int_0^\infty dr_A r_A^{-1} F_{00}(r_A), \quad (30)$$

and

$$T = \int dV_t [-\tfrac{1}{2}\nabla_t^2 \chi_3(A, t)] \chi_4(B, t), \quad (31)$$

$$T = n_3 \zeta_3 V_2 - \tfrac{1}{2}\zeta_3^2 S - \tfrac{1}{2}(n_3 + l_3)(n_3 - l_3 - 1) \times \int_0^\infty dr_A r_A^{-2} F_{00}(r_A). \quad (32)$$

IV. COULOMB INTEGRALS

The development of the Coulomb integrals follows similar lines as those described above. The angular dependence is exhibited in the form

$$C = N_5 N_6 \int dV_2 \sum_{lm} \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{lm}(\theta_{A2}\varphi_{A2}) f_{lm}(r_{A2}) \times r_{B2}^{n_b-2} \exp(-\beta r_{B2}) [(2l_5+1)(2l_6+1)]^{-1/2} \times Y_{l_5 m_5}(\theta_{B2}\varphi_{B2}) Y_{l_6 m_6}(\theta_{B2}\varphi_{B2}). \quad (33)$$

Firstly, the spherical harmonics on center B are

combined by using Eq. (7) to yield $Y_{LM}(\theta_B\varphi_B)$. Secondly, the latter is transferred from center B to center A through Eq. (11) giving $Y_{KM}(\theta_A\varphi_A)$. Thirdly, the latter is combined with Y_{lm} to yield a sum of terms containing $Y_{\Lambda\mu}$:

$$C = N_5N_6 \sum_{l=|l_1-l_2|}^{l_1+l_2}{}' \sum_{m}^{(m_1,m_2)} \int dV_2 f_{lm}(r_{A2}) \sum_{L=|l_5-l_6|}^{l_5+l_6}{}' \sum_{M}^{(m_5,m_6)} \sum_{K=|M|}^{L} \sum_{\Lambda=|l-K|}^{l+K}{}' \sum_{\mu}^{(M,m)} r_{A2}^{K} r_{B2}^{n_b-L-2} \exp(-\beta r_{B2}) \times R^{L-K}(2L+1)p_K(LM)q_{LM}(l_5m_5, l_6m_6) \times q_{\Lambda\mu}(KM, lm)\left(\frac{2\Lambda+1}{4\pi}\right)^{1/2} Y_{\Lambda\mu}(\theta_{A2}\varphi_{A2}). \quad (34)$$

Integrating over the angular variable φ_{A2} gives $\delta_{\mu 0}$, implying $M = m$ and the following orthogonality conditions:

$$\operatorname{sgn}(m_1)\operatorname{sgn}(m_2)|(|m_1| \pm |m_2|)| = \operatorname{sgn}(m_5)\operatorname{sgn}(m_6)|(|m_5| \pm |m_6|)|. \quad (35)$$

Again this equality must be satisfied by some choice of the ± signs for the total integral to be nonzero.

Performing the remaining integrations in this case now yields the final Coulomb result:

$$C = \sum_{l=|l_1-l_2|}^{l_1+l_2}{}' \sum_{m}^{(m_1,m_2)} \int_0^\infty dr_A f_{lm}(r_A) G_{lm}(r_A), \quad (36)$$

where the new charge distribution function G is defined by

$$G_{lm}(r_A) = N_5N_6 \sum_{L=|l_5-l_6|}^{l_5+l_6}{}' \sum_{M}^{(m_5,m_6)} \delta_{Mm} \sum_{K=|m|}^{L} \sum_{\Lambda=|K-l|}^{K+l}{}' (2L+1)p_K(Lm)q_{Lm}(l_5m_5, l_6m_6)q_{\Lambda 0}(Km, lm) \times R^{L-K-1} r_A^{K+1} B_{\Lambda, n_b-L-1}(r_A, R; \beta) \quad (37)$$

Comparison of G with the hybrid charge distribution F, in Eq. (25), reveals that the constants and functions required are all identical. Thus, tables of the constants p and q and a routine for the calculation of the B functions are all that is required to generate both F and G.

In passing, it should be noted that the charge distribution function G_{00} can be used to evaluate the nuclear attraction integral

$$V_1 = \int dV_t r_{At}^{-1} \chi_5(B,t)\chi_6(B,t) \quad (38)$$

from the expression

$$V_1 = \int_0^\infty dr_A r_A^{-1} G_{00}(r_A). \quad (39)$$

In addition, the accuracy of the procedure can be partially assessed by examining the value obtained for the one-center overlap integral:

$$\int dV_t \chi_5(B,t)\chi_6(B,t) = \int_0^\infty dr_A G_{00}(r_A) = \delta_{l_5l_6}\delta_{m_5m_6}N_5N_6[(2l_5+1)(2l_6+1)]^{-1/2}n_b! \times \beta^{-n_b-1}. \quad (40)$$

V. EXCHANGE INTEGRALS

The exchange integral E is written as follows:

$$E = \int dV_2 U_{AB}(2)\chi_3(A,2)\chi_4(B,2), \quad (41)$$

where the two-center, one-electron potential U_{AB} has the form

$$U_{AB}(2) = \int dV_2 \chi_7(A,1)\chi_8(B,1)r_{12}^{-1}. \quad (42)$$

Thus, the exchange integral differs from the hybrid integral of Eq. (3) only in the use of the two-center potential function U_{AB} instead of the one-center potential U_A.

The expansion for r_{12}^{-1} in Eq. (10) is first introduced giving a sum of spherical harmonics, Y_{lm}:

$$U_{AB}(2) = N_7N_8 \int dV_1 \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left(\frac{4\pi}{2l+1}\right)\sigma^l\gamma^{-l-1} \times Y_{lm}(\theta_{A2}\varphi_{A2})\, Y_{lm}(\theta_{A1}\varphi_{A1}) r_{A1}^{n_7-1} \exp(-\zeta_7 r_{A1}) \times r_{B1}^{n_8-1} \exp(-\zeta_8 r_{B1}) [(2l_7+1)(2l_8+1)]^{-1/2} \times Y_{l_7m_7}(\theta_{A1}\varphi_{A1}) Y_{l_8m_8}(\theta_{B1}\varphi_{B1}), \quad (43)$$

where σ and γ signify, respectively, the smaller and greater of r_{A1} and r_{A2}. The similarity of this expression with Eq. (19) for the hybrid integral suggests similar handling of the two cases. Therefore, Eq. (7) is used to combine Y_{lm} with $Y_{l_7m_7}$ to give Y_{LM}. The function $Y_{l_8m_8}$ is transferred to center A using Eq. (11) to give Y_{Km_8}. Finally, this is combined with Y_{LM} to yield $Y_{\Lambda\mu}$:

$$U_{AB}(2) = N_7N_8 \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \int dV_1 \sigma^l\gamma^{-l-1}(2l+1)^{-1/2} \times Y_{lm}(\theta_{A2}\varphi_{A2}) \sum_{L=|l_7-l|}^{l_7+l}{}' \sum_{M}^{(m,m_7)} \sum_{K=|m_8|}^{l_8} \sum_{\Lambda=|L-K|}^{L+K}{}' \sum_{\mu}^{(M,m_8)} r_{A1}^{n_7+K-1} \exp(-\zeta_7 r_{A1})\, r_{B1}^{n_8-l_8-1} \exp(-\zeta_8 r_{B1}) \times R^{l_8-K}(2L+1)p_K(l_8m_8)q_{LM}(l_7m_7, lm) \times q_{\Lambda\mu}(LM, Km_8)(2\Lambda+1)^{1/2} Y_{\Lambda\mu}(\theta_{A1}\varphi_{A1}). \quad (44)$$

Integrating over φ_{A1} from Eq. (6) gives $\delta_{\mu 0}$ and the requirement that $M = m_8$. The remaining integrations give the result

$$U_{AB}(2) = \sum_{m}^{(m_7,m_8)} \sum_{l=|m|}^{\infty} \left(\frac{4\pi}{(2l+1)}\right)^{1/2} \times Y_{lm}(\theta_{A2}\varphi_{A2})X_{lm}(r_{A2}), \quad (45)$$

where the exchange charge distribution function X_{lm} is defined by

$$X_{lm}(r) = \int_0^\infty dt e_l(t) F'_{lm}(rt), \tag{46}$$

where

$$e_l(t) = t^l, \quad 0 \le t \le 1, \tag{47}$$

$$e_l(t) = t^{-l-1}, \quad 1 \le t \le \infty, \tag{48}$$

and the prime on the function F'_{lm} is to indicate that the parameter subscripts 3 and 4 in the definition of F in Eq. (25) are to be read 7 and 8 for use in Eq. (46).

When the two-center potential U_{AB} is inserted into Eq. (41), the reduction of the exchange integral follows exactly the procedure outlined above for the hybrid integral, giving the final result

$$E = \sum_m^{(m_7,m_8)} \sum_{l=|m|}^{\infty} \int_0^\infty dr_A X_{lm}(r_A) F_{lm}(r_A), \tag{49}$$

which contains the orthogonality condition that the equation

$$m_4 = \operatorname{sgn}(m)\operatorname{sgn}(m_3)|(|m| \pm |m_3|)| \tag{50}$$

or equivalently,

$$\operatorname{sgn}(m_3)\operatorname{sgn}(m_4)|(|m_3| \pm |m_4|)| = \operatorname{sgn}(m_7)\operatorname{sgn}(m_8)|(|m_7| \pm |m_8|)| \tag{51}$$

must be satisfied in order for the total integral to be nonzero.

The two-center hybrid charge distribution functions F_{lm} can therefore be used with an infinite series to recover the exchange integrals. Since the final integration is to be performed numerically, the functions F_{lm} can be assumed to be tabulated for certain values of r_A over the range of the integration variable. The function X_{lm} is defined in such a way that it can be computed using the same set of tabulated function values as are needed in Eq. (24) for the hybrids.

VI. AUXILIARY FUNCTIONS

A. The Function $B_{\Lambda n}$

The definition of the function $B_{\Lambda n}$ can be written in terms of its integral representation:

$$B_{\Lambda,n}(r_A, R; \zeta) = (2\Lambda+1)^{1/2} \int_{|R-r_A|}^{R+r_A} dr_B r_B^n \exp(-\zeta r_B) \times \mathcal{P}_\Lambda^0(\cos\theta_A). \tag{52}$$

This is transformed into a sum over the special functions[16] I_v as follows[2]:

$$B_{\Lambda,n}(r_A, R; \zeta) = \sigma^{n+1} \exp(-\zeta\gamma) \sum_{u=0}^{n+\Lambda} \left(\frac{\gamma}{\sigma}\right)^{u-\Lambda} \times \sum_{v=0}^{n+2\Lambda-u} (\zeta\sigma)^v I_v(\zeta\sigma) W_{uv}(\Lambda, n), \tag{53}$$

where σ and γ represent, respectively, the smaller and greater of r_A and R, and the constants W_{uv} are given by

$$W_{uv}(\Lambda, n) = 2^v \left[(v+1)! \binom{2v}{v}\right]^{-1} \sum_{g=0}^{\Lambda} \sum_{h=h_0}^{n+2\Lambda-g-u} Q_{uvgh}(\Lambda, n)(-1)^{h+v} \times \left[\binom{g+h}{g}\binom{g+h+v+1}{g+h}\right]^{-1} \times \sum_{i=0}^{v} (-1)^i \binom{v}{i}\binom{h+i}{h}\binom{g+v-i}{g}, \tag{54}$$

where

$$h_0 = \max[\Lambda - g, \Lambda - u, v - g], \tag{55}$$

and the constants Q are defined:

$$Q_{uvgh}(\Lambda, n) = 2^{1/2}(2\Lambda+1)(-1)^{n+\Lambda+u+v} \binom{\Lambda}{g}^2 \times \sum_{j=j_0}^{j_1} \sum_{k=k_0}^{k_1} 2^j \binom{n}{j}\binom{\Lambda-g}{k}\binom{g}{\Lambda+j+k-h} \times \binom{n+\Lambda-g-j-k}{u+h-\Lambda-j-k}, \tag{56}$$

in which

$$j_0 = \max[0, g+h-2\Lambda], \tag{57}$$

$$j_1 = \min[n, g+h-\Lambda, u+h-\Lambda], \tag{58}$$

$$k_0 = \max[0, h-\Lambda-j], \tag{59}$$

$$k_1 = \min[\Lambda-g, g+h-\Lambda-j, h+u-\Lambda-j]. \tag{60}$$

Although the lower summation limit of the index v in Eq. (53) is explicitly zero, a more precisely defined limit has been discussed[24] and is $\max[0, u-n]$. The constants W_{uv} need be computed once and stored within a computer peripheral memory for use in computing the functions B.

The most time-consuming operation arising in the evaluation of the functions B involves the computation of the functions I_v.

These can be related to the previously described[16] functions f_μ. The recurrence relation

$$I_v(x) = \frac{(2v+1)(2v-1)}{x^2}[I_{v-2}(x) - I_{v-1}(x)], \tag{61}$$

with the starting functions,

$$I_0(x) = x^{-1}\sinh(x), \tag{62}$$

$$I_{-1}(x) = \cosh(x), \tag{63}$$

can be used with a 16-digit double-precision computer word to yield no less than ten significant

figures whenever

$$x \geq (4v_{max} - 3)v_{max}/100 \tag{64}$$

is satisfied: v_{max} is the largest index value required. When x is too small to use the relation in Eq. (61), then the continued fraction[16,25]

$$I_v(x) = r_v(x)I_{v-1}(x), \tag{65}$$

where

$$r_v(x) = \left(1 + \frac{x^2 r_{v+1}(x)}{(2v+1)(2v+3)}\right)^{-1}, \tag{66}$$

can be used quite efficiently and the number of terms required to obtain the same accuracy is given by the integer t satisfying the equation

$$t > 2.5 + \frac{7.5x}{v_{max}}. \tag{67}$$

Since the I_v functions can be related to the functions E_n of Eq. (17):

$$I_v(x) = \frac{(2v+1)!}{(v!)^2} \exp(x) \sum_{n=0}^{v} E_{n+v}(2x)(-1)^n \binom{v}{n}, \tag{68}$$

an alternative representation of the B functions can be written:

$$B_{\Lambda,n}(r_A, R; \zeta) = \sigma^{n+1} \exp(\zeta\sigma - \zeta\gamma) \sum_{u=0}^{n+\Lambda} \left(\frac{\gamma}{\sigma}\right)^{u-\Lambda} \times \sum_{v=v_0}^{n+2\Lambda-u} E_v(2\zeta\sigma) P_{uv}(\Lambda, n), \tag{69}$$

where σ and γ are again, respectively, the smaller and greater of r_A and R; the index v_0 is given by

$$v_0 = \max[0, \Lambda - u]; \tag{70}$$

and the constants P_{uv} are defined by

$$P_{uv}(\Lambda, n) = \sum_{g=g_0}^{\Lambda} \sum_{h=h_1}^{h_2} Q_{uvgh}(\Lambda, n) \binom{g}{v-h}, \tag{71}$$

with

$$g_0 = \max[0, \Lambda - v], \tag{72}$$

$$h_1 = \max[\Lambda - g, \Lambda - u, v - g], \tag{73}$$

$$h_2 = \min[n + 2\Lambda - u - g, v]. \tag{74}$$

The constants P_{uv} are simpler to compute than W_{uv} of Eq. (54), and the former can be computed with absolute accuracy since only a sum of integers is involved. The availability of two distinct representations of the B functions provides a good means for checking computational accuracy.

B. The Functions A_n and E_n

The functions A_n of Eq. (18) are obtained through the recursion relation

$$A_n(x) = [nA_{n-1}(x) + \exp(-x)]/x \tag{75}$$

with the starting function given by

$$A_0(x) = x^{-1} \exp(-x). \tag{76}$$

The functions E_n of Eq. (17) are needed for the evaluation of the one-center charge distribution function f_{lm} in Eq. (16) and can also be used for the evaluation of the B functions. The recursion relation

$$E_n(x) = [nE_{n-1}(x) - \exp(-x)]/x \tag{77}$$

can be employed with the starting function

$$E_0(x) = x^{-1}[1 - \exp(-x)], \tag{78}$$

when the maximum index value required n_{max} and the variable x satisfy the equation

$$x \geq (n_{max} + 6)n_{max}/80. \tag{79}$$

This will guarantee ten significant figures out of a 16-digit computer word. When x is too small to satisfy this relation, the recursive procedure in Eq. (77) loses too many significant figures and the inverse recursion is required:

$$E_n(x) = [xE_{n+1}(x) + \exp(-x)]/(n+1). \tag{80}$$

The starting function can be obtained[1] by using a Taylor's series expansion:

$$E_n(x) = \sum_{k=0}^{\infty} \frac{(\epsilon - x)^k}{k!} E_{n+k}(\epsilon), \tag{81}$$

about fixed values ϵ; but this requires the storage of tables of function values $E_n(\epsilon)$ for closely spaced intervals ϵ. In addition to the infinite series[1,11]

$$E_n(x) = n! \exp(-x) \sum_{k=0}^{\infty} \frac{x^k}{(n+k+1)!}, \tag{82}$$

the starting function can be obtained by setting

$$E_{n_{max}+m}(x) = 0 \tag{83}$$

and recurring downwards with Eq. (80). If m is taken to satisfy the equation

$$m > 5 + n_{max}/2, \tag{84}$$

this ensures accuracy for the required set of E functions. For x greater than $2n + 20$, $E_n(x)$ has the asymptotic value[11]

$$E_n(x) \sim n! x^{-n-1}. \tag{85}$$

VII. DISCUSSION

As can be seen from Eq. (25) for hybrid integrals, a set of B functions must be computed which depends only on χ_4 at center B. This set of function

values can then be coupled with all possible orbitals on center A to form all two-center charge distribution quantities needed. In the case of the Coulomb integrals, a new set of B functions is needed for each new two-orbital charge distribution on center B. However, the resulting function G of Eq. (37) is used with all possible orbital choices on center A; in this way, the time required per integral is kept low.

Another feature arising with Coulomb integrals is that the summation parameter L appears as an argument of the second index of the functions B. Thus, a table of B-function values is needed; however, all of these functions have the same arguments r_A, R, and β. Thus, only one set of auxiliary functions I_v or E_v need be computed to produce the full array of required B functions. Since the calculation of the I_v or E_v functions is the time-limiting step, the time required for computing B functions is kept from becoming excessive.

The final integration over r_A indicated in Eqs. (24) and (36) is performed numerically by splitting the range into two intervals, namely, $(0, R)$ and (R, ∞). This is a natural choice since the calculation of the B functions splits into the same two ranges. Gauss-Legendre quadrature[26a] is employed in the first range after a suitable change of variable. In the second range, since the functions B contain an explicit exponential dependence of $\exp(-\zeta r_A)$ and for hybrid integrals an additional exponential factor embedded in F, a Gauss–Laguerre procedure[26b] could be used to take account of this property. However, because of the presence of different orbital exponents for each charge distribution, a different set of integration points would be required for each new charge distribution. Therefore, to make efficient use of the charge distribution concept, a Gauss–Legendre process is better suited to the second integration range, since all integrals can be evaluated using the same set of numerical grid points in this case. It should be noted that the argument of the I or E functions required for evaluating the B functions in the outer integration range is a constant: ζR. A partial check on the over-all accuracy of the numerical integration schemes is provided by the use of Eq. (40).

To obtain the exchange charge distribution function X_{lm} of Eq. (46), the integration is split into the two ranges $(0, R/r)$ and $(R/r, \infty)$. This takes cognizance of the fact that the functions F_{lm} are tabulated for a specific set of integration points over the two ranges $(0, R)$ and (R, ∞). The exchange integral can thus be evaluated by performing the quadratures in both Eqs. (46) and (49) by using the already tabulated function values. This is tantamount to a final double numerical integration plus the infinite series. The fact that the hybrid charge distribution functions F_{lm} can be reused for this purpose is encouraging, but the previous exchange scheme[3] has an advantage in that it involves an infinite series with only one final numerical integration.

The unified treatment for the Coulomb and hybrid integral types makes double use of the one-center charge distribution functions f_{lm} of Eq. (16). The two charge distributions F_{lm} and G_{lm} of Eqs. (25) and (37) require all the same auxiliary functions and the same constants. The latter are quite simple and only small arrays of them are needed. Exploitation of these features offers a considerable savings in the computer evaluation of these integrals. Furthermore, all the two-center, one-electron integrals (overlap, nuclear attraction, and kinetic energy) can be obtained concurrently by making use of the various charge distribution functions calculated for the two-electron integrals.

---

* Work supported by the Department of the Navy, Naval Ordnance Systems Command, under Contract No. N00017-62-C-0604.

1 D. M. Silver and K. Ruedenberg, J. Chem. Phys. **49**, 4306 (1968).
2 R. E. Christoffersen and K. Ruedenberg, J. Chem. Phys. **49**, 4285 (1968).
3 E. L. Mehler and K. Ruedenberg, J. Chem. Phys. **50**, 2575 (1969).
4 K. Ruedenberg, J. Chem. Phys. **19**, 1459 (1951); *Molecular Orbitals in Chemistry, Physics and Biology*, P. O. Löwdin and B. A. Pullmann, Eds. (Academic, New York, 1964), p. 215.
5 C. C. J. Roothaan, J. Chem. Phys. **19**, 1445 (1951).
6 K. Ruedenberg, C. C. J. Roothaan, and W. Jaunzemis, J. Chem. Phys. **24**, 201 (1956).
7 C. C. J. Roothaan, J. Chem. Phys. **24**, 947 (1956).
8 K. O-Ohata and K. Ruedenberg, J. Math. Phys. **7**, 547 (1966).
9 K. J. Miller, J. Math. Phys. **9**, 1292 (1968).
10 I. I. Guseinov, J. Phys. B. **3**, 1399 (1970).
11 A. C. Wahl, P. E. Cade, and C. C. J. Roothaan, J. Chem. Phys. **41**, 2578 (1964).
12 F. E. Harris and H. H. Michels, Advan. Chem. Phys. **13**, 205 (1967).
13 I. Shavitt and M. Karplus, J. Chem. Phys. **43**, 398 (1965).
14 A. C. Wahl and R. H. Land, Intern. J. Quantum Chem. **1S**, 375 (1967); J. Chem. Phys. **50**, 4725 (1969).
15 S. Huzinaga, Progr. Theoret. Phys. **40**, Suppl. 52 (1967).
16 D. M. Silver and K. Ruedenberg, J. Chem. Phys. **49**, 4301 (1968).
17 M. B. Milleus, M. Twerdochlib, and J. O. Hirschfelder, J. Chem. Phys. **45**, 13 (1966).
18 E. W. Hobson, *The Theory of Spherical and Ellipsoidal Harmonics* (Cambridge U. P., Cambridge, England, 1931), Sec. 89.
19 R. J. Buehler and J. O. Hirschfelder, Phys. Rev. **83**, 628 (1951).
20 P. R. Fontana, J. Math. Phys. **2**, 825 (1961).
21 R. M. Pitzer, C. W. Kern, and W. N. Lipscomb, J. Chem. Phys. **37**, 267 (1962).
22 Y. N. Chiu, J. Math. Phys. **5**, 283 (1964).
23 K. Ruedenberg, K. O-Ohata, and D. G. Wilson, J. Math. Phys. **7**, 539 (1966).
24 W. England and K. Ruedenberg, J. Chem. Phys. **54**, 2291 (1971); in this reference, the correct lower limit for λ should be 0 and that for δ should be $\max[0, \lambda - n]$.
25 F. J. Corbato, J. Chem. Phys. **24**, 452 (1956).
26 *Handbook of Mathematical Tables*, M. Abramowitz and I. A. Stegun, Eds. (Natl. Bur. Std. Appl. Math. Ser. 55, Washington, D.C. 1964): (a) p. 887, Eq. (25. 4. 29); (b) p. 890, Eq. (25. 4. 45).

Linear Random Operator Equations in Mathematical Physics. II

G. Adomian
Department of Mathematics, University of Georgia, Athens, Georgia 30601
(Received 2 September 1970, Revised Manuscript Received 25 January 1971)

This paper is a continuation of Paper I [J. Math. Phys. 11, 1069 (1970)]. A general expression is determined for the stochastic Green's function (SGF) for two-point correlation functions, and various useful relationships are determined between the stochastic Green's functions for various statistical measures and between the stochastic Green's functions, random Green's functions, and ordinary Green's functions. In the author's dissertation and earlier papers, SGF was given as an ensemble average of the product of random Green's functions. This random Green's function is now specified in terms of an ordinary Green's function for a deterministic operator and a resolvent kernel which can be calculated for the random part of the stochastic operator. Hence that SGF is determinable which yields the desired statistical measure of the solution process directly. Second, the two-point correlation function of the solution process is found for the perturbation case. It is also demonstrated that, in the event that perturbation theory is adequate to deal with the randomness involved, the correct two-point correlation of the solution process is easily specialized from the general expression, i.e., the results of perturbation theory are obtained from the SGF of Adomian when perturbation theory is applicable.

1. GENERAL STOCHASTIC GREEN'S FUNCTION FOR CORRELATIONS

The present author[1] has defined the "stochastic Green's function" (SGF) for correlations as the kernel G_H relating the output (or solution process) correlation R_y to the input correlation function R_x in the expression

$$R_y(t_1, t_2) = \iint G_H(t_1, t_2, \tau_1, \tau_2) R_x(\tau_1, \tau_2) d\tau_1 d\tau_2. \tag{1.1}$$

A very detailed example, for the special case where stationarity could be assumed throughout[2] gave the spectral density for a randomly sampled random process and the well-known results of filter theory in the limiting case of a deterministic filter. Our purpose now is to look at the kernel G_H in a more comprehensive manner. Using terminology and symbols of Paper I, we can write the stochastic differential equation $\mathfrak{L}y = x$, where $\mathfrak{L}$ is a stochastic (differential) operator involving stochastic process coefficients $a_\nu(t, \omega)$, $t \in T$, $\omega \in (\Omega, \mathfrak{F}, \mu)$ as

$$y(t) = F(t) - \int K(t, \tau) y(\tau) d\tau, \tag{1.2}$$

where

$$F(t) = \int l(t, \tau) x(\tau) d\tau + \Sigma c_\nu \Phi_\nu.$$

Then

$$\begin{aligned} R_y(t_1, t_2) &= \langle y(t_1) \overset{*}{y}(t_2) \rangle \\ &= \langle (F(t_1) - \int K(t_1, \tau_1) y(\tau_1) d\tau_1) \\ &\times (\overset{*}{F}(t_2) - \int \overset{*}{K}(t_2, \tau_2) \overset{*}{y}(\tau_2) d\tau_2) \rangle \\ &= \langle F(t_1) \overset{*}{F}(t_2) \rangle - \int \langle K(t_1, \tau_1) \overset{*}{F}(t_2) y(\tau_1) \rangle d\tau_1 \\ &\quad - \int \langle \overset{*}{K}(t_2, \tau_2) F(t_1) \overset{*}{y}(\tau_2) \rangle d\tau_2 \\ &\quad + \iint \langle K(t_1, \tau_1) \overset{*}{K}(t_2, \tau_2) y(\tau_1) \overset{*}{y}(\tau_2) \rangle d\tau_1 d\tau_2 \end{aligned} \tag{1.3}$$

Using Adomian's iteration procedure in Paper I, we can write Eq. (2) in terms of iterated kernels as used by Sibul[3] thus:

$$y(t) = F(t) - \sum_{m=0}^{\infty} \int (-1)^{m+1} K_{m+1}(t, \tau) F(\tau) d\tau, \tag{1.4}$$

where $K_m(t, \tau)$ is defined by the recurrence formula

$$K_m(t, \tau) = \int K(t, \tau_1) K_{m-1}(\tau_1, \tau) d\tau_1, \tag{1.5}$$

with $K_1 = K$.

Thus

$$\begin{aligned} y(t) &= F(t) - \int K(t, \tau) y(\tau) d\tau \\ &= F(t) - \int K(t, \tau) [y_0 - y_1 + y_2 + \cdots] d\tau \\ &= F(t) - \int K(t, \tau) y_0(\tau) d\tau + \int K(t, \tau) y_1(\tau) d\tau - \cdots \\ &= y_0 - y_1 + y_2 - \cdots \\ &= F(t) - \int K(t, \tau) F(\tau) d\tau \\ &\quad + \int K(t, \tau_1) K(\tau_1, \tau) F(\tau) d\tau \cdots \\ &= F(t) + \sum_{m=0}^{\infty} \int (-1)^{m+1} K_{m+1}(t, \tau) F(\tau) d\tau. \end{aligned}$$

If the sum is uniformly convergent, then summation and integration can be interchanged[3] in (1.4).[4] Defining the resolvent kernel $\Gamma(t, \tau) = \sum_{m=0}^{\infty} (-1)^m K_{m+1}(t, \tau)$ allows us to write very conveniently

$$y(t) = F(t) + \int \Gamma(t, \tau) F(\tau) d\tau. \tag{1.6}$$

Writing $R_y(t_1, t_2)$, we now have

$$\begin{aligned} R_y(t_1, t_2) &= \langle F(t_1) \overset{*}{F}(t_2) \rangle - \int \langle \Gamma(t_1, \tau_1) \overset{*}{F}(t_2) F(\tau_1) \rangle d\tau_1 - \int \langle \overset{*}{\Gamma}(t_2, \tau_2) F(t_1) \overset{*}{F}(\tau_2) \rangle d\tau_2 \\ &\quad + \iint \langle \Gamma(t_1, \tau_1) \overset{*}{\Gamma}(t_2, \tau_2) F(\tau_1) \overset{*}{F}(\tau_2) \rangle d\tau_1 d\tau_2. \end{aligned} \tag{1.7}$$

In order to separate out $\langle F(\tau_1) \overset{*}{F}(\tau_2) \rangle$, we can rewrite (1.7) as

$$R_y(t_1,t_2) = \iint\langle F(\tau_1)\overset{*}{F}(\tau_2)\rangle\delta(\tau_1-t_1)\delta(\tau_2-t_2)d\tau_1 d\tau_2 - \iint\langle\Gamma(t_1,\tau_1)\rangle\langle F(\tau_1)\overset{*}{F}(\tau_2)\rangle\delta(\tau_2-t_2)d\tau_1 d\tau_2$$
$$- \iint\langle\overset{*}{\Gamma}(t_2,\tau_2)\rangle\langle F(\tau_1)\overset{*}{F}(\tau_2)\rangle\delta(\tau_1-t_1)d\tau_1 d\tau_2 + \iint\langle\Gamma(t_1,\tau_1)\overset{*}{\Gamma}(t_2,\tau_2)\rangle\langle F(\tau_1)\rangle\overset{*}{F}(\tau_2)\rangle d\tau_1 d\tau_2, \tag{1.8}$$

where

$$\langle F(\tau_1)\overset{*}{F}(\tau_2)\rangle = R_F(\tau_1,\tau_2) = \iint G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)R_x(\sigma_1,\sigma_2)d\sigma_1 d\sigma_2. \tag{1.9}$$

Substituting (9) into (8), we get

$$R_y(t_1,t_2) = \iiiint G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)R_x(\sigma_1,\sigma_2)$$
$$\times\delta(\tau_1-t_1)\delta(\tau_2-t_2)\,d\tau_1 d\tau_2 d\sigma_1 d\sigma_2 - \iiiint\langle\Gamma(t_1,\tau_1)\rangle G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)R_x(\sigma_1,\sigma_2)\delta(\tau_2-t_2)$$
$$\times d\tau_1 d\tau_2 d\sigma_1 d\sigma_2 - \iiiint\langle\overset{*}{\Gamma}(t_2,\tau_2)\rangle G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)R_x(\sigma_1,\sigma_2)\delta(\tau_1-t_1)d\tau_1 d\tau_2 d\sigma_1 d\sigma_2$$
$$+ \iiiint\langle\Gamma(t_1,\tau_1)\overset{*}{\Gamma}(t_2,\tau_2)\rangle G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)R_x(\sigma_1,\sigma_2)d\tau_1 d\tau_2 d\sigma_1 d\sigma_2,$$

which is the same as the general expression

$$R_y(t_1,t_2) = \iint G_H(t_1,t_2,\sigma_1,\sigma_2)R_x(\sigma_1,\sigma_2)d\sigma_1 d\sigma_2,$$

where

$$G_H = \iint G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)\delta(\tau_1-t_1)\delta(\tau_2-t_2)d\tau_1 d\tau_2 - \iint\langle\Gamma(t_1,\tau_1)\rangle G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)\delta(\tau_2-t_2)$$
$$\times d\tau_1 d\tau_2 - \iint\langle\overset{*}{\Gamma}(t_2,\tau_2)\rangle G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)\delta(\tau_1-t_1)d\tau_1 d\tau_2 + \iint\langle\Gamma(t_1,\tau_1)\overset{*}{\Gamma}(t_2,\tau_2)\rangle$$
$$\times G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)d\tau_1 d\tau_2 \tag{1.10}$$

is the stochastic Green's function[5] if two-point correlations are used for the statistical measures of the input (forcing function) or output (solution process or dependent variable). [We have, as before, used statistical independence of the random coefficients and the forcing function to separate ensemble averages involving Γ and $F(t)$.] When there is no random term ($R = 0$) the last three terms of G_H are zero, so

$$R_y(t_1,t_2) = \iint G(t_1,\sigma_1)\overset{*}{G}(t_2,\sigma_2)R_x(\sigma_1,\sigma_2)d\sigma_1 d\sigma_2,$$

where G's are, of course, ordinary (deterministic) Green's functions.

2. RELATIONSHIPS BETWEEN KERNEL FUNCTIONS (OR SGF'S FOR VARIOUS STATISTICAL MEASURES)

In I, the SGF's were given for various statistical measures of input and output [see Eqs. (I. 2. 1) for $R_y(t_1,t_2)$ or (I. 2. 3) for $R_y(\beta)$ (assuming stationarity) or (I. 2. 4) for the spectral density (also assuming stationarity holds)]. Equation (1.10) in this paper seems to show a more complicated kernel. Thus

$$R_y(t_1,t_2) = \iint G_H(t_1,t_2,\sigma_1,\sigma_2)R_x(\sigma_1,\sigma_2)d\sigma_1 d\sigma_2,$$

where the SGF G_H is given by

$$G_H = G(t_1,\sigma_1)\overset{*}{G}(t_2,\sigma_2) - \int\langle\Gamma(t_1,\tau_1)\rangle G(\tau_1,\sigma_1)$$
$$\times\overset{*}{G}(t_2,\sigma_2)d\tau_1 - \int\langle\overset{*}{\Gamma}(t_2,\tau_2)\rangle G(t_1,\sigma_1)$$
$$\times\overset{*}{G}(\tau_2,\sigma_2)d\tau_2 + \iint\langle\Gamma(t_1,\tau_1)\overset{*}{\Gamma}(t_2,\tau_2)\rangle$$
$$\times G(\tau_1,\sigma_1)\overset{*}{G}(\tau_2,\sigma_2)d\tau_1 d\tau_2. \tag{2.1}$$

This kernel is of course identical to the corresponding kernel in Paper I. There, the H is a stochastic operator and $h(t,\sigma)$ is a random Green's function, not the Green's function G corresponding to the deterministic operator L^{-1}.[6] From (2.1) in Paper I we had

$$G_H(t_1,t_2,\sigma_1,\sigma_2) = \langle h(t_1,\sigma_1)h^*(t_2,\sigma_2)\rangle,$$

which is the same as (1.1) above. Hence we see immediately that

$$h(t,\sigma) = G(t,\sigma) - \int\Gamma(t,\tau)G(\tau,\sigma)d\tau, \tag{2.2}$$

a rather simple relation between the various Green's functions: the random Green's function h, a random quantity from which the SGF is easily found, the deterministic Green's function G (or sometimes l), and the resolvent kernel. Thus the results generalize and make more useful some of the results of the author.[2]

This expression clearly shows we can indeed compute the SGF for any statistical measure, e.g.,

for $R_y(t_1, t_2)$, as soon as h can be determined (by the indicated average of a product of h functions); and h can be determined since it depends on the known G and the resolvent kernel Γ, which can be found for reasonable operators R. Thus, for a given stochastic differential equation, after deciding we want a particular statistical measure (s.m.) of the solution process, we calculate the appropriate SGF which yields the desired s.m. in terms of the s.m. of the given random input.

3. PERTURBATION CASE FOR CORRELATIONS

In the event that perturbation theory is adequate to deal with the randomness involved (see I), we can let $R = \epsilon\mathfrak{L}_1$, where $\langle\mathfrak{L}_1\rangle = 0$ is the general expression for the stochastic Green's function. First, however, let us see the results to be expected by extending the conventional approach as used for the expectation $\langle y\rangle$ to the case of correlation measures $R_y(t_1, t_2) = \langle y(t_1)y(t_2)\rangle$:

$$\begin{aligned} y &= L^{-1}x - \epsilon L^{-1}\mathfrak{L}_1 y \\ &= L^{-1}x - \epsilon L^{-1}\mathfrak{L}_1[y_0 + \epsilon y_1 + \epsilon^2 y_2 + O(\epsilon^3)] \\ &= L^{-1}x - \epsilon L^{-1}\mathfrak{L}_1 L^{-1}x + \epsilon^2 L^{-1}\mathfrak{L}_1 L^{-1}\mathfrak{L}_1 L^{-1}x \\ &\quad - O(\epsilon^3). \end{aligned}$$

If $x = g_0 + \epsilon g_1 + \epsilon^2 g_2$, with $\langle g_1\rangle = \langle g_2\rangle = 0$, absorbing the means into $\langle g_0\rangle$, if they exist, leads immediately to[1]

$$\langle y\rangle = L^{-1}\langle x\rangle + \epsilon^2 L^{-1}\langle\mathfrak{L}_1 L^{-1}\mathfrak{L}_1\rangle L^{-1}\langle x\rangle,$$
$$\langle y\rangle = [1 + \epsilon^2 L^{-1}\langle\mathfrak{L}_1 L^{-1}\mathfrak{L}_1\rangle]L^{-1}\langle g_0\rangle,$$

assuming R and x are uncorrelated, as in I. In the same manner we can extend to correlations $R_y(t_1, t_2)$:

$$y(t) = L^{-1}(t)x(t) - \epsilon L^{-1}(t)\mathfrak{L}_1(t)L^{-1}(t)x(t) + \epsilon^2 L^{-1}(t)\mathfrak{L}_1(t)L^{-1}(t)\mathfrak{L}_1(t)L^{-1}(t)x(t), \tag{3.1}$$

$$y(t) = L^{-1}g_0 + \epsilon L^{-1}g_1 + \epsilon^2 L^{-1}g_2 - \epsilon L^{-1}\mathfrak{L}_1 L^{-1}g_0 - \epsilon^2 L^{-1}\mathfrak{L}_1 L^{-1}g_1 + \epsilon^2 L^{-1}\mathfrak{L}_1 L^{-1}\mathfrak{L}_1 L^{-1}g_0,$$

$$\begin{aligned} R_y(t_1, t_2) &= \langle L^{-1}(t_1)g_0(t_1)L^{-1}(t_2)g_0(t_2)\rangle + \epsilon\langle L^{-1}(t_1)g_0(t_1)L^{-1}(t_2)g_1(t_2)\rangle + \epsilon^2\langle L^{-1}(t_1)g_0(t_1)L^{-1}(t_2)g_2(t_2)\rangle \\ &\quad - \epsilon\langle L^{-1}(t_1)g_0(t_1)L^{-1}(t_2)\mathfrak{L}_1(t_2)L^{-1}(t_2)g_0(t_2)\rangle - \epsilon^2\langle L^{-1}(t_1)g_0(t_1)L^{-1}(t_2)\mathfrak{L}_1(t_2)L^{-1}(t_2)g_1(t_2)\rangle \\ &\quad + \epsilon^2\langle L^{-1}(t_1)g_0(t_1)L^{-1}(t_2)\mathfrak{L}_1(t_2)L^{-1}(t_2)\mathfrak{L}_1(t_2)L^{-1}(t_2)g_0(t_2)\rangle + \epsilon\langle L^{-1}(t_1)g_1(t_1)L^{-1}(t_2)g_0(t_2)\rangle \\ &\quad + \epsilon^2\langle L^{-1}(t_1)g_1(t_1)L^{-1}(t_2)g_1(t_2)\rangle - \epsilon^2\langle L^{-1}(t_1)g_1(t_1)L^{-1}(t_2)\mathfrak{L}_1(t_2)L^{-1}(t_2)g_0(t_2)\rangle \\ &\quad + \epsilon^2\langle L^{-1}(t_1)g_2(t_1)L^{-1}(t_2)g_0(t_2)\rangle - \epsilon\langle L^{-1}(t_1)\mathfrak{L}_1(t_1)L^{-1}(t_1)g_0(t_1)L^{-1}(t_2)g_0(t_2)\rangle \\ &\quad - \epsilon^2\langle L^{-1}(t_1)\mathfrak{L}_1(t_1)L^{-1}(t_1)g_0(t_1)g_0(t_1)L^{-1}(t_2)g_1(t_2)\rangle - \epsilon^2\langle L^{-1}(t_1)\mathfrak{L}_1(t_1)L^{-1}(t_1)g_1(t_1)L^{-1}(t_2)g_0(t_2)\rangle \\ &\quad + \epsilon^2\langle L^{-1}(t_1)\mathfrak{L}_1(t_1)L^{-1}(t_1)\mathfrak{L}_1(t_1)L^{-1}(t_1)g_0(t_1)L^{-1}(t_2)g_0(t_2)\rangle. \end{aligned} \tag{3.2}$$

The fourth, fifth, ninth, twelth, and thirteenth terms vanish because $\langle\mathfrak{L}_1\rangle = 0$. Rewriting in terms of the Green's function $l(t, \tau)$ rather than the operator L^{-1} and rearranging in powers of ϵ, we obtain

$$\begin{aligned} R_y(t_1, t_2) &= \iint l(t_1, \tau_1)l(t_2, \tau_2)[\langle g_0(\tau_1)g_0(\tau_2)\rangle + \epsilon\langle g_0(\tau_1)g_1(\tau_2)\rangle + \epsilon\langle g_1(\tau_1)g_0(\tau_2)\rangle + \epsilon^2\langle g_0(\tau_1)g_2(\tau_2)\rangle \\ &\quad + \epsilon^2\langle g_1(\tau_1)g_1(\tau_2)\rangle + \epsilon^2\langle g_2(\tau_1)g_0(\tau_2)\rangle]d\tau_1 d\tau_2 + \epsilon^2\iiiint l(t_1, \tau_1)l(t_2, \tau_2)l(\tau_2, \tau_3)l(\tau_3, \tau_4) \\ &\quad \times \langle\mathfrak{L}_1(\tau_2)\mathfrak{L}_1(\tau_3)\rangle\langle g_0(\tau_1)g_0(\tau_4)\rangle d\tau_1\cdots d\tau_4 + \epsilon^2\iiiint l(t_1, \tau_1)l(\tau_1, \tau_2)l(\tau_2, \tau_3)l(t_2, \tau_4) \\ &\quad \times \langle\mathfrak{L}_1(\tau_1)\mathfrak{L}_1(\tau_2)\rangle\langle g_0(\tau_3)g_0(\tau_4)\rangle d\tau_1\cdots d\tau_4. \end{aligned} \tag{3.3}$$

Rearranging the order of the last two terms and of the repeated τ's to see the symmetry better, we find

$$\begin{aligned} R_y(t_1, t_2) &= \iint l(t_1, \tau_1)l(t_2, \tau_2)[\langle g_0(\tau_1)g_0(\tau_2)\rangle + \epsilon\langle g_0(\tau_1)g_1(\tau_2)\rangle + \epsilon\langle g_1(\tau_1)g_0(\tau_2)\rangle + \epsilon^2\langle g_0(\tau_1)g_2(\tau_2)\rangle \\ &\quad + \epsilon^2\langle g_1(\tau_1)g_1(\tau_2)\rangle + \epsilon^2\langle g_2(\tau_1)g_0(\tau_2)\rangle]d\tau_1 d\tau_2 + \epsilon^2\iiiint l(t_1, \tau_1)l(\tau_1, \tau_1')l(\tau_1', \tau_1'')l(t_2, \tau_2) \\ &\quad \times \langle\mathfrak{L}_1(\tau_1)\mathfrak{L}_1(\tau_1')\rangle\langle g_0(\tau_1'')g_0(\tau_2)\rangle d\tau_1 d\tau_1' d\tau_1'' d\tau_2 + \epsilon^2\iiiint l(t_2, \tau_2)l(\tau_2, \tau_2')l(\tau_2', \tau_2'')l(t_1, \tau_1)\rangle \\ &\quad \times \langle\mathfrak{L}_1(\tau_2)\mathfrak{L}_1(\tau_2')\rangle\langle g_0(\tau_1)g_0(\tau_2'')\rangle d\tau_2 d\tau_2' d\tau_2'' d\tau_1 \end{aligned} \tag{3.4}$$

4. PERTURBATION RESULTS FROM STOCHASTIC GREEN'S FUNCTION

We now use Adomian's stochastic Green's function (SGF) [for correlation measures of input and output from Eq. (1.10)] to verify the perturbation case, i.e., the case where randomness is relatively insignificant, and hence could be handled by conventional perturbation theory. To calculate the SGF, we need the resolvent kernel Γ, i.e.,

$$\Gamma(t_1,\tau_1)=\sum_m(-1)^m K_{m+1}(t_1,\tau_1).$$

Since $K_1(t_1,\tau_1)=G(t_1,\tau_1)R(\tau_1)$ and R is zero mean, clearly

$$\langle K_1\rangle=0,$$

and

$$-K_2(t_1,\tau_1)=-\int K(t_1,\tau_1')K(\tau_1',\tau_1)d\tau_1'$$
$$=-\int G(t_1,\tau_1')\epsilon\mathfrak{L}_1(\tau_1')G(\tau_1',\tau_1)\epsilon\mathfrak{L}_1(\tau_1)d\tau_1',$$

which we get by replacing R with $\epsilon\mathfrak{L}_1$ (see Paper I). Hence

$$\langle\Gamma(t_1,\tau_1)\rangle=0+\langle-K_2(t_1,\tau_1)\rangle+\mathcal{O}(\epsilon^3).$$

Thus, to order ϵ^2,

$$\langle\Gamma(t_1,\tau_1)\rangle=-\epsilon^2\int G(t_1,\tau_1')G(\tau_1',\tau_1)\langle\mathfrak{L}_1(\tau_1')\times\mathfrak{L}_1(\tau_1)\rangle d\tau_1'.$$

The four terms of the SGF G_H are now easily determined. The first term is simply $G(t_1,\sigma_1)G(t_2,\sigma_2)$. Since $x(t)=g_0(t)+\epsilon g_1(t)+\epsilon^2 g_2(t)$, we have

$$R_x(\sigma_1,\sigma_2)=\langle x(\sigma_1)x(\sigma_2)\rangle=\langle g_0(\sigma_1)g_0(\sigma_2)\rangle+\epsilon\langle g_0(\sigma_1)g_1(\sigma_2)\rangle+\epsilon^2\langle g_0(\sigma_1)g_2(\sigma_2)\rangle+\epsilon\langle g_1(\sigma_1)g_0(\sigma_2)+\epsilon^2\langle g_1(\sigma_1)g_1(\sigma_2)\rangle+\epsilon^2\langle g_2(\sigma_1)g_0(\sigma_2)\rangle.$$

We see[7] that

$$R_y(t_1,t_2)=\iint G(t_1,\sigma_1)G(t_2,\sigma_2)R_x(\sigma_1,\sigma_2)d\sigma_1 d\sigma_2$$

gives exactly the double integral terms of Eq. (3.4). The remaining fourfold integral terms come from the terms of G_H which involve the resolvent kernel Γ, specifically, the second and third since the fourth is higher in ϵ than we are interested.

The second term of G_H is

$$-\int\langle\Gamma(t_1,\tau_1)\rangle G(\tau_1,\sigma_1)G(t_2,\sigma_2)d\tau_1,$$

into which we substitute the calculated $\langle\Gamma\rangle$ from above. Hence the second term for G_H becomes

$$\epsilon^2\iint G(t_1,\tau_1')G(\tau_1',\tau_1)G(\tau_1,\sigma_1)G(t_2,\sigma_2)\times\langle\mathfrak{L}_1(\tau_1')\mathfrak{L}_1(\tau_1)\rangle d\tau_1'd\tau_1.$$

The third term is

$$-\int\Gamma(t_2,\tau_2)G(t_1,\sigma_1)G(\tau_2,\sigma_2)d\tau_2$$

or

$$\epsilon^2\iint G(t_2,\tau_2')G(\tau_2',\tau_2)G(\tau_2,\sigma_2)G(t_1,\sigma_1)\times\langle\mathfrak{L}_1(\tau_2')\mathfrak{L}_1(\tau_2)\rangle d\tau_2'd\tau_2,$$

which when used in the expression for $R_y(t_1,t_2)$ obviously is identical to the fourfold integral terms of Eq. (3.4). Hence we have verified that the results of perturbation theory can be obtained from the SGF of Adomian when perturbation theory is applicable.

5. PERTURBATION RESULTS FROM THE RANDOM GREEN'S FUNCTION $h(t,\tau)$

The random Green's function $h(t,\tau)$ was given by

$$h(t,\tau)=G(t,\tau)-\int\Gamma(t,\sigma)G(\sigma,\tau)d\sigma;\qquad(5.1)$$

hence $y(t)=\int h(t,\tau)x(\tau)d\tau$. Consequently,

$$y(t)=\int G(t,\tau)x(\tau)d\tau-\iint\Gamma(t,\sigma)G(\sigma,\tau)x(\tau)d\sigma\,d\tau;$$

averaging, we have

$$\langle y(t)\rangle=\int G(t,\tau)\langle x(\tau)\rangle d\tau-\iint\langle\Gamma(t,\sigma)G(\sigma,\tau)x(\tau)\rangle d\sigma\,d\tau.$$

Expanding the resolvent kernel $\Gamma(t,\sigma)$ in terms of iterated kernels, we have

$$\langle y(t)\rangle=\int G(t,\tau)\langle x(\tau)\rangle d\tau-\iint G(t,\tau_1)\langle R(\tau_1)\rangle G(\tau_1,t)\langle x(\tau)\rangle d\tau_1 d\tau+\iiint G(t,\tau_1)G(\tau_1,\tau_2)\langle R(\tau_1)R(\tau_2)\rangle\times G(\tau_2,\tau)\langle x(\tau)\rangle d\tau_2 d\tau_1 d\tau-\iiint\int G(t_1,\tau_1)G(\tau_1,\tau_2)G(\tau_2,\tau_3)\langle R(\tau_1)R(\tau_2)R(\tau_3)\rangle G(\tau_3,\tau)\langle x(\tau)\rangle\times d\tau_3 d\tau_2 d\tau_1 d\tau+\cdots.$$

If $R=\epsilon\mathfrak{L}_1+\epsilon^2\mathfrak{L}_2$ and $x=g_0+\epsilon g_1+\epsilon^2 g_2=g$, as before, we have

$$\langle y(t)\rangle=\int G(t,\tau)\langle(g_0+\epsilon g_1+\epsilon^2 g_2)\rangle d\tau-\iint G(t,\tau_1)\langle\epsilon\mathfrak{L}_1(\tau_1)\rangle G(\tau_1,\tau)\langle g_0+\epsilon g_1+\epsilon^2 g_2\rangle d\tau_1 d\tau-\iint G(t,\tau_1)\langle\epsilon^2\mathfrak{L}_2(\tau_1)\rangle G(\tau_1,\tau)g_0 d\tau_1 d\tau+\iiint G(t,\tau_1)G(\tau_1,\tau_2)\langle\epsilon^2\mathfrak{L}_1(\tau_1)\mathfrak{L}_1(\tau_2)\rangle G(\tau_2,\tau)\times\langle g_0+\epsilon g_1+\epsilon^2 g_2\rangle d\tau_2 d\tau_1 d\tau+O(\epsilon^3)$$

or, equivalently,

$$\langle y(t)\rangle = L^{-1}\langle g_0 + \epsilon g_1 + \epsilon^2 g_2\rangle - \epsilon L^{-1}\langle \mathfrak{L}_1\rangle L^{-1}\langle g_0 + \epsilon g_1\rangle - \epsilon^2 L^{-1}\langle \mathfrak{L}_2\rangle L^{-1} g_0 + \epsilon^2 L^{-1}\langle \mathfrak{L}_1 L^{-1}\mathfrak{L}_1\rangle \times L^{-1} g_0 + O(\epsilon^3).$$

If $\langle \mathfrak{L}_1\rangle = \langle \mathfrak{L}_2\rangle = 0$,

$$\langle y(t)\rangle = L^{-1}\langle g\rangle + \epsilon^2 L^{-1}\langle \mathfrak{L}_1 L^{-1}\mathfrak{L}_1\rangle L^{-1} g_0$$

or, if $g_1 = g_2 = 0$ so that $g_0 = g$,

$$\langle y(t)\rangle = (1 + \epsilon^2 L^{-1}\langle \mathfrak{L}_1 L^{-1}\mathfrak{L}_1\rangle) L^{-1} g$$

as derived in Paper I. We have already demonstrated that the correlation result, for the case where perturbation theory is valid, can be derived from the SGF. It clearly could be found by writing $h(t, \tau)$.

ACKNOWLEDGMENTS

This work has been supported by the National Aeronautics and Space Administration under Grant No. NGR11-003-020 and by the office of Naval Research, under Contract No. N00014-69-A-0423-Themis.

[1] G. Adomian, J. Math. Phys. 11, 1069 (1970).
[2] G. Adomian, Ph. D. thesis (UCLA, 1961) (unpublished).
[3] L. H. Sibul, Ph. D. thesis (Pennsylvania State University, 1968) (unpublished).
[4] A separate paper will deal with rates of convergence and comparison with hierarchy methods.
[5] Obviously some integrations can be carried out, but we leave the expression this way.
[6] l has also been used in the author's previous work.
[7] $G(t, \tau) = l(t, \tau)$.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Linear Random Operator Equations in Mathematical Physics. III

G. Adomian

Department of Mathematics, University of Georgia, Athens, Georgia 30601

(Received 2 September 1970; Revised Manuscript Received 25 January 1971)

The problem of wave motion in a stochastic medium is treated as an application of stochastic operator theory and as a generalization of Papers I and II (and previous work by the author) to the case of partial differential equations and random fields without monochromaticity assumptions and closure approximations. Connections to the theory of partial coherence are considered. The stochastic Green's function for the two-point correlation of the solution process can be determined so the correlation can be obtained. Spectral spreading in a "hot" medium is easily demonstrable and can be calculated.

INTRODUCTION

The problem of wave motion in a stochastic or randomly inhomogeneous or fluctuating medium arises in a number of interesting contexts in physics and as a natural generalization of Paper I (Ref. 1) to the case of partial differential equations. The refractive index is assumed to be a random point function or stochastic process (SP) rather than a random variable. Use of stochastic distributions is, of course, suggested; however, it is desirable to keep the formulation initially simple since there already exist a number of complexities not present in usual treatments. (For the same reason the nonlinear stochastic problem is deferred.) Nearly all studies of wave propagation in a random continuum utilize the monochromatic or quasi-monochromatic assumption of harmonic time dependence and essentially no spectral spreading, and therefore proceed immediately to a reduced wave equation or Helmholtz equation. Thus the field quantity becomes a functional of a random process $k(\bar{x})$ rather than $k(\bar{x}, t)$ or, more completely, $k(\bar{x}, t, \omega)$, where $\omega \in (\Omega, \mathfrak{F}, \mu)$, a probability space. (See, e.g., Beran and Parrent[2] or Beran.[3]) Keller,[4] e.g., considered the scalar (reduced) wave equation $(\nabla^2 + k^2 n^2(\bar{x}))u = g(\bar{x})$, where $g(\bar{x})$ is the source distribution and there exists an appropriate condition on u and ∇u (radiation condition). k is the propagation constant for the medium, and n is the refractive index. Let $n^2(\bar{x}) = 1 + \mu(\bar{x})$, where $\mu(\bar{x})$ is a zero-mean SP. Then $(\nabla^2 + k^2)u + k^2\mu(\bar{x})u = g(\bar{x})$ or $\mathfrak{L}u = g$, where $\mathfrak{L}$ is a stochastic operator separable into the sum of a deterministic operator $L = \nabla^2 + k^2$ and a random operator R. The deterministic operator $L = \nabla^2 + k_0^2$. The Green's function $G(\bar{x} - \bar{x}') = G(r) = \exp(ik_0 r)/4\pi r = \exp(ik_0|x - x'|)/4\pi|x - x'|$. In a uniform or nonrandom medium, $n = 1$ and $(\nabla^2 + k^2)u = g$. The stochastic medium may, of course, be considered an ensemble of possible media with a probability distribution giving probabilities for various members of the ensemble.

The medium may not be known precisely, and the objective is to determine what is likely; it may be too complex to specify, or it may be randomly fluctuating. Most results involving stochastic equations in physics and engineering have been obtained by averaging procedures, closure, or truncation approximations (hierarchy methods, perturbation theories, etc.), self-consistent field approximations, and restriction to very special processes. Many of these have correlated well

$$\langle y(t)\rangle = L^{-1}\langle g_0 + \epsilon g_1 + \epsilon^2 g_2\rangle - \epsilon L^{-1}\langle \mathfrak{L}_1\rangle L^{-1}\langle g_0 + \epsilon g_1\rangle - \epsilon^2 L^{-1}\langle \mathfrak{L}_2\rangle L^{-1} g_0 + \epsilon^2 L^{-1}\langle \mathfrak{L}_1 L^{-1}\mathfrak{L}_1\rangle \times L^{-1} g_0 + O(\epsilon^3).$$

If $\langle \mathfrak{L}_1\rangle = \langle \mathfrak{L}_2\rangle = 0$,

$$\langle y(t)\rangle = L^{-1}\langle g\rangle + \epsilon^2 L^{-1}\langle \mathfrak{L}_1 L^{-1}\mathfrak{L}_1\rangle L^{-1} g_0$$

or, if $g_1 = g_2 = 0$ so that $g_0 = g$,

$$\langle y(t)\rangle = (1 + \epsilon^2 L^{-1}\langle \mathfrak{L}_1 L^{-1}\mathfrak{L}_1\rangle) L^{-1} g$$

as derived in Paper I. We have already demonstrated that the correlation result, for the case where perturbation theory is valid, can be derived from the SGF. It clearly could be found by writing $h(t, \tau)$.

ACKNOWLEDGMENTS

This work has been supported by the National Aeronautics and Space Administration under Grant No. NGR11-003-020 and by the office of Naval Research, under Contract No. N00014-69-A-0423-Themis.

[1] G. Adomian, J. Math. Phys. 11, 1069 (1970).
[2] G. Adomian, Ph. D. thesis (UCLA, 1961) (unpublished).
[3] L. H. Sibul, Ph. D. thesis (Pennsylvania State University, 1968) (unpublished).
[4] A separate paper will deal with rates of convergence and comparison with hierarchy methods.
[5] Obviously some integrations can be carried out, but we leave the expression this way.
[6] l has also been used in the author's previous work.
[7] $G(t, \tau) = l(t, \tau)$.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Linear Random Operator Equations in Mathematical Physics. III

G. Adomian

Department of Mathematics, University of Georgia, Athens, Georgia 30601

(Received 2 September 1970; Revised Manuscript Received 25 January 1971)

The problem of wave motion in a stochastic medium is treated as an application of stochastic operator theory and as a generalization of Papers I and II (and previous work by the author) to the case of partial differential equations and random fields without monochromaticity assumptions and closure approximations. Connections to the theory of partial coherence are considered. The stochastic Green's function for the two-point correlation of the solution process can be determined so the correlation can be obtained. Spectral spreading in a "hot" medium is easily demonstrable and can be calculated.

INTRODUCTION

The problem of wave motion in a stochastic or randomly inhomogeneous or fluctuating medium arises in a number of interesting contexts in physics and as a natural generalization of Paper I (Ref. 1) to the case of partial differential equations. The refractive index is assumed to be a random point function or stochastic process (SP) rather than a random variable. Use of stochastic distributions is, of course, suggested; however, it is desirable to keep the formulation initially simple since there already exist a number of complexities not present in usual treatments. (For the same reason the nonlinear stochastic problem is deferred.) Nearly all studies of wave propagation in a random continuum utilize the monochromatic or quasi-monochromatic assumption of harmonic time dependence and essentially no spectral spreading, and therefore proceed immediately to a reduced wave equation or Helmholtz equation. Thus the field quantity becomes a functional of a random process $k(\bar{x})$ rather than $k(\bar{x}, t)$ or, more completely, $k(\bar{x}, t, \omega)$, where $\omega \in (\Omega, \mathfrak{F}, \mu)$, a probability space. (See, e.g., Beran and Parrent[2] or Beran.[3]) Keller,[4] e.g., considered the scalar (reduced) wave equation $(\nabla^2 + k^2 n^2(\bar{x}))u = g(\bar{x})$, where $g(\bar{x})$ is the source distribution and there exists an appropriate condition on u and ∇u (radiation condition). k is the propagation constant for the medium, and n is the refractive index. Let $n^2(\bar{x}) = 1 + \mu(\bar{x})$, where $\mu(\bar{x})$ is a zero-mean SP. Then $(\nabla^2 + k^2)u + k^2\mu(\bar{x})u = g(\bar{x})$ or $\mathfrak{L}u = g$, where $\mathfrak{L}$ is a stochastic operator separable into the sum of a deterministic operator $L = \nabla^2 + k^2$ and a random operator R. The deterministic operator $L = \nabla^2 + k_0^2$. The Green's function $G(\bar{x} - \bar{x}') = G(r) = \exp(ik_0 r)/4\pi r = \exp(ik_0|x - x'|)/4\pi|x - x'|$. In a uniform or nonrandom medium, $n = 1$ and $(\nabla^2 + k^2)u = g$. The stochastic medium may, of course, be considered an ensemble of possible media with a probability distribution giving probabilities for various members of the ensemble.

The medium may not be known precisely, and the objective is to determine what is likely; it may be too complex to specify, or it may be randomly fluctuating. Most results involving stochastic equations in physics and engineering have been obtained by averaging procedures, closure, or truncation approximations (hierarchy methods, perturbation theories, etc.), self-consistent field approximations, and restriction to very special processes. Many of these have correlated well

with experiment. However, extrapolation without better understanding is dangerous, and a proper stochastic formulation is desirable.

GENERAL WAVE EQUATION[5]

The above approach is inadequate for a number of reasons. From the Maxwell equations

$$\begin{aligned}
&\nabla \times \mathcal{E} + \frac{\partial B}{\partial t} = 0,\\
&\nabla \times \nabla \times \mathcal{E} + \nabla \times \frac{\partial B}{\partial t} = 0,\\
&\nabla \times \nabla \times \mathcal{E} + \mu \frac{\partial}{\partial t} \nabla \times H = 0,\\
&\nabla \times \nabla \times \mathcal{E} + \mu \frac{\partial}{\partial t} (J + \frac{\partial D}{\partial t}) = 0,\\
&\nabla \times \nabla \times \mathcal{E} + \mu \frac{\partial^2 \epsilon \mathcal{E}}{\partial t^2} = -\mu \frac{\partial J}{\partial t},\\
&\text{grad div}\mathcal{E} - \nabla^2 \mathcal{E} + \mu \frac{\partial^2 \epsilon \mathcal{E}}{\partial t^2} = -\mu \frac{\partial J}{\partial t}, \qquad (1)
\end{aligned}$$

In a charge free medium, $\text{div}\epsilon\mathcal{E} = 0$. If ϵ is constant, $\text{div}\mathcal{E} = 0$; hence the first term vanishes in (1). More generally, $\text{div}D = \rho$; hence $\nabla \cdot \epsilon\mathcal{E} = \rho$ or $\epsilon \nabla \cdot \mathcal{E} = \rho - \nabla\epsilon \cdot \mathcal{E}$. Hence $\nabla \cdot \mathcal{E} = (\rho/\epsilon) - (\nabla\epsilon/\epsilon) \cdot \mathcal{E} = \rho/\epsilon - \mathcal{E} \cdot \nabla \ln\epsilon$. Consequently, $\text{grad div}\mathcal{E} = \nabla(\rho/\epsilon) - \nabla(\mathcal{E} \cdot \nabla \ln \epsilon)$. The wave equation becomes

$$\nabla^2 \mathcal{E} + \nabla(\mathcal{E} \cdot \nabla \ln\epsilon) - \mu \frac{\partial^2 \epsilon \mathcal{E}}{\partial t^2} = \nabla(\frac{\rho}{\epsilon}) + \mu \frac{\partial J}{\partial t} = g, \qquad (2)$$

where g is simply the source term (possibly random) and zero in a nonconducting medium with $\rho = 0$, the second term is almost always neglected, and ϵ is generally moved before the time derivative, i.e., taken as time independent. A reasonable approximation to the latter often can be based on time variations in ϵ or refractive index being small compared with the propagation time of the wave (e.g., Keller[4]). Sibul[6] assumes variations in ϵ over the distance of a characteristic radiation wavelength to be small, i.e., the spatial gradient of ϵ over a wavelength is negligible or $|\nabla\epsilon|/\epsilon \ll 1/\lambda$. Generally $\epsilon = \epsilon(\overline{r}, t, \omega)$, $[\omega \in (\Omega, \mathfrak{F}, \mu)]$. [In Beran's ground glass example,[2] $\epsilon = \epsilon(\overline{r}, \omega)$ so that no time fluctuation is involved and the second term is neglected to write $\nabla^2\mathcal{E} - \mu_0\epsilon(\overline{r}, \omega)\partial^2\mathcal{E}/\partial t^2 = g$]. Making both assumptions makes the problem nonstochastic and therefore devoid of interest. The monochromatic assumption leads to $\nabla^2\mathcal{E} + k^2\mathcal{E} = g$, i.e., one assumes there will be no spectral spreading. We will also drop the second term for simplicity and concentrate on the effect of the monochromatic assumption. Hence we write $\nabla^2\mathcal{E} - (\partial^2/\partial t^2)\mu_0\epsilon\mathcal{E} = g$ without assuming harmonic time fluctuation.

SCALAR AND VECTOR WAVE EQUATIONS[5]

If we assume harmonic time dependence, refractive index a function of space only, and one dimension for the moment, the equation becomes

$$d^2\psi(x)/dx^2 + k^2n^2(x)\psi(x) = g \text{ or}$$
$$d^2\psi/dx^2 + k^2[1 + \mu(x)]\psi(x) = g.$$

If x is t, this is the equation of a random harmonic oscillator (one with a randomly varying spring constant). We will see that this equation can be solved without assuming a Markovian $\mu(x)$. We will assume for simplicity that μ is zero mean and Gaussian, but even that purely for convenience. We need not assume Brownian motion or replace operators by their averages, thus neglecting fluctuations in the operator. We will deal with the medium as a continuum. However, a set of discrete randomly distributed scattering points can be treated by letting $\mu(x) = a \sum_{j=1}^{n} \delta(x - x_j)$, where the x_j are n correlated random variables. We can then treat any distribution of scatterers or the limit $n \to \infty$. Finally we remark that if $\mu(x)$ is the Uhlenbeck–Ornstein process, i.e., zero mean, stationary, Gaussian, and Markov SP with given correlation function $\langle\mu(x)\mu(x')\rangle = \epsilon^2 \exp(-|x - x'|/L)$, or, letting L be a unit length and writing $\mu(x)$ as $\epsilon\mu(x)$, we can use the correlation function $\exp(-|x - x'|)$. The probability density of the stationary $U - 0$ process $\mu(x)$ is $W(\mu) = (2\pi)^{-1/2} \exp(-\mu^2/2)$, where $W(\mu)$ is the stationary normalized solution of the Fokker–Planck equation

$$\frac{\partial}{\partial x} W(x, \mu) = \frac{\partial}{\partial \mu} (\mu W) + \frac{\partial^2}{\partial \mu^2} W.$$

This paper will consider the scalar wave equation. [It is hoped that a subsequent treatment of the vector equation will follow where wave motion is described by a vector function $\overline{u}(\overline{x}, t, \omega)$, with $\omega \in (\Omega, \mathfrak{F}, \mu)$ and $\overline{u}$ satisfying the wave equation and auxiliary (initial or boundary) conditions.] Thus we take L as a deterministic invertible linear partial differential operator, possibly with constant coefficients for simplicity, and R as a stochastic operator, again linear, possibly involving partial differential operations with coefficients which are zero-mean stochastic processes (mean values if any are absorbed into L). (The possible variations of nonlinear stochastic partial differential equations must be deferred). The source term may be a stochastic process including the case of a deterministic source function. The initial conditions may be stochastic also. These latter cases of randomness have been treated by a number of authors and are discussed by Syski in a recent book.[7]

The monochromatic assumption assumes a harmonic source causes a harmonic field, hence the time factor $\exp(-i\omega t)$ cancels out, and we conventionally write the Helmholtz equation $\nabla^2\psi(\overline{r}, \omega) + k^2n^2(\overline{r}, \omega)\psi(\overline{r}, \omega) = g(\overline{r})$, where k is a real positive number (free-space wavenumber), $n(\overline{r}, \omega)$, the index of refraction, is a (real) random function of position only (with mean square of 1), and g is a nonrandom source. Also n^2 is then written $1 + \mu(\overline{r}, \omega)$, where μ is a zero-mean (homogeneous isotropic) SP (a random function of position) on which various assumptions are then made (Gaussian, realizable, etc.). We will deal with the more general equation avoiding restrictive assumptions as far as possible.

The determination of the probability distribution after transformation of a statistically known SP is an unsolved problem except for special cases (Kac and Siegert.[8] When the transformation is itself stochastic—a stochastic operator—the conventional approaches are inadequate, though a general procedure has been discussed by Adomian.[9] A well-known technique of conventional approaches is that of the Fokker–Planck–Kolmogorov equations, i.e., deriving a differential equation satisfied by the desired probability density function—which works for Markov inputs (and some extensions; see Ref. 9). However, for stochastic operators the procedure is inadequate. It is often quite satisfactory to deal with moments, correlations, covariances, spectral densities, etc., which we do in this paper. Since we speak of general SP's rather than Brownian motions, white noise, etc., it is possible to ignore most of the literature, although appropriate connections should be made to the large volume of application related literature.

CONNECTION TO THEORY OF PARTIALLY COHERENT STATES

Beran and Parrent[2] and Beran[3] have discussed some interesting and closely related work. Let us relate it to the work which follows. Assuming an ensemble of systems with identical macroscopic properties where, because of ignorance or for convenience, microscopic properties are ignored, we can inquire only into average properties while instantaneous time variations may be quite different for each individual system in the ensemble. Thus in classical statistical mechanics we find it desirable to apply a statistical description, though, in principle at least, it is supposed possible to follow the system dynamics in detail. Similarly in electromagnetic theory, a statistical theory deals with averages of certain functions of the electromagnetic field. These averages are called statistical measures.[9] One such statistical measure (s.m.) has been called the mutual coherence function (in optics—see Refs. 2 and 3). We will symbolize it by[10] $\Gamma_{12}(\tau)$ and define

$$\Gamma_{12}(\tau) = \langle V_1(t+\tau)\overset{*}{V}_2(t)\rangle,$$

where $V_1(t)$ and $V_2(t)$ are the (complex) field at two points P_1 and P_2, with the brackets meaning an average over t, and τ is a time delay. Thus $\Gamma_{12}(\tau) = \langle V_1(\bar{x}_1, t+\tau)\overset{*}{V}_2(\bar{x}_2, t)\rangle$ and $\Gamma_{11}(\tau) = \langle V_1(\bar{x}_1, t+\tau)\overset{*}{V}_1(\bar{x}_1, t)\rangle$. Thus V is a SP. The distribution function $P_n(V_1(\bar{x}_1, t_1), V_2(\bar{x}_2, t_2), \cdots, V_n(\bar{x}_n, t_n))\, dV_1(\bar{x}_1, t_1)\cdots dV_n(\bar{x}_n, t_n)$ is the probability that the field will have value between $V_1(\bar{x}_1. t_1)$ and $V_1(\bar{x}_1, t_1) + dV_1(\bar{x}_1, t_1)$ at $\bar{x}_1, t_1$, between V_2 and $V_2 + dV_2$ at $\bar{x}_2, t_2$, etc.[9]

Then $\langle V_1(\bar{x}_1, t+\tau)\overset{*}{V}_1(\bar{x}_1, t)\rangle$ is a correlation or second-order moment. $\Gamma_{12}(\tau) = \langle V_1(\bar{x}_1, t+\tau)\overset{*}{V}_2(\bar{x}_2, t)\rangle$ is a cross-correlation function or the so-called mutual coherence function. Only under very severe restrictions, however, will $\Gamma_{12}(\tau)$ be adequate since it implies stationarity of the field—which is generally nonstationary. (Necessary and sufficient conditions for stationarity of a stochastic process under stochastic transformation will be discussed elsewhere). Thus

$$\Gamma_{12}(\bar{x}_1, t_1, \bar{x}_2, t_2) \text{ or } \Gamma_{12}(t_1, t_2) = \langle V_1(\bar{x}_1, t_1, \omega)\overset{*}{V}_2(\bar{x}_2, t_2, \omega)\rangle,$$

where $\omega \in \Omega$ on a probability space becomes simply $\Gamma_{12}(\bar{x}_1, \bar{x}_2, \tau)$ or $\Gamma_{12}(\tau)$ if we do have stationarity ($\tau = t_1 - t_2$). The Fourier transform of $\Gamma_{12}(\tau)$ is a spectral density (or power spectrum), and in this connection is also called the mutual power spectrum. $\Gamma_{12}(t_1, t_2)$ is simply $R_{12}(t_1, t_2)$ or correlation for space positions $\bar{x}_1$ and $\bar{x}_2$. When $\bar{x}_1 = \bar{x}_2$, we have $R_{11}(t_1, t_2)$ or simply $R(t_1, t_2)$, the time correlation function at one position in space, i.e., $\langle V(\bar{x}, t_1)\overset{*}{V}(\bar{x}, t_2)\rangle$ as discussed in Ref. 1 by Adomian. For the simple source-free equation

$$\nabla^2 V(\bar{x}, t, \omega) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} n^2(\bar{x}, t, \omega) V(\bar{x}, t, \omega),$$

for example, we can define the time correlation $\Gamma(t_1, t_2)$, or $R(t_1, t_2)$ in Ref. 1, equal to $\langle V(\bar{x}, t_1)\overset{*}{V}(\bar{x}, t_2)\rangle$, or the space correlation $\Gamma(\bar{x}_1, \bar{x}_2) = \langle V_1(\bar{x}_1, t)\overset{*}{V}_2(\bar{x}_2, t)\rangle$, or the cross correlation $\Gamma(\bar{x}_1 t_1, \bar{x}_2, t_2) = \langle V_1(\bar{x}_1, t_1)\overset{*}{V}_2(\bar{x}_2, t_2)\rangle$, where V_1 is the field at $\bar{x}_1$, etc.

The concept of partial coherence is useful almost everywhere where electromagnetic radiation is involved, and particularly so in the case of lasers. Strictly monochromatic radiation is coherent, i.e., $\Gamma_{12}(\tau) = 1$ (See Ref. 2, p. 47, for a discussion of temporal and spatial aspects of coherence). Radiation of finite spectral width cannot be coherent; spectral spreading means partial coherence, and radiation may be incoherent even for very narrow spectral width (the so-called quasimonochromatic case). We will avoid the usual time approximations and see the effect of the medium on the spectra.

EQUATIONS SATISFIED BY THE MUTUAL COHERENCE FUNCTION

For the simplest wave equation $\nabla_1^2 V = (1/c^2)(\partial^2 V/\partial t^2)$, we have $\Gamma_{12}(\tau) = \langle V_1(t+\tau)\overset{*}{V}_2(t)\rangle$. Then, operating with the Laplacian with respect to P_1 or $\bar{x}_1$, we have

$$\nabla_1^2\Gamma_{12}(\tau) = \langle \nabla_1^2 V_1(t+\tau)\overset{*}{V}_2(t)\rangle = \left\langle \frac{\partial^2 V_1(t+\tau)}{c^2\partial\tau^2}\overset{*}{V}_2(t)\right\rangle = \frac{\partial^2}{c^2\partial\tau^2}\langle V_1(t+\tau)\langle\overset{*}{V}_2(t)\rangle.$$

Hence $\nabla_1^2\Gamma_{12}(\tau) = (\partial^2/c^2\partial\tau^2)\Gamma_{12}(\tau)$ as given by Beran, i.e., a differential equation satisfied by Γ_{12}.

Similarly,

$$\nabla_2^2\Gamma_{12}(\tau) = \langle V_1(t+\tau)\nabla_2^2 \overset{*}{V}_2(t)\rangle$$
$$= \left\langle V_1(t+\tau)\ \frac{\partial^2 \overset{*}{V}_2(t)}{c^2\partial\tau^2}\right\rangle.$$

Replacing the ensemble average by the time average

$$\lim_{T\to\infty}\ \frac{1}{2T}\int_{-T}^{T}(\ )dt$$

and integrating twice by parts, we obtain

$$\nabla_2^2\Gamma_{12}(\tau) = \left\langle \frac{\partial^2 V_1(t+\tau)}{c^2\partial t^2}\ \overset{*}{V}_2(t)\right\rangle,$$

where the integrated terms vanish at the limits because time derivatives are assumed finite. Also $\partial^2 V_1(t+\tau)/c^2\partial t^2 = \partial^2 V_1(t+\tau)/c^2\partial\tau^2$. Thus $\nabla_2^2\Gamma_{12}(\tau) = (\partial^2/c^2\partial\tau^2)\Gamma_{12}(\tau)$. Therefore,

$$\nabla_s^2\,\Gamma_{12}(\tau) = \frac{\partial^2}{c^2\partial\tau^2}\ \Gamma_{12}(\tau), \qquad s = 1, 2,$$

and $\Gamma_{12}(\tau)$ depends of course on $\bar{x}_1, \bar{x}_2, \tau$.

The case of spatially and time varying index of refraction $n(\bar{x}, t, \omega)$ is much more difficult even for a simplified and source-free equation

$$\nabla^2 V(\bar{x}, t, \omega) = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\, n^2(\bar{x}, t, \omega)\, V(\bar{x}, t, \omega).$$

If n^2 is time independent as in Beran's ground glass case, it can be moved ahead of the derivative, but, otherwise, we define $\Gamma_{12}(t_1, t_2) = \langle V_1(t_1)\overset{*}{V}_2(t_2)\rangle$ and consider the Laplacian with respect to $\bar{x}_1$ of the correlation Γ_{12}. Thus

$$\nabla_1^2\Gamma_{12}(t_1, t_2) = \langle \nabla_1^2 V_1(\bar{x}_1, t_1)\overset{*}{V}_2(\bar{x}_2, t_2)\rangle$$
$$= \left\langle \frac{1}{c^2}\frac{\partial^2}{\partial t_1^2}\, n^2(\bar{x}_1, t_1) V_1(\bar{x}_1, t_1)\overset{*}{V}_2(\bar{x}_2, t_2)\right\rangle$$
$$= \frac{1}{c^2}\frac{\partial^2}{\partial t_1^2}\langle n^2(\bar{x}_1, t_1) V_1, (\bar{x}_1, t_1)\overset{*}{V}_2(\bar{x}_2, t_2)\rangle.$$

Now, since V is not statistically independent of n, the ensemble average on the right is not separable, so without unjustifiable assumptions of so-called local independence or closure approximations, we cannot get a determinate equation governing Γ_{12} as before. In the time-independent but spatially random case (Ref. 2, p. 87) of propagation through ground glass, the results are similar. We cannot exactly specify the ground glass, and must consider an ensemble of possible glasses to get the average results of many experiments (see also the atmospheric example in Chap. 4 of Ref. 9. Thus in the star twinkling or scintillation problem[11] we can only calculate statistical properties of the direction and intensity having chosen a random medium with statistical properties corresponding to the real atmosphere. Since n is random, we cannot specify an exact direction or intensity at a given t. Often one assumes the index does not change appreciably with time because of the velocity involved. Consequently $n = n(\bar{x}, \omega)$ rather than $n(\bar{x}, t, \omega)$, so it is the same as the ground glass problem). The result is

$$\nabla_1^2\Gamma_{12}(\tau) = \frac{n^2(\bar{x}_1, \omega)}{c^2}\,\frac{\partial^2\Gamma_{12}(\tau)}{\partial\tau^2},$$

i.e., this approach does not lead to a determinate equation involving averages of n for $\Gamma_{12}(\tau)$. This is of no use whatsoever. What we want is an equation connecting the field correlation to the correlation of n, or more generally, to the source correlation in terms of a stochastic Green's function (see Adomian, Refs. 1, 9, 12, 13) involving statistics of n. If no source term is present, we still have initial conditions involving randomness. In both cases we get a correlation of the field (output) in terms of a correlation (of an "input" given random quantity such as source or initial conditions) with a stochastic Green's function involving statistics of the medium. These correlations—or expectations such as $\langle V\rangle$—are not obtained by simply averaging the stochastic equation. This and the nature of the usual closure approximations have been thoroughly discussed by Adomian.[14] (If the ensemble average involving n^2 for the randomly time-varying case could be separated out, we would have $\langle n^2\rangle\Gamma_{12}(\tau)$, i.e., Γ_{12} would be the solution of an averaged equation.) The iteration method of Ref. 1 will be extended to solve this problem. Thus, e.g., defining $\Gamma_{11}(\tau) = \langle V_1(t+\tau)\overset{*}{V}_1(t)\rangle$, we have

$$\nabla_1^2\langle V_1(t+\tau)\overset{*}{V}_1(t)\rangle = \langle(\nabla_1^2 V_1(t+\tau))\overset{*}{V}_1(t)$$
$$+\ V_1(t+\tau)\nabla_1^2\overset{*}{V}_1(t)\rangle$$
$$= \frac{1}{c^2}\frac{\partial^2}{\partial\tau^2}\langle n^2(\bar{x}_1, t+\tau) V(\bar{x}_1, t+\tau)\overset{*}{V}_1(\bar{x}_1, t)\rangle$$
$$+\ \langle V_1(t+\tau)\times\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\, n^2(\bar{x}_1, t)\overset{*}{V}_1(\bar{x}_1, t)\rangle,$$

where the last term is treated as the Ry term of Ref. 1 and iterated to the source term.

GENERAL PROCEDURE[15]

The scalar version of (2) with the complication of the second term neglected can be written (not bothering to write ω)

$$\nabla^2 y(\bar{r}, t) - \frac{\partial^2}{\partial t^2}\, a(\bar{r}, t) y(\bar{r}, t) = x(\bar{r}, t),$$

where $a(\bar{r}, t) = \mu\epsilon(\bar{r}, t)$. Let $a(\bar{r}, t) = \langle a\rangle + \alpha(\bar{r}, t)$, i.e., separate a into a deterministic part $\overline{\mu\epsilon}$ or usually $\mu\bar{\epsilon}$, and a randomly fluctuating part α, where α is a zero-mean SP. In order to identify $\overline{\mu\epsilon}$ in such a way as to yield familiar Green's functions, we write $\epsilon = \epsilon_0 + \epsilon_r$, where ϵ_0 is the free-space constant. Then $\langle\mu\epsilon\rangle = \langle\mu\epsilon_0\rangle + \langle\mu\epsilon_r\rangle = (1/c^2)$ $+ \langle\mu\epsilon_r\rangle$ and $(\partial^2/\partial t^2)(\overline{\mu\epsilon} + \alpha) = (\partial^2/\partial t^2)(1/c^2 +$ $\langle\mu\epsilon_r\rangle + \alpha) = (1/v^2)(\partial^2/\partial t^2) + (\partial^2/\partial t^2)\alpha$, where v

is the (deterministic) velocity $c^2/(1 + c^2\langle\mu\epsilon_r\rangle)$. The equation is in the same form $\mathcal{L}y = x$ as in Ref. 1 with $\mathcal{L} = L + R$ except the operators are partial differential operators. L is now the d'Alembertian operator $\Box^2 = \nabla^2 - (1/v^2)\,\partial^2/\partial t^2$ and $R = \partial^2/\partial t^2$. The Green's function L^{-1} is found from the usual one by substituting the velocity v for c to take account of the average $\langle\epsilon_r\rangle$. x is not necessarily stochastic but assumed so for generality. α is a SP dependent on space and time, i.e., a random field (Ref. 9). As in Ref. 1, α and x are statistically independent. We take α to be a real SP, although no difficulty is encountered in making it complex. We will assume that α and x are either wide-sense stationary (w.s.s.) (i.e., stationary to order two)(or "reducible to w.s.s. in time" processes—to be defined shortly). No assumption is made restricting the statistical properties of α and x in the spatial variable $\bar{r}$ except that α and x are second-order[16] processes—they need not be stationary in $\bar{r}$. Physical considerations will restrict the manner of space variation of the medium, e.g., the mean square amplitude of the fluctuation of $\alpha(\bar{r}, t, \omega)$ may vary with height (as in tropospheric communication problems). [Since we allow the processes to be reducible to stationary[17] rather than necessarily stationary, the statistical properties of α and of x may vary slowly with time; it would, of course, be still more general to remove even this restriction and allow nonstationary processes. It appears possible to remove this restriction as well since the solution is usually nonstationary in any event. The general expression for $R_y(t_1, t_2)$ for the nonstationary case has been derived by Adomian (see Papers I and II). However, in the interest, of clarity we do not attempt to go too far with generality here.] The scalar equation used is adequate for sound waves in a random medium; for electromagnetic waves it would also be desirable to consider changes in polarization due to the random medium so that one might want to look at the vector wave equation as well. If α and x are w.s.s. but not zero means, $\langle\alpha\rangle$ can be included in the deterministic part as long as the deterministic Green's function can be found; a nonzero mean for the source is handled by superposition since we confine ourselves to a linear theory.

A few parenthetical remarks will be made before proceeding with the solution. We can solve the problem in either time or frequency domain. We could use spectral representations, e.g.,

$$\alpha(\bar{r}, t, \omega) = \int_{-\infty}^{\infty} e^{iut} A(\bar{r}, u, \omega)\, du,$$

$$x(\bar{r}, t, \omega) = \int_{-\infty}^{\infty} e^{izt} X(\bar{r}, z, \omega)\, dz,$$

i.e., integral canonical expressions[18], or in Stieltjes form

$$\alpha = \int e^{iut} dA_0(u, \omega),$$

$$x = \int e^{izt} dX_0(z, \omega),$$

where dA_0 and dX_0 are SP's with orthogonal increments. However, for clarity and connection to Paper I (i.e., Ref. 1), we will consider the time domain.

DETERMINATION OF THE STATISTICAL MEASURES OF THE SOLUTION OF THE WAVE EQUATION AND THE SPECTRAL SPREADING

A paraticularly simple and elegant form of the stochastic Green's function for the spectral density (a particular statistical measure) was found by Adomian[9] using a spectral representation. Sibul[6] extended this approach (using it to find coherence functions for the solution of the wave equation) because it conveniently reveals the spectral spreading caused by a randomly time varying medium. This spectral broadening effect of a randomly fluctuating medium demonstrates that the widely used monochromatic assumption is neither generally appropriate nor necessary. When it exists, the spectral density is an interesting and convenient statistical measure (s.m.) and the other second-order s.m.'s are easily found from it by taking Fourier transforms (e.g., variance, mutual coherence). The procedure is to solve for the spectral representation of the solution (integral canonical expansion of Pugachev[18]). We will further examine these solutions considering the wave equation

$$\nabla^2 y(\bar{r}, t, \omega) - \frac{\partial^2}{\partial t^2}\left(\frac{1}{c^2} + \alpha(\bar{r}, t, \omega)\right) y(\bar{r}, t, \omega) = x(\bar{r}, t, \omega),$$

where $t \in T$ represents time, $\bar{r} \in R^3$, $\omega \in \Omega$ on a probability space $(\Omega, \mathfrak{F}, \mu)$. The quantities x and α, and consequently y, are all stochastic processes (random functions of space and time). Assuming weak or wide-sense stationarity for α and x, we would, for example, write the correlation function

$$R_x(\tau) = \langle x(\bar{r}, t, \omega)\overset{*}{x}(r, t + \tau, \omega)\rangle$$

for the input $x(t)$.

Suppose $y(\bar{r}, t, \omega)$, or $y(\bar{r}, t)$, suppressing the ω for brevity, is representable as a Fourier integral with respect to the time variable, i.e.,

$$y(t) = \int_{-\infty}^{\infty} Y(f)\, \exp(2\pi i f t)\, df$$

If necessary we can ensure this existence by defining a new function $\exp(-\xi t^2)\, y(\bar{r}, t)$ with ξ sufficiently small so that there is no substantial change for finite t but rapid decrease as $t \to \pm\infty$. Similarly

$$\begin{aligned} \alpha(\bar{r}, t) &= \int_{-\infty}^{\infty} A(\bar{r}, u)\, \exp(2\pi i u t)\, du, \\ x(\bar{r}, t) &= \int_{-\infty}^{\infty} X(\bar{r}, v)\, \exp(2\pi i v)\, dv. \end{aligned} \tag{3}$$

If α and x are w.s.s. (wide-sense stationary) with zero means, their integral expansions are the above. (The stationarity requirement will be discussed further shortly.) The zero means constitute no loss of generality. If $\langle\alpha\rangle$ is nonzero, the mean is included in the deterministic L, and $\langle x\rangle$, if nonzero, can be handled by superposition.

The integrals should be written as Stieltjes integrals, e.g., $\alpha(\bar{r}, t) = \int \exp(2\pi iut)\, dA_0(\bar{r}, u)$, but, for simplicity, the above integral expressions are used with the understanding A and X may be generalized functions.

The scalar wave equation is rewritten as

$$\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) y(\bar{r}, t, \omega) = x(\bar{r}, t, \omega) + \frac{\partial^2}{\partial t^2}\alpha(\bar{r}, t, \omega) y(\bar{r}, t, \omega).$$

(The operators L and R of Ref. 1 are given by the d'Alembertian operator and by $(\partial^2/\partial t^2)\alpha$, respectively.)

Substituting the integral expansions for α and x, multiplying both sides by $\exp(-2\pi ist)$, and integrating leads to the spectral representation of the wavefunction $Y(\bar{r}, s, \omega)$.[6,9] Thus the first term is $\int dt\, \exp(-2\pi ist)\nabla^2 y(r, t) = 2\pi \nabla_2^2 Y(r, s)$, by interchanging the integration and ∇^2 operators. The second term is $-(1/c^2)\int dt\, \exp(-2\pi ist) \times (\partial^2/\partial t^2) y(\bar{r}, t)$, which after integrating by parts[19] yields $(8\pi^3 s^2/c^2) Y(\bar{r}, s)$. The source term is $\int dt\, \exp(-2\pi ist)\, x(\bar{r}, t) = 2\pi X(s)$. The last term is $(2\pi/c^2) \iint \exp(2\pi ist)\, (\partial^2/\partial t^2) \times A(\bar{r}, u) \exp(2\pi iut)\, y(r, t)\, du\, dt$. Integrating by parts yields $(8\pi^3 s^2/c^2) \int du\, A(\bar{r}, u) \int dt\, y(\bar{r}, t) \exp[-2\pi i (s - u)t]$ or $(8\pi^3 s^2/c^2) \int du\, A(\bar{r}, u) Y(\bar{r}, s - u)$. Let $k = 2\pi s/c$ to get the spectral representation

$$\nabla^2 Y(\bar{r}, s) + k^2 Y(\bar{r}, s) = X(\bar{r}, s) - k^2 \int_{-\infty}^{\infty} A(\bar{r}, u) Y(\bar{r}, s - u)\, du.$$

The left side is simply the Helmholtz equation for the spectral representation (or Fourier integral representation) $Y(\bar{r}, s, \omega)$. In order for the result to be valid, a number of quantities must vanish as $t \to \pm\infty$. We will see this again in a moment in the time domain approach. In general, it cannot occur if the forcing function is really w.s.s.; however, this is a mathematical idealization implying activity from $t = -\infty$ to $t = +\infty$, which is physically unreasonable. Hence we assert that $x(\bar{r}, t, \omega)$ is actually reducible to stationary in the sense of Pugachev, i.e., x is of the form $x(t, \omega) = g(t)z(t, \omega) + f(t)$, where z is a stationary SP and g and f are real and nonrandom time functions. In particular, we can take f to be zero and select g such that the undesired quantities all vanish as $t \to \pm\infty$, e.g., $g(t) = \exp(-\zeta t^2)$. Solution of the Helmholtz equation is known for a number of boundary conditions. For these conditions, L^{-1} is taken as the inverse operator, and $F(\bar{r}, s, \omega)$ will denote $L^{-1}X(\bar{r}, s, \omega)$, i.e., $F(\bar{r}, s)$ is the solution if $\alpha = 0$. We have the integral equation

$$Y(\bar{r}, s, \omega) = F(\bar{r}, s, \omega) - L^{-1}k^2 \int_{-\infty}^{\infty} A(\bar{r}, u, \omega) \times Y(\bar{r}, s - u, \omega)\, du.$$

Leaving out the variables $\bar{r}$ and ω for notational simplicity, we have

$$Y(s) = F(s) - L^{-1}k^2 \int_{-\infty}^{\infty} A(u) Y(s - u)\, du$$

or finally, with a change of variable which simplifies the iterative solution, we have

$$Y(s) = F(s) - L^{-1}k^2 \int A(s - u) Y(u)\, du \qquad (4)$$

The solution of (4) can be written in the form

$$Y(\bar{r}, s, \omega) = F(\bar{r}, s, \omega) + \int_m \int_{-\infty}^{\infty} \Gamma(\bar{r}, \bar{r}', s, u, \omega) \times F(\bar{r}', u, \omega)\, d\bar{r}'\, du,$$

where the resolvent kernel $\Gamma(\bar{r}, \bar{r}', s, u)$, omitting ω, is related to the Fourier representation A of the stochastic index of refraction $\alpha(t)$ and the $\bar{r}'$ integration is over the volume of the stochastic medium.

In the time domain, with $L^{-1}x = F$, we write immediately

$$y(\bar{r}, t, \omega) = F(\bar{r}, t, \omega) + L^{-1}\frac{\partial^2}{\partial t^2}\alpha(\bar{r}, t, \omega) y(\bar{r}, t, \omega), \qquad (5)$$

where L^{-1} is the inverse of the operator $\nabla^2 - (1/c^2)(\partial^2/\partial t^2)$. Denoting the Green's function by $G(t, \tau)$,[20] the last term is rewritten as $\int G(t, \tau)(\partial^2/\partial t^2)\alpha(\tau) y(\tau)\, d\tau$, i.e., the random operator R is $-(\partial^2/\partial t^2)\alpha(t)$. After integrating twice by parts, we can write

$$y(t) = F(t) + \int [\partial^2 G(t, \tau)/\partial \tau^2]\alpha(\tau) y(\tau) d\tau \qquad (6)$$

if quantities

$$G(t, \tau)\frac{\partial}{\partial \tau}\alpha(\tau) y(\tau)$$

and

$$\frac{\partial G(t, \tau)}{\partial \tau}\alpha(\tau) y(\tau)$$

vanish as $t \to \pm\infty$, which we suppose does happen either because of the initial conditions (G and G' zero) or because α is reducible to stationary.

Now in (6) let $y(t) = y_0(t) - y_1(t) + y_2(t) - \cdots$, we obtain

$$y_0 = F(t) = L^{-1}x,$$

$$y_1 = -\int \frac{\partial^2 G(t, \tau)}{\partial \tau^2}\alpha(\tau) F(\tau)\, d\tau,$$

$$y_2 = \iint \frac{\partial^2 G(t, \tau)}{\partial \tau^2}\frac{\partial^2 G(\tau, \sigma)}{\partial \sigma^2}\alpha(\tau)\alpha(\sigma) F(\sigma)\, d\tau\, d\sigma,$$

$$y_3 = -\iiint \frac{\partial^2 G(t, \tau)}{\partial \tau^2}\frac{\partial^2 G(\tau, \sigma)}{\partial \sigma^2}\frac{\partial^2 G(\sigma, \gamma)}{\partial \gamma^2} \times \alpha(\tau)\alpha(\sigma)\alpha(\gamma) F(\gamma)\, d\sigma\, d\tau\, d\gamma,$$

etc.

(or in a less useful operator form we could write

$$y = L^{-1}x - L^{-1}\frac{\partial^2}{\partial t^2}\alpha y_0 + L^{-1}\frac{\partial^2}{\partial t^2}\alpha y_1 - \cdots,$$

where

$$y_0 = L^{-1}x, \quad y_1 = -L^{-1}\frac{\partial^2}{\partial t^2}\alpha L^{-1}x, \text{ etc.},$$

i.e., each term can be determined from the preceding term, or $y = \sum_{n=0}^{\infty}(-T\alpha)^n L^{-1}x$, where T is the operator $L^{-1}\partial^2/\partial t^2$). The general term is

$$\int\cdots\int \frac{\partial^2 G(t,\tau_1)}{\partial\tau_1^2}\frac{\partial^2 G(\tau_1,\tau_2)}{\partial\tau_2^2}\cdots\frac{\partial^2 G(\tau_{n-1},\tau_n)}{\partial\tau_n^2} \times \alpha(\tau_1)\alpha(\tau_2)\cdots\alpha(\tau_n)F(\tau_n)\,d\tau_1\cdots d\tau_n,$$

with an appropriate minus sign depending on whether n is even or odd.

Clearly the procedure works as in Ref. 1. If we find $\langle y\rangle$, the ensemble averages in each term separate into averages involving α's and the average of F. For the two-point correlation $R_y(t_1,t_2)$, we must consider the term-by-term product $y(t_1)\overset{*}{y}(t_2)$ before averaging. Again each term leads to an average involving products of α's (correlations of α in the Gaussian case) and correlation of the input F. Thus there is no difficulty in obtaining $R_y(t_1,t_2)$.

However, if the solution is stationary (a very special circumstance) and we wish to show the spectral spreading, in which case the simpler correlation $R_y(\tau)$ is sufficient, then the Fourier transform of all the terms in the product will be needed; hence Sibul perfers to use the spectral approach immediately. This author prefers a time domain approach valid in the nonstationary case, i.e., looking at $R_y(t_1,t_2)$ or coherence functions.

The most direct approach is to use the stochastic Green's function (SGF).[21] We write

$$\Gamma(t,\tau) = \sum_{m=0}^{\infty}(-1)^m K_{m+1}(t,\tau), \text{ with } K_1 = K$$

as before;

$$K(t,\tau) = \frac{\partial^2 G(t,\tau)}{\partial\tau^2}\alpha(\tau),$$

$$K_2(t,\tau) = \int K(t,\tau_1)K(\tau_1,\tau)\,d\tau_1 = \int\frac{\partial^2 G(t,\tau_1)}{\partial\tau_1^2}\alpha(\tau_1)\frac{\partial^2 G(\tau_1,\tau)}{\partial\tau^2}\alpha(\tau)\,d\tau_1,$$

$$K_3(t,\tau) = \int K(t,\tau_1)K_2(\tau_1,\tau)\,d\tau_1, \text{ etc.}$$

The random Green's function $h(t,\tau) = G(t,\tau) - \int\Gamma(t,\sigma)G(\sigma,\tau)\,d\sigma$ can now be written from which we determine the SGF, or we can use Eq. (II. 1. 10) to write $G_H(t_1,t_2,\sigma_1,\sigma_2)$ from Γ above. For Γ we have

$$\begin{aligned}\Gamma(t,\tau) &= K(t,\tau) - K_2(t,\tau) + K_3(t,\tau)\cdots\\ &= K(t,\tau) - \int K(t,\tau_1)K(\tau_1,\tau)d\tau_1\\ &+ \iint K(t,\tau_1)K(\tau_1,\tau_2)K(\tau_2,\tau)d\tau_1 d\tau_2 - \cdots\\ &= \frac{\partial^2 G(t,\tau)}{\partial\tau^2}\alpha(\tau) - \int\frac{\partial^2 G(t,\tau_1)}{\partial\tau_1^2}\frac{\partial^2 G(\tau_1,\tau)}{\partial\tau^2}\\ &\times\alpha(\tau_1)\alpha(\tau)d\tau_1 + \iint\frac{\partial^2 G(t,\tau_1)}{\partial\tau_1^2}\frac{\partial^2 G(\tau_1,\tau_2)}{\partial\tau_2^2}\\ &\times\frac{\partial^2 G(\tau_2,\tau)}{\partial\tau^2}\alpha(\tau_1)\alpha(\tau_2)\alpha(\tau)\,d\tau_1 d\tau_2 - \cdots.\end{aligned}$$

Thus we can determine the SGF either for the spectral density s.m. if it exists, or immediately the more general two-point correlation (and mutual coherence functions); thus $R_y(t_1,t_2) = \iint G_H(t_1,t_2,\sigma_1,\sigma_2)R_x(\sigma_1,\sigma_2)\,d\sigma_1 d\sigma_2$, where G_H is found from $h(t,\tau)$, the random Green's function.[1,9]

The first term of G_H (which we do not write out) shows the results for waves propagating in a *deterministic* medium. The other terms of G_H involving statistics of Γ show the effects of spectral spreading due to the stochastic medium. These are the terms lost by a monochromatic assumption. The calculation for a specific case presents considerable difficulty but can be made knowing the statistics (i.e., s.m.) of α (such as correlation if α is Gaussian). This problem has been considered substantially only by Sibul.[22]

The simplest calculation of the spectral spreading should result (if one determines first that stationarity exists in the solution process or wavefunction—the necessary and sufficient conditions will be discussed in another paper) if the spectral density is calculated [see Eq. (I. 2. 4)]. From

$$\Phi_y(f) = \int K_H(s,f)\Phi_x(s)\,ds,$$

where the stochastic Green's function K_H is

$$K_H(s,f) = \iiint_{-\infty}^{\infty}\langle h(t,\tau)\overset{*}{h}(t+\beta,\tau+\sigma)\rangle\exp(2\pi i f\beta) \times\exp(-2\pi i s\sigma)\,d\tau\,d\beta\,d\sigma.$$

In the more general nonstationary case, we make the time domain iterative treatment, and, if we assume Gaussian behavior for the index of refraction, we observe that the odd terms vanish in the series (terms involving products of odd numbers of α's) and the even terms are negative. Thus in forming products $y(t_1)y(t_2)$ for correlations, the contribution of the spectral spreading or nonmonochromatic terms of G_H (i.e., the last three of the four term expression) are all positive.

Our procedure involves no assumption of statistical independence of the solution SP or wavefunction and the stochastic index of refraction, and makes no closure approximations.[14]

ACKNOWLEDGMENTS

The author thanks the reviewer for some valuable comments and also expresses his appreciation to L. H. Sibul, formerly the author's student and now a valued collaborator. This work has been supported by the National Aeronautics and Space Administration (NGR11-003-020) and by the office of Naval Research (Contract No. N00014-69-A-0423-Themis).

[1] G. Adomian, J. Math. Phys. **11**, 1069 (1970).
[2] M. J. Beran and G. B. Parrent, *Theory of Partial Coherence* (Prentice-Hall, Englewood Cliffs, N.J., 1964).
[3] M. J. Beran, *Statistical Continuum Theories* (Interscience, New York, 1968).
[4] J. B. Keller, Proc. Symp. Appl. Math. **16**, 145 (1964).
[5] This section is presented, even though well known, in order to clarify some of the underlying assumptions which become significant in the stochastic case later. μ is, of course, the permeability. It has also been used for probability measure in this series and, in the next section, on scalar and vector wave equations, for the random part of the index of refraction. The meaning is always clear from context.
[6] L. H. Sibul, Ph.D. thesis, Pennsylvania State University, 1968.
[7] R. Syski, in *Modern Nonlinear Equations*, edited by T. L. Saaty (McGraw-Hill, New York, 1967), Chap. 8.
[8] M. Kac and A. J. F. Siegert, J. Appl. Phys. **18**, 383 (1947).
[9] G. Adomian, Ph.D. thesis, UCLA, 1961.
[10] We have previously (Paper II) used Γ for the resolvent kernel and will continue to do so. It cannot be confused with the mutual coherence function, which we will specifically identify as such if referred to.
[11] Actually two sources of scintillation are present in problems of this nature—one due to variations in the atmosphere which makes light rays enter the observer's eye from different directions at different instants of time and the second, unimportant with stars or point targets but very significant for complex aircraft targets in radar detection and tracking systems, due to the fact that the target is not a point source but a set of complex moving vibrating scattering surfaces. Both a fluctuation in mean intensity and an apparent fluctuation in angle of arrival result.
[12] G. Adomian, Rev. Mod. Phys. **35**, 185 (1963).
[13] G. Adomian, Proc. Symp. Appl. Math. **16**, 1 (1964).
[14] G. Adomian, "The Closure Approximations in Hierarchy Equations," J. Stat. Phys. (to be published).
[15] It should be clear from context here, and in the earlier section on the general wave equation, that μ is the permeability, although it has been used with other meanings. Also, ϵ is the dielectric constant, although it is used as a small parameter in perturbation results elsewhere in this series.
[16] $X(t)$ is said to be second order if, for all $t \in T$, $E\{|X(t)|^2\}$ exists; then $E\{X(t)\}$ exists.
[17] See the next section.
[18] V. S. Pugachev, *Theory of Random Functions* (Addison-Wesley, Reading, Mass., 1965).
[19] Conditions for validity to be discussed.
[20] Given, for example, in Friedman, *Principles and Techniques of Applied Mathematics* (Wiley, New York, 1956), p. 300. The Green's function, for L^{-1}, is found from $\Box^2 G = \delta(x_1 - x_1')\delta(x_2 - x_2')\delta(x_3 - x_3')\delta(t - t')$, where $G(x_1, x_2, x_3, t)$, or $G(\bar{r}, t)$ satisfies the equation and initial conditions $G(\bar{r}, 0) = G_t(\bar{r}, 0) = 0$ and such that G is bounded for all t as either x_1, x_2, or $x_3 \to \pm\infty$.
[21] Relationships between the random Green's function h, the SGF G_H, the ordinary Green's function $G(t, \tau)$ and the resolvent kernel Γ have been discussed in Paper II.
[22] A following paper by Sibul and Adomian will calculate the spectral spreading and the mutual coherence and related quantities.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

A Second-Order JWKB Approximation with One Turning Point and Two Singular Points: Stability of an Accelerating Liquid Sphere

E. Y. Harper
Bell Telephone Laboratories, Incorporated, Whippany, New Jersey 07981

and

I-Dee Chang
Stanford University, Palo Alto, California 94305

and

G. W. Grube
Bell Telephone Laboratories, Incorporated, Whippany, New Jersey 07981

(Received 6 January 1971)

A formal higher-order matching procedure is employed to obtain a second-order asymptotic solution, of the JWKB type, to a Legendre-like differential equation with a large parameter. The equation has two second-order poles and a first-order turning point. In addition to the usual nonuniformity, the second-order JWKB approximation exhibits a divergent integral at these points. Eigenfunctions and eigenvalues, valid to the second order of approximation, are found by simultaneously matching the latter approximation to a turning-point expansion and two boundary-layer expansions. The solutions, which heretofore have not been described, are appropriate to the neutral stable surface waves manifest by an accelerating liquid sphere.

I. INTRODUCTION

We seek solutions to the differential equation

$$\frac{d}{dx}(1 - x^2)\frac{d\eta}{dx} - (2 - B_o x)\eta = 0 \tag{1a}$$

that are regular on the closed interval

$$-1 \le x \le 1. \tag{1b}$$

Such solutions may be compared to the Legendre polynomials P_n, which under the same restriction,

ACKNOWLEDGMENTS

The author thanks the reviewer for some valuable comments and also expresses his appreciation to L. H. Sibul, formerly the author's student and now a valued collaborator. This work has been supported by the National Aeronautics and Space Administration (NGR11-003-020) and by the office of Naval Research (Contract No. N00014-69-A-0423-Themis).

[1] G. Adomian, J. Math. Phys. **11**, 1069 (1970).
[2] M. J. Beran and G. B. Parrent, *Theory of Partial Coherence* (Prentice-Hall, Englewood Cliffs, N.J., 1964).
[3] M. J. Beran, *Statistical Continuum Theories* (Interscience, New York, 1968).
[4] J. B. Keller, Proc. Symp. Appl. Math. **16**, 145 (1964).
[5] This section is presented, even though well known, in order to clarify some of the underlying assumptions which become significant in the stochastic case later. μ is, of course, the permeability. It has also been used for probability measure in this series and, in the next section, on scalar and vector wave equations, for the random part of the index of refraction. The meaning is always clear from context.
[6] L. H. Sibul, Ph.D. thesis, Pennsylvania State University, 1968.
[7] R. Syski, in *Modern Nonlinear Equations*, edited by T. L. Saaty (McGraw-Hill, New York, 1967), Chap. 8.
[8] M. Kac and A. J. F. Siegert, J. Appl. Phys. **18**, 383 (1947).
[9] G. Adomian, Ph.D. thesis, UCLA, 1961.
[10] We have previously (Paper II) used Γ for the resolvent kernel and will continue to do so. It cannot be confused with the mutual coherence function, which we will specifically identify as such if referred to.
[11] Actually two sources of scintillation are present in problems of this nature—one due to variations in the atmosphere which makes light rays enter the observer's eye from different directions at different instants of time and the second, unimportant with stars or point targets but very significant for complex aircraft targets in radar detection and tracking systems, due to the fact that the target is not a point source but a set of complex moving vibrating scattering surfaces. Both a fluctuation in mean intensity and an apparent fluctuation in angle of arrival result.
[12] G. Adomian, Rev. Mod. Phys. **35**, 185 (1963).
[13] G. Adomian, Proc. Symp. Appl. Math. **16**, 1 (1964).
[14] G. Adomian, "The Closure Approximations in Hierarchy Equations," J. Stat. Phys. (to be published).
[15] It should be clear from context here, and in the earlier section on the general wave equation, that μ is the permeability, although it has been used with other meanings. Also, ϵ is the dielectric constant, although it is used as a small parameter in perturbation results elsewhere in this series.
[16] $X(t)$ is said to be second order if, for all $t \in T$, $E\{|X(t)|^2\}$ exists; then $E\{X(t)\}$ exists.
[17] See the next section.
[18] V. S. Pugachev, *Theory of Random Functions* (Addison-Wesley, Reading, Mass., 1965).
[19] Conditions for validity to be discussed.
[20] Given, for example, in Friedman, *Principles and Techniques of Applied Mathematics* (Wiley, New York, 1956), p. 300. The Green's function, for L^{-1}, is found from $\Box^2 G = \delta(x_1 - x_1')\delta(x_2 - x_2')\delta(x_3 - x_3')\delta(t - t')$, where $G(x_1, x_2, x_3, t)$, or $G(\bar{r}, t)$ satisfies the equation and initial conditions $G(\bar{r}, 0) = G_t(\bar{r}, 0) = 0$ and such that G is bounded for all t as either x_1, x_2, or $x_3 \to \pm\infty$.
[21] Relationships between the random Green's function h, the SGF G_H, the ordinary Green's function $G(t, \tau)$ and the resolvent kernel Γ have been discussed in Paper II.
[22] A following paper by Sibul and Adomian will calculate the spectral spreading and the mutual coherence and related quantities.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

A Second-Order JWKB Approximation with One Turning Point and Two Singular Points: Stability of an Accelerating Liquid Sphere

E. Y. Harper
Bell Telephone Laboratories, Incorporated, Whippany, New Jersey 07981

and

I-Dee Chang
Stanford University, Palo Alto, California 94305

and

G. W. Grube
Bell Telephone Laboratories, Incorporated, Whippany, New Jersey 07981

(Received 6 January 1971)

A formal higher-order matching procedure is employed to obtain a second-order asymptotic solution, of the JWKB type, to a Legendre-like differential equation with a large parameter. The equation has two second-order poles and a first-order turning point. In addition to the usual nonuniformity, the second-order JWKB approximation exhibits a divergent integral at these points. Eigenfunctions and eigenvalues, valid to the second order of approximation, are found by simultaneously matching the latter approximation to a turning-point expansion and two boundary-layer expansions. The solutions, which heretofore have not been described, are appropriate to the neutral stable surface waves manifest by an accelerating liquid sphere.

I. INTRODUCTION

We seek solutions to the differential equation

$$\frac{d}{dx}(1 - x^2)\frac{d\eta}{dx} - (2 - B_o x)\eta = 0 \tag{1a}$$

that are regular on the closed interval

$$-1 \le x \le 1. \tag{1b}$$

Such solutions may be compared to the Legendre polynomials P_n, which under the same restriction,

Eq. (1b), are the only bounded solutions of

$$\frac{d}{dx}(1-x^2)\frac{dP}{dx}+n(n+1)P=0 \tag{2}$$

and which correspond to the eigenvalues, $n = 0, 1, 2, \cdots$, the positive integers.

The purpose of this paper is to obtain asymptotic estimates of the eigenvalues and the corresponding eigenfunctions appropriate to Eq. (1a). The analysis is initiated by considering the result of the JWKB approximation. This asymptotic approximation displays singular behavior at a turning point near $x = 0$ as well as at two "vortex" points $x = \pm 1$, where the differential equation exhibits boundary-layer behavior. Moreover, when carried to a second order of approximation, the JWKB expansion displays another nonuniformity through the appearance of a divergent integral. These difficulties are resolved by constructing a composite expansion which employs various asymptotic solutions in their respective regions of validity. The requirement that these asymptotic representations match to a certain order is sufficient to determine unknown constants in each expansion including, in particular, the eigenvalues $(B_o)_n$.

The procedure for matching the JWKB and vortex point solutions is generally referred to as the method of matched asymptotic expansions.[1] In this case the JWKB approximation corresponds to the "outer" expansion, while the approximations near the vortex points play the role of "inner" expansions. For reasons of consistency as well as simplicity, the turning point is treated in like fashion. Although other techniques have been outlined for higher-order approximations of the JWKB type with turning points,[2] a survey of the existing literature[3] reveals that matching to higher order has been done only infrequently and for simpler problems than the one treated here.[4]

In the case of Eq. (1a) the eigenfunctions correspond to stationary waves of small amplitude on the surface of a liquid sphere of unit radius, whose center of mass is undergoing constant acceleration.[5] In terms of a system of spherical coordinates, $(1, \theta, \phi)$, with origin fixed at the center of mass, the liquid globe accelerates along the polar axis $\theta = 0, \pi$, which is an axis of symmetry, $\partial/\partial\phi = 0$. Points on the surface of the sphere corresponding to positive values of the variable $x = \cos\theta$ are in the direction of motion. The parameter B_o, which is real and positive, corresponds to the ratio of the gravitational to the surface tension force and is known as the Bond number. The eigenvalues or critical Bond numbers $(B_o)_n$ are those for which the corresponding eigenfunctions are neutrally stable, that is, neither oscillate nor grow with time. In particular, the lowest critical Bond number $(B_o)_1$ is that below which surface waves of arbitrary form oscillate with time but do not grow. Under this condition the accelerating sphere is said to be stable to small disturbances.

II. THE JWKB APPROXIMATION

We make the change of variable

$$\eta = Y/(1-x^2)^{1/2} \tag{3}$$

in Eq. (1a) and consider approximate solutions of the resulting equation

$$\frac{d^2Y}{dx^2}+\left(\frac{1}{(1-x^2)^2}+\frac{2-B_ox}{(1-x^2)}\right)Y=0, \tag{4}$$

under the same restriction on the regularity of Y on the closed interval $-1 \le x \le 1$. The JWKB approximation is an asymptotic representation, for large B_o, of the form

$$Y \approx C \exp\left[\sqrt{B_o}\left(\int\phi_0 dx+\frac{1}{\sqrt{B_o}}\int\phi_1 dx + \frac{1}{B_o}\int\phi_2 dx+\cdots\right)\right]. \tag{5}$$

We therefore define the small parameter

$$\epsilon = B_o^{-1/3} \tag{6}$$

and consider first the approximation appropriate to the region $-1 < x < 0$:

$$Y \approx A\,[(1-x^2)^{1/4}/x^{1/4}]\sin[\epsilon^{-3/2}i\alpha(x) + \phi + \epsilon^{3/2}i\beta(x)], \tag{7a}$$

where

$$i = \sqrt{-1},$$

$$\alpha(x) = \int_0^x\left(\frac{\xi}{1-\xi^2}\right)^{1/2}d\xi, \tag{7b}$$

$$\beta(x) = \int_{-x_0}^x \frac{35\xi^4-34\xi^2-5}{32\xi^{5/2}(1-\xi^2)^{3/2}}d\xi, \tag{7c}$$

and where x_o is an arbitrary constant, $0 < x_0 < 1$, and ϕ is a constant of integration which appears as a phase angle in the region under consideration. The JWKB approximation for Y, Eq. (7a), is not uniform in x because of the singularity in amplitude at $x = 0$ and the divergence, in the second approximation, of $\beta(x)$ at $x = \pm 1$ [the first JWKB approximation to the function η, Eq. (1a), is singular at the vortex points]. We therefore consider other approximations valid in the region of the turning point, and the vortex point $x = -1$. In the next section we consider the turning point solution, which, when matched to the JWKB approximation, serves to determine the phase angle ϕ.

III. THE TURNING POINT

Inspection of Eq. (4) reveals that an approximation for large B_o is adequate when $x = 0(1)$, but will offer a poor approximation when x is sufficiently small. We therefore magnify the region of nonuniformity by defining a stretched variable

$$\bar{x} = B_o^m x \tag{8a}$$

in terms of which Eq. (4) becomes

$$\frac{d^2Y}{d\bar{x}^2} + B_o^{-2m}[1 + 2\bar{x}^2 B_o^{-2m} + (2 - B_o^{1-m}\bar{x}) \times (1 - \bar{x}^2 B_o^{-2m})]Y = O(B_o^{-4m}). \quad (8b)$$

In the first approximation

$$m = \tfrac{1}{3}, \quad \bar{x} = x/\epsilon, \quad (9a)$$

and

$$\frac{d^2Y}{dx^2} = \bar{x}Y, \quad (9b)$$

so that

$$Y \approx \mathcal{C}\mathrm{Ai}(x) = \mathcal{C}\mathrm{Ai}\left(\frac{x}{\epsilon}\right) \quad (10)$$

where Ai is the Airy function. The approximation [Eq. (10)] replaces the JWKB approximation in the region of nonuniformity, $\bar{x} = 0(1)$, and will be referred to as an inner solution.

IV. MATCHING AT THE TURNING POINT

We now match the asymptotic form of Eq. (10) as $\bar{x} \to -\infty$ with that of Eq. (6) as $x \to 0$. We define the variables

$$y = -x, \quad \bar{y} = y/\epsilon \quad (11)$$

in terms of which the expansion of the inner solution away from the turning point is

$$\mathcal{C}\mathrm{Ai}(\bar{y}) \sim \frac{\mathcal{C}}{\sqrt{\pi}} \frac{\epsilon^{1/4}}{y^{1/4}} \sin(\epsilon^{-3/2}\tfrac{2}{3}y^{3/2} + \tfrac{1}{4}\pi - \epsilon^{3/2}\tfrac{5}{48}y^{-3/2}) \quad \text{as } \bar{y} \to \infty. \quad (12)$$

Under the change of variable

$$\xi = -\eta, \quad (13)$$

the integral $\alpha(x)$, appearing in the JWKB approximation, has the form

$$\alpha(x) = -i\int_0^y \left(\frac{\eta}{1-\eta^2}\right)^{1/2} d\eta \sim -i\tfrac{2}{3}y^{3/2} + O(y^{7/2}) \quad \text{as } y \to 0. \quad (14)$$

The integral $\beta(x)$ is singular in the limit $y \to 0$ and is therefore expanded by adding and subtracting the divergent part first, as follows:

$$\beta(x) = i\left(\int_{x_0}^y F(\eta)d\eta - \int_{x_0}^y \frac{5}{32\eta^{5/2}}d\eta\right), \quad (15a)$$

where

$$F(\eta) = \frac{35\eta^4 - 34\eta^2 - 5[1 - (1-\eta^2)^{3/2}]}{32\eta^{5/2}(1-\eta^2)^{3/2}}, \quad (15b)$$

whence

$$\beta(x) = i\left[\left(\tfrac{5}{48}(y^{-3/2} - x_0^{-3/2}\right) - \int_0^{x_0} F(\eta)d\eta + \int_0^y F(\eta)d\eta\right]. \quad (15c)$$

We now take account of the fact that

$$F(\eta) \sim -\tfrac{83}{64}\,1/\eta^{1/2} + O(\eta^{3/2}) \quad (16a)$$

as $\eta \to 0$, to obtain the result

$$\beta(x) \sim i\left[\tfrac{5}{48}(y^{-3/2} - \kappa^{-3/2}) - J + O(y^{1/2})\right], \quad (16b)$$

where

$$J = \int_0^{x_0} F(\eta)d\eta \quad (16c)$$

is a convergent integral. The behavior of the JWKB approximation near $y = 0$ is thus

$$Y(y) \sim \frac{\mathcal{A}}{e^{i\pi/4}} \frac{1}{y^{1/4}} \sin\{\epsilon^{-3/2}\tfrac{2}{3}y^{3/2} + \phi - \epsilon^{3/2}\tfrac{5}{48}[(y^{-3/2} - x_0^{-3/2}) - J]\} \quad \text{as } y \to 0. \quad (17)$$

We proceed formally[1] and express both the outer expansion, Eq. (7a), and the inner expansion, Eq. (10), in terms of an intermediate variable, $\hat{y} = y/\sqrt{\epsilon}$ appropriate to the overlap domain. The inner and outer expansions are matched to $O(\epsilon^{3/2})$ in the limit $\epsilon \to 0$, $\hat{y}$ fixed. This limit requires that the inner variable $\bar{y} = y/\epsilon \to \infty$, while the outer variable $y \to 0$. The formal matching procedure thus requires the equivalence of Eqs. (12) and (17), with the results

$$\frac{\mathcal{A}}{e^{i\pi/4}} = \epsilon^{1/4}\frac{\mathcal{C}}{\sqrt{\pi}} \quad (18a)$$

and

$$\phi = \tfrac{1}{4}\pi - \epsilon^{3/2}(\tfrac{5}{48}1/x_0^{3/2} + J). \quad (18b)$$

V. THE VORTEX POINT APPROXIMATION

We define a magnified coordinate

$$\bar{s} = B_0 s = s/\epsilon^3, \quad (19)$$

where $s = x + 1$ and in terms of which Eq. (4) becomes

$$\frac{d^2Y}{d\bar{s}^2} + \frac{1}{2\bar{s}}\left(\frac{1}{2\bar{s}} + 1\right)Y = O(\epsilon^3). \quad (20)$$

Under the changes of variable

$$t = (2\bar{s})^{1/2} \quad (21)$$

and

$$Y = tp, \quad (22)$$

the equation for the leading approximation becomes

$$\frac{d^2p}{dt^2} + \frac{1}{t}\frac{dp}{dt} + p = 0, \quad (23)$$

with the result

$$Y \approx \kappa(2\bar{s})^{1/2} J_0(2\bar{s})^{1/2}, \quad (24)$$

where J_0 is the Bessel function of the first kind of order zero.

We choose to normalize the eigenfunction η in such a way that

$$\eta(x=-1)=(-1)^n, \quad n=1,2,3,\cdots, \tag{25}$$

where the introduction and choice of the index n will become clear with the matching of vortex and JWKB approximation. Under the above normalization we have

$$Y \approx (-1)^n (2s)^{1/2} J_0[\epsilon^{3/2}(2s)^{1/2}]. \tag{26}$$

The use of the term "vortex point" is meant to reflect the physical significance of the boundary layer defined by $\bar{s}=O(1)$. In that small region the drop appears flat, and terms representing the curvature of the sphere do not enter in the first approximation, Eq. (23). The resulting solution is of the special class of three-dimensional waves having cylindrical symmetry.[6]

VI. MATCHING AT THE VORTEX POINT

We proceed to match the asymptotic behavior of the boundary-layer approximation, as $\bar{s}\to\infty$, with the JWKB approximation as $s\to 0$. The asymptotic behavior of the former approximation is

$$Y \sim \epsilon^{3/4}(2s)^{1/4}(2/\pi)^{1/2} \sin[-\epsilon^{-3/2}(2s)^{1/2} - \tfrac{1}{4}\pi + \epsilon^{3/2}(1/8\sqrt{2})s^{-1/2} - n\pi], \tag{27}$$

where the index n has been shifted from the amplitude to the phase through the relation

$$(-1)^n \sin\alpha = \sin\{\alpha - n\pi\}, \quad n=1,2,3,\cdots. \tag{28}$$

Under the change of variable

$$u=\xi+1 \tag{29}$$

the integral $\alpha(x)$, appearing in the JWKB approximation, may be represented as

$$\alpha(x) = -iA + i\int_0^s \left(\frac{1-u}{2u-u^2}\right)^{1/2} du \tag{30a}$$

where

$$A=\int_0^1 \left(\frac{\eta}{1-\eta^2}\right)^{1/2} d\eta = \frac{1}{2}\frac{\Gamma(\frac{3}{4})\,\Gamma(\frac{1}{2})}{\Gamma(\frac{5}{4})} = 1.198, \tag{30b}$$

and with an asymptotic form

$$\alpha(x) \sim -iA + i\sqrt{2}\, s^{1/2} + O(s^{3/2}) \quad \text{as } s\to 0. \tag{31}$$

The integral $\beta(x)$ is singular in the limit $s\to 0$. As in Sec. IV, we add and subtract the divergent part before expanding, as detailed below:

$$\beta(x) = -i\left(\int_{1-x_0}^{s} G(u)du - \frac{1}{16\sqrt{2}}\int_{1-x_0}^{s}\frac{du}{u^{3/2}}\right), \tag{32a}$$

where

$$G(u)=\frac{35(u-1)^4 - 34(u-1)^2 - 5 + \sqrt{2}\,[(1-u)^{5/2}(2-u)^{3/2}]}{32u^{3/2}\,(1-u)^{5/2}(2-u)^{3/2}}, \tag{32b}$$

whence

$$\beta(x) = -i\left(\frac{1}{8\sqrt{2}}[s^{-1/2} - (1-x_0)^{-1/2}] - \int_0^{1-x_0} G(u)du + \int_0^s G(u)du\right). \tag{32c}$$

We take account of the fact that

$$G(u) \sim -\frac{85}{64\sqrt{2}}\,\frac{1}{u^{1/2}} + O(u^{1/2}) \tag{32d}$$

as $u\to 0$, to obtain the result

$$\beta(x) \sim -i\{(1/8\sqrt{2})[s^{-1/2} - (1-x_0)^{-1/2}] - M + O(s^{1/2})\}, \tag{33a}$$

where

$$M=\int_0^{1-x_0} G(u)du \tag{33b}$$

is a convergent integral. The behavior of the JWKB approximation near $s=0$ is thus

$$Y \sim \epsilon^{1/4}(\mathcal{C}/\sqrt{\pi})(2s)^{1/4} \sin(\epsilon^{-3/2}(A - \sqrt{2}\, s^{1/2}) + \phi + \epsilon^{3/2}\{(1/8\sqrt{2})[s^{-1/2} - (1-x_0)^{-1/2}] - M\}). \tag{34}$$

When Eqs. (27) and (34) are matched, we obtain the result

$$\mathcal{C} = \epsilon^{1/2}\sqrt{2} \tag{35a}$$

and

$$\epsilon^{-3/2}A + \phi - \epsilon^{3/2}(1/8\sqrt{2})\,[(1-x_0)^{-1/2} + M] + \tfrac{1}{4}\pi - n\pi = 0, \tag{35b}$$

where ϕ is given by Eq. (18b). Equation (35b) is satisfied only for discrete values of ϵ, which, through Eq. (6), determine the eigenvalues $(B_o)_n$. The equation for the eigenvalues is

$$(B_o)_n = \left(\frac{(n+\frac{1}{2})\pi + [(n+\frac{1}{2})^2\pi^2 + 4AQ]^{1/2}}{2A}\right)^2, \quad n=1,2,3,\cdots, \tag{36}$$

where

$$Q=\{(1/8\sqrt{2})[(1-x_0)^{-1/2} + M] + \tfrac{5}{48}x_0^{-3/2} + J\}. \tag{37}$$

It is important to note that Eq. (36) is a second-order approximation in which the quantity Q, deriving from the retention of the higher-order term $\beta(x)$ of the JWKB expansion, serves to correct the first approximation

$$(B_o)_n = [(n+\tfrac{1}{2})\pi/A]^2, \quad n=1,2,3,\cdots. \tag{38}$$

Furthermore, the numerical value of Q is negative and is of such magnitude that the smallest real value of $(B_o)_n$ corresponds to $n = 1$. Thus, the second-order correction, in conjunction with the definition of B_o as a real number, serves to initialize the index n, which we refer to henceforth as the mode number. Finally, it is clear from Eq. (7) that the quantity Q is independent of the particular choice of x_0, $0 < x_0 < 1$, since a change in its value will simply be compensated by an appropriate change in the integration constant ϕ. [x_0 is usually chosen to be zero. However, because the integral $B(x)$ is singular, such a choice is not possible.]

VII. CALCULATION OF THE EIGENVALUES

The constant Q appearing in Eq. (37) was determined by choosing, without loss of generality, the limit of integration

$$x_0 = \tfrac{1}{2} \tag{39a}$$

and the associated values

$$J = \int_0^{1/2} F(\eta)d\eta = -1.898, \tag{39b}$$

$$M = \int_0^{1/2} G(u)du = -1.690, \tag{39c}$$

with the result

$$Q = -1.847. \tag{40}$$

The numerical values of J and M were determined by integrating Eq. (39c) once and Eq. (39b) twice, by parts. The remaining integrals, whose integrands are finite at the lower limit, were then evaluated numerically.

The eigenvalues corresponding to the first ten modes are given in Table I, for both the first and second approximations, by Eqs. (38) and (36), respectively. Also shown are the results of a numerical procedure which is detailed in Ref. 5. Because the JWKB approximation is valid for large mode numbers, the second approximation provides a significant improvement over the first approximation to the lowest eigenvalues.

VIII. THE EIGENFUNCTIONS

In order to complete the description of the eigenfunctions, we treat the domain $0 < x < 1$, where the JWKB approximation displays exponential behavior

$$Y \approx \hat{\mathfrak{a}}[(1-x^2)^{1/4}/x^{1/4}] \exp\{-[\epsilon^{-3/2}\alpha(x) + \epsilon^{3/2}\beta(x)]\}, \tag{41}$$

in a fashion identical to that displayed in the previous sections. The approximation [Eq. (41)] is matched to the turning-point approximation at $x = 0$,

$$Y \approx \epsilon^{1/2}\sqrt{2}\,\mathrm{Ai}(x/\epsilon), \tag{42}$$

TABLE I. First ten eigenvalues. $(B_o)_n$.

Mode number n	First approximation Eq. (38)	Second approximation Eq. (36)	Numerical ref. 5
1	15.47	12.19	11.22
2	42.70	39.84	38.36
3	84.22	81.13	79.45
4	139.2	136.2	134.4
5	208.0	204.9	203.0
6	290.5	287.5	285.6
7	386.7	383.7	381.7
8	496.7	493.8	491.7
9	620.5	617.5	615.4
10	758.0	755.1	752.9

and the appropriate boundary-layer approximation at $x = 1$,

$$Y \approx \hat{\kappa}(2\hat{s})^{1/2} I_0[\epsilon^{-3/2}(2\hat{s})^{1/2}], \qquad \hat{s} = (1-x), \tag{43}$$

where I_0 represents the modified Bessel function of the first kind of order zero. The matching serves to determine both the amplitude factors $\hat{\mathfrak{a}}$ and $\hat{\kappa}$. The first-order approximation to the eigenfunctions in five overlapping regions, extending continuously from $x = -1$ to $x = +1$ and shown

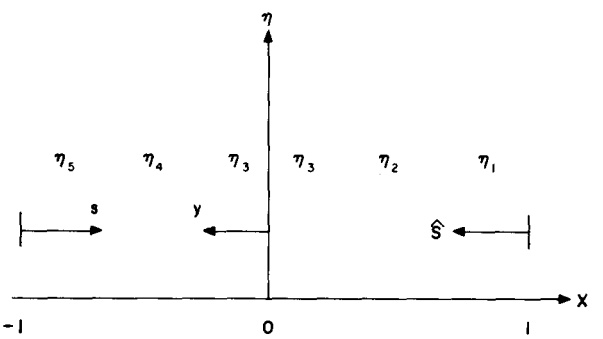

FIG. 1. Overlapping regions of the composite approximation.

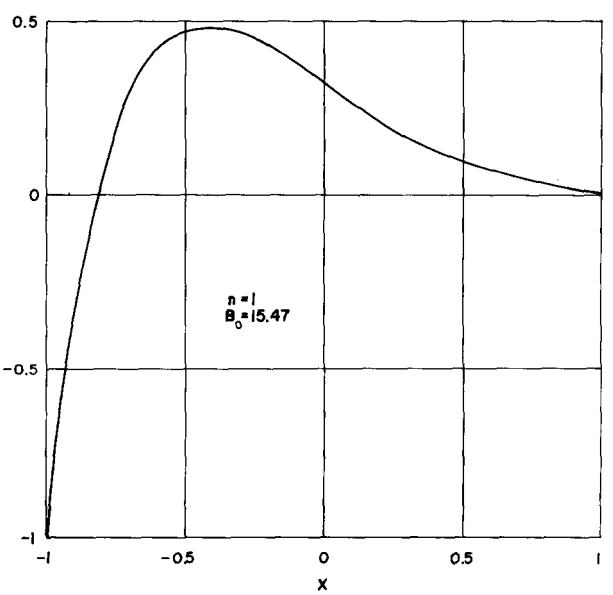

FIG. 2. First-order composite approximation to the first neutral stable mode.

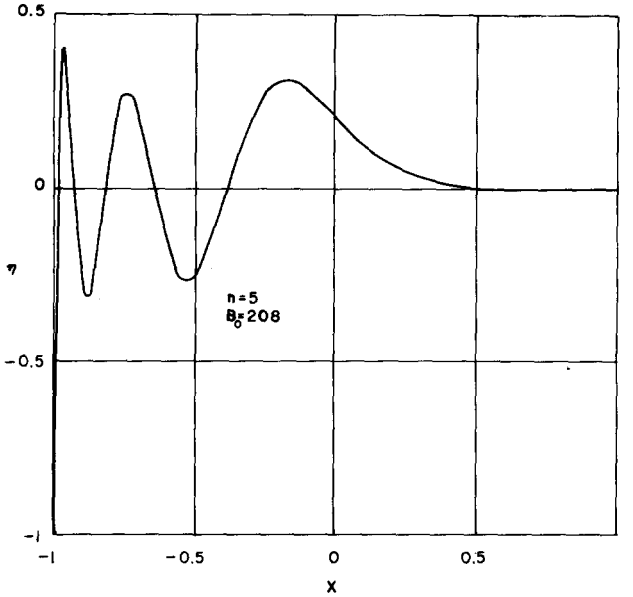

FIG. 3. First-order composite approximation to the fifth neutral stable mode.

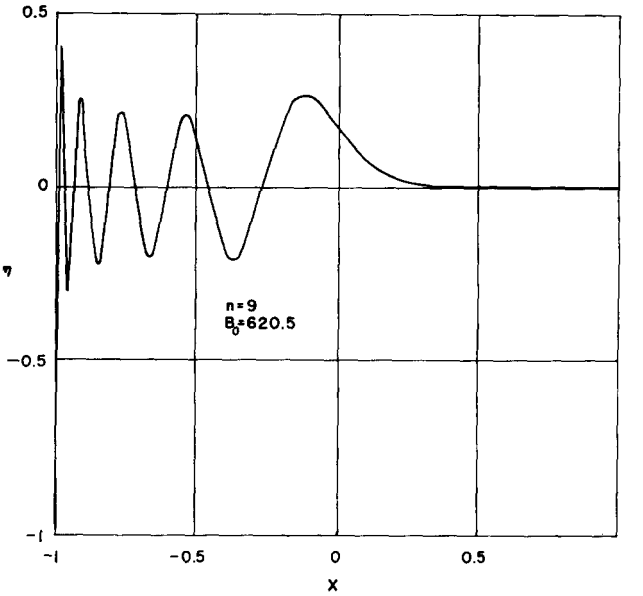

FIG. 4. First-order composite approximation to the ninth neutral stable mode.

schematically in Fig. 1, is summarized below:

$$\eta_5 \approx (-1)^n J_0(2B_o s)^{1/2},$$

$$\eta_4 \approx B_o^{-1/4}\left(\frac{2}{\pi}\right)^{1/2} \frac{\sin\{\sqrt{B_o}\int_0^y [\xi/(1-\xi^2)]^{1/2} d\xi + \frac{1}{4}\pi\}}{y^{1/4}(1-y)^{1/4}},$$

$$\eta_3 \approx B_o^{-1/6}\sqrt{2}A_i(B_o^{1/3}x), \qquad (44)$$

$$\eta_2 \approx B_o^{-1/4} \frac{1}{(2\pi)^{-1/2}} \frac{\exp\{-\sqrt{B_o}\int_0^x [\xi/(1-\xi^2)]^{1/2} d\xi\}}{x^{1/4}(1-x)^{1/4}},$$

$$\eta_1 \approx e^{-A\sqrt{B_o}} I_o(2B_o \hat{s})^{1/2}.$$

First-order composite approximations to the eigenfunctions, constructed by numerically evaluating η_1 through η_5 and joining the resulting curves at arbitrary points in the overlap domains, are shown in Figs. 2–4.

As was mentioned in the Introduction, the eigenfunctions correspond to the amplitudes of small, axially symmetric, stationary waves on the surface of an accelerating liquid sphere. These waves appear as rings on the hemispherical surface, $x = \cos\theta < 0$, when the sphere accelerates in the direction $\theta = 0$. The development of Eq. (1a) is detailed in Ref. 1, where it is shown that an accelerating liquid sphere is subject to instability on the surface $x < 0$ when the Bond number exceeds the lowest critical value $(B_o)_1$.

ACKNOWLEDGMENTS

The authors wish to thank Dr. P. Frost and Dr. J. McHugh[3] for several useful discussions.

[1] J. D. Cole, *Perturbation Methods in Applied Mathematics* (Blaisdell, Waltham, Mass., 1968).
[2] N. Fröman, Arkiv Fysik 32, No. 32 (1967).
[3] J. McHugh, "Historical Survey of Ordinary Linear Differential Equations with Large Parameter," Arch. Hist. Exact Sci., (to be published) (1971).
[4] K. O. Friedrichs, "Advances in Ordinary Differential Equations. II." Lecture Notes, Courant Institute, New York University (unpublished).
[5] I-Dee Chang, E. Y. Harper, and G. W. Grube, "The Breakup of Liquid Drops. I. The Stability of an Accelerating Liquid Sphere" (unpublished).
[6] J. J. Stoker, *Water Waves* (Interscience, New York, 1957).

Solution of the Schrödinger Equation in the Hardy–Lebesgue Space

Evangelos K. Ifantis
Nuclear Research Center "Democritos," Aghia Paraskevi, Attikis, Athens, Greece
(Received 5 August 1970; Revised Manuscript Received 12 April 1971)

We present in this paper a uniform technique for the study of differential and difference equations in the Hardy–Lebesgue space, i.e., the Hilbert space consisting of analytic functions in the unit disk, taking the Schrödinger equation as an example. The approach followed is based on the representation of the Hardy–Lebesgue space by means of the unilateral shift operator, and reduces the problem of solving the Schrödinger equation to a perturbation problem of non-self-adjoint operators in an abstract separable Hilbert space.

I. INTRODUCTION

The Hardy–Lebesgue space $\mathfrak{H}_2(D)$ is a Hilbert space consisting of analytic functions in the unit disk D of the complex plane $\mathbb{C}$. Hilbert spaces of analytic functions are very suitable for the formulation and solution of many problems in function theory.[1] They have the advantage that every element is represented by exactly one function and not by a class of equivalent functions as is done in L_2 spaces of complex-valued functions. For these reasons, papers related to the theory of spaces of analytic functions appear quite often.

On the other hand, problems of physical interest lead to differential equations which must be studied in a Hilbert space of analytic functions.[2] In particular, the space $\mathfrak{H}_2(\mathfrak{D})$ was used recently as an appropriate space for the representation of some commutators[3] and the construction of interesting self-adjoint operators.[4] Another reason which suggests the study of differential and difference equations in $\mathfrak{H}_2(\mathfrak{D})$ is that this space contains the class of polynomials and is therefore suitable for the problem of "polynomial solutions."

In this article, taking and studying extensively, as an example, the ordinary Schrödinger-type differential equation, we present a uniform technique for the study of differential and difference equations in $\mathfrak{H}_2(\mathfrak{D})$. The approach we follow is based on the representation of the space $\mathfrak{H}_2(\mathfrak{D})$ by means of the unilateral shift operator. This representation transforms the problem of solving differential and difference equations in $\mathfrak{H}_2(\mathfrak{D})$ to a perturbation problem of the unilateral shift operator.

The technique is related to the theory of tridiagonal operators[5] (in particular the theory of oscillator phase operators[6]) and gives results which are not so easily obtained in the classical theory of differential and difference equations.

II. THE REPRESENTATION OF THE HARDY–LEBESGUE SPACE

Denote by $\mathfrak{H}$ an abstract separable Hilbert space over the complex field $\mathbb{C}$, by $\mathfrak{H}_2(\mathfrak{D})$ the Hardy–Lebesgue space, consisting of all analytic functions $f(z) = \sum_{n=1}^{\infty} a(n) z^{n-1}$, $|z| < 1$, with the additional property $\sum_{n=1}^{\infty} |a(n)|^2 < \infty$, by $\{e_n\}_1^{\infty}$ an orthonormal basis in $\mathfrak{H}$, and by V the unilateral shift operator V: $Ve_n = e_{n+1}$. The following statements, which we shall use later, are well known[5]:

1. Every value z in the unit disk ($|z| < 1$) is a proper value of the adjoint of V and the set of proper elements $f_z = \sum_{n=1}^{\infty} z^{n-1} e_n$ forms a complete system in $\mathfrak{H}$, in the sense that if f is orthogonal to f_z for every z: $|z| < 1$, then $f = 0$.

2. The mapping

$$f(z) = (f_z, f), \quad f \in \mathfrak{H}, \tag{1}$$

is an isomorphism from $\mathfrak{H}$ onto $\mathfrak{H}_2(\mathfrak{D})$. Thus the space $\mathfrak{H}_2(\mathfrak{D})$ with the scalar product $(f_1(z), f_2(z))_{\mathfrak{H}_2(\mathfrak{H})} = (\overline{f_1}, \overline{f_2})_{\mathfrak{H}}$ becomes a separable Hilbert space with the functions z^{n-1}, $n = 1, 2, \cdots$, forming a complete orthonormal system corresponding to the basis $\{e_n\}_1^{\infty}$ in $\mathfrak{H}$.

3. If (1) holds, then

$$zf(z) = (f_z, Vf), (1/z)[f(z) - f(0)] = (f_z, V^*f). \tag{2}$$

Proposition 1: If C_0 is a diagonal operator, defined as

$$C_0 e_n = n e_n, \quad n = 1, 2, \cdots,$$

then

$$z \frac{df(z)}{dz} = (f_z, \{C_0 - I\} f) \tag{3a}$$

and

$$z^2 \frac{d^2 f(z)}{dz^2} = (f_z, \{C_0^2 - 3C_0 + 2I\} f), \tag{3b}$$

where I is the identity operator on $\mathfrak{H}$.

Proof: The operators C_0 and C_0^2 have a self-adjoint extension[7] in $\mathfrak{H}$ and the elements f_z: $|z| < 1$ belong[5] to the definition domains $\mathfrak{D}(C_0)$ and $\mathfrak{D}(C_0^2)$ of C_0 and C_0^2. The relation (3b) follows by differentiation of the relation

$$f(z) + zf'(z) = \sum_{n=1}^{\infty} n z^{n-1} (e_n, f),$$

which is in fact the relation (3a).

Corollary: The operator $z^2 d^2/dz^2$ in $\mathfrak{H}_2(\mathfrak{D})$ corresponds to the self-adjoint operator

$$A = C_0^2 - 3C_0 + 2I$$

in $\mathfrak{H}$. [In general Euler-type differential operators in $\mathfrak{H}_2(\mathfrak{D})$ are represented by diagonal operators in $\mathfrak{H}$.]

Proposition 2: Let $\phi(z) = \sum_{n=1}^{\infty} C_n z^n \in \mathfrak{H}_2(\mathfrak{D})$. Then the multiplication operator Φ on $\mathfrak{H}_2(\mathfrak{D})$,

$$\Phi : \Phi(f(z)) = \phi(z) f(z), \quad f(z) \in \mathfrak{H}_2(\mathfrak{D}),$$

is represented on $\mathfrak{H}$ by the operator

$$\overline{\phi(V)} = \sum_{n=1}^{\infty} \overline{C}_n V^n.$$

Proof: Define the operator $\phi(V)$ on the set $\{e_n\}_1^{\infty}$ as

$$\phi(V) e_k = \sum_{n=1}^{\infty} C_n V^n e_k = \sum_{n=1}^{\infty} C_n e_{n+k}, \; k = 1, 2, \cdots.$$

Since $\sum_{n=1}^{\infty} |C_n|^2 < \infty$, $\phi(V)$ is defined on $\{e_n\}_1^{\infty}$ and is bounded on every linear combination of elements of $\{e_n\}_1^{\infty}$. Therefore, since it is defined on a dense set in $\mathfrak{H}$, it can be uniquely extended on all elements of $\mathfrak{H}$. Proposition 2 follows now from the first of the relations (2).

Proposition 3: The equation

$$z^2 \frac{d^2 f(z)}{dz^2} + \phi(z) f(z) = 0 \tag{4}$$

has a solution in $\mathfrak{H}_2(\mathfrak{D})$ if and only if the null space of the operator

$$T = \overline{\phi(V)} + A$$

is not empty.

This follows from Statement 2 because of Propositions 1 and 2.

III. THE OPERATOR T

Theorem 1: The null space of T is not empty.

Proof: The operator T has a pure point spectrum (see the Appendix) and, since it is densely defined,

$$\mathrm{Sp}(T) = \overline{\mathrm{Sp}(T^*)}, \tag{5}$$

where $\mathrm{Sp}(T)$ means spectrum of T. The theorem follows from the observation that e_1 is a proper element of T^* with proper value zero.

Theorem 2: In case $C_1 \neq 0$, the proper element, which corresponds to the proper value zero of the operator T, is uniquely determined.

Proof: The proof is very easy if we observe that

$$(V^m f, e_n) = \begin{cases} 0 & \text{for } n \leq m \\ (f, e_{n-m}) & \text{for } n > m \end{cases}$$

and

$$(Af, e_n) = \begin{cases} 0 & \text{for } n \leq 2 \\ a(n) \neq 0 & \text{for } n > 2, \end{cases}$$

where $a(n) = (n-1)(n-2), n = 1, 2, \cdots$.

Let $[\overline{\phi(V)} + A] f = 0$. Since $C_1 \neq 0$, the inner product by e_2 gives $(f, e_1) = 0$. Consequently,

$$\overline{C}_1 (f, e_2) + a(3)(f, e_3) = 0,$$
$$\overline{C}_1 (f, e_3) + \overline{C}_2 (f, e_2) + a(4)(f, e_4) = 0,$$
$$\vdots$$

and with the normalization $(f, e_2) = 1$ the terms (f, e_n) for $n > 2$ can be recursively found, i.e.,

$$(f, e_3) = -\overline{C}_1 / a(3),$$
$$(f, e_4) = \overline{C}_1^2 / a(3) a(4) - \overline{C}_2 / a(4),$$

and so forth. The solution of Eq. (4) is given from (1), i.e.,

$$f(z) = (f_z, f) = z - \frac{C_1}{a(3)} z^2 + \left(\frac{C_1^2}{a(3) a(4)} - \frac{C_2}{a(4)} \right) z^2 + \cdots.$$

For $C_1 \neq 0$, Eq. (4) is of the form

$$\frac{d^2 f(z)}{dz^2} + \left(\frac{a_1}{z} + W(z) \right) f(z) = E f(z). \tag{6}$$

This according to the above theorems means the following.

Conclusion 1: For $a_1 \neq 0$ and $W(z) \in \mathfrak{H}_2(\mathfrak{D})$, every value $E \neq \infty$ is an eigenvalue of the Eq. (6) in the space $\mathfrak{H}_2(\mathfrak{D})$, and the determination of the corresponding eigenfunction in terms of a series is straightforward.

Example 1: Consider the equation

$$\frac{d^2 f(z)}{dz^2} + \left(\frac{a}{z} + Cz + b \right) f(z) = 0,$$
$$a, b, c = \text{real numbers} \neq 0$$

The operator in $\mathfrak{H}$ is $A + aV + bV^2 + cV^3$.

We find recursively the components of the proper element, corresponding to the proper value zero as follows:

$$(Af, e_2) + a(Vf, e_2) = 0,$$
$$\text{i.e.,} \quad a(f, e_1) = 0 \quad \text{or} \quad (f, e_1) = 0,$$
$$a(3)(f, e_3) + a(f, e_2) = 0,$$
$$\text{or} \quad 2(f, e_3) + a(f, e_2) = 0$$

with the normalization $(f, e_2) = 1$.

We have

$$(f, e_3) = -a/2;$$

consequently,

$(f, e_4) = a^2/12 - b/6,$

$(f, e_5) = a\cdot b/18 - c/12 - a^3/144,$ a.s.o.

The proper element f is

$$f = e_2 - (a/2)e_3 + (a^2/12 - b/6)e_4 + \cdots,$$

and the unique in $\mathfrak{H}_2(\mathfrak{D})$ solution of the equation is

$$f(z) = z - (a/2)z^2 + (a^2/12 - b/6)z^3 + \cdots.$$

IV. PERTURBED POTENTIALS OF THE FORM $1/z^n, n \geq 2$

Consider the equation

$$z^3 \frac{d^2f(z)}{dz^2} + \left(\sum_{n=1}^{\infty} C_n z^n\right) f(z) = 0. \tag{7}$$

The operator in $\mathfrak{H}$, which corresponds to Eq. (7) in $\mathfrak{H}_2(\mathfrak{D})$, is $VA + \sum_{n=1}^{\infty} \overline{C}_n V^n$ or

$$V\cdot\left(A + \sum_{n=1}^{\infty} \overline{C}_n V^{n-1}\right), \tag{8}$$

and due to $V^*V = I$ the null space of the operator (8) is not empty if and only if the value $-\overline{c}_1$ is a proper value of the operator

$$A + \sum_{n=2}^{\infty} \overline{C}_n V^{n-1}. \tag{9}$$

Theorem 3: The proper values of the operator (9) are included in the discrete set $a(n) = (n-1)(n-2), n = 1, 2, \cdots,$ i.e.,

$$E_n \subseteq a(n), \quad n = 1, 2, 3, \cdots. \tag{10}$$

Proof: The assumption that there exists a proper value $E \neq a(n), n = 1, 2, \cdots,$ with corresponding proper element f leads easily to $(f, e_1) = (f, e_2) = \cdots = 0,$ i.e., $f = 0.$

Proposition 4: The equality in the relation (10) does not in general hold.

Proof: Consider the operator

$$A + V - \tfrac{1}{2}V^2 \tag{11}$$

and assume that $a(n)$, for a fixed n, say $n = 3$, is a proper value of (11). Then, because of the discretenes of the spectrum of the operator (11) and due to the relation (5), it must be also a proper value of the operator

$$A + V^* - \tfrac{1}{2}V^{*2} \tag{12}$$

Let $1, x_1, x_2, \cdots, x_n, \cdots$ be the components of a proper element of (12) corresponding to the proper value $a(3) = 2$. Then, we must have

$$2x_2e_3 + a(4)x_3e_4 + \cdots + a(n)x_{n-1}e_n + \cdots$$
$$+ x_1e_1 + x_2e_2 \cdots + x_ne_n + \cdots$$
$$- \tfrac{1}{2}x_2e_1 - \tfrac{1}{2}x_3e_2 - \cdots - \tfrac{1}{2}x_ne_{n-1} - \tfrac{1}{2}x_{n+1}e_n \cdots$$
$$= 2\cdot(e_1 + x_1e_2 + x_2e_3 + \cdots + x_{n-1}e_n + \cdots)$$

and

$$x_1 - \tfrac{1}{2}x_2 = 2, \tag{13}$$

$$x_2 - \tfrac{1}{2}x_3 = 2x_1, \tag{14}$$

$$2x_2 + x_3 - \tfrac{1}{2}x_4 = 2x_2, \tag{15}$$

$$\vdots$$

$$a(n)x_{n-1} + x_n - \tfrac{1}{2}x_{n+1} = 2x_{n-1}. \tag{16}$$

For $x_3 \neq 0$ it follows from (13) and (14) that $x_3 = -8$ and from (15) that $x_4 = -16$. Thus, it follows from the general relation (16) that, for $n > 2, x_{n+1} \neq 0$ because $a(n) > 2$ for $n > 3$. It is easy to see that $\lim |x_n| = \infty$ as $n \to \infty$. This contradicts the assumption that f is an element of $\mathfrak{H}$. Thus $x_3 = 0$, i.e., f must lie in one of the invariant subspaces of the operator (12) spanned by the elements e_1, e_2, e_3. But this is impossible because of (13) and (14).

Proposition 5: There exist special cases for which the equality in the relation (10) holds.

For instance, it is easy to see that if f is a proper element of the operator $A + \mu\cdot V^*$ with the proper value $a(n)$ then $(f, e_{n+1}) = (f, e_{n+2}) = \cdots = 0,$ i.e., f must lie in the supspace spanned by the elements $e_1, e_2, \cdots, e_n$. On the other hand, it is easy to see that for every $a(n)$ the coefficients of an element can always be determined such that it is a proper element of $A + \mu\cdot V^*$. Thus the proper values of $A + \mu\cdot V$ are exactly the values $a(n) = (n-1)\cdot(n-2), \ n = 1, 2, 3, \cdots.$

Example 2: Consider the equation

$$\frac{d^2f(x)}{dx^2} + \lambda \exp(-k^2x)f(x) = Ef(x), \quad x\in[0, \infty]. \tag{17}$$

If we make the transformation $z = \exp(-k^2x)$, the above equation takes the form

$$z^2 \frac{d^2f(z)}{dz^2} + z\frac{df(z)}{dz} + \mu z f(z) = \epsilon f(z), \tag{18}$$

where $\epsilon = E/k^4, \mu = \lambda/k^4,$ and $z \in [0, 1]$.

Equation (18) due to the relations (2a), (3a), and (3b) is equivalent to the operator equation

$$(B + \mu\cdot V)f = \epsilon f;$$

where

$$B : Be_n = b(n)e_n, \quad n = 1, 2, \cdots,$$

and

$$b(n) = n^2 - 2n + 2, \quad n = 1, 2, \cdots.$$

Therefore, due to the example in Proposition 5, we have

$$E_n = k^4(n^2 - 2n + 2), \quad n = 1, 2, \cdots .$$

We observe that, for $n > 1$, $(f, e_1) = 0$. This means that

$$f(z) \underset{z\to 0}{=} f(x), \quad x\to\infty .$$

i.e., for $E_n = k^n(n^2 - 2n + 2)$, $n = 2, 3, \cdots$, Eq. (17) has solutions which satisfy the condition $f(\infty) = 0$.

Consider now the equation

$$z^K \frac{d^2f(z)}{dz^2} + \left(\sum_{n=1}^{\infty} C_n z^n\right) f(z) = 0. \tag{19}$$

The operator in $\mathfrak{H}$ which corresponds to Eq. (19) in $\mathfrak{H}_2(\mathfrak{D})$ is the following:

$$V^{K-2}A + \sum_{n=1}^{\infty} \overline{C}_n V^n, \quad K > 3, \quad C_1 \neq 0. \tag{20}$$

It is easy to see that the null space of the operator (20) is empty. In fact, the assumption that there exists a proper element f with proper value zero leads to $(f, e_1) = (f, e_2) = \cdots = 0$, i.e., $f = 0$.

Conclusion 2: The equation

$$\frac{d^2f(z)}{dz^2} + \left(\frac{a_n}{z^n} + \cdots + \frac{a_1}{z} + W(z)\right) f(z) = Ef(z), \tag{21}$$

for $a_n \neq 0, n > 2$, has no solution in $\mathfrak{H}_2(\mathfrak{D})$.

V. CONCLUDING REMARKS

(I) We have studied extensively a peculiar eigenvalue problem for the ordinary Schrödinger-type differential equation (21).

We require that $f(z) = \sum_{n=1}^{\infty} c_n z^{n-1}$ be analytic in the unit disk and satisfy the condition $\sum_{n=1}^{\infty} |c_n|^2 < \infty$, i.e., $f(z)$ belongs to the Hardy-Lebesgue space $\mathfrak{H}_2(\mathfrak{D})$.

For every $W(z) \in \mathfrak{H}_2(\mathfrak{D})$ it is shown that:

(A) For $a_n = 0$, $n \geq 1$, a nonuniquely determined solution always exists.

(B) For $a_1 \neq 0$, $a_n = 0, n > 1$, a unique solution in $\mathfrak{H}_2(\mathfrak{D})$ always exists.

(C) For $a_n \neq 0$, $n > 2$, there is no solution in $\mathfrak{H}_2(\mathfrak{D})$.

(D) For $a_2 \neq 0$ and $a_n = 0$ for $n > 2$, a solution exists only for at most a countable set of real values of the parameter a_2.

It is well known from the classical theory of differential equations that Eq. (21) in the (A) case has two linearly independent solutions analytic in the unit disk. Also, in the (B) case the methods of classical analysis give easily the result that only one solution analytic in the unit disk exists. But that the solutions belong to the space $\mathfrak{H}_2(\mathfrak{D})$ is for the classical analysis an other problem which is very difficult in the cases (C) and (D).

(II) The study of the inhomogeneous differential equations with the free term being an element in $\mathfrak{H}_2(\mathfrak{D})$ is straightforward. We note that in some cases the generalized Green's function can be easily constracted. For instance, in Example 2, we can take, without loss of generality, $|\mu| < 1$. Then, because of

$$\|B^{-1}\| = \sup_n (n^2 - 2n + 2)^{-1} = 1,$$

we have

$$B + \mu V = B(I + \mu B^{-1}V),$$

with

$$\|\mu B^{-1} V\| \leq |\mu| < 1.$$

Thus

$$(B + \mu V)^{-1} = (I + \mu B^{-1}V)^{-1}B^{-1}$$
$$= \sum_{n=0}^{\infty} (-1)^n (\mu B^{-1}V)^n B^{-1}.$$

(III) The method which we follow for the study of the Schrödinger equation can be applied for the study of differential equations of higher order than the second and the study of equations of different kind as well.

For instance, the operator M defined by

$$Me_n = \mu^n e_n, \quad n = 1, 2, \cdots,$$

is represented in $\mathfrak{H}_2(\mathfrak{D})$ by the operator

$$B : Bf(z) = f(\mu \cdot z).$$

This is convenient for the study of geometrical difference equations. We shall examine as an example the case of the homogeneous geometrical difference equation

$$(az + b)f(\mu \cdot z) = (cz + d)f(z), \quad |\mu| < 1. \tag{22}$$

The operator equation corresponding to (22) is

$$V \cdot (\bar{a}M^* - \bar{c}I)f + \bar{b}M^* f = \bar{d}f. \tag{23}$$

It is not difficult to see that the operator in Eq. (23) is one of the cases which predicts Proposition 5. Thus we have

$$d = b\mu^{n-1}, \quad n = 1, 2, \cdots .$$

For $a = 0$, $b = 1$, $c = 1$, Eq. (22) takes the simple form

$$f(\mu z) = (d - z)f(z). \tag{24}$$

The iteration method of the classical theory gives us the solution which satisfies the condition $f(0) \neq 0$, say $f(0) = 1$. The solution is given as follows:

$$f(z) = 1/\prod_{k=1}^{\infty}(d - \mu^k z), \quad d = \mu^{n-1}, \quad n = 1, 2, \cdots.$$

But $f(0) = 1$ means according to the correspondence (1) that $(f, e_1) = 1$. We observe that for $d = \mu^{n-1}$, where $n \geq 2$, the iteration method cannot give a solution because in that case $f(0) = 0$. We thus have solutions of Eq. (22) and (24) which the iteration method of the classical theory does not give.

We remark that only for $d = b$ has Eq. (22) a solution in $\mathfrak{K}_2(\mathfrak{D})$ satisfying the condition $f(0) = 1$. This result is also given by the iteration method of the classical theory. However, this method can hardly justify[8] the assumption $d = b$.

(IV) Consider the diagonal operators A_i, $i = 0, 1, \cdots, k$, defined as

$$A_i e_n = a_i(n) e_n, \quad n = 1, 2, \cdots, \quad i = 1, 2, \cdots, k,$$

and define the operator T as

$$T = \sum_{i=0}^{k} A_i V^i, \qquad V^0 = I. \tag{25}$$

T represents in $l_2(1, \infty)$ a k-order difference equation. If $a_i(n)$, $i = 1, 2, \cdots, k$, are bounded and $a_0(n)$ unbounded, we conclude from the theorem in the Appendix that the spectrum of T is discrete. Moreover, in a similar way to that in theorem (B), we have

$$\mathrm{Sp}(T) \subseteq a_0(n), \quad n = 1, 2, \cdots. \tag{26}$$

If $a_i(n)$, $i = 0, 1, \cdots, k$, are bounded and $\lim a_i(n)$ as $n \to \infty$ exists and is bounded, T represents a Poincaré-type difference equation. For the point spectrum (if it is not empty) we conclude also the relation (26). In any case, we localize the point spectrum within a discrete set of values.

APPENDIX: GAP PERTURBATION OF BOUNDED OPERATORS

Theorem: If T_0 is bounded, if A is normal with a completely continuous inverse, and if there is a gap, in the sense that a circle of radius $\alpha \geq \| T_0 \|$ can be drawn within the set of the regular points of A, then $T_0 + A$ has a pure point spectrum.

In order to prove this theorem, we use the following.

Lemma: If there is a circle $R(\alpha)$ of radius $\alpha \geq \| T_0 \|$ within the resolvent set R_s of the operator A, then there exists a complex vector λ such that

$$\| (A + \lambda I)^{-1} \cdot T_0 \| < 1. \tag{A1}$$

Proof: Since A^{-1} is normal and completely continuous by hypothesis, A has a complete orthonormal set of proper elements $\{e_n\}_1^{\infty}$, i.e.,

$$Ae_n = a_n e_n, \quad \lim |a_n| = \infty \text{ as } n \to \infty,$$

and

$$(A + \lambda I)^{-1} e_n = (\lambda + a_n)^{-1} e_n, \quad \lambda \in R_s;$$

hence

$$\| (A + \lambda I)^{-1} \| = \sup |a_n + \lambda|^{-1} = 1/\inf |a_n + \lambda|$$

and

$$\| (A + \lambda I)^{-1} T_0 \| \leq \| T_0 \| (\inf |a_n + \lambda|)^{-1}.$$

(A1) holds therefore if

$$\inf |a_n + \lambda| > \| T_0 \|. \tag{A2}$$

In fact, the vector λ causes a translation of the spectrum $\{a_n\}$ in the complex plane. Thus, if one takes the vector OA as λ[O is the intersection of the coordinate axis and A the center of the circle $A(\alpha)$ of radius α], then the points $a_n + \lambda$ lie on peripheries of circles containing the circle $A(\alpha)$, i.e., (A2) holds.

Proof of the theorem: Due to the above lemma, we can accept that $\| A^{-1} T_0 \| < 1$ without loss of generality, i.e., the operator $(T_0 + A)^{-1} = (I + A^{-1}T_0)^{-1}A^{-1}$ exists and is completely continuous (because A^{-1} is completely continuous). $T_0 + A$ has, therefore, a discrete spectrum in the sense that it consists only of isolated proper values (see Ref. 9).

[With respect to the nature of the spectrum of $\phi(V) + A$, A can be considered, without restriction of the generality, as an operator with compact resolvent.]

---

1 V. P. Khavin, *Spaces of Analytic Functions* (Progress in Mathematics 1)(Plenum, New York, 1968).
2 S. Schweber, Ann. Phys. (N.Y.) **41**, 205 (1967).
3 I. T. Todorov, *Derivation and Solution of an Infinite-Component Wave Equation for the Relativistic Coulomb Problem*, Lectures presented at the 1969 Battell Seattle Rencontres in Mathematics and Physics (preprint of the Institute for Advanced Study, Princeton, N.J.) (to be published by Springer-Verlag, Berlin-Heidelberg, New York).
4 J. C. Garrison and J. Wong, J. Math. Phys. **11**, 2242 (1970).
5 E. K. Ifantis, J. Math. Phys. **11**, 3138 (1970).
6 E. K. Ifantis, J. Math. Phys. **12**, 1021 (1971).
7 P. C. Deliyannis and E. K. Ifantis, J. Math. Phys. **10**, 421 (1969).
8 H. Meschkowski, *Differenzengleichungen* (Vandenhoeck und Reprecht, Göttingen, 1959), p. 202.
9 T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, Berlin, 1966), p. 187.

Reduction of Group Representations. V*

John R. Gabriel
Argonne National Laboratory, Argonne, Illinois 60439
(Received 22 February 1971)

This paper shows how to use information which can be obtained by use of the Todd Coxeter algorithm and related techniques, to reduce a group representation. The method reduces a representation of $\mathcal{G}$ given a reduction for a subgroup $\mathcal{H}$ of finite index in $\mathcal{G}$. If the character table for $\mathcal{G}$ is given, only rational algebraic processes and square roots are used. If the character table for $\mathcal{G}$ is not known it can be found by solution of eigenvalue equations, using the class sums, which are obtained in the course of the calculation without scanning the whole group.

INTRODUCTION

Previous papers in this series which will be called I–IV have made extensive use of solutions of the eigenvalue problem to extract idempotents from the commutator algebra.[1–4]

This is objectionable because the eigenvalue calculation is essentially numerical and approximate. Recent work on the study of abstract groups using presentations[5] has shown that it is possible to obtain extensive information about the group from knowledge of the generators and defining relations[6,7]; this paper uses such knowledge in the reduction.

Here we shall assume that we are given an abstract group $\mathcal{G}$ which has a subgroup $\mathcal{H}$, that it is desired to reduce a representation of $\mathcal{G}$ which is already reduced w.r.t. $\mathcal{H}$, that the index of $\mathcal{H}$ in $\mathcal{G}$ is finite, that finite sets of generators for $\mathcal{H}$ and $\mathcal{G}$ are given, that character tables for both groups are known,[8–10] that one element from each class of $\mathcal{G}$ is known (the last two restrictions may be relaxed at the expense of additional work) and that the expansion of $\mathcal{G}$ in cosets w.r.t. $\mathcal{H}$ is known.

This may seem to be a great deal to ask for, but with the exception of the reduction w.r.t. $\mathcal{H}$ it is accessible by modern methods for study of finite groups. The reduction w.r.t. $\mathcal{H}$ is achieved by starting with a cyclic subgroup of $\mathcal{H}$ which can be reduced easily and proceeding inductively along a chain of subgroups, using the methods of this paper.

PRELIMINARIES

We shall need some preliminary results.

Lemma 1: Let $\mathcal{G}$ be expanded in cosets w.r.t. $\mathcal{H}$ as

$$\mathcal{G} = \mathcal{H}R_1 \cup \mathcal{H}R_2 \cup \cdots \cup \mathcal{H}R_m$$

with

$$R_1 = E. \tag{1}$$

If $C_{\mathcal{H}}$ commutes with every element of $\mathcal{H}$, then $C_{\mathcal{G}}$ defined by

$$C_{\mathcal{G}} = \frac{1}{m}\sum_{i=1}^{m} R_i^{-1} C_{\mathcal{H}} R_i \tag{2}$$

commutes with every element of $\mathcal{G}$.

Proof: Since $C_{\mathcal{H}}$ commutes with $\mathcal{H}$,

$$C_{\mathcal{H}} = H^{-1} C_{\mathcal{H}} H \quad \text{for} \quad H \text{ in } \mathcal{H} \tag{3}$$

Therefore,

$$C_{\mathcal{H}} = \frac{1}{h}\sum_{H \text{ in } \mathcal{H}} H^{-1} C_{\mathcal{H}} H, \tag{4}$$

where h is the order of $\mathcal{H}$.

Substituting in (2), we have

$$C_{\mathcal{G}} = \frac{1}{mh}\sum_{i=1}^{m}\sum_{H \text{ in } \mathcal{H}} R_i^{-1} H^{-1} C_{\mathcal{H}} H R_i. \tag{5}$$

Because of (1), Eq. (5) shows that

$$C_{\mathcal{G}} = \frac{1}{g}\sum_{G \text{ in } \mathcal{G}} G^{-1} C_{\mathcal{H}} G, \tag{6}$$

which commutes with every element of G.

Lemma 2: If S_σ is an element of the class σ of $\mathcal{G}$ and

$$C_{\mathcal{H}}^{\sigma} = \frac{1}{h}\sum_{H \text{ in } \mathcal{H}} H^{-1} S_\sigma H, \tag{7}$$

then

$$C = \frac{1}{m}\sum_{i=1}^{m} R_i^{-1} C_{\mathcal{H}}^{\sigma} R_i \tag{8}$$

is a class average over the class σ in $\mathcal{G}$.

Proof: Essentially the same as the proof of Lemma 1.

Lemma 3: If ϵ_α is the projection operator for the representation Γ_α of $\mathcal{H}$ in the reduction of the irreducible (w.r.t. $\mathcal{G}$) representation Γ_β of $\mathcal{G}$ w.r.t. the subgroup $\mathcal{H}$ of $\mathcal{G}$, then

$$C = \frac{1}{m}\sum_{i=1}^{m} R_i^{-1} \epsilon_\alpha R_i \tag{9}$$

is equal to

$$(d_\alpha/d_\beta)\epsilon_\beta, \tag{10}$$

where ϵ_β is the projection operator for the irreducible representation Γ_β of $\mathcal{G}$ which contains the given representation Γ_α of the subgroup $\mathcal{H}$ of $\mathcal{G}$.

Proof: Let S_β be the space that affords Γ_β and contains Γ_α. Since R_i is in $\mathcal{G}$ and ϵ_α leaves a subspace of S_β invariant, $R_i^{-1}\epsilon_\alpha R_i$ leaves $R_i^{-1}S_\alpha$, which is a subspace of S_β, invariant. Therefore, each of the m terms in (9) leaves S_β invariant, and so C leaves S_β invariant.

But C commutes with every element of $\mathcal{G}$ and S_β is irreducible w.r.t. $\mathcal{G}$, so that

$$C = \lambda 1 \quad \text{in } S_\beta; \tag{11}$$

taking traces, we see that

$$\lambda = d_\alpha/d_\beta \quad \text{and} \quad C = (d_\alpha/d_\beta)\epsilon_\beta, \tag{12}$$

where d_α and d_β are the dimensions of Γ_α and Γ_β.

Corollary: Let the spaces $S(\alpha, p)$ and $S(\alpha, p')$ be irreducible w.r.t. $\mathfrak{IC}$, and let $e^\alpha_{pp'}$ be the mapping from $S(\alpha, p')$ to $S(\alpha, p)$. If $S(\alpha, p)$ and $S(\alpha, p')$ afford the same representation of $\mathfrak{IC}$ and not merely equivalent representations, then $e^\alpha_{pp'}$ is represented by a unit submatrix in the $\alpha, p; \alpha p'$ position and zeros everywhere else.

Let $S(\beta, q)$, $S(\beta, q')$, and $e^\beta_{qq'}$ be defined analogously for $\mathcal{G}$.

Then, if $S(\alpha, p) \subset S(\beta, q)$ and $S(\alpha, p') \subset S(\beta q')$,

$$e_{qq'} = \frac{d_\beta}{d_\alpha}\frac{1}{m}\sum_{i=1}^{m} R_i^{-1} e^\alpha_{pp'} R_i. \tag{13}$$

Proof: The rhs of (13) maps $S(\beta, q')$ onto $S(\beta, q)$ and by Schur's lemma must be square and nonsingular. If Γ_β has *the same representation* in $S(\beta, q)$ and $S(\beta, q')$, then e^β_{qq}, is the $d_\beta \times d_\beta$ unit submatrix. Note that if $S(\alpha, p)$ and $S(\alpha, p')$ belong with inequivalent representations Γ_β and $\Gamma_{\beta'}$ of $\mathcal{G}$, then the rhs of (13) must be zero.

Lemma 4: If an element T of the group is of order n, i.e., $T^n = E$ and it has a spectral decomposition

$$T = \sum \omega^r \epsilon_r, \quad \text{where} \quad \omega = \exp(2\pi i/n), \tag{14}$$

then

$$\epsilon_r = \frac{1}{n}\sum_{k=1}^{n} \omega^{-kr} T^k. \tag{15}$$

Proof: From the orthogonality of the characters for the cyclic group of order n.

Lemma 5: If S_1 is the space projected by the projection operator ϵ_1 and S_2 is projected by ϵ_2, then the intersection S_{12} of S_1 and S_2 has a basis consisting of the eigenvectors of $\epsilon_1\epsilon_2$ with eigenvalue unity.

Proof: Vectors in S_{12} are obviously simultaneous eigenvectors of ϵ_1 and ϵ_2. All vectors x which obey $\epsilon_1\epsilon_2 x = x$ are simultaneous eigenvectors of ϵ_1 and ϵ_2 because if

$$\epsilon_2 x = y \quad \text{and} \quad \epsilon_1 y = \lambda x, \tag{16}$$

then, since $|\epsilon x| < |x|$ unless $\epsilon x = x$, we have $\lambda < 1$ unless $y = x$.

The equation $\epsilon_1\epsilon_2 x = x$ may be solved by a wide variety of rational methods,[11,12] which are described in detail in the references given. For the sake of completeness the following solution for x is given, which depends only on rational operations. There are better methods for numerical work, however, such as inverse iteration. For symbolic calculations the two-step integer-preserving process is preferable.[13,14] Our conceptually simple method is as follows.

If $\epsilon_1\epsilon_2 x = x$, then $(\epsilon_1\epsilon_2 - 1)x = 0$. Then nonsingular matrices P and Q may be found such that

$$\epsilon_1\epsilon_2 - 1 = P\begin{bmatrix} 1_r & 0 \\ 0 & 0 \end{bmatrix} Q, \tag{17}$$

where 1_r is the $r \times r$ unit submatrix and r is the rank of $(\epsilon_1\epsilon_2 - 1)$. The solutions x are the columns of X where

$$X = Q^{-1}\begin{bmatrix} 0 \\ 1_{n-r} \end{bmatrix}, \tag{18}$$

in which 1_{n-r} is the $(n-r) \times (n-r)$ unit submatrix.

THE CLASS SUMS IN $\mathcal{G}$

The next step in the calculation is to calculate the class sums in $\mathcal{G}$, because these can be used to construct a projection operator ϵ_β which selects the space S_β containing *all* the occurrences of the irreducible representation Γ_β of $\mathcal{G}$. This is useful for three reasons:

(i) S_β is the smallest space containing Γ_β which is invariant w.r.t. $\mathcal{G}$ and its commutator algebra $\mathcal{C}(\mathcal{G})$. Thus it is the smallest version of the problem in microcosm.

(ii) If S_β is of dimension n, because of (1) the problem can be done by using $n \times n$ matrices, which may be considerably smaller than those operating in the whole space. Since the storage requirements are $O(n^2)$ and running time is $O(n^3)$ for most linear algebra calculations, this allows substantial savings in computer resources used.

(iii) If the character table for $\mathcal{G}$ is not known, it may be found from the class sums.[8-10]

Let S_σ be an element of $\mathcal{G}$ belonging to the class σ. Let

$$C^\sigma_{\mathfrak{IC}} = \frac{1}{h}\sum_{H \text{ in } \mathfrak{IC}} H^{-1} S_\sigma H. \tag{19}$$

By Lemma 2,

$$C^\sigma = \frac{1}{m}\sum_{i=1}^{m} R_i^{-1} C^\sigma_{\mathcal{G}} R_i \tag{20}$$

is a class average in $\mathcal{G}$.

It is not necessary to perform the sum over $\mathfrak{IC}$ in order to obtain $C^\sigma_{\mathfrak{IC}}$. The alternative is the following:

Since $C^\sigma_{\mathfrak{IC}}$ is an element of $\mathcal{C}_{\mathfrak{IC}}$, we have

$$C^\sigma_{\mathfrak{IC}} = \sum_{\alpha p q} \lambda^{\sigma\alpha}_{pq} e^\alpha_{pq}, \tag{21}$$

where

$$\lambda^{\sigma\alpha}_{pq} = \frac{1}{d_\alpha h}\sum_{H \text{ in } \mathfrak{IC}} \mathrm{Tr}(H^{-1} S_\sigma H e^\alpha_{qp}) \tag{22}$$

because

$$e^\alpha_{pq} e^{\alpha'}_{rs} = \delta_{\alpha\alpha'}\delta_{qr} e^\alpha_{ps} \tag{23}$$

and

$$\mathrm{Tr}\,(e^{\alpha}_{pp}) = d_\alpha. \tag{24}$$

Since e^{α}_{qp} is in $\mathfrak{C}_{\mathcal{H}}$,

$$\lambda^{\sigma\alpha}_{pq} = \frac{1}{d_\alpha h}\sum_{H \text{ in } \mathcal{H}} \mathrm{Tr}\,(H^{-1}S_\sigma e^{\alpha}_{qp}\mathcal{H}) \tag{25}$$

$$= \frac{1}{d_\alpha}\,\mathrm{Tr}\,(S_\sigma e^{\alpha}_{qp}). \tag{26}$$

Thus Eqs. (16) and (22) offer two alternatives for calculation of the $\lambda^{\sigma\alpha}_{pq}$. The optimal choice depends on the order h of the group $\mathcal{H}$ and the number of "units" e^{α}_{pq}.

Note that if S_σ is in $\mathcal{H}$,

$$\lambda^{\sigma\alpha}_{pq} = \frac{\chi^{\alpha}_{\sigma}}{d_\alpha}\,\delta_{pq}. \tag{27}$$

Having found the coefficients $\lambda^{\sigma\alpha}_{pq}$ for C^σ, we may perform the mapping from $\mathfrak{C}_{\mathcal{H}}$ to $\mathfrak{C}_{\mathcal{G}}$ by Eq. (6). Using the results of Lemma 1, we have

$$C_{\mathcal{G}} = \sum_{\alpha pq} \lambda^{\sigma\alpha}_{pq} f^{\alpha}_{pq}, \tag{28}$$

where

$$f^{\alpha}_{pq} = \frac{1}{m}\sum_{i=1}^{n} R_i^{-1} e^{\alpha}_{pq} R_i. \tag{29}$$

Since at this stage we do not know a basis in which a space $S(\alpha,p)$ belongs to a given space $S(\beta,q)$, we cannot use Lemma 3. However, the f^{α}_{pq} may be expanded in terms of the e^{α}_{pq}, because $\mathfrak{C}_{\mathcal{G}} \subset \mathfrak{C}_{\mathcal{H}}$. We have

$$f^{\alpha}_{pq} = \sum_{\alpha' p' q'} \phi(\alpha,p,q;\alpha',p',q') e^{\alpha'}_{p'q'}, \tag{30}$$

$$\phi(\alpha,p,q;\alpha',p',q') = \frac{1}{m d_{\alpha'}}\sum_{i=1} \mathrm{Tr}\,(R_i^{-1} e^{\alpha}_{pq} R_i e^{\alpha'}_{q'p'}) \tag{31}$$

so that $C^{\sigma}_{\mathcal{G}}$ may be written

$$C^{\sigma}_{\mathcal{G}} = \sum_{\alpha pq} \mu^{\sigma\alpha}_{pq} e^{\alpha}_{pq}, \tag{32}$$

where

$$\mu^{\sigma\alpha}_{pq} = \sum_{\alpha' r' s'} \frac{1}{d_\alpha}\,\mathrm{Tr}(S_\sigma e^{\alpha'}_{s'r'}) \frac{1}{m}\sum_{i=1}^{m} \times \mathrm{Tr}\,(R_i^{-1} e^{\alpha'}_{r's'} R_i e^{\alpha}_{qp}). \tag{33}$$

THE PROJECTION OPERATOR FOR S_β

Having found the coefficients in the expansion (32) for C_σ, we note that the eigenvalue of C_σ in Γ_β is $\chi^{\beta}_{\sigma}/d_\beta$, where d_β is the dimension of Γ_β. Therefore,

$$C_\sigma = \sum_\beta (\chi^{\beta}_{\sigma}/d_\beta)\epsilon_\beta. \tag{34}$$

If the χ^{β}_{σ} are known, Eq. (34) can be inverted to give

$$\epsilon_\beta = (d_\beta/g)\sum_\sigma \chi^{\beta}_{\sigma} C_\sigma n_\sigma, \tag{35}$$

where n_σ is the number of elements in σ of $\mathcal{G}$.

If the χ^{β}_{σ} are not known, they can be found from the structure constants for the class algebra by solution of eigenvalue problems analogously to the methods of Papers III and IV. This matter is also discussed in Refs. 8–10.

The projection operator ϵ_β differs from the ϵ_β of Lemma 3 in that it selects all the n_β occurrences of Γ_β in the representation, not just one.

Our next task is to study the eigenvectors of ϵ_β. Write

$$\epsilon_\beta = \sum_{\alpha pq} \lambda^{\alpha}_{pq} e^{\alpha}_{pq}. \tag{36}$$

We need eigenvectors of ϵ_β having eigenvalue unity. Let

$$\epsilon_\beta = \sum_\alpha \epsilon^{\alpha}_{\beta}, \tag{37}$$

where

$$\epsilon^{\alpha}_{\beta} = \sum_{pq} \lambda^{\alpha}_{pq} e^{\alpha}_{pq}. \tag{38}$$

Then

$$\epsilon^{\alpha}_{\beta}\epsilon^{\alpha'}_{\beta} = \delta_{\alpha\alpha'}\epsilon^{\alpha}_{\beta}. \tag{39}$$

by the usual argument about mutually exclusive idempotents, and so we may start with the most convenient $\epsilon^{\alpha}_{\beta}$ in a search for bases suitable to Lemma 3.

If the reduction of Γ_β w.r.t. $\mathcal{H}$ is

$$\Gamma_\beta = \sum a_{\beta\alpha}\Gamma_\alpha \tag{40}$$

and S_β contains Γ_β n_β times, then the subspace S^{α}_{β} projected by $\epsilon^{\alpha}_{\beta}$ contains $\Gamma_\alpha a_{\beta\alpha}$ n_β times. Let the coefficients λ^{α}_{pq} in $\epsilon^{\alpha}_{\beta}$ form a $p_{\max}(\alpha) \times p_{\max}(\alpha)$ matrix Λ^α, where $p_{\max}(\alpha)$ is the number of times Γ_α appears in the whole space. Since

$$e^{\alpha}_{pq} e^{\alpha}_{rs} = \delta_{qr} e^{\alpha}_{ps}, \tag{41}$$

The matrix Λ^α is isomorphic to $\epsilon^{\alpha}_{\beta}$ so that $(\Lambda^\alpha)^2 = \Lambda^\alpha$. This implies that the columns of Λ^α are eigenvectors of Λ^α belonging to eigenvalue unity, and if they are orthonormalized, together with their orthogonal complement, they define a matrix U^α such that

$$U^\alpha \Lambda^\alpha U^{\alpha-1} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \tag{42}$$

where 1 is the $a_{\beta\alpha}n_\beta \times a_{\beta\alpha}n_\beta$ unit matrix.

The matrix U^α defines an element V^α of $\mathfrak{C}_{\mathcal{H}}$,

$$V^\alpha = \sum_{pq} u^{\alpha}_{pq} e^{\alpha}_{pq}, \tag{43}$$

whose first $a_{\beta\alpha}n_\beta d_\alpha$ rows give a basis $x(\alpha,p,i)$

related to the old basis $x'(\alpha,p',i)$ by

$$x(\alpha,p,i)=\sum_{p'}u^{\alpha}_{pp'}x'(\alpha,p',i) \tag{44}$$

which displays the reduction of S_β w.r.t. $\mathfrak{K}$.

If an α exists for which $a_{\beta\alpha}=1$,[15] then the corresponding n_β spaces $S(\alpha,p)$, $p=1\cdots n$, each belong to a different $S(\beta,q)$. Each one of them satisfies the condition for Lemma 3, and a corresponding e^{β}_{qq} may be generated by the algorithm given therein. The e^{β}_{qq} are primitive idempotents for the n_β irreducible components $S(\beta,q)$, $q=1\cdots n_\beta$, of the space S_β. Similarly, if $e^{\alpha}_{pp'}$ maps $S(\alpha,p')$ onto $S(\alpha,p)$ it generates an $e^{\beta}_{qq'}$, which may be used in the style of Papers III and IV to ensure the same representation in each $S(\beta,q)$.

If there is no $a_{\beta\alpha}=1$ belonging to S_β, then more work must be done. The trouble arises because there is some mapping in $\mathfrak{C}_{\mathfrak{K}}$ but not in $\mathfrak{C}_{\mathcal{G}}$, which must be applied to the $x(\alpha,p,i)$ of Eq. (44) to give spaces $S(\alpha,p'')$ which belong to unique $S(\beta,q)$ instead of having vectors which are sums over q values.

The solution to this problem is somewhat lengthy but simple in essence. It depends on the fact that a set of orthogonal vectors which span an irreducible representation of $\mathfrak{C}_{\mathcal{G}}$ in S_β belong each to a different q value in the spaces $S(\beta,q)$. Thus our problem may be solved by reducing the representation of $\mathfrak{C}_{\mathcal{G}}$ in S_β to find a set of first vectors for the spaces $S(\beta,q)$. The reduction is done in the spirit of III and IV by studying the commutator algebra of $\mathfrak{C}_{\mathcal{G}}$, i.e., the group algebra $\mathfrak{A}(\mathcal{G})$ of $\mathcal{G}$. Because $\mathcal{G}$ is a group, the results of Lemmas 4 and 5 allow us to avoid the eigenvalue calculations which disfigure III and IV.

Consider an element C of $\mathfrak{C}_{\mathcal{G}}$. S_β is invariant w.r.t. C because C cannot map between inequivalent irreducible representations of $\mathcal{G}$.

The space of $S_\alpha(1)$ spanned by all the $p_{max}(\alpha)$ first vectors of Γ_α in the whole space is invariant w.r.t. $\mathfrak{C}_{\mathfrak{K}}$ and so *a fortiori* w.r.t. $\mathfrak{C}_{\mathfrak{K}}$. The intersection $S^{\alpha}_{\beta}(1)$ of S_β and $S_\alpha(1)$ is thus also invariant w.r.t. $\mathfrak{C}_{\mathcal{G}}$. It is spanned by the $n_\beta a_{\beta\alpha}$ vectors $x(\alpha,p,1)$, $p=1\cdots a_{\alpha\beta}n_\beta$, of Eq. (44). It contains the $n_\beta\times n_\beta$ matrix algebra irreducible representation of $\mathfrak{C}_{\mathcal{G}}$ $a_{\beta\alpha}$ times.

The last step in the reduction which divides $S^{\alpha}_{\beta}(1)$ into its irreducible components w.r.t. $\mathfrak{C}$ must be done by appeal to $\mathcal{G}$.

Let R be an element of $\mathcal{G}$ not in $\mathfrak{K}$, preferably a generator, with spectral decomposition

$$R=\sum_{\rho}\rho\epsilon_\rho \tag{45}$$

Since $CR=RC$, the spaces projected by the ϵ_ρ are invariant w.r.t. $\mathfrak{C}_{\mathcal{G}}$. Calculate the ϵ_ρ by the method of Lemma 4. Let S_ρ be the space projected by ϵ_ρ. Choose S_ρ so that the intersection S' of S_ρ and $S^{\alpha}_{\beta}(1)$ is neither null nor $S^{\alpha}_{\beta}(1)$. Then S' affords a step in the reduction of $S^{\alpha}_{\beta}(1)$ w.r.t. $\mathfrak{C}_{\mathcal{G}}$. If S' has dimension $>n_\beta$, then continue, using another generator of $\mathcal{G}$. If the generators are not known, then the coset multipliers R_i may be used. The reduction must terminate when the generators or the R_i are exhausted, if not before.

Once S' with dimension n_β has been found, an orthogonal basis in S' may be constructed. Call the basis $x(\alpha,p,1)$, $p=1\cdots n$. Because S' affords the $n_\beta\times n_\beta$ irreducible matrix representation of $\mathfrak{C}_{\mathcal{G}}$, these $x(\alpha,p,1)$ are suitable first vectors for the n_β occurrences of Γ_β in S_β, and also suitable first vectors for n_β representations Γ_α of $\mathfrak{K}$, each one entirely in the corresponding Γ_β.

Let

$$\epsilon^{\alpha}_{pp}(1)=x(\alpha,p,1)x^{\dagger}(\alpha,p.1);$$

then $\epsilon^{\alpha}_{pp}(1)$ maps vectors in $S(\alpha,p)$ onto other vectors in $S(\alpha,p)$ so that

$$\frac{d_\alpha}{h}\sum_{H\text{ in }\mathfrak{K}}H^{-1}\epsilon^{\alpha}_{pp}(1)H \tag{47}$$

is e^{α}_{pp} in the new basis. It may be expanded in terms in the e^{α}_{pq} in the old basis, which we shall label $e^{\alpha}_{p'q'}$, by

$$e^{\alpha}_{pp}=\sum\psi(\alpha,p,p;\alpha,p',q')e^{\alpha}_{p'q'}, \tag{48}$$

where

$$\psi(\alpha,p,p;\alpha,p',q')=\frac{1}{d_\alpha}\mathrm{Tr}\,[e^{\alpha}_{pp}(1)e^{\alpha}_{q'p'}] \tag{49}$$

$$=\frac{1}{d_\alpha}\mathrm{Tr}\,[x(\alpha,p,1)x^{\dagger}(\alpha,p,1)e^{\alpha}_{q'p'}], \tag{50}$$

which may be calculated in terms of the mapping from the old $x(\alpha,p',i)$ onto the new $x(\alpha,p,i)$.

Once e^{α}_{pp} has been constructed, Lemma 2 gives the e^{β}_{pp} at once. Similar construction of

$$\epsilon^{\alpha}_{pp'}(1)=x(\alpha,p,1)x^{\dagger}(\alpha,p',1), \tag{51}$$

which couples vectors in $S(\beta p)$ and $S(\beta p')$, gives the off-diagonal units for $\mathfrak{C}_{\mathcal{G}}$ by the corollary to Lemma 2.

Construction of a basis in which all n^2_β units e^{α}_{pq} are represented by $d_\beta\times d_\beta$ unit submatrices proceeds, just as in Papers III and IV of this series, by transforming the bases for each $S(\beta,q)$, $q=2\cdots n\beta$, to make the off-diagonal e^{α}_{pq} multiples of the unit submatrix.

POSSIBLE APPLICATIONS IN PHYSICS

The work reported in this paper is part of the development of tools necessary for a molecular analogue of the Racah shell model theory, which

has been so successful in dealing with spherical systems.

Many of the details of the theory are not yet clear, because it is a significant problem to replace the infinitesimal generator techniques used in calculation of Racah coefficients with an appropriate mix of Lie group and finite group methods to deal with the subgroup chain from $SU(n)$ to the molecular symmetry group. Some of the possible techniques for dealing with this have been discussed elsewhere.[16-18]

ACKNOWLEDGMENTS

I am grateful to J. Cannon for drawing my attention to related work by J. D. Dixon[19] and to the referee for suggesting various ways in which the original version of this paper could be improved.

---

* Work supported by the U.S. Atomic Energy Commission.

[1] J. R. Gabriel, J. Math. Phys. **5**, 494 (1964).
[2] J. R. Gabriel, J. Math. Phys. **9**, 973 (1968).
[3] J. R. Gabriel, J. Math. Phys. **10**, 1789 (1969).
[4] J. R. Gabriel, J. Math. Phys. **10**, 1932 (1969).
[5] (Footnote suggested by referee.) A presentation is a set of abstract generators and relations between them which define the group, e.g., $B^7 = (AB)^2 = (A^{-1}B)^3 = (A^2B^2)^4 = 1$ for generators A and B
[6] J. Leech, in *Computational Problems in Abstract Algebra*, Proceedings of a Conference in 1967 (Pergamon, Oxford, 1970), pp. 21-41.
[7] J. Neubuser, in Ref. 6, pp. 1-19.
[8] J. McKay, in Ref. 6, pp. 89-100.
[9] C. Brott and J. Neubuser, in Ref. 6, pp. 101-10.
[10] J. Dixon, Numerische Math. **10**, 446 (1967).
[11] L. Fox, *Introduction to Numerical Linear Algebra* (Oxford U.P., London, 1964).
[12] J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Oxford U.P., London, 1965).
[13] E. H. Bareiss, Math. Computation **22**, 565 (1968); "Computional Solutions of Matrix Problems over an Integral Domain" Argonne National Lab. Technical Memorandum TM222.
[14] J. Lipson, In *Proceedings of 1968 Summer Institute on Symbolic Mathematical Computation*, edited by R. Tobey (IBM, Boston, 1969), pp. 233-306.
[15] E. P. Wigner [*Spectroscopic and Group Theoretical Methods in Physics*, edited by F. Bloch *et al.* (North-Holland, Amsterdam, 1968), p. 131] gives conditions for $\alpha_{\beta\alpha} = 1$.
[16] J. R. Gabriel, J. Chem. Phys. **51**, 1533 (1969).
[17] J. R. Gabriel, J. Chem. Phys. **51**, 3713 (1969).
[18] J. R. Gabriel, J. Computational Phys. **2**, 336 (1968).
[19] J. D. Dixon, Math. Computation (to be published).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Fourier Transform Methods in Linear Transport Theory*

K. M. Case
The Rockefeller University, New York, New York 10021

and

R. D. Hazeltine
Institute for Advanced Study, Princeton, New Jersey 08540

(Received 3 December 1970)

We generalize a three-dimensional Fourier transform method presented previously, to solve various forms of the linearized transport equation in planar geometry. Infinite-space problems are in general easily treated by our procedures. Half-space problems may also be solved analytically in, at least, the following cases: (i) separable scattering kernel (arbitrary particle speed); (ii) one-speed, anistropic scattering with rotation-invariant kernel; (iii) one-dimensional energy-dependent kernel of Kac; (iv) multigroup transport with down scattering only. The general importance of recursion relations to problems with nonseparable kernels is emphasized. A comparison is made between our methods and the two-dimensional singular eigenfunction approach, and a criterion is presented for the analytic solubility of any problem of the general form considered.

1. INTRODUCTION

We are concerned with the analytical solution of boundary value problems involving the linearized transport equation

$$\left(1 + \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)\psi(\mathbf{x},\mathbf{v},t) = c\int d^3\mathbf{v}' f(\mathbf{v},\mathbf{v}')\psi(\mathbf{x},\mathbf{v}',t) + q(\mathbf{x},\mathbf{v},t), \quad \mathbf{x}\in V. \tag{1.1}$$

Here ψ, the phase-space density, is to be determined in some region V of $\mathbf{x}$ space with boundary S, given the boundary data

$$\psi(\mathbf{x},\mathbf{v},t) = \psi_S(\mathbf{x},\mathbf{v},t), \quad \mathbf{x}\in S, \quad \mathbf{v} \text{ inwards}. \tag{1.2}$$

The scattering kernel f and source function q are, like ψ_S, presumed to be given.

It is well known that the one-dimensional, time-independent, one-speed version of Eq. (1.1), with a variety of kernels f, may readily be solved by the "singular eigenfunction" technique.[1] There have recently appeared in the literature several formulations which extend this technique to a wider class of problems. Kaper,[2] for example, allows the one-speed angular density $\psi(\mathbf{x},\Omega)$ to vary in the transverse direction. (By "transverse," we mean perpendicular to the normal of the bounding surface. These directions are well defined since the methods under discussion are limited in applicability to problems in which the boundary de-

has been so successful in dealing with spherical systems.

Many of the details of the theory are not yet clear, because it is a significant problem to replace the infinitesimal generator techniques used in calculation of Racah coefficients with an appropriate mix of Lie group and finite group methods to deal with the subgroup chain from $SU(n)$ to the molecular symmetry group. Some of the possible techniques for dealing with this have been discussed elsewhere.[16-18]

ACKNOWLEDGMENTS

I am grateful to J. Cannon for drawing my attention to related work by J. D. Dixon[19] and to the referee for suggesting various ways in which the original version of this paper could be improved.

---

* Work supported by the U.S. Atomic Energy Commission.

[1] J. R. Gabriel, J. Math. Phys. **5**, 494 (1964).
[2] J. R. Gabriel, J. Math. Phys. **9**, 973 (1968).
[3] J. R. Gabriel, J. Math. Phys. **10**, 1789 (1969).
[4] J. R. Gabriel, J. Math. Phys. **10**, 1932 (1969).
[5] (Footnote suggested by referee.) A presentation is a set of abstract generators and relations between them which define the group, e.g., $B^7 = (AB)^2 = (A^{-1}B)^3 = (A^2B^2)^4 = 1$ for generators A and B
[6] J. Leech, in *Computational Problems in Abstract Algebra*, Proceedings of a Conference in 1967 (Pergamon, Oxford, 1970), pp. 21-41.
[7] J. Neubuser, in Ref. 6, pp. 1-19.
[8] J. McKay, in Ref. 6, pp. 89-100.
[9] C. Brott and J. Neubuser, in Ref. 6, pp. 101-10.
[10] J. Dixon, Numerische Math. **10**, 446 (1967).
[11] L. Fox, *Introduction to Numerical Linear Algebra* (Oxford U.P., London, 1964).
[12] J. H. Wilkinson, *The Algebraic Eigenvalue Problem* (Oxford U.P., London, 1965).
[13] E. H. Bareiss, Math. Computation **22**, 565 (1968); "Computional Solutions of Matrix Problems over an Integral Domain" Argonne National Lab. Technical Memorandum TM222.
[14] J. Lipson, In *Proceedings of 1968 Summer Institute on Symbolic Mathematical Computation*, edited by R. Tobey (IBM, Boston, 1969), pp. 233-306.
[15] E. P. Wigner [*Spectroscopic and Group Theoretical Methods in Physics*, edited by F. Bloch *et al.* (North-Holland, Amsterdam, 1968), p. 131] gives conditions for $\alpha_{\beta\alpha} = 1$.
[16] J. R. Gabriel, J. Chem. Phys. **51**, 1533 (1969).
[17] J. R. Gabriel, J. Chem. Phys. **51**, 3713 (1969).
[18] J. R. Gabriel, J. Computational Phys. **2**, 336 (1968).
[19] J. D. Dixon, Math. Computation (to be published).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Fourier Transform Methods in Linear Transport Theory*

K. M. Case
The Rockefeller University, New York, New York 10021

and

R. D. Hazeltine
Institute for Advanced Study, Princeton, New Jersey 08540

(Received 3 December 1970)

We generalize a three-dimensional Fourier transform method presented previously, to solve various forms of the linearized transport equation in planar geometry. Infinite-space problems are in general easily treated by our procedures. Half-space problems may also be solved analytically in, at least, the following cases: (i) separable scattering kernel (arbitrary particle speed); (ii) one-speed, anistropic scattering with rotation-invariant kernel; (iii) one-dimensional energy-dependent kernel of Kac; (iv) multigroup transport with down scattering only. The general importance of recursion relations to problems with nonseparable kernels is emphasized. A comparison is made between our methods and the two-dimensional singular eigenfunction approach, and a criterion is presented for the analytic solubility of any problem of the general form considered.

1. INTRODUCTION

We are concerned with the analytical solution of boundary value problems involving the linearized transport equation

$$\left(1 + \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)\psi(\mathbf{x},\mathbf{v},t) = c\int d^3\mathbf{v}' f(\mathbf{v},\mathbf{v}')\psi(\mathbf{x},\mathbf{v}',t) + q(\mathbf{x},\mathbf{v},t), \quad \mathbf{x}\in V. \tag{1.1}$$

Here ψ, the phase-space density, is to be determined in some region V of $\mathbf{x}$ space with boundary S, given the boundary data

$$\psi(\mathbf{x},\mathbf{v},t) = \psi_S(\mathbf{x},\mathbf{v},t), \quad \mathbf{x}\in S, \quad \mathbf{v} \text{ inwards}. \tag{1.2}$$

The scattering kernel f and source function q are, like ψ_S, presumed to be given.

It is well known that the one-dimensional, time-independent, one-speed version of Eq. (1.1), with a variety of kernels f, may readily be solved by the "singular eigenfunction" technique.[1] There have recently appeared in the literature several formulations which extend this technique to a wider class of problems. Kaper,[2] for example, allows the one-speed angular density $\psi(\mathbf{x},\Omega)$ to vary in the transverse direction. (By "transverse," we mean perpendicular to the normal of the bounding surface. These directions are well defined since the methods under discussion are limited in applicability to problems in which the boundary de-

pends upon only one spatial variable, e.g., half-space and slab problems.) Similarly, Klinc and Kuščer[3] follow Kaper but, in addition, allow for (exponential) time variation of ψ. Finally, Cercignani[4] presented a one-dimensional formulation which, because it uses an energy-dependent scattering kernel, involves similar techniques.

Common to the analyses of these and other[5] authors (which analyses, it may be remarked, consider only separable scattering kernels), is the apparent need for a fairly high level of mathematical sophistication. In particular, the various extensions of the one-dimensional singular eigenfunction technique typically involve complex singular eigenfunctions, defined on a certain two-dimensional region G of the complex plane. In order, firstly, to prove the various completeness and orthogonality properties of these eigenfunctions, and secondly, to reduce final "answers" to more tractable form, it is found necessary to invoke the theory of generalized analytic functions.[6]

In previous discussion[7] of the work of Kaper, hereafter referred to as I, we argued that the two-dimensional eigenfunction procedure is unnecessarily complicated. Specifically, we showed that a comparatively very simple Fourier transform procedure yields the solution to any boundary value problem of the form which Kaper considers. The method expounded in I inherently requires no completeness or orthogonality proofs; it entirely avoids the mathematical complexity of generalized analytic functions; and, most significantly, it provides, directly, solutions in the form of contour integrals. These solutions were shown to be equivalent to, but much more easily evaluated than, the two-dimensional integrals which Kaper's method yields.

The discussion in I, like the work of Kaper, was restricted to the time-independent, one-speed version of Eq. (1.1), with isotropic scattering ($f = \text{const}$). The purpose of the present study is to determine the degree to which these restrictions may be relaxed.

Our conclusions may be stated here. We shall find, first of all, that whenever f has the separable form

$$f(\mathbf{v},\mathbf{v}') = f_0(\mathbf{v})g(\mathbf{v}'), \tag{1.3}$$

it is almost trivial to extend the Fourier transform method to include exponential time dependence and arbitrary particle speed. Thus, our contention that the use of generalized analytic functions is uncalled for in linear transport theory seems as applicable to the work of Klinc and Kuščer, and of Cercignani, as it was to that of Kaper.

Secondly, we examine the extension of the Fourier transform technique to nonseparable kernels. Our attention is restricted to kernels which may be represented in the form

$$f(\mathbf{v},\mathbf{v}') = g(\mathbf{v}')\sum_n f_n\varphi_n(\mathbf{v})\varphi_n^*(\mathbf{v}'), \tag{1.4}$$

where the f_n are constants, the asterisk denotes complex conjugation, and the sum may include a finite or infinite number of terms. In this case we shall find that an explicit prescription for the solution of Eq. (1.1) may be given, in general, only when the region V includes all space; the half-space or slab problem with anisotropic scattering is not generally amenable to analytic solution. Such a prescription *can* be given, however, if appropriate linear combinations $\hat{\varphi}_m$ of the functions φ_n satisfy a three-term recursion relation of the form

$$v_k\hat{\varphi}_n(\mathbf{v}) = a_n(\mathbf{k})\hat{\varphi}_{n+1}(\mathbf{v}) + b_n(\mathbf{k})\hat{\varphi}_{n-1}(\mathbf{v}), \tag{1.5}$$

where v_k is the component of $\mathbf{v}$ parallel to the transform-variable vector $\mathbf{k}$. The requirement (1.5) will be seen to hold for a variety of scattering kernels. In particular, for any one-speed problem in which

$$f(\Omega,\Omega') = f(\Omega\cdot\Omega'), \qquad \Omega \equiv \mathbf{v}/|\mathbf{v}|, \tag{1.6}$$

Eq. (1.5) merely expresses the well-known recursion formula for Legendre polynomials.

We may remark that equations analogous to Eq. (1.5), but expressed in terms of the variables ζ and ζ' of two-dimensional singular eigenfunction theory, will be (if they exist at all) extremely unwieldy. Indeed, even the degenerate kernel $g(\zeta)$ of Ref. 2 is quite complicated, due to the appearance of the Jacobian of the transformation $\Omega \to \zeta$; a theory of orthogonal functions for the two-dimensional region G, which corresponds to the Legendre theory for the line $(-1, 1)$, is entirely lacking. Hence, consideration of anisotropic scattering provides yet another reason for not using the variable ζ and the singular eigenfunctions associated with it.

To summarize, we hope to demonstrate the following: (i) that the use of Fourier transforms gives *in general* a simpler and more direct procedure for solving Eqs. (1.1) and (1.2), than does the use of two-dimensional singular eigenfunctions; (ii) that the general problem with anisotropic scattering is analytically soluble, in most cases (an exception is considered in Sec. 5), only if the kernel may be separated in terms of functions to which three-term recursion relations of the form (1.5) apply.

A Fourier transform formulation of the general problem defined by Eqs. (1.1), (1.2), and (1.4) is presented in Sec. 2. In Secs. 3 and 4 we treat special cases of Eq. (1.4) for which finite boundary problems are analytically soluble. Finally, we consider in Sec. 5 a problem (involving a kernel due to Kac) for the analytical solution of which the Fourier transform procedure yields no prescription. It is verified that in this case, and in any other case which lacks appropriate recursion relations, the singular eigenfunction approach is also unavailing; thus the above-stated necessity of such relations is confirmed.

2. GENERAL FORMULATION

We study in this section the general equations (1.1) and (1.2), assuming only that the scattering kernel f may be expanded in the manner of Eq. (1.4). The formulation presented here generalizes that of I in a fairly obvious way, and therefore some of the details will be omitted.

We confine our attention to the temporal Fourier transform of the density

$$\hat{\psi}(\mathbf{x},\mathbf{v},\omega) = \int_0^\infty dt e^{-i\omega t}\psi(\mathbf{x},\mathbf{v},t). \tag{2.1}$$

The ω dependence will be left implicit below. According to Eqs. (1.1) and (1.2),

$$(1 + i\omega + \mathbf{v}\cdot\nabla)\hat{\psi} = c\int d^3\mathbf{v}' f(\mathbf{v},\mathbf{v}')\hat{\psi}(\mathbf{x},\mathbf{v}') + q(\mathbf{x},\mathbf{v}), \quad \mathbf{x}\in V, \tag{2.2}$$

$$\psi(\mathbf{x}_S,\mathbf{v}) = \psi_S(\mathbf{x}_S,\mathbf{v}), \quad \mathbf{x}_S\in S, \quad \mathbf{v}\text{ inwards}. \tag{2.3}$$

In Eq. (2.2), q represents, of course, the sum of any source which may be present and the initial value contribution $-\psi(t=0)$; it remains a given quantity. The collisionless Green's function

$$G(\mathbf{x}-\mathbf{x}',\mathbf{v}) \equiv \frac{1}{(2\pi)^3}\int d^3\mathbf{k}\,\frac{e^{+i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{1+i\omega+i\mathbf{k}\cdot\mathbf{v}} \tag{2.4}$$

allows us to write the system (2.2) and (2.3) in terms of the integral equation

$$\psi(\mathbf{x},\mathbf{v}) = \int_V d^3\mathbf{x}' G(\mathbf{x}'-\mathbf{x},\mathbf{v})[cp(\mathbf{x}',\mathbf{v}) + q(\mathbf{x}',\mathbf{v})] + \mathbf{v}\cdot\int_S \hat{n}d^2\mathbf{x}_S G(\mathbf{x}_S-\mathbf{x},\mathbf{v})\hat{\psi}_S(\mathbf{x}_S,\mathbf{v}). \tag{2.5}$$

Here we have introduced the abbreviation

$$p(\mathbf{x},\mathbf{v}) \equiv \int d^3\mathbf{v}' f(\mathbf{v},\mathbf{v}')\hat{\psi}(\mathbf{x},\mathbf{v}'), \tag{2.6}$$

and $\hat{n}$ denotes the inward normal to the region V, which region is at this point completely arbitrary. In writing the known function $\hat{\psi}_S$ in the last term of Eq. (2.5), we have used the fact that

$$G(\mathbf{x}_S-\mathbf{x},\mathbf{v}) = 0, \quad \mathbf{x}\in V, \quad \mathbf{v}\cdot\hat{n} < 0. \tag{2.7}$$

This relation can be seen to follow from Eq. (2.4), provided we assume, as is consistent with Eq. (2.1), that $\mathrm{Im}(\omega) \leq 0$.

We now, as usual, presume Eq. (2.5) to hold, not only for $\mathbf{x}\in V$, but in all space (thus extending the domain of definition of $\hat{\psi}$), and take its three-dimensional Fourier transform. With the convention

$$\tilde{\psi}(\mathbf{k},\mathbf{v}) \equiv \int d^3\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}}\hat{\psi}(\mathbf{x},\mathbf{v}), \tag{2.8}$$

and the definition

$$\tilde{p}_V(\mathbf{k},\mathbf{v}) \equiv \int_V d^3\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}}p(\mathbf{x},\mathbf{v}), \tag{2.9}$$

we obtain in this way

$$\tilde{\psi}(\mathbf{k},\mathbf{v}) = \frac{c\tilde{p}_V(\mathbf{k},\mathbf{v}) + \tilde{q}(\mathbf{k},\mathbf{v})}{1+i\omega-\mathbf{k}\cdot\mathbf{v}} + \frac{\mathbf{v}}{1+i\omega-i\mathbf{k}\cdot\mathbf{v}} \cdot\int_S \hat{n}d^2\mathbf{x}_S e^{i\mathbf{k}\cdot\mathbf{x}}\psi_S(\mathbf{x}_S,\mathbf{v}). \tag{2.10}$$

We recall here that in the case of isotropic scattering,[7] $\tilde{p}_V$ is independent of $\mathbf{v}$, so that the velocity average of Eq. (2.10) provides a simple relation between $\tilde{p}$ and $\tilde{p}_V$; for planar geometries $\tilde{p}_V$ may be determined from this relation and, with Eq. (2.10) for $\tilde{\psi}$, our problem is solved. In the present case of anisotropic scattering, Eq. (1.4) provides the expansion

$$\tilde{p}(\mathbf{k},\mathbf{v}) = \sum_n f_n\rho^n(\mathbf{k})\varphi_n(\mathbf{v}), \tag{2.11}$$

where

$$\rho_n(\mathbf{k}) \equiv \int d^3\mathbf{v} g(\mathbf{v})\varphi_n^*(\mathbf{v})\tilde{\psi}(\mathbf{k},\mathbf{v}). \tag{2.12}$$

Now Eq. (2.10) yields an algebraic *system* of relations between ρ^n and ρ_V^n, where the latter quantity, defined by the convention of Eq. (2.5), may be written as

$$\rho_V^n(\mathbf{k}) = \int d^3\mathbf{k}'\Delta_V(\mathbf{k}-\mathbf{k}')\rho^n(\mathbf{k}'), \tag{2.13}$$

with

$$\Delta_V(k) \equiv (2\pi)^{-3}\int_V d^3\mathbf{x} e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{2.14}$$

Explicitly, upon multiplying Eq. (2.10) by $g\varphi_n^*$ and integrating over $\mathbf{v}$, we obtain

$$\rho^n(\mathbf{k}) = \sum_m [\delta_{nm} - \Lambda_{nm}(\mathbf{k})]\rho_V^m(\mathbf{k}) + B^n(\mathbf{k}). \tag{2.15}$$

Here B^n is the known contribution from the initial conditions, boundary data, and sources:

$$B^n(\mathbf{k}) \equiv \int d^3\mathbf{v} g(\mathbf{v})\varphi_n^*(\mathbf{v})(1+i\omega-i\mathbf{k}\cdot\mathbf{v})^{-1} \times (\tilde{q}(\mathbf{k},\mathbf{v}) + \mathbf{v}\cdot\int_S \hat{n}d^2\mathbf{x}_S e^{i\mathbf{k}\cdot\mathbf{x}_S}\psi_S(\mathbf{x}_S,\mathbf{v})), \tag{2.16}$$

and Λ_{nm} denotes the matrix dispersion function

$$\Lambda_{nm} = \delta_{nm} - cf_m\int d^3\mathbf{v} g(\mathbf{v})\frac{\varphi_n^*(\mathbf{v})\varphi_m(\mathbf{v})}{1+i\omega-i\mathbf{k}\cdot\mathbf{v}}. \tag{2.17}$$

We see from Eq. (2.13) that Eq. (2.15) represents a (possibly infinite) set of coupled integral equations for the $\rho^n(\mathbf{k})$. If these equations can be solved, then $\tilde{p}$ (and hence $\tilde{p}_V$) is known from Eq. (2.11), and Eq. (2.10) provides $\tilde{\psi}$. The question therefore is, under what circumstances can we determine the ρ^n from Eq. (2.15)?

One situation in which Eq. (2.15) is immediately soluble (in theory!) is clear: when the region V includes all space. Then $\Delta_V(\mathbf{k}) = \delta(\mathbf{k})$ and the equation reduces to

$$\sum_m \Lambda_{nm}\rho^m = B^n. \tag{2.18}$$

Thus, in the (translation-invariant) infinite-space case, our basic problem reduces, unsurprisingly, to the purely algebraic task of inverting the matrix Λ_{nm}; we need only require

$$\det|\Lambda_{nm}| \neq 0, \quad \text{for} \quad \mathbf{k} \text{ real.} \tag{2.19}$$

(We should note that this requirement can be relaxed, as in fact it must be for regenerative, $c > 1$, transport. The technical modifications needed to treat the $c > 1$ case may be found, for example, in Refs. 1 and 8.)

In considering more complicated geometries, we confine our attention to the simplest nontrivial case: half-space problems. In the next section we will show that when the scattering kernel separates as in Eq. (1.3), these problems can be solved, provided only that the dispersion function Λ is decomposable into factors each of which is analytic in an appropriate region of the $\mathbf{k}\cdot\hat{n}$ plane. Clearly, in the more general case considered here, a *matrix* factorization of Λ_{nm} would be required. That is, one would need matrices Λ_{+nm} and Λ_{-nm}, each of whose elements are analytic in the appropriate half-plane of the complex variable $\mathbf{k}\cdot\hat{n}$, and such that

$$\Lambda_{nm} = \sum_k \Lambda_{+nk}(\Lambda_-^{-1})_{km}. \tag{2.20}$$

While the existence of matrices $\Lambda_\pm$ of this form has been studied,[9] a prescription for their construction is entirely lacking, and Eq. (2.20) may not be presumed to solve Eq. (2.15).

We might remark here that one could imagine particular properties of the Λ_{nm} which would allow immediate solution of Eq. (2.15). For example, if each element Λ_{nm} of the nth row has the same cuts in the complex $\mathbf{k}\cdot\hat{n}$ plane, and if the ratio of boundary values $\Lambda_{nm}^+/\Lambda_{nm}^-$ across each cut is independent of the column index m, then Eq. (2.15) may be solved by the procedure of I. Alternatively, if the matrix $T_{mn}(\mathbf{k})$, corresponding to the transformation which brings Λ_{nm} into Jordan canonical form, were to be a rational function of $\mathbf{k}\cdot\hat{n}$, then again Eq. (2.15) could be solved by conventional procedures. There is, in fact, one case of some importance in which Λ_{nm} is (effectively) in Jordan canonical form from the start; this case will be discussed in Sec. 5. However, examination of Eq. (2.17) reveals that such properties as these for Λ_{nm} are quite exceptional.

We conclude that the matrix equation (2.15) is not in general amenable to analytic solution. There is, nonetheless, one class of scattering kernels, in addition to the separable case of Eq. (1.3), which are *not* exceptional, and for which Eq. (2.15) may be solved: kernels characterized by the existence of recursion relations of the form (1.5). Kernels of this form will be considered in Secs. 4 and 5, where the explicit solutions to various half-space problems will be constructed. It will suffice here to draw attention to the fact that Eq. (1.5) permits us to express all the ρ_V^n in terms of ρ_V^0; upon substituting this expression into the "zeroth component" of Eq. (2.15), we obtain a single integral equation for ρ_V^0. This equation is of conventional form and may be solved by, essentially, the usual[7] prescription.

3. SEPARABLE SCATTERING KERNELS

Of course all the complications discussed at the end of the previous section are irrelevant when the scattering kernel is separable [as in Eq. (1.3)]. To treat this case, we may begin with Eqs. (2.8)–(2.10). If we define, in addition, the integrated density

$$\tilde{\rho}(\mathbf{k}) \equiv \int d^3\mathbf{v}' g(\mathbf{v}')\tilde{\psi}(\mathbf{k}, \mathbf{v}'), \tag{3.1}$$

then, upon multiplying Eq. (2.10) by g and integrating over $\mathbf{v}$, we immediately obtain

$$\tilde{\rho}(\mathbf{k}) = \tilde{\rho}_V(\mathbf{k})[1 - \Lambda(\mathbf{k})] + B(\mathbf{k}). \tag{3.2}$$

The dispersion function here is

$$\Lambda(\mathbf{k}) \equiv 1 - c\int d^3\mathbf{v} f_0(\mathbf{v})(1 + i\omega - i\mathbf{k}\cdot\mathbf{v})^{-1}, \tag{3.3}$$

and, as usual, B represents the known contributions from the last two terms of Eq. (2.10).

We reiterate our basic approach: Eq. (3.2) is to be solved for $\rho_V(\mathbf{k})$. Then Eq. (2.10), with $p_V \equiv f_0\rho_V$, provides the complete solution to the problem.

This procedure (including the inverse Fourier transform with respect to $\mathbf{k}\cdot\hat{n}$) has already been carried out explicitly, and for a variety of regions V, in the special case $|\mathbf{v}| = 1$, $\omega = 0, f = \text{const.}$[7,8] The only essential differences between that case and the more general one considered here are those evident in Eq. (3.3) for Λ. We shall, nonetheless, discuss the solution to Eq. (3.2) in some detail, both for the sake of completeness and because the function theoretic arguments of the previous analysis require generalization.

We begin by observing that infinite-space problems are once again trivial to solve from Eq. (3.2), since we have in this case ($\rho_V = \rho$)

$$\tilde{\rho}(\mathbf{k}) = B(\mathbf{k})/\Lambda(\mathbf{k}), \tag{3.4}$$

which is well defined so long as [cf. the remark following Eq. (2.19)]

$$\Lambda(\mathbf{k}) \neq 0, \quad \mathbf{k} \text{ real.} \tag{3.5}$$

Next, we recall[1,8] that slab problems can always be treated, at least in the wide-slab approximation, whenever the half-space problem is soluble. Hence we may restrict our attention here to half-space problems and assume the region V to be defined by $\{x > 0, -\infty < y, z < \infty\}$. For convenience we denote the normal component of $\mathbf{k}$ by k: $\mathbf{k}\cdot\hat{n} = k_x \equiv k$; dependence upon the transverse components $\mathbf{k}_t \equiv (k_y, k_z)$ will be left implicit wherever possible. We have, then, from Eq. (2.14),

$$\Delta_V(\mathbf{k}) = \frac{1}{2\pi i}\frac{\delta(\mathbf{k}_t)}{k + i0}, \tag{3.6}$$

whence

$$\rho_V(k) = \rho_+(k), \tag{3.7}$$

where the + subscript refers to a conventional decomposition of $\rho = \rho_+ + \rho_-$ into functions analytic, respectively, above and below the real k axis. Equation (3.2) may now be written as

$$\Lambda(k)\rho_+(k) = -\rho_-(k) + B(k). \tag{3.8}$$

Now suppose (at this point the procedure of I is somewhat generalized) we can find a function $X(k)$, which is analytic in the k plane cut along the real axis, and such that its boundary values $X^\pm$ on the cut satisfy

$$X^+(k)/X^-(k) = \Lambda(k), \quad k \text{ real}. \tag{3.9}$$

Then, according to Eq. (3.8),

$$X^+(k)\rho_+(k) + X^-(k)\rho_-(k) = B(k)X_-(k), \quad k \text{ real}. \tag{3.10}$$

For suitably behaved $B(k)$, Eq. (3.10) determines the $\rho_\pm$ in a well-known[10] way. We define the function

$$\mathfrak{F}(k) \equiv X(k) \begin{cases} \rho_+(k), & \mathrm{Im}k > 0, \\ -\rho_-(k), & \mathrm{Im}k < 0. \end{cases} \tag{3.11}$$

This function is evidently analytic in the cut k plane, its discontinuity across the cut being given by Eq. (3.10):

$$\mathfrak{F}^+(k) - \mathfrak{F}^-(k) = B(k)X_-(k), \quad k \text{ real}. \tag{3.12}$$

The analytic properties of $\mathfrak{F}$ and Eq. (3.12) imply that

$$\mathfrak{F}(k) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} dk' \frac{B(k')X^-(k')}{k'-k} + E(k), \tag{3.13}$$

provided the integral exists. Here E denotes an entire function which may be determined from the Liouville theorem. Specifically, by anticipating the fact that

$$\lim_{k\to\infty} X(k) = 1 \tag{3.14}$$

and, further, requiring the inverse Fourier transform of $\rho(k)$ to exist in the "classical" sense[11]

$$\lim_{k\to\infty} \rho(k) = 0, \tag{3.15}$$

we easily find that $E \equiv 0$. The solution to the general half-space problem is thus provided by

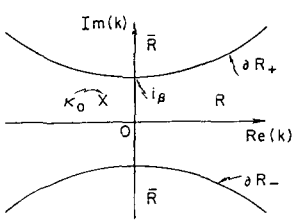

Fig. 1. Region of analyticity R, with boundaries $\partial R_\pm$. κ_0 denotes a root of Λ.

Eqs. (3.11) and (3.13):

$$\rho_V(k) = \rho_+(k) = \frac{1}{2\pi i X^+(k)}\int_{-\infty}^{\infty} dk' \frac{B(k')X^-(k')}{k'-k-i0}. \tag{3.16}$$

Of course, there remains the construction of the function X—to which we now turn our attention.

We assume for simplicity that Eq. (3.5) holds, and that $\Lambda(k)$ is sufficiently smooth for its logarithm to satisfy a Hölder condition on the real line. It should be noted, however, that no assumption is made here concerning the behavior of Λ for complex k; in this respect our treatment is more general than is customary. Since it is evident that

$$\lim_{k\to\infty} \Lambda(k) = 1, \tag{3.17}$$

the function

$$\Gamma(k) \equiv \frac{1}{2\pi i}\int_{-\infty}^{\infty} dk' \frac{\ln\Lambda(k')}{k'-k} \tag{3.18}$$

is analytic in the cut plane and vanishes at $k = \infty$. The discontinuity of Γ across the cut is, by the Plemelj formulas,[10]

$$\Gamma^+ - \Gamma^- = \ln\Lambda, \quad k \text{ real}, \tag{3.19}$$

so that if we define

$$X(k) = e^{\Gamma(k)}, \tag{3.20}$$

then X has all the properties we have required above. In particular, Eq. (3.14) is obviously valid. It follows that Eqs. (2.10), (3.16), and (3.20) provide the explicit solution to the general half-space problem with separable scattering kernel.

To see how the discrete and continuum "modes," typical of linear transport solutions, are contained in Eqs. (3.18) and (3.20), we must specialize to the (usual) case in which Λ is analytic in some open neighborhood of the real k axis. We call the region of analyticity R and its complement $\bar{R}$; a typical configuration is depicted in Fig. 1. It is evident that the function $X(k)$ may be analytically continued into functions Λ_+ or Λ_- which have cuts, not along the real axis, but rather on the ∂R_+, respectively: we have merely appropriately to deform the integration contour in Eq. (3.18), taking proper account of the possible vanishing of Λ in R. After replacing, in Eq. (3.16), the functions $X^\pm$ by their analytic continuations $\Lambda_\pm$, and performing the inverse Fourier transform, we clearly obtain discrete and continuum modes in a well-known way from, respectively, the zeros and cuts of the $\Lambda_\pm$. (For the details of how this works out in a particular case, see, for example, I.)

A further simplification is permitted here. We observe from Eq. (3.3) that the function Λ is analytic almost nowhere within the region $\bar{R}$. On the other hand, there will generally exist a function, $\hat{\Lambda}(k)$, which coincides with Λ for $k \in R$, but which, unlike Λ, may be analytically continued into the region $\bar{R}$. Since our problem is to solve Eq. (3.2) for real k, we may *immediately* replace Λ by $\hat{\Lambda}$

and thereby ignore all the mathematical pathologies of the former function. Examples of the form of $\hat{\Lambda}$ are given explicitly below; for the present we note that $\hat{\Lambda}$ is typically analytic in a region $\hat{R}$, which includes the entire complex plane with the exception of two cuts $l_{\pm}$, as depicted in Fig. 2. Thus, assuming the replacement $\Lambda \to \hat{\Lambda}$ to have been made, we see that the integrals along the contours $\partial R_{\pm}$ in such equations as (3.21) may be replaced by ordinary branch-cut integrals; the consequent gain in simplicity is substantial.

It may be remarked here that one reason for the mathematical complexity of two-dimensional singular eigenfunction methods is that they require detailed consideration of the function Λ, rather than $\hat{\Lambda}$: in such methods, Fig. 1 (or, more precisely, its image under the map $\zeta = -i/k$), rather than Fig. 2, plays the essential role. The theory of generalized analytic functions is required because the basic domain of the singular eigenfunctions is (the image of) the "pathological" region $\bar{R}$, rather than the analyticity region R.

We conclude this section by considering two specific problems, both of which have been treated in the literature from the point of view of two-dimensional singular eigenfunctions.

One-speed, isotropic scattering[2,3]:

Here

$$\Lambda(\mathbf{k}) = 1 - \frac{c}{4\pi}\int \frac{d\Omega}{1 + i\omega - i\mathbf{k}\cdot\Omega}. \tag{3.21}$$

Assuming real $\mathbf{k}_t$ and ω, it is clear that the analyticity region R exists in this case, as it may be expected to exist in any one-speed formulation. For $\bar{k} \in R$, we may straightforwardly evaluate the integral and obtain $\Lambda = \hat{\Lambda}$, $k \in R$, with

$$\hat{\Lambda}(\mathbf{k}) \equiv 1 + \frac{ic}{2(k^2 + B^2)^{1/2}} \ln \frac{l + i\omega + i(k^2 + B^2)^{1/2}}{l + i\omega - i(k^2 + B^2)^{1/2}}. \tag{3.22}$$

(Here the conventional notation $|\mathbf{k}_t| = B$ has been used.) This function is the obvious $\omega \neq 0$ generalization of the function denoted by $\Lambda_3(k)$ in I. It has the simple analytic structure indicated in Fig. 2, with branch points at $k = \pm i\sqrt{B^2 + (l + i\omega)^2}$, and at most two zeros $\pm \kappa_0$, depending upon the value of ω. There is no difficulty in applying our general factorization procedure of Eqs. (3.17)–(3.20), and half-space problems characterized by Eq. (3.21) may be presumed solved by Eq. (3.16). [Similarly, Eq. (3.4) solves the infinite-space problem.] For further details, the reader may consult I; we are content here to remark that the inclusion of nonzero ω has essentially two effects: (i) the roots $\hat{\Lambda}(\kappa_0) = 0$, and hence the discrete modes, will not always exist; (ii) for certain ranges of ω and B, the discrete mode need not dominate the continuum modes for large x.

Many-speed problems:

It is evident from Eq. (3.3) that when the velocity integral includes arbitrarily large values of v_x, the analyticity region R need not include an open neighborhood of the real k axis. While this fact has no effect on the general argument of Eqs. (3.17)–(3.20), it may be expected to complicate the succeeding analysis. It is interesting to note that a problem considered by Cercignani,[4] using singular eigenfunctions, is constructed precisely so as to avoid this complication. Cercignani begins with a one-dimensional equation slightly different from Eq. (1.1). We consider here the three-dimensional form

$$\left(\frac{\partial}{\partial t} + \nu(v) + \mathbf{v}\cdot\nabla\right)\psi(\mathbf{x}, \mathbf{v}, t) = f_0(v)\int d^3\mathbf{v}'\, g(\mathbf{v}')\psi \times (\mathbf{x}, \mathbf{v}', t) + q(\mathbf{x}, \mathbf{v}, t). \tag{3.23}$$

The sole effect on our analysis of including a velocity-dependent collision frequency ν is to replace Eq. (3.3) by

$$\Lambda(\mathbf{k}) = 1 - c\int d^3\mathbf{v}\, \frac{f_0(\mathbf{v})}{\nu(\mathbf{v}) + i\omega - i\mathbf{k}\cdot\mathbf{v}}. \tag{3.24}$$

Now it is assumed in Ref. 4 that $(\nu - \nu_m)/v$, with ν_m the minimum of ν, is monotone nonincreasing, and further, that

$$\lim_{v\to\infty} \nu/v \equiv a \neq 0. \tag{3.25}$$

It is clear from Eq. (3.27) that these assumptions, with $a > 0$, guarantee the analyticity of Λ in an open neighborhood of the real k axis, i.e., the usual region R exists. It follows that not only the general formulation of Eqs. (3.17)–(3.20) (which, we reemphasize, demands no analyticity properties of Λ), but also the simplifications discussed following those equations, will go through without difficulty. For definiteness, we specialize to the particular f_0 used by Cercignani. In this case the function $\hat{\Lambda}$ has the form

$$\hat{\Lambda}(k) = 1 - \int_0^\infty dv^4 e^{-v^2} \frac{\nu^2(v)}{\bar{\nu}} F(kv),$$

$$F(kv) \equiv \frac{i}{kv}\left\{\left[1 + \left(\frac{\nu + i\omega}{kv}\right)^2\right] \ln \frac{\nu + i\omega - ikv}{\nu + i\omega + ikv} + \frac{2i(\nu + i\omega)}{kv}\right\}. \tag{3.26}$$

It is easily verified that F has its only singularities, branch-points, at $k = \pm i(\nu + i\omega)/v$. From the

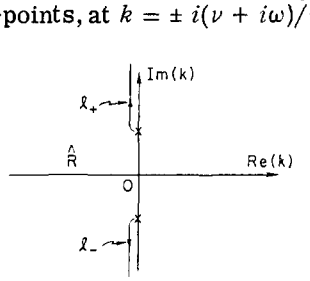

Fig. 2. Region of analyticity $\hat{R}$, with cuts $l\pm$.

assumed properties of ν we find that $\hat{\Lambda}$ may be taken to have two cuts of the general form depicted in Fig. 2. In particular $\hat{\Lambda}$ is analytic in the region $\mathrm{Im}k < a$.

To summarize the results of this section: Problems with separable kernels always lead to equations of the form (3.2), the solution of which provides, via Eq. (2.10), the complete solution to the problem. The infinite-space version of Eq. (3.2) is trivially solved by Eq. (3.4), and the solution to the general half-space problem is provided by Eq. (3.16). These solutions are of particularly simple form when the dispersion function has certain analytic properties. Finally, we have shown that the dispersion function does indeed have these properties in cases recently discussed in the literature.

4. ONE-SPEED PROBLEMS WITH ANISOTROPIC SCATTERING

A. General Method of Solution

In this section we return to the general, anisotropic scattering problem, assuming now that the velocity vector (denoted here by $\boldsymbol{\Omega}$) has unit magnitude, and that the scattering kernel has the rotation-invariant form of Eq. (1.7). Since such a kernel may always be expanded in the manner of Eq. (1.4), we may use the general results of Sec. 2, which are easily specialized to the one-speed case.

Specifically, we write

$$f(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') = \sum_l \frac{2l+1}{2\pi} f_l P_l(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}'), \tag{4.1}$$

where P_l is the Legendre polynomial of order l, and

$$f_l = 2\pi \int_{-1}^{1} dx\, f(x) P_l(x). \tag{4.2}$$

The addition theorem

$$P_l(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^m(\boldsymbol{\Omega}) Y_l^{m*}(\boldsymbol{\Omega}'), \tag{4.3}$$

permit us to write

$$f(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') = \sum_{l,m} f_l Y_l^m(\boldsymbol{\Omega}) Y_l^{m*}(\boldsymbol{\Omega}'), \tag{4.4}$$

just as in Eq. (1.4). In Eq. (4.4), Y_l^m is the usual spherical harmonic, and we abbreviate:

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} = \sum_{l,m}.$$

We now identify the φ_n of Sec. 2 with the Y_l^m, and appropriately adopt our previous results. The ρ^n of Sec. 2 become

$$\rho_l^m(\mathbf{k}) \equiv \int d\boldsymbol{\Omega}\, Y_l^{m*}(\boldsymbol{\Omega}) \psi(\mathbf{k}, \boldsymbol{\Omega}). \tag{4.5}$$

These quantities must satisfy our basic matrix relation, Eq. (2.15), which now has the form

$$\rho_l^m = \sum_{k,n} [\delta_{lk}\delta_{mn} - \Lambda_{lk}^{mn}] \rho_{Vk}^n + B_k^n, \tag{4.6}$$

where the dispersion matrix is

$$\Lambda_{lk}^{mn} \equiv \delta_{lk}\delta_{mn} - c f_l \int d\boldsymbol{\Omega}\, \frac{Y_l^{m*}(\boldsymbol{\Omega}) Y_k^n(\boldsymbol{\Omega})}{1 + i\omega - i\mathbf{k}\cdot\boldsymbol{\Omega}}, \tag{4.7}$$

and B_k^n is given by the obvious modification of Eq. (2.16). Finally, we may recall that ρ_{Vl}^m is related to ρ_l^m by Eq. (2.13) and that our problem is solved once we have determined the quantity

$$\tilde{\rho}_V(\mathbf{k}, \boldsymbol{\Omega}) = \sum_{l,m} f_l \rho_{Vl}^m(\mathbf{k}) Y_l^m(\boldsymbol{\Omega}). \tag{4.8}$$

It is not obvious that the system of equations (4.6), for the ρ_{Vl}^m is any more tractable than the more general version (2.15). (Both systems are of course trivial in the infinite-space case). The point is that in the present case it will suffice to consider only the $m = l = 0$ member of this system. This latter equation may be written in the form

$$\rho^0(\mathbf{k}) = c \sum_l (2l+1) f_l F_l(|k|) \rho_V^l(\mathbf{k}) + B(k), \tag{4.9}$$

where we have introduced the notation

$$\rho^l(\mathbf{k}) \equiv \int d\boldsymbol{\Omega}\, \psi(\mathbf{k}, \boldsymbol{\Omega}) \rho_l(\hat{k}\cdot\boldsymbol{\Omega}), \tag{4.10}$$

$$= \frac{4\pi}{2l+1} \sum_m \rho_l^m(\mathbf{k}) Y_l^m(\hat{k}), \tag{4.11}$$

and the functions F_l are defined by

$$\frac{1}{4\pi} \int d\boldsymbol{\Omega}\, \frac{Y_l^m(\boldsymbol{\Omega})}{1 + i\omega - i\mathbf{k}\cdot\boldsymbol{\Omega}} = F_l(|k|) Y_l^m(\hat{k}). \tag{4.12}$$

[We use the notation $|k| = (k_x^2 + k_y^2 + k_z^2)^{1/2}$ to prevent confusion with the $k = k_x$ of Sec. 3.]

A procedure for solving the infinite-space ($\rho_V^l = \rho^l$) version of Eq. (4.9) is well known[12]: one uses the recursion relation for Legendre polynomials

$$\mathbf{k}\cdot\boldsymbol{\Omega} P_n(\hat{k}\cdot\boldsymbol{\Omega}) = |k| \frac{(n+1)P_{n+1}(\hat{k}\cdot\boldsymbol{\Omega}) + nP_{n-1}(\hat{k}\cdot\boldsymbol{\Omega})}{2n+1} \tag{4.13}$$

to deduce, from Eq. (2.2), a recursion relation for the ρ^l, which functions may then be written in terms of the single unknown function ρ^0. In the case of nontrivial geometry,[1] the identical procedure clearly yields an equation relating to ρ^0 to ρ_V^0. This relation has the form

$$\rho^0(\mathbf{k}) - [1 - \Lambda(\mathbf{k})]\rho_V^0(\mathbf{k}) = \sum_n (2n+1) f_n F_n(|k|) \sum_{l=0}^{n=1} a_{nl}(\mathbf{k}) [q_l(\mathbf{k}) + S_l(\mathbf{k})] + B(\mathbf{k}), \tag{4.14}$$

with

$$\Lambda(\mathbf{k}) \equiv 1 - c\sum_n (2n+1) f_n F_n(|k|) h_n(1/i|k|). \quad (4.15)$$

Here the a_{nl} are determined by (we write $\nu = 1/i|k|$ for convenience)

$$(n+1)a_{n+1,0} + na_{n-1,l} - (1 + i\omega - cf_n(2n+1) \times \nu a_{nl} = 0,$$

$$a_{n+1,n} = -\frac{(2n+1)}{n+1}\nu, \; a_{n+2,n} = -\frac{(2n+3)(2n+1)}{(n+2)(n+1)} \times (1 + i\omega - cf_{n+1}); \quad (4.16)$$

and the h_n[13,14] by

$$(n+1)h_{n+1} + nh_{n-1} - (1 + i\omega - cf_n)(2n+1)\nu h_n = 0, \quad h_0 = 1, \quad h_{-1} = 0. \quad (4.17)$$

We also have

$$q_l(\mathbf{k}) = \int d\Omega \, \rho_l(\hat{k}\cdot\Omega)\, \tilde{q}(\mathbf{k}, \Omega), \quad (4.18)$$

$$S_l(\mathbf{k}) = \int d\Omega \rho(\hat{k}\cdot\Omega)\Omega \cdot \int_S \hat{n} d^2\mathbf{x}_S e^{i\mathbf{k}\cdot\mathbf{x}_S} \psi(\mathbf{x}_S, \Omega). \quad (4.19)$$

Notice that the S_l of Eq. (4.19) are unknown functions (since ψ rather than ψ_S appears in the integrand); we nonetheless temporarily regard them as known. In this case, Eq. (4.14) is identical in form to Eq. (3.2), and assuming only that $\ln\Lambda$ is Hölder continuous for real $\mathbf{k}$, we may immediately apply the general theory of Sec. 3 to obtain the solution to, for example, a half-space problem, in terms of the S_l. Now the recursion relation (4.13) implies[12] that

$$\rho_V^n(\mathbf{k}) = h_n(1/i|k|)\rho_V^0(\mathbf{k}) + \sum_{l=0}^{n-1} a_{nl}(\mathbf{k})\,[q_l(\mathbf{k}) + S_l(\mathbf{k})], \quad (4.20)$$

and it is furthermore evident from Eq. (4.11) that

$$\rho_{Vl}^m(\mathbf{k}) = \frac{2l+1}{4\pi} \int d\hat{k}\, Y_l^m(\hat{k})\, \rho^l(\mathbf{k}). \quad (4.21)$$

Hence the quantity $\tilde{p}_V$ is given by [cf. Eq. (4.8)]:

$$\tilde{p}_V(\mathbf{k}, \Omega) = \sum_{l,m} f \frac{2l+1}{4\pi} Y_l^m \int d\hat{k}\, Y_l^m(\hat{k}) \times \left(h_l(1/i|k|)\rho_V^0 + \sum_{n=0}^{l-1} a_{ln}(\mathbf{k})(q_n + S_n)\right) \quad (4.22)$$

$$= \sum_l f_l \left(\frac{2l+1}{4\pi}\right)^2 \int d\hat{k}\, P_l(\hat{k}\cdot\Omega)\left(h_l(1/i|k|)\rho_V^0 + \sum_{m=0}^{l-1} a_{lm}(q_m + S_m)\right). \quad (4.23)$$

Finally, the angular density is given by Eqs. (4.23) and (2.10):

$$\tilde{\psi}(\mathbf{k}, \Omega) = \frac{\tilde{p}_V(\mathbf{k}, \Omega)}{1 + i\omega - i\mathbf{k}\cdot\Omega} + B(\mathbf{k}, \Omega), \quad (4.24)$$

and there remains only the evaluation of the S_l. The final task may be accomplished by substituting Eqs. (4.23) and (4.24) into Eq. (4.19); we then obtain a purely algebraic system of linear equations for the S_l. This system is not as formidable as it may at first appear. In particular, for half-space problems we easily find

$$S_l(\mathbf{k}) = \int d\Omega \Omega_x P_l(k\cdot\Omega) \int \frac{dk_x'}{2\pi} \tilde{\psi}(\mathbf{k}_x', \mathbf{k}_t, \Omega). \quad (4.25)$$

Notice that the k_x dependence (which in planar geometry is crucial) of this expression is contained entirely in the Legendre polynomial. Hence the half-space S_l involve only (unknown) constants multiplying known functions of k_x. (In the infinite-space case, of course, all the S_l are zero.)

In summary, we have solved the system (4.6) by using the recursion relation (4.13) to reduce it to the simple form of Eq. (3.2), and by then applying our usual method. Since, however, the modifications induced by the need for recursive procedures are not trivial, we next discuss ways in which such formulas as Eqs. (4.14) and (4.15) may be simplified.

B. Some Simplifications

We consider first the expression (4.15), for Λ, which is conveniently rewritten as $\Lambda = \lim \Lambda_N$ as $N \to \infty$, where

$$\Lambda_N = 1 - c\sum_{n=0}^{N} (2n+1) f_n F_n h_n. \quad (4.26)$$

It is easily shown[12] that the F_n satisfy

$$(n+1)F_{n+1} + nF_{n-1} - (1 + i\omega)(2n+1)\nu F_n = -\nu\delta_{n0}. \quad (4.27)$$

In fact, as is clear from Eq. (4.12), the F_n can be written in explicit form:

$$F_n = \frac{1}{i|k|} Q_n\left(\frac{1 + i\omega}{i|k|}\right), \quad (4.28)$$

where Q_n is the Legendre function of the second kind, but Eq. (4.27) will be most useful here. By combining Eqs. (4.17) and (4.27), we may write

$$\Lambda_N = 1 - \frac{1}{\nu}\sum_{n=0}^{N}\{(1 + i\omega)(2n+1)\nu F_n h_n - [(n+1)h_{n+1} + nh_{n-1}]F_n\}$$

$$= -\frac{1}{\nu}\sum_{n=0}^{N}\{[(n+1)F_{n+1}h_n - nh_{n-1}F_n] - [nF_{n-1}h_n - (n+1)h_{n+1}F_n]\}$$

$$= \frac{N+1}{\nu}(h_{N+1}F_N - h_N F_{N+1}). \quad (4.29)$$

We conclude that Eq. (4.15) may be replaced by

$$\Lambda(k) = \lim_{n\to\infty} (n+1)\left[h_{n+1}(1\ i|k|)Q_n\left(\frac{1+i\omega}{i|k|}\right) - h_n(1\ i|k|)\,Q_{n+1}\left(\frac{1+i\omega}{i|k|}\right)\right]. \quad (4.30)$$

We note that in many cases of practical importance, the sum in Eq. (4.15) will be finite, so that Eq. (4.29), rather than Eq. (4.30), may be used.

Similarly, we may use the result, Eq. (4.16), to reduce the double sum in Eq. (4.14) to a single sum. Thus, in order to evaluate

$$C_N(\mathbf{k}) \equiv \sum_{n=0}^{N} (2n+1) f_n F_n \sum_{l=0}^{N-1} a_{nl}(q_l + S_l), \quad (4.31)$$

we rearrange terms:

$$C_N(\mathbf{k}) = \sum_{l=0}^{N-1} \Gamma_l (q_l + S_l), \quad (4.32)$$

with

$$\Gamma_l \equiv \sum_{n=l+1}^{N} (2n+1) f_n F_n a_{nl} = (2l+3) f_{l+1} F_{l+1} a_{l+1,l} + \sum_{n=l+2}^{N} (2n+1) f_n F_n a_{nl}. \quad (4.33)$$

Now the summation range in Eq. (4.33) is such that Eq. (4.16) always holds. It follows that we may combine Eqs. (4.27) and (4.16) to perform the sum in Eq. (4.33), using precisely the same procedure as was applied to $\Lambda(k)$, above. The result is

$$C_N(k) = \sum_{l=0}^{N-1} (q_l + S_l)\{(2l+3) f_{l+1} F_{l+1} a_{l+1,l} + (ik/c)[(N+1)(F_{N+1} a_{N,l} - F_N a_{N+1,l}) + (l+2)F_{l+1} a_{l+2,l} - F_{l+2} a_{l+1,l})]\}. \quad (4.34)$$

Notice that we already have, in Eq. (4.16) explicit expressions for $a_{l+1,1}$ and $a_{l+2,l}$.

Thus our basic problem has been reduced to fairly tractable form. Using the technique of Sec. 3, we are to solve the equation

$$\rho^0(\mathbf{k}) - [1 - \Lambda(\mathbf{k})]\,\rho_V^0(\mathbf{k}) = B(\mathbf{k}) + C(\mathbf{k}), \quad (4.35)$$

where Λ is given by Eq. (4.30), and $C \equiv \lim C_N$ as $N \to \infty$ by Eq. (4.34).

5. CONCLUSIONS

We have emphasized that the formalism presented in Sec. 2 serves, generally, only to reformulate our original problem, and not to solve it. Thus the integro-differential equation (1.1) is reduced to the set of coupled integral equations (2.15); but, aside from the trivial infinite-space case, the latter can be solved analytically only in particular circumstances. On the other hand, the types of scattering kernels for which Eq. (2.15) is soluble are by no means restricted to those [Eqs. (1.3) and (1.4)] discussed in the two previous sections. Before summarizing our general conclusions, we wish to mention two types of many-speed problems which are amenable to analytic solution.

A. One-Dimensional Kac Model

Restricting x and v to one dimension, and setting $\omega = 0$ for simplicity, we have to solve

$$\left(1 + v\frac{\partial}{\partial x}\right)\psi(x,v) = c\int dv' f(v,v')\psi(x,v') + q(x,v), \quad x \in V, \quad (5.1)$$

$$\psi(x,v) = \psi_S(x,v), \quad x \in S, \quad v \text{ inwards}. \quad (5.2)$$

For the scattering kernel f we use a slight generalization of one due to Kac[15]:

$$f(v,v') = e^{-v'^2}\sum_l f_l H_l(v) H_l(v'),$$

where the H_n, which of course correspond to the φ_n of Sec. 2, are Hermite polynomials.[16] The crucial point here is that the H_n satisfy the recursion relation

$$vH_n(v) = nH_{n-1}(v) + \tfrac{1}{2} H_{n+1}(v). \quad (5.3)$$

It is clear that this relation allows us to use the procedure outlined in Sec. 3 to derive equations formally identical to Eqs. (4.14)–(4.23), which equations may then be solved in the usual way. In fact the formalism necessary to reduce Eqs. (5.1) and (5.2) to the standard form of Eq. (3.2) differs so little from that of the previous section that we omit the details here. One significant difference, however, between the one-speed anisotropic scattering case and the Kac model is worthy of note: The latter is characterized by the dispersion relation

$$\Lambda(k) = 1 - c\sum_n G_n(k) g_n(k), \quad (5.4)$$

where

$$G_n(k) \equiv \int dv e^{-v^2}\frac{H_n(v)}{1-ikv} \quad (5.5)$$

and the g_n satisfy [cf. Eq. (4.17)]

$$(1 - c\pi^{1/2}2^n n!\, f_n)g_n - ik(ng_{n-1} + \tfrac{1}{2} g_{n+1}) = 0, \quad g_{-1} = 0, \quad g_0 = 1. \quad (5.6)$$

Notice that the G_n of Eq. (5.5), unlike the F_n of Eqs. (4.12), are evidently not analytic in any open neighborhood of the real k axis. Hence we have, in Eq. (5.4), an example of a dispersion function to which only the very general technique of Eqs. (3.16)–(3.20) need apply; some of the analytical simplifications discussed in Sec. 3 may not be possible.

B. Multigroup Problems[17]

The formalism of Sec. 2 is trivially generalizable to the case in which the ψ of Eq. (2.1) is a column vector $\psi_j(\mathbf{x},\Omega)$, the index j referring to a discrete set of speeds $|v_j|$. Explicitly, a general multigroup problem may be expressed as

$$\sum_j (\sigma_{ij} + i\omega + \delta_{ij}\Omega\cdot\mathbf{V})\psi_j(\mathbf{x},\Omega) = \sum_j c_{ij} \int d\Omega' f(\Omega\cdot\Omega')\psi_j(\mathbf{x},\Omega') + q_i(\mathbf{x},\Omega), \tag{5.7}$$

$$\psi_i(\mathbf{x},\Omega) = \psi_i^S(\mathbf{x},\Omega), \quad \mathbf{x}\in S, \quad \Omega \text{ inwards}. \tag{5.8}$$

Here the matrix σ_{ij} may be presumed to be diagonal, with $\sigma_{ij} > 0$; it is this feature which makes the procedures of Sec. 2 so easily applicable. On the other hand, of course, the resulting version of Eq. (2.15) is again only soluble, in general, where V includes all space.

Since the character of Eqs. (5.7) and (5.8) is so similar to that of problems we have studied above, we need not consider it in any further detail. It may be remarked, however, that there is one case of some importance in which the equations can be solved in nontrivial geometry. Specifically, if

$$c_{ij} = 0, \quad \text{for} \quad i < j, \tag{5.9}$$

then the $i = 1$ component of Eq. (5.7) is identical to Eq. (2.2), with the kernel of Eq. (4.1), and is therefore soluble (in, for example, a half-space) by the method of Sec. 4. Then, considering the other ($i = 1, 2, \cdots$) components in order, we see that each is of the standard, one-group, form, since the coupled terms may be presumed known and lumped with q_i.

That the condition (5.9), which corresponds to down scattering only, grossly simplifies the solution to infinite-space problems is, of course, well known.

C. Conclusions

We have already noted that there exist scattering kernels for which our half-space procedures are not applicable. An example is the three-dimensional kernel of Kac[18]:

$$f(\mathbf{v},\mathbf{v}') = e^{-v'^2}\sum_{i=0}^{4} f_i g_i(v) g_i(v'), \quad g_0 = 1,$$
$$g_{1,2,3} = \sqrt{2}\,(v_x, v_y, v_z),$$
$$g_4 = (2/\sqrt{3})(v^2 - \tfrac{3}{2}). \tag{5.10}$$

For this case, the formalism of Sec. 2 provides solutions only to infinite-space problems; the half-space prescription of Sec. 4 is of no use since the g_i satisfy four-term, rather than three-term, recursion relations.

This circumstance suggests that we examine the range of applicability of two-dimensional singular eigenfunction methods. But it is easily seen that such methods are analogously restricted. Consider, for example, an essential step in the singular eigenfunction solution of one-speed half-space problems with isotropic scattering.[2] In terms of the basic complex variable ζ,

$$\zeta \equiv \frac{\mu}{1 - i\mathbf{k}_t\cdot\Omega}, \tag{5.11}$$

whose domain for physical Ω is a bounded region G of the complex plane (G corresponds, under the map $k_x = -i/\zeta$, to the region $\overline{k}$ of Fig. 1), one must determine that function $X(\zeta)$ which is analytic in a certain subdomain $G^+ \subset G$, and which satisfies

$$X(\zeta)\frac{\partial\Lambda}{\partial\zeta^*} = \Lambda(\zeta)\frac{\partial X}{\partial\zeta^*}, \quad \zeta\in G^+. \tag{5.12}$$

Here Λ is the appropriate dispersion function; it is characterized by being analytic almost nowhere inside the region G. For anisotropic scattering, Eq. (5.12) becomes a matrix equation, for the solution of which the methods of Ref. 2 are neither applicable nor generalizable.

The essential reasons for the inability of singular eigenfunction methods to treat a matrix dispersion function are quite analogous to those for the general insolubility of Eq. (2.15). This analogy between the singular eigenfunction and Fourier transform approaches can be carried further: just as in Sec. 4, the existence of appropriate recursion relations would allow us to reduce such matrix equations as (5.12) to ordinary, "scalar," equations, and our problem could be solved by, essentially, the isotropic scattering methods.

This recursive procedure is in fact commonly applied to the solution of one-dimensional ($\zeta = \mu$) problems.[1] When $\zeta \neq \mu$ as in Eq. (5.11), however, one must ask how recursion relations are to be obtained. The answer, in the one-speed case, is clear: We must return to the original variables Ω, in terms of which we have the well-known formula of Eq. (4.13). In other words, as was remarked in Sec. 1, the variable ζ, by making Legendre theory only very indirectly accessible, has the primary effect of obscuring the analysis.

We may summarize by stating that two-dimensional singular eigenfunction techniques are substantially less well-suited to the solution of three-dimensional problems with anisotropic scattering than the Fourier transform method. In particular, such techniques will not provide solutions to problems involving the scattering kernel, Eq. (5.10), of Kac.

Our general conclusions, already stated in Sec. 1, may be reiterated here. The Fourier transform prescription formulated in I is readily generalized to the solution of a wide class of problems of the form of Eqs. (1.1) and (1.2), in planar geometry. Specifically, any problem of this form can be solved analytically if and only if the corresponding

form of Eq. (2.15) can be solved. It clearly, and unsurprisingly, follows that "any" infinite-space problem is amenable to analytic solution. More significant is the fact that half-space problems are also analytically soluble, by the relatively elementary methods of Secs. 3–5, in, among other cases, (i) all those discussed in the literature from the singular eigenfunction point of view; (ii) the general case of rotation-invariant, anisotropic scattering. The most important situation to which our general approach can be applied only in infinite space is the case of three-dimensional, arbitrary-speed problems with nonseparable kernels, e.g., the Kac problem. The difficulty here is that we lack appropriate recursion relations. We have noted that, for analogous reasons, the two-dimensional singular eigenfunction approach is also inapplicable to problems of this type. Finally, we may remark that the relative complexity of two-dimensional singular eigenfunction methods, which was previously observed in the simple case of I, becomes particularly severe as more general scattering kernels are considered.

ACKNOWLEDGMENT

One of us (K.M.C.) would like to thank the Institute for Advanced Study for the hospitality extended to him as a visitor during part of the time when this work was done.

---

* Work supported in part by the U.S. Atomic Energy Commission, under Contract No. AT(30-1)-3927.

1 See, for example, K. M. Case and P. F. Zweifel, *Linear Transport Theory* (Addison-Wesley, Reading, Mass., 1967).
2 H. G. Kaper, J. Math. Phys. **10**, 286 (1969).
3 T. Klinc and I. Kuščer, "Effect of Lateral Leakage on Neutron Waves" (unpublished).
4 C. Cercignani, Ann. Phys. (N.Y.) **40**, 454 (1966).
5 For example: R. C. Erdmann and A. Sotoodehnia, J. Math. Anal. Appl. **31**, 603 (1970).
6 I. N. Vekua, *Generalized Analytic Functions* (Addison-Wesley, Reading, Mass., 1962).
7 K. M. Case and R. D. Hazeltine, J. Math. Phys. **11**, 1126 (1970).
8 R. D. Hazeltine, thesis (University of Michigan, 1968) (unpublished).
9 See, for example, I. C. Gohberg and M. G. Krein, Am. Math. Soc. **14**, 217 (1960).
10 See, for example, N. I. Muskhelishvili, *Singular Integral Equations* (Noordhoff, Groningen, The Netherlands, 1953).
11 Here we restrict our consideration to the "least singular" solution, in the sense of K. M. Case, J. Math. Phys. **7**, 12 (1966). For regenerative transport, the least singular solution does not satisfy Eq. (3.15), which is unsurprisingly from physical considerations.
12 I. Waller, Arkiv. Mat. Astron. Fysik **34A**, No. 3 (1947). We are grateful to the referee for drawing our attention to this reference.
13 J. Mika, Nucl. Sci. Eng. **11**, 415 (1961).
14 C. Inönu, "Case Eigenfunctions and the Theory of Orthogonal Polynomials," talk presented at the Blacksburg Conference on Transport Theory, 1969 (unpublished).
15 M. Kac, in *Proceedings of the Third Berkeley Symposium on Mathematics, Statistics and Probability* (University of California Press, Berkeley, Calif., 1956), Vol. 3, pp. 171-193.
16 We use the normalization convention of P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).
17 C. E. Siewert and P. S. Shieh, J. Nucl. Energy **21**, 383 (1967).
18 See G. E. Uhlenbeck and G. W. Ford, *Lectures in Statistical Mechanics* (American Mathematical Society, Providence, R. I., 1963), p. 93. See also P. L. Bhatnagar, E. P. Gross, and M. Krook, Phys. Rev. **94**, 511 (1954).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Markov Approach to Density Fluctuations Due to Transport and Scattering. I. Mathematical Formalism*

K. M. van Vliet
Centre de Recherches Mathématiques, Université de Montréal, Montréal 101, Canada
(Received 5 October 1970)

A kinetic approach to fluctuations and correlations of stochastic processes depending on a continuous set of parameters y is presented. In particular, we consider particle densities $n^p(y,t)$ which may refer to macroscopic densities in position space, or to microscopic quantities such as distributions in phase space, or occupancies of quantum states of which the labeling is continuous (as with Bloch states in solids). In a Markovian sense such processes are infinite dimensional. We describe the fluctuating particle densities in a Hilbert space: the analog of de Groot's a-space for non-spatial-dependent variables. Mainly, we employ a Langevin description; i.e., we start from presumed phenomenological equations, amended with source densities $\xi^p(y,t)$. A theorem is derived for the density–density or two-point covariance function (Λ theorem). In its general form, the theorem applies to the nonequilibrium steady state. It closely resembles the generalized g-r theorem for finite-dimensional processes. However, the solutions may involve extra parts stemming from stochastic boundary conditions and constraints. Simplifications for the thermal equilibrium case and the connection with generalized Onsager's relations are discussed. A variety of expressions for the spectral intensities $\Sigma^{pq}(y,y',\omega)$ are derived. In order to justify the Langevin procedure as well as to calculate the source terms and generalized Fokker-Planck moments, we consider the master-rate functional $W_{\gamma\gamma'}$ for transitions $\gamma \to \gamma'$ of the over-all state. Expressions are given for transitions involving change of species and scattering due to one- or two-body collisions. These determine uniquely the quantities entering into the Λ theorem. The statistical-mechanical basis for our formalism is discussed in some detail.

1. INTRODUCTION

Fluctuation phenomena can be classified as microscopic or macroscopic, depending on whether the quantities under consideration refer to the microscopic (many-body) state or to thermodynamic observables which are averages over a finite volume of phase space or over a range of quantum states. The early studies on fluctuations at the beginning of this century involved macroscopic observables such as voltage fluctuations in a resistor, studied by de Haas and Lorentz in 1913 and Nyquist in 1928, temperature fluctuations studied by Gibbs in 1902, and shot noise in electron emission studied by Schottky in 1918. In recent years several phenomena have been added to the macroscopic list, such as electron fluctuations in conductors or semiconductors, fluctuations due to spontaneous and stimulated emission in masers and lasers, photon flux fluctuations, polarization fluctuations in ferroelectric materials, etc. The first-mentioned effect, electron fluctuations in solids, has been extensively studied by the author. Though such fluctuations require a picture close to the microscopic point of view, we were largely able to use macroscopic methods, since the variables of the problem are seldom the occupancies of the individual quantum states, but lumped quantities, such as the number of electrons in a range $(\mathcal{E}, \mathcal{E} + d\mathcal{E})$. On the other hand, fluctuations caused by intraband scattering and hot-electron effects, among others, require a microscopic point of view.

The original studies of Brownian motion provide, to some extent, an example of microscopic fluctuations, though these studies are incomplete in a full microscopic sense, as we indicate below.

Both for macroscopic and microscopic phenomena, statistical studies can be based on the Gibbsian ensemble point of view or on the kinetic point of view of nonequilibrium statistical mechanics. The latter is much wider in scope in that it encompasses phenomena outside thermal equilibrium, i.e., a final state in which driving forces causing a steady particle and (or) energy transport are present, while it also accounts for the approach to this final state. Whereas the ensemble method historically has been rooted in cumbersome arguments about ergodicity (or nowadays in statistical formalisms exceeding the scope of physics proper, such as information theory), the kinetic point of view finds its origin and justification in the Liouville equation or its quantum equivalent, the von Neumann equation, the detailed steps being likewise elaborate (cf. Sec. 1B).

A. Phenomenological Kinetic Description

Presently, we consider the kinetics underlying the fluctuations in a given system from a pure phenomenological point of view. Both a steady-state situation and an equilibrium situation exist only because transitions and (or) transport, caused by interactions and (or) force fields, give rise to random fluxes to and from the equilibrium or steady state. In a steady-state situation the *sum totals* of these fluxes balance, whereas in equilibrium *detailed balancing* for any pair of opposing transitions occurs. The consequences of this feature for the fluctuations are far reaching, as we shall also see in this paper.

All physical quantities in a system not subject to rigid constraints exhibit random fluctuations about a given state of that system. The word "state" is used here in a rather broad sense; its specific meaning depends on the stochastic variables which we want to examine. In one sense, it may refer to a macroscopic thermodynamic characterization of the system by variables $a_i(t)$, which for the sake of argument are assumed to be all extensive, such as energy, particle numbers, charge, etc., and which have exchange with external systems (reservoirs) or other parts of the same system. The kinetic regression equations for the $\dot{a}_i$ are considered in irreversible thermodynamics, and the stochastic path of the vector $\mathbf{a} = \{a_i\}$ can be pictured in the a-space (de Groot and Mazur[1]).

Secondly, the "state" may refer to a specification of the coordinates of the system in μ-space, which are subject to change if the molecules interact with obstacles or with each other. Obviously, the μ-space path is only relevant for systems in which the interactions are weak, as, e.g., assumed in Brownian motion. The regression equations for $\dot{\mathbf{v}}$ and $\dot{\mathbf{r}}$ are the ordinary friction-type equations discussed in the standard papers on the subject[2-4] (in particular, Ref. 2).

Finally, we may be interested in the stochastic behavior of observables, requiring a microscopic characterization, such as the spin-deviation number in a ferromagnet or the number of Bloch electrons of certain band index and $\mathbf{k}$ vector. The "state" of the system in this case is the many-body state in the regular quantum-mechanical sense; however, we adhere to the view that the pure state is inaccessible to measurement and meaningless, so that an ensemble description is required.[5] The actual state fluctuates over the ensemble, and the time evolution for the state is discussed in Sec. 1B below. Often, however, the regression equations can be formulated without a complete many-body description. In the case of spin, the dynamics of spin waves may suffice; stochastic equations for creation and annihilation operators were derived by Lax.[6] For the case of Bloch electrons, the Boltzmann equation may be applicable.

Generally, the kinetic equations pertaining to the above-mentioned examples may be quite nonlinear. We assume, however, that the fluctuations of the variables, denoted as α_i, are small, so that linearized equations for the return to equilibrium (or steady state) apply. In order that the description be Markovian complete, the set of equations must be first order in the time (if not so, add $\dot{\alpha}_i \equiv \beta_i$ as variables). Finite-dimensional processes with equations of the form

$$\frac{\partial}{\partial t}\langle \alpha_i(t)\rangle_{\text{cond}} + \sum_j M_{ij}\langle \alpha_j(t)\rangle_{\text{cond}} = 0, \qquad (1.1)$$

with $i = 1, 2, \cdots, m$, have been extensively investigated, both in the mathematical literature[7,8] and in a physical context.[9,10] The subscript cond stands here for a conditional average, taken over an ensemble with fixed values at $t = 0$. The averaged stochastic equations (1.1) are identical in form to the equations for externally imposed changes α_i, according to what is sometimes called "Onsager's principle"[11] (e.g., a fluctuating charge ΔQ in an RC network decays in the ensemble in the same manner as applied excess charge); hence we refer to Eqs (1.1) as the phenomenological equations. It has been shown that (1.1) is equivalent to a Langevin description,[2-4,12] i.e., a set of regression equations, nonconditional in the ensemble, of the form

$$\frac{\partial \alpha_i(t)}{\partial t} + \sum_j M_{ij}\alpha_j(t) = \xi_i(t), \qquad (1.1')$$

provided the source terms have no memory of themselves:

$$\langle \xi_i(t)\ \xi_i(t')\rangle = B_{ij}\delta(t-t'). \qquad (1.2)$$

These equations describe well most of the examples alluded to above; in particular, fluctuations in the thermodynamic a-space are of this form.[1,10]

The aim of this paper is to consider processes in which the stochastic variables depend, besides on t, on a continuous vector y of a domain $\mathfrak{D}$ in some space $\mathfrak{R}^l$. Thus, we consider phenomenological equations of the form

$$\sum_q \mathsf{L}^{pq}[\langle \alpha^q(y,t)\rangle_{\text{cond}}] = 0, \qquad (1.3)$$

where

$$\mathsf{L}^{pq} = \Lambda^{pq} + \partial/\partial t, \qquad (1.4)$$

and where Λ^{pq} is an (integro)differential operator with respect to y. We further assume that an equivalent Langevin description applies, viz.,

$$\sum_q \mathsf{L}^{pq}[\alpha^q(y,t)] = \xi^p(y,t), \qquad (1.3')$$

in which the source terms have no memory:

$$\langle \xi^p(y,t)\ \xi^q(y',t')\rangle = \Xi^{pq}(y,y')\ \delta(t-t'); \qquad (1.5)$$

the quantities Ξ satisfy the obvious symmetry rule

$$\Xi^{pq}(y,y') = \Xi^{qp}(y'y). \qquad (1.6)$$

Equations of this nature occur in a number of cases.

First, we need this form for macroscopic variables in nonhomogeneous systems. Then, $y = \mathbf{r}$, where $\mathbf{r}$ is the position vector in the system. As an example, we can consider charge flow in the presence of gradients. Then $\Lambda = 1/\tau + \boldsymbol{\beta}\cdot\nabla + \gamma\nabla^2$. Or, we can consider stochastic electromagnetic fields.[13(a)] However, we shall confine ourselves to variables which are proportional to particle densities, $n^p(y)$, with $\alpha \equiv \Delta n^p(y)$, where $p = 1, 2, \ldots, s$ defines the species. It is by no means certain that a Langevin description (1.3′) for spatially dependent processes always exists. In fact, any Langevin description must be justified by other Markovian techniques (cf. Sec. 1B).

Secondly, and of more fundamental importance, processes of the type (1.3) occur in classical or quantum microscopic considerations. Thus, for a classical plasma we may consider the densities $n^p(\mathbf{r}, \mathbf{v}, t)$ in μ-space; in this case $y = \{\mathbf{r}, \mathbf{v}\}$, and the regression equation may be the Boltzmann equation, Vlasov equation, etc., depending on the model under consideration. We thus deal with *fluctuating distributions* $\Delta n^p(\mathbf{r}, \mathbf{v}, t)$. Such a description applies also to any Brownian motion process, and is far more precise than the idea that $\mathbf{r}$ and $\mathbf{v}$ are themselves fluctuating variables.

[Perhaps we should refer to the description (1.3) as "second Brownian motion", to indicate the contrast with the original theories (see also Ref.13(b).] In quantum systems it is most convenient to describe the many-body state $|\gamma\rangle$ in the formalism of second quantization. Since in a large system one or more quantum numbers, say $\{y\}$, will be dense, it is appropriate to consider the occupation numbers $n^p(y)$; $|\gamma\rangle \equiv |\{n^p(y)\}\rangle$, where p denotes the further discrete quantization of the states. For the example of Bloch electrons given above, $y = \mathbf{k}$, p denotes the band index and spin. If such processes are, in addition, spatially dependent, we consider the occupancies $n^p(\mathbf{k}, \mathbf{r})$, where $y = \{\mathbf{k}, \mathbf{r}\}$ is a semiclassical set of coordinates, such as occurs in the Wannier Hamiltonian in solid-state physics.

Processes (1.3) are considerably more complex than the first-mentioned processes (1.1). The processes considered here are $(\infty)^s$ dimensional in a Markovian sense. Nevertheless, the finite-dimensional methods of processes (1.1) have been applied to processes (1.3) with some success, both by van Vliet and Fassett[14] and by Lax.[15] The first authors used coarse graining in the domain $\mathfrak{D}$ of y, whereas Lax wrote differential operators as occurring in Λ in the form of integral operators (which is always possible using the δ function and its derivatives[16]) and subsequently interprets the integral operators as matrix operators of continuously infinite rank. [This procedure is, in the author's opinion, as unfortunate as the use of transformation theory in quantum mechanics in order to declare a wavefunction $\Psi(\mathbf{r})$ to be a column matrix $\langle\Psi|\mathbf{r}\rangle$ in the "$\mathbf{r}$ representation".[17]] A rigorous mathematical method will be given here. The quantities $\Delta n^p(y,t) \equiv \alpha^p(y,t)$ will be pictured as stochastic elements in a separable Hilbert space, which is the analog of de Groot's a-space for finite-dimensional processes. Complications, not existing in the finite-dimensional case, arise from the boundary conditions for the domain $\mathfrak{D}$ of y and from constraints.

In the main part of the paper (Secs. 2–6) we assume that the phenomenological equations are given and that the functions Ξ^{pq} are known; i.e., we have found a way of expressing the effect of all physical interactions in a set of "Langevin kernels". This is less preposterous than it seems to be: The advantages (or shortcomings?) of a Langevin treatment are that in various instances one can get by without detailed microscopic specifications. We are then interested in the following quantities:

$$F_2^{pq}(y,y') \equiv \langle n^p(y,t)\, n^q(y't)\rangle \tag{1.7}$$

(density–density or two-point correlation functions[18]);

$$\Gamma^{pq}(y,y') \equiv \langle \Delta n^p(y,t)\, \Delta n^q(y',t)\rangle \tag{1.8}$$

(density–density or two-point covariance functions);

$$\Phi^{pq}(y,y',t) \equiv \langle \Delta n^p(y,t)\, \Delta n^q(y',0)\rangle \tag{1.9}$$

(time-displaced density–density covariance functions);

$$\Sigma^{pq}(y,y',\omega) = 2\int_{-\infty}^{\infty} e^{-i\omega t}\Phi^{pq}(y,y',t)\,dt \tag{1.10}$$

(spectral intensity functions).

In Sec. 2 we derive an operator theorem for Γ, called the Λ theorem; it expresses Γ in Λ and Ξ. This is the main theorem which allows the correlations to be found from a kinetic viewpoint. In Sec. 3 we elaborate on the solutions of the Λ theorem and consider extensions. In Sec. 6 we state results for the spectral intensities in terms of Green's operators (the resolvent of Λ), which are essentially a reformulation of some results of Ref. 14 in a more rigorous and complete form.

Sections 4 and 5 deal with auxiliary properties. In Sec. 4, the approach to equilibrium is discussed. By imposing that the equilibrium distribution $\langle n^p(y, t\to\infty)\rangle$ agrees with statistical mechanics, conditions for Ξ are implied. In Sec. 5 specific equilibrium properties are considered, quite analogously to the method of Ref. 9. Moreover, the kernels Ξ^{pq} are shown to be identical with generalized Onsager coefficients, so that Ξ may be known from models in irreversible thermodynamics of nonhomogeneous systems. This point is not further pursued in this paper.

B. Detailed Kinetic Description

Finally, when it comes to a justification of the Langevin description, as well as to general forms to compute the source kernels Ξ^{pq}, we must go back to the foundations of the kinetic method. The basic kinetic equations for the evolution of a point in Γ space, or of a many-body quantum state, are the Liouville and the von Neumann equations, respectively. Using suitable diagram techniques (van Hove,[19] Prigogine and Résibois,[20] Balescu[21]) or projection techniques (Zwanzig[22]), one can arrive at a generalized master equation (ME), which is still time reversible. This equation has two advantages, however, over the original equations from which it is derived. First, it is relatively easy to investigate the limiting behavior for $t\to\pm\infty$; van Hove has shown that the density matrix for a closed system, with appropriate initial conditions, leads indeed to a microcanonical ensemble. Secondly, it is relatively easy to obtain an irreversible Markovian ME if the "standard" assumptions are made (initial random-phase assumption, large-system limit, weak coupling, separation of time scales for duration of interactions and relaxations). The ME relates the evolution of the ensemble probability $p(\gamma) = \langle\gamma|\rho|\gamma\rangle$, where ρ is the density operator, to the transition rates per unit time, $W_{\gamma\gamma'} \equiv W(\gamma\to\gamma')$. [More precisely, it gives the evolution of the conditional probability $P(\gamma, t|\gamma^*, t^*)$.] In the quantum picture, which is more easily understood than the

classical picture (cf. Fujitta[23]) $|\gamma\rangle$ is again the occupation-number state $|\{n^p(y)\}\rangle$.

The average occupancies $\langle n^p(y)\rangle$ follow from the first moments of the ME via the generalized first-order Fokker-Planck (FP) moments A^p. Hence, one obtains the phenomenological equations, *which do not have to be assumed, but are a consequence of the ME*. As a detailed example, van Hove[24] derived the Boltzmann equation for Bloch electrons in a state $\mathbf{k}$, assuming that changes of the total many-body state $|\gamma\rangle = |\{n^1(\mathbf{k})\}, \{n^2(\mathbf{q})\}\rangle$ occur due to electron–phonon interaction (see also Ref. 25).

Likewise, one can obtain a kinetic equation for the two-point time-displaced covariance functions from the second-order moments of the ME, which involve generalized second-order FP moments B^{pq}. For $t \to \infty$, this leads to an expression for Γ which can be expected to be identical with the Λ theorem of this paper (though this is not established here). The connection relies on the fact that the generalized FP moments B^{pq} are (almost) identical with the Langevin kernels Ξ^{pq}.

Despite the vast literature on the ME, we note that no appropriate, sufficiently general form exists for our present purpose. The quantum case has not been extended so far to nonhomogeneous systems, to the author's knowledge. Thus, in van Hove's derivation of the Boltzmann equation, the transport or "streaming" terms are missing. The classical forms by Prigogine and co-workers deal with Fourier-transformed distribution functions. Only Severne[26] gives a discussion which includes streaming terms in nonhomogeneous systems. A form involving distribution functions in action-angle variables was recently given by Leaf and Schieve.[27] Basically, however, the Liouville equation is not symmetrized with respec to particle interchange, and the reduced distribution functions do not lead to an occupation number form for points (or cells) in Γ space, though an ME for the functional $p(\gamma)$ with $\gamma = \{n^p(\mathbf{v}, \mathbf{r})\}$ can easily be conjectured. We plan to return to this in a future paper.

The present paper circumvents this problem in the following manner. Mainly, we operate on the Langevin level, i.e., we work with given phenomenological equations (Secs. 2-6). However, in order to find Ξ, we assume the existence of a "master-rate functional" $W_{\gamma\gamma'} \equiv W[n^p(y) \to n^{p\prime}(y)]$, in Secs. 7 and 8. We shall argue that streaming is of no importance for $W_{\gamma\gamma'}$; hence $W_{\gamma\gamma'}$ depends only on the nature of the transitions and scattering, whether involving one-body collisions (with fixed obstacles), two-body collisions, or other interactions, and is therefore known for most classical or quantum processes. In Sec. 7 the connection between Ξ and the generalized second-order Fokker–Planck moments is established. The argument is analogous to that for ordinary Langevin equations, except that proper care must be given to the streaming terms. Finally, in Sec. 8 we derive some general formulas for the generalized second-order FP moments, *which then give* Ξ; in addition, we find the generalized first-order FP moments, *which must corroborate the collisional part of the phenomenological operator* Λ, *a posteriori*. If this corroboration fails, it indicates that neither a phenomenological description (1.3), nor an associated Langevin description (1.3′), as supposed in the preceding sections, exists. Applications, both microscopic and macroscopic, are considered in the following paper.[28]

I. LANGEVIN-LEVEL DESCRIPTION

2. DERIVATION OF A THEOREM FOR THE DENSITY–DENSITY OR TWO-POINT COVARIANCE FUNCTION

We consider the generalized Langevin equations of the form (1.3′), where $y = \mathbf{r}$ for macroscopic processes, and $y = \mathbf{k}$, or $\mathbf{k}, \mathbf{q}$, or $\mathbf{k}, \mathbf{r}$, or $\mathbf{v}, \mathbf{r}$, etc., for microscopic processes, as discussed in the preceding section. It is advantageous to write the set of equations (1.3′) in the shorter form

$$\mathsf{L}\alpha(y,t) = \xi(y,t), \tag{2.1}$$

where $\alpha = \{\alpha^p\} \equiv \{\Delta n^p\}$ and $\xi = \{\xi^p\}$ are vectors in an s-dimensional space $\mathcal{S}^s$ and $\mathsf{L} = [\mathsf{L}^{pq}]$ is a generalized dyadic operator.[29] The stochastic variables α^p and ξ^p are defined on the domain $y \in \mathfrak{D}$ in $\mathfrak{R}^l$, with t as a parameter. The sources ξ^p are uncorrelated in time, but not in the coordinates y.

We consider the idealized circumstances that the $\alpha^p(y,t)$ are square integrable in the sense of Lebesgue. Thus, as in the problem of electron spin in quantum mechanics, we define a product space $\mathcal{S}^s \otimes \mathfrak{L}^2(\mathfrak{D}, \mathfrak{R}^l)$, which is a Hilbert space $\mathfrak{H}$ with elements $\alpha(y,t)$. The adjoint elements are denoted as $\alpha^\dagger(y,t)$. We remarked already that the Hilbert space $\mathfrak{H}$ for a process $\alpha^p(y,t)$ is a generalization of the thermodynamic a-space.

The scalar product in $\mathfrak{H}$ is defined as

$$(\alpha,\beta) = \sum_p \int_{\mathfrak{D}} \beta^{p*}(y,t)\alpha^p(y,t)d^l y = \int_{\mathfrak{D}} \beta^\dagger(y,t)\alpha(y,t)d^l y = (\beta,\alpha)^*. \tag{2.2}$$

The Langevin equations (2.1) are a transformation in the space $\mathfrak{H}$. If L is a differential operator, strictly speaking, the α's must be confined to a subensemble guaranteeing absolute continuity or similar properties, so that the operations exist. Since such a subensemble is everywhere dense in $\mathfrak{H}$, there is always a neighboring element which may serve as a substitute to idealize the process.

For a Markovian complete system, we write, in accord with (1.4)

$$\mathsf{L} = \Lambda + \mathsf{I}\partial/\partial t, \tag{2.3a}$$

$$\tilde{\mathsf{L}} = \tilde{\Lambda} - \mathsf{I}\partial/\partial t, \tag{2.3b}$$

where I is the idem operator and $\tilde{L}$ and $\tilde{\Lambda}$ are adjoint[30] operators. At present, we consider the case that Λ is linear, i.e., additive and homogeneous. The latter aspect also involves the boundary conditions (bc). Thus, a *"Markovian-linear" process excludes the case of stochastic boundary conditions on the surface* $\mathbf{S}$ *of* $\mathfrak{D}$. Such processes can be quite well *"response linear,"* however, as is discussed in Sec. 3C.

For any two elements we then have

$$(\Lambda\alpha,\beta) = (\alpha,\tilde{\Lambda}\beta), \tag{2.4}$$

and from (2.3)

$$\int_0^{t_1} dt(L\alpha,\beta) - \int_0^{t_1} dt(\alpha,\tilde{L}\beta)$$
$$= (\alpha(y,t_1),\beta(y,t_1)) - (\alpha(y,0),\beta(y,0)), \tag{2.5}$$

which is a Green's theorem, relative to the time evolution in the space $\mathfrak{K}$. The matrix Green's functions of the system (being square matrices) are conventionally defined by

$$Lg(y,t;y',t') = I\delta(t-t')\delta(y-y'), \tag{2.6a}$$

$$\tilde{L}\tilde{g}(y,t;y',t') = I\delta(t-t')\delta(y-y'), \tag{2.6b}$$

satisfying the homogenous bc and adjoint bc. In addition, we introduce Green's operators[31] by

$$g(t,t')\gamma(y,t') = \int g(y,t;y',t')\gamma(y',t')\,d^l y', \tag{2.7a}$$

$$\tilde{g}(t,t')\gamma(y,t') = \int \tilde{g}(y,t;y',t')\gamma(y',t')\,d^l y', \tag{2.7b}$$

so that according to Eqs. (2.6)

$$Lg(t,t') = \tilde{L}\tilde{g}(t,t') = I\delta(t-t'), \tag{2.8}$$

or for arbitrary γ

$$\tilde{L}\tilde{g}(t,t')\gamma(y,t') = \delta(t-t')\gamma(y,t'). \tag{2.8'}$$

The condition for reciprocity can be expressed as

$$g(y,t;y',t') = \tilde{g}^{\dagger}(y',t';y,t), \tag{2.9}$$

or

$$((g(t,t')\beta(y,t'),\gamma(y,t)) = (\beta(y,t'),\tilde{g}(t',t)\gamma(y,t)). \tag{2.9'}$$

The solution of (2.1) is now obtained in the standard way,[32] with the result

$$(\alpha(y,t),\gamma(y,t)) = \int_0^{t+0} dt'(g(t,t')\xi(y,t'),\gamma(y,t))$$
$$+ (g(t,0)\alpha(y,0),\gamma(y,t)),$$

which holds for arbitrary $\gamma(y,t)$, so that

$$\alpha(y,t) = \int_0^{t+0} dt'\; g(t,t')\xi(y,t') + g(t,0)\alpha(y,0). \tag{2.10}$$

The operator equations (2.8), together with Eqs. (2.3), can also be solved formally, the solution being

$$g(t,t') = H(t-t')\,e^{-\Lambda(t-t')}, \tag{2.11}$$

where H is the unit step function. In addition we introduce the resolvent $(\Lambda+s)^{-1}$, which plays a central role in these problems. Let $\varphi_k(y)$ and $\psi_l(y)$ be eigenstates of Λ and $\tilde{\Lambda}$ in $\mathfrak{K}$ with eigenvalues λ_k and μ_l, respectively. We then have the decomposition[33]

$$G(s) \equiv \frac{1}{\Lambda+s} = \sum_k \frac{P_k}{\lambda_k+s} \quad \text{or} \quad \int_0^{\infty} \frac{dP(\lambda)}{\lambda+s}, \tag{2.12}$$

where P_k are the projectors, i.e., for any $f(y)$, $P_k f = (f,\psi_k)\varphi_k$.[34] It is clear that the resolvent is the Laplace transform of the Green's operator $g(t,t')$:

$$g(t,0) = \frac{1}{2\pi i}\oint_C G(s)\,e^{st}\,ds = \sum_k P_k H(t)\,e^{-\lambda_k t}, \tag{2.13}$$

where C is a counterclockwise path enclosing all poles. Accordingly, we must substitute into (2.10)

$$g(t,t')\xi(y,t') = g(t-t',0)\xi(y,t')$$
$$= \sum_k (\xi(t'),\psi_k)\varphi_k(y)\,e^{-\lambda_k(t-t')}H(t-t'). \tag{2.14}$$

Next, we consider the tensor product space $\mathfrak{K}^{(2)} = \mathfrak{K}\otimes\mathfrak{K}$, with elements

$$\alpha\otimes\beta = \alpha(y)\beta^{\mathrm{tr}}(y') \equiv \Phi(y,y') \equiv [\Phi^{pq}(y,y')]. \tag{2.15}$$

The scalar product is defined by

$$(\Psi,\Phi) = \sum_{pq}\iint \Phi^{*pq}\Psi^{pq}\,d^l y\,d^l y' = \iint \Phi^{*}:\Psi\,d^l y\,d^l y'; \tag{2.16}$$

hence

$$(\alpha\beta^{\mathrm{tr}},\gamma\delta^{\mathrm{tr}}) = (\alpha,\gamma)\,(\beta,\delta). \tag{2.17}$$

From (2.10) we form the average, conditional to given $\alpha(y,0)$; using (2.14), we obtain

$$\langle\alpha(y,t)\alpha^{\mathrm{tr}}(y',t')\rangle_{\mathrm{cond}} = \sum_{kl}\int_0^{t+0}\int_0^{t'+0} ds\,ds'$$
$$\times e^{-\lambda_k t-\lambda_l t'}\,e^{\lambda_k s+\lambda_l s'}(\langle\xi(y,s)\xi^{\mathrm{tr}}(y',s')\rangle,\psi_k\psi_l^{\mathrm{tr}})$$
$$\times \varphi_k(y)\varphi_l^{\mathrm{tr}}(y') + \text{initial term}, \tag{2.18}$$

where the average on the ξ's is unconditional since this is a rapidly fluctuating variable with zero mean $\langle\xi\rangle = 0$. We shall make the change in notation $t'\to t$, $t\to t+u$. We write for the time-displaced covariance functions in accord with Eq. (1.9)

$$\Phi(y,y',u) = \lim_{t\to\infty}\langle\alpha(y,t+u)\alpha^{\mathrm{tr}}(y',t)\rangle_{\mathrm{cond}}; \tag{2.19}$$

and in particular for the stationary covariance functions

$$\Gamma(y,y') = \lim_{t\to\infty,\, u\to 0} \langle \alpha(y, t+u)\alpha^{\mathrm{tr}}(y', t)\rangle_{\mathrm{cond}}; \tag{2.20}$$

finally for the sources in accord with Eq. (1.5)

$$\Xi(y,y')\delta(t-t') = \langle \xi(y,t)\xi^{\mathrm{tr}}(y',t')\rangle. \tag{2.21}$$

We make further the customary change in variables $s' - s \to s''$, and $s' \to s' - 0$. Then (2.18) reads

$$\langle \alpha(y,t+u)\alpha^{\mathrm{tr}}(y',t)\rangle = \sum_{kl} e^{-(\lambda_k+\lambda_l)t} e^{-\lambda_k u} \int_0^t ds' \times \int_{s'-t-u}^{s'+0} ds''\, e^{(\lambda_k+\lambda_l)s'} e^{-\lambda_k s''} \delta(s'') \times (\Xi, \psi_k\psi_l^{\mathrm{tr}})\varphi_k(y)\varphi_l^{\mathrm{tr}}(y'). \tag{2.22}$$

In order that we do not end on the top of the δ function with the integral over ds'', it is necessary that $u > 0$, if s' covers the interval $(0, t)$ (see Fig. 1).[35] The integral over s' can now be carried out and the limit for $t \to \infty$ can be taken. This limit exists provided all $\mathrm{Re}\lambda_k > 0$. (*For the present we exclude eigenvalues zero.*)

We obtain

$$\Phi(y,y',u) = \sum_{kl} e^{-\lambda_k u} \frac{\varphi_k(y)\varphi_l^{\mathrm{tr}}(y')}{\lambda_k+\lambda_l} (\Xi, \psi_k\psi_l^{\mathrm{tr}}), \quad u > 0. \tag{2.23}$$

The covariance functions will be taken as the limit for $u \to 0+$:

$$\Gamma(y,y')\Big|_{\mathrm{right}} = \sum_{kl} \frac{\varphi_k(y)\varphi_l^{\mathrm{tr}}(y')}{\lambda_k+\lambda_l} (\Xi, \psi_k\psi_l^{\mathrm{tr}}). \tag{2.24a}$$

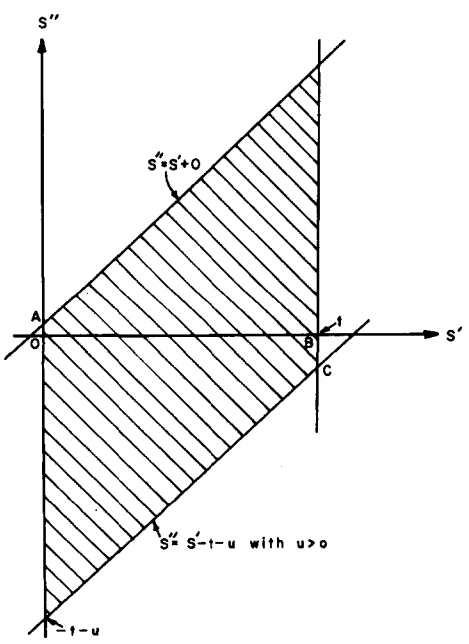

FIG. 1. Pertaining to the integral of Eq. (2.22).

In order to also obtain the left-hand side (lhs) limit, we use the fact that, for a stationary process, $\Phi(u) = \Phi^{\mathrm{tr}}(-u)$. Thus, taking the limit when the argument $\to 0-$, we have

$$\Gamma(y,y')\Big|_{\mathrm{left}} = \sum_{kl} \frac{\varphi_l(y)\varphi_k^{\mathrm{tr}}(y')}{\lambda_k+\lambda_l} (\Xi, \psi_k\psi_l^{\mathrm{tr}}). \tag{2.24b}$$

Since we can interchange the summation indices, the double sums in Eqs. (2.24a) and (2.24b) are equal. However, from pure dimensional analysis, we can expect that neither limit exists strictly speaking, but has a singularity $\delta(y-y')$ (cf. Ref. 14).

We corroborate this by accepting Eqs. (2.24) formally, and by taking an internal product with $\psi_m\psi_n^{\mathrm{tr}}$ in the space $\mathfrak{K}^{(2)}$. The required integral (2.16) exists and is finite; using biorthogonality, we obtain

$$(\Gamma, \psi_m\psi_n^{\mathrm{tr}}) = (\Xi, \psi_m\psi_n^{\mathrm{tr}})/(\lambda_m + \lambda_n). \tag{2.25}$$

This is an integral equation for Γ, which is easily converted to an operator equation involving Λ. We write

$$\begin{aligned} \lambda_n\psi_n^* &= \mu_n^*\psi_n^* = \tilde{\Lambda}^*\psi_n^*, \\ \lambda_m\psi_m^\dagger &= \mu_m^*\psi_m^\dagger = \psi_m^\dagger\tilde{\Lambda}^\dagger, \end{aligned} \tag{2.26}$$

where the operator works to the left in the latter case. Thus, multiplying both sides of (2.25) with $(\lambda_m + \lambda_n)$ and substituting (2.26), we obtain

$$(\Gamma, \tilde{\Lambda}_y\psi_m(y)\psi_n^{\mathrm{tr}}(y') + \psi_m(y)\psi_n^{\mathrm{tr}}(y')\tilde{\Lambda}_{y'}^{\mathrm{tr}}) = (\Xi, \psi_m\psi_n^{\mathrm{tr}}). \tag{2.27}$$

The elements $\psi_m\psi_n^{\mathrm{tr}}$ form a basis in $\mathfrak{K}^{(2)}$. Thus, (2.27) yields for arbitrary $\Psi(y,y')$

$$(\Gamma, \tilde{\Lambda}_y\Psi + \Psi\tilde{\Lambda}_{y'}^{\mathrm{tr}}) = (\Xi, \Psi). \tag{2.28}$$

We can view $\tilde{\Lambda}_{(2)}{}^{\to} + {}^{\leftarrow}\tilde{\Lambda}_{y'}^{\mathrm{tr}}$ as a tranformation operator in $\mathfrak{K}^{(2)}$, which has an adjoint. Accordingly, the lhs of (2.28) is also

$$(\Gamma, \tilde{\Lambda}_y\Psi + \Psi\tilde{\Lambda}_{y'}^{\mathrm{tr}}) = (\Lambda_y\Gamma + \Gamma\Lambda_{y'}^{\mathrm{tr}}, \Psi). \tag{2.29}$$

Comparing (2.28) and (2.29), we arrive at the "Λ theorem":

$$\Lambda_y\Gamma(y,y') + \Gamma(y,y')\Lambda_{y'}^{\mathrm{tr}} = \Xi(y,y'). \tag{2.30}$$

3. DISCUSSION OF THE Λ THEOREM AND EXTENSIONS

The Λ theorem is the extension of the generalized generation-recombination (gr) theorem derived in the fifties by van Vliet and Blok,[36] using the Fokker–Planck equation. Then, for a multivariate Markov process $\mathbf{N}(t) = \{N^p(t)\}$ of the type (1.1), we obtain

$$\langle \Delta\mathbf{N}\, \Delta\mathbf{N}^{\mathrm{tr}}\rangle M^{\mathrm{tr}} + M\langle \Delta\mathbf{N}\, \Delta\mathbf{N}^{\mathrm{tr}}\rangle = B^0, \tag{3.1}$$

where $\langle \Delta \mathbf{N}\, \Delta \mathbf{N}^{\mathrm{tr}} \rangle$ is the covariance matrix, M is the phenomenological relaxation matrix, and B^0 is composed of the steady-state second-order FP moments (Lax's diffusion matrix[9]).

The Λ theorem enables us to obtain the correlations if the Langevin source kernels Ξ are known. The latter contain the interactions as we discussed in the Introduction (see, further, Sec. 7).

Since the Λ theorem operates in the product space $\mathfrak{K}^{(2)}$, it is generally much more complex in structure than the phenomenological equations. Typically, if Λ is a three-dimensional integrodifferential operator of ordinary space, the density correlations Γ are governed by an equation of the same order but of a six-dimensional space. In thermal equilibrium the equation for Γ can be reduced to one of a three-dimensional space, however (see Sec. 5).

Instead of the correlation strength of the sources, we could also have used their white spectral densities, since from the Wiener-Khintchine theorem and Eq. (2.21), we find

$$\Sigma_{\xi\xi}(y,y',\omega) = 2\int_{-\infty}^{\infty} e^{-i\omega t'} \langle \xi(y,t+t')\xi^{\mathrm{tr}}(y',t)\rangle dt' = 2\Xi(y,y'). \tag{3.2}$$

A. Formal solutions

A formal solution of the Λ theorem is always available in the form of the series expansion, Eqs. (2.24). This result is not easily evaluated, except when the domain is large and plane waves suffice as eigenstates. For a single-variable problem ($s = 1$) in ordinary n-dimensional space ($y = \mathbf{r}$), we have

$$\Gamma(\mathbf{r},\mathbf{r}') = \frac{1}{(2\pi)^{2n}} \iint \frac{e^{i(\mathbf{k}\cdot\mathbf{r}+\mathbf{l}\cdot\mathbf{r}')}}{\lambda(\mathbf{k})+\lambda(\mathbf{l})}\, d^n k\, d^n l \times \iint \Xi(\boldsymbol{\rho},\boldsymbol{\rho}')\, e^{-i(\mathbf{k}\cdot\boldsymbol{\rho}+\mathbf{l}\cdot\boldsymbol{\rho}')} d^n\rho\, d^n\rho'. \tag{3.3}$$

Returning to the general case, we can write Eqs. (2.24) in the shorter notation:

$$\Gamma(y,y') = \sum_{kl} \frac{\mathsf{P}_{k,y}\Xi(y,y')\mathsf{P}^{\mathrm{tr}}_{l,y'}}{\lambda_k+\lambda_l} \equiv \iint \mathfrak{K}(yy',zz')\,\Xi(z,z')\,d^l z\, d^l z' = \mathsf{K}_{yy'}\Xi(y,y'), \tag{3.4}$$

where evidently $\mathfrak{K}$ is the Green's function and K is the Green's operator relevant to the Λ theorem. We note the following decomposition of K:

$$\mathsf{K} = \sum_{kl} \mathsf{P}_{k,y}\mathsf{P}^{\mathrm{tr}}_{l,y'}/(\lambda_k+\lambda_l). \tag{3.5}$$

In Sec. 5 we prove that in thermal equilibrium the two terms in the Λ theorem are equal. This tremendous simplification means that in this case the solution can be given in terms of the Green's operator associated with Λ, i.e., the resolvent $\mathsf{G}(s=0)$:

$$\Gamma(y,y') = \tfrac{1}{2}\int \mathfrak{G}(y,0;y'')\Xi(y'',y')\,d^l y' = \tfrac{1}{2}\mathsf{G}_y(0)\Xi(y,y'), \tag{3.6}$$

with [cf. (2.12)]

$$\tfrac{1}{2}\mathsf{G}(0) = \sum_k \mathsf{P}_k/2\lambda_k \;(= \sum_{kl} \mathsf{P}_k\mathsf{P}_l^{\mathrm{tr}}/2\lambda_k), \tag{3.7}$$

where $\mathfrak{G}(y,s;y'')$ is the Laplace-transformed Green's function used by van Vliet and Fassett[14]; the last expression in (3.7) is given for comparison with (3.5).[37]

Another form of the solution will yet be stated. We go back to (2.23), and write this equation as

$$\Phi(y,y',u) = \sum_{kl}\int_0^\infty dt\, e^{-\lambda_k(t+u)}e^{-\lambda_l t}H(u)\varphi_k(y)\varphi_l^{\mathrm{tr}}(y')(\Xi,\psi_k\psi_l^{\mathrm{tr}}) = \int_0^\infty dt\, e^{-\lambda_k(t+u)}e^{-\lambda_l(t)}H(u)\mathsf{P}_{k,y}\Xi(y,y')\mathsf{P}^{\mathrm{tr}}_{l,y'}, \tag{3.8a}$$

$$= (\mathrm{alt})\int_u^\infty dt\, e^{-\lambda_k t}\, e^{-\lambda_l(t-u)}\mathsf{P}_{k,y}\Xi(y,y')\mathsf{P}^{\mathrm{tr}}_{l,y'}. \tag{3.8b}$$

In view of (2.13) this becomes

$$\Phi(y,y',u) = \int_o^\infty dt\; \mathsf{g}_y(t+u,0)\Xi(y,y')\mathsf{g}_{y'}^{\mathrm{tr}}(t,0) \tag{3.9a}$$

$$= (\mathrm{alt})\int_u^\infty dt\; \mathsf{g}_y(t)\,\Xi\,\mathsf{g}_{y'}^{\mathrm{tr}}(t-u), \tag{3.9b}$$

with $u > 0$ in both expressions. In practice this is a formidable integral (over t, y, and y'). For the variance, both (3.9a) and (3.9b) give the result

$$\Gamma(y,y') = \int_0^\infty dt\; \mathsf{g}_y(t,0)\Xi(y,y')\mathsf{g}_{y'}^{\mathrm{tr}}(t,0). \tag{3.10}$$

We notice that $\Gamma(y,y') = \Gamma^{\mathrm{tr}}(y',y)$, as it should be.

B. Connection with the Two-Point Distribution Functions of BBGKY

The correlation functions are connected to the covariance functions by

$$F_2^{pq}(y_1,y_2) = \Gamma^{pq}(y_1,y_2) + \langle n^p(y_1)\rangle\langle n^q(y_2)\rangle = \Gamma^{pq}(y_1,y_2) + F_1^p(y_1)\,F_1^q(y_2), \tag{3.11}$$

where F_1 is the solution of the steady-state phenomenological equations. *Our correlation functions are not identical with the two-point distribution functions f_2 of the BBGKY procedure* which follow from the canonical ensemble or by integration of the Liouville equation. The connection is easily shown to be

$$F_2^{pq}(y_1,y_2) = f_2^{pq}(y_1,y_2) + \delta^{pq} f_1^p(y_1)\,\delta(y_1-y_2), \tag{3.12}$$

where $f_1 \equiv F_1$ is the one-point distribution function. We note the correct normalization: The lhs

is normalized to N^pN^q, the first term on the rhs is normalized to N^pN^q $(p \neq q)$ or to $N^p(N^p-1)$ $(p=q)$, and the second term to $\delta^{pq}N^p$. Comparing with (3.11), we have also

$$\Gamma^{pq}(y_1,y_2) = f_2^{pq}(y_1,y_2) - f_1^p(y_1)f_1^q(y_2) + \delta^{pq}f_1^p(y_1)\delta(y_1-y_2). \tag{3.13}$$

The simplest truncation rule of the BBGKY hierarchy to lowest order involves the assumption of molecular chaos: $f_2^{pq}(y_1,y_2) \to f_1^p(y_1)f_1^q(y_2)$. This means that

$$\Gamma^{pq} \to \delta^{pq}f_1^p(y_1)\,\delta(y_1-y_2). \tag{3.14}$$

This remaining covariance has nothing to do with physical interactions; it stems purely from a "dimensional singularity". The reason for (3.14) is easily demonstrated. For the case $y = \mathbf{r}$

$$\int_{\delta V}\int_{\delta V}\langle \Delta n(\mathbf{r})\Delta n(\mathbf{r}')\rangle dV dV' = \langle(\Delta N_{\delta V})^2\rangle = O(N_{\delta V}) = O(\bar{n}\delta V), \tag{3.15}$$

or[38]

$$\frac{\langle \Delta n(\mathbf{r})\Delta n(\mathbf{r}')\rangle}{\langle n(\mathbf{r})\rangle\langle n(\mathbf{r}')\rangle} = O(1/\bar{n}\delta V) \begin{cases} \to \delta(\mathbf{r}-\mathbf{r}') \text{ if } |\mathbf{r}-\mathbf{r}'| \to 0. \\ \to 0 \text{ if } |\mathbf{r}-\mathbf{r}'| \to \infty \end{cases} \tag{3.16}$$

Moreover, (3.14) is directly verified for the case that particles are distributed at random over K elements of a volume V according to the multinomial distribution, with $K, V \to \infty$.[39]

C. Differential Operators with Stochastic Boundary Conditions

Interactions at the boundary may sometimes result in stochastic boundary conditions. Examples for macroscopic situations are easily furnished; e.g., when a steady diffusive flow occurs, the average gradient $\langle \nabla_0 \alpha \rangle$ is zero at the boundary, but the instantaneous gradient can be stochastic, $\nabla_0\alpha(\mathbf{r}_0, t) = v(\mathbf{r}_0, t)$, where $\mathbf{r}_0$ is a surface position coordinate. In a microscopic description in phase space this situation will not occur [expressions for the particle and energy transfer, like $\int \mathbf{v}n(\mathbf{r},\mathbf{k},t)d^3k$ have instantaneous validity, but a macroscopic expression like $\mathbf{J} = D\nabla n(\mathbf{r})$ has not]. Therefore, the following results have only macroscopic significance, i.e., $y = \mathbf{r}$.

We write the stochastic boundary conditions on the surface $\mathbf{S}$ of $\mathfrak{D}$ as

$$l\alpha(y_0,t) = v(y_0,t), \tag{3.17}$$

where $y_0 \in \mathbf{S}$ and l is a surface operator. The effect of v will appear in the bilinear concomitant of the Green's theorem relevant to Λ:

$$(\Lambda\alpha,\beta) - (\alpha,\tilde{\Lambda}\beta) = \oint C[\alpha,\beta^*]dS. \tag{3.18}$$

We assume that C contains a term of the form $\beta^\dagger m^\dagger l\alpha$, where m is another surface operator. With homogeneous bc $l\mathfrak{g} = 0$, and suitable adjoint bc of $\tilde{\mathfrak{g}}$, the bilinear concomitant gives

$$\oint C[\alpha(y_0,t'),\tilde{\mathfrak{g}}^*(y_0,t';y,t)]dS = \oint \mathfrak{g}(y,t;y_0,t')m^\dagger_{y_0}v(y_0,t')dS_{y_0} \equiv h_S(t,t')\,v(y_0,t'), \tag{3.19}$$

where h_S is introduced for convenience as a surface Green's operator. The result analogous to (2.10) is now

$$\alpha(y,t) = \mathfrak{g}(t,0)\alpha(y,0) + \int_0^{t+0} dt'[\mathfrak{g}(t,t')\xi(y,t') + h_S(t,t')v(y_0,t')]. \tag{3.20}$$

Similar to (2.21) we have the equation

$$\Upsilon(y_0,y_0')\delta(t-t') = \langle v(y_0,t)v(y_0',t')\rangle, \tag{3.21}$$

whereas we assume that v and ξ are uncorrelated.

Instead of (3.9), we obtain in a similar fashion

$$\Gamma(y,y') = \int_0^\infty dt[\mathfrak{g}_y(t,0)\Xi(y,y')\mathfrak{g}^{tr}_{y'}(t,0) + h_{Sy}(t,0)\Upsilon(y_0,y_0')h^{tr}_{Sy'}(t,0)]. \tag{3.22}$$

However, the boundary term often does not contribute to the correlations. If we operate on (3.22) with $\Lambda_y \to + \leftarrow \Lambda_{y'}$, we find that the last term yields zero, i.e., is a solution of the homogeneous equation

$$\Lambda_y H + H\Lambda_{y'} = 0, \tag{3.23}$$

whereas the volume term yields again the Λ theorem. To see this, we only need Eqs. (2.6), (2.3), and

$$\lim_{t\to\infty}\mathfrak{g}(y,t;y',t') = 0, \tag{3.24}$$

$$\lim_{t\to t'+0}\mathfrak{g}(y,t;y't') = \delta(y-y'). \tag{3.25}$$

Further examination indicates that the surface part of (3.22) can only contribute to the covariance of two surface points, as long as $\langle \xi v\rangle = 0$.

D. Integral Operators and Constraints

The macroscopic transport equations of mathematical physics which are first order in the time are often integral equations, although they may appear in a diffusion approximation (for an example, see Ref. 28). The microscopic equations are certainly of an integral nature.

The solutions of the Λ theorem were formally stated in Eqs. (3.4) and (3.6), with the help of Green's functions $\mathfrak{K}(y,y';z,z')$ and $\mathfrak{G}(y,0;y')$ pertaining to $\Lambda_y \to + \leftarrow \Lambda_{y'}$ and Λ_y, respectively. These Green's functions always exist unless $\lambda = 0$ is an eigenvalue of Λ. This means that the homogeneous equation $\Lambda\varphi = 0$ has a solution other than the

trivial solution $\varphi = 0$. Clearly, in that case there is also a nontrivial solution H in $\mathfrak{K}^{(2)}$ of Eq. (3.23).

This unfortunate situation is not the exception but the rule when dealing with integral transport equations. If the phenomenological equations are linear in $n^p(y)$, rather than *linearized* in $\alpha^p(y)$, as is, e.g., the case for the Boltzmann equation of a classical gas, the equation $\Lambda[\gamma(y)] = 0$ always has a solution, viz., the steady state $n_0^p(y)$. [The same argument does not apply to differential equations, since $n(y)$ and $\alpha(y)$ satisfy different boundary conditions.] If the domain $\mathfrak{D}$ under consideration is large, this solution is not bothersome, however. The normalized eigenfunction φ_0 associated with $\lambda = 0$ is of order $V^{-1/2}$, where V is the volume of $\mathfrak{D}$. Thus, for $V \to \infty$, φ_0 approaches the trivial solution and must be discarded. For finite V, a Green's function exists only if the following holds.[40] Let Θ be a solution of the adjoint homogeneous equation to the Λ theorem:

$$\tilde{\Lambda}_y \Theta(y,y') + \Theta(y,y')\tilde{\Lambda}^{\mathrm{tr}}_{y'} = 0; \tag{3.26}$$

then we require that

$$(\Theta, \Xi) = 0. \tag{3.27}$$

For the linear Boltzmann case we show in Appendix A that this condition is met. We can thus construct Green's operators in the extended sense. The defining equations for these operators are

$$\Lambda_y \mathsf{K}_{yy'} + \mathsf{K}_{yy'}\Lambda^{\mathrm{tr}}_{y'} = \mathsf{I} - |\mathrm{H}(y,y')\rangle\langle\Theta(y,y')|, \tag{3.28}$$

$$\Lambda \mathsf{G}(0) = \mathsf{I} - |\varphi_0\rangle\langle\psi_0| = \mathsf{I} - \mathsf{P}_0; \tag{3.29}$$

this follows easily from the standard definition for the extended Green's functions.[41] *It thus follows immediately that the expansions for* K *and* G(0), *Eqs. (3.5) and (3.7), are still correct providing the terms with* $\lambda_k = \lambda_l = 0$ *are omitted* (signified by the use of $\sum'$ instead of $\sum$). Likewise, Eqs. (2.23), (2.24), and (3.3) can be maintained, if $\sum$ is replaced by $\sum'$, thereby revalidating our method of Sect. 2.

Lax[15] indicated that we may wish to use the solution of the homogeneous equation, which can be added at liberty to the particular solution (2.24), in order to satisfy certain constraints. In particular, one may want to satisfy the canonical particle constraint

$$\int_D n^p(y)d^l y = N \quad \text{or} \quad \int_D \alpha^p(y)d^l y = 0, \tag{3.30}$$

with, as a consequence,

$$\int_D \int_D \Gamma(y,y')d^l y d^l y' = 0. \tag{3.31}$$

In the linear Boltzmann case, the solution of the homogeneous Λ theorem is simply $\langle \mathbf{n}(y)\rangle\langle \mathbf{n}^{\mathrm{tr}}(y)\rangle$. Denoting by Γ_∞ the solution without constraint, we find that

$$\Gamma(y,y') = \Gamma_\infty(y,y') - \langle \mathbf{n}(y)\rangle\langle \mathbf{n}^{\mathrm{tr}}(y')\rangle N^{-2} \times \int_D \int_D \Gamma_\infty d^l y d^l y'. \tag{3.32}$$

Lax also arrived at these rules by performing a transformation on the random variables which decouples them so that Γ_∞ is diagonal. This permits an easy discussion of the $\lambda = 0$ case. There is essentially no necessity for this procedure, as long as one proves (3.27). Equations of the nature of (3.32), connecting canonical and grand canonical averages, have also been derived by us by statistical-mechanical procedures.

4. APPROACH TO THE STEADY STATE

We shall find an expression for the conditional covariance, using a method analogous to Refs. 2 and 4.

The solution (2.10) will be written in the form

$$\chi(y,t) \equiv \alpha(y,t) - g(t,0)\alpha(y,0) = \int_0^{t+0} dt''\, g(t,t'')\xi(y,t''). \tag{4.1}$$

The covariance function of the quantities χ is denoted by

$$\mathrm{X}_t(y,y') = \langle \chi(y,t)\chi^{\mathrm{tr}}(y',t)\rangle_{\mathrm{cond}} = \langle \alpha(y,t)\alpha^{\mathrm{tr}}(y',t)\rangle_{\mathrm{cond}} - g_y(t,0)\alpha(y,0)\alpha^{\mathrm{tr}}(y',0)g^{\mathrm{tr}}_{y'}(t,0). \tag{4.2}$$

The rhs is given by the main term $\left(\sum_{kl}\right)$ in Eq. (2.18). We substitute the results of Eqs. (2.22) and (2.25) and find

$$\mathrm{X}_t(y,y') = \sum_{kl}[1 - e^{-(\lambda_k + \lambda_l)t}]\,(\Gamma, \psi_k\psi_l^{\mathrm{tr}})\varphi_k(y)\varphi_l^{\mathrm{tr}}(y') = \sum_{kl}[1 - e^{-(\lambda_k+\lambda_l)t}]\mathsf{P}_{k,y}\Gamma(y,y')\mathsf{P}^{\mathrm{tr}}_{l,y'}, \tag{4.3}$$

where P_k and P_l are again projectors of Λ. Substituting back (2.13), we arrive at the following connection between the conditional covariance X_t and the steady-state covariance Γ:

$$\mathrm{X}_t(y,y') = \Gamma(y,y') - g_y(t,0)\Gamma(y,y')g^{\mathrm{tr}}_{y'}(t,0). \tag{4.4}$$

As in Ref. 2, one can find the conditional Markov functional $P[\alpha(y,t)\,|\,\alpha(y,0)]$ in the Gaussian approximation. Clearly

$$P[\alpha(y,t)\,|\,\alpha(y,0)] = P[\chi(y,t)]. \tag{4.5}$$

Let the characteristic functional be $F[\hat{\omega}(y)]$, defined by the *functional* integration:

$$F[\hat{\omega}(y,t)] = \int \delta\chi P[\chi(y,t)]e^{2\pi i(\chi,\hat{\omega})}, \tag{4.6a}$$

with inversion

$$P[\chi\,(y,t)] = \int \delta\hat{\omega} F[\hat{\omega}(y,t)]e^{-2\pi i(\chi,\hat{\omega})}. \tag{4.6b}$$

Using (4.1), (4.4), and (4.5), we obtain

$$P[\alpha(y,t)\,|\,\alpha(y,0)] = \int \delta\hat{\omega}\, \exp\{-2\pi i([\alpha(y,t) - g_y(t,0)\alpha(y,0)], \hat{\omega}(y)) - \tfrac{1}{2}([\Gamma(y,y') - g_y(t,0)\Gamma(y,y')g^{tr}_{y'}(t,0)], \hat{\omega}(y)\hat{\omega}^{tr}(y'))\}. \quad (4.7)$$

Though the Green's functions decrease monotonically with t, we cannot speak of the familiar "exponentially smoothed" path; the formal result (4.7) is much more complex.

5. THERMAL EQUILIBRIUM PROPERTIES

In thermal equilibrium important simplifications occur; the argument is closely parallel to that for processes in a finite-dimensional vector space[9] and is a modification of Onsager's original argument.[42] From Eqs. (4.1) we have

$$\langle \chi(y,t)\alpha^{tr}(y',0)\rangle = \langle \alpha(y,t)\alpha^{tr}(y',0)\rangle - g_y(t)\langle \alpha(y,0)\alpha^{tr}(y',0)\rangle = \Phi(y,y',t) - g_y(t)\Gamma(y,y') \approx 0. \quad (5.1)$$

The result is zero for times larger than the collision time [compare the rhs of Eq. (4.1)]. Likewise we obtain

$$\langle \chi(y',t)\alpha^{tr}(y,0)\rangle = \Phi(y',y,t) - g_{y'}(t)\Gamma(y,y') \approx 0. \quad (5.2)$$

For a stationary process we noted before

$$\Phi^{tr}(y',y,t) = \Phi(y,y',-t); \quad (5.3)$$

for a microscopically reversible process, in addition, we note

$$\Phi(y,y',-t) = \Phi(y,y',t). \quad (5.4)$$

Whence from (5.10) -(5.4) we obtain for such a process

$$g_y(t)\Gamma(y,y') = \Gamma(y,y')g^{tr}_{y'}(t). \quad (5.5)$$

Since this is true for all t, it is also true for the Laplace-transformed result

$$G_y(s)\Gamma(y,y') = \Gamma(y,y')G^{tr}_{y'}(s). \quad (5.5')$$

When we operate on this with $(\Lambda_y \rightarrow)$ $(\leftarrow \Lambda^{tr}_{y'})$, we find alternately

$$\Lambda_y\Gamma(y,y') = \Gamma(y,y')\Lambda^{tr}_{y'}. \quad (5.6)$$

Thus the two terms in the Λ theorem are equal as we contemplated before, and we have

$$\Lambda_y\Gamma(y,y') = \tfrac{1}{2}\Xi(y,y'). \quad (5.7)$$

Equation (5.6), valid for all y, y' and all components of Λ, is a set of generalized Onsager relations. To see this, we must show that the dyad $\Lambda_y\Gamma(y,y')$, or the dyad Ξ, is a generalized conductance in flow equations derived from entropy transport. To this purpose, we define the conjugate variables to α by the functional derivative $k^{-1}\delta S/\delta\alpha = \delta \log P[\alpha(y)]/\delta\alpha$. For the thermal equilibrium case these variables are related to the intensive variables associated with the local entropy production. From Eqs. (4.6) and (4.7) it follows that the conjugate variables ("forces") have the same distribution as the functions $\hat{\omega}$ if $t \rightarrow \infty$; i.e.,

$$P\left[\frac{\delta \log P}{\delta\alpha}\right] = \lim_{t\rightarrow\infty} F[\hat{\omega}(\dot{y},t)] \equiv F[\omega(y)]. \quad (5.8)$$

Further we find

$$\langle \omega(y)\alpha^{tr}(y')\rangle = \int \left(\frac{\delta \log P}{\delta\alpha}\right)_y \alpha^{tr}(y')\delta\alpha = -\Im\delta(y-y'). \quad (5.9)$$

as is found by integration by parts; $\Im$ is the unit matrix. Consequently, from (5.7) and (5.9) we obtain

$$\Lambda_y\langle \alpha(y)\alpha^{tr}(y')\rangle\, \delta(y'-y'') = -\tfrac{1}{2}\Xi(y,y')\langle \omega(y')\alpha^{tr}(y'')\rangle. \quad (5.10)$$

We integrate over d^3y' and use (2.3a) and (2.1). This gives

$$\left\langle \left(\frac{\partial\alpha(y,t)}{\partial t} - \tfrac{1}{2}\int \Xi(y,y')\omega(y',t)d^3y'\right)\alpha^{tr}(y'',t)\right\rangle = 0. \quad (5.11)$$

This means the quantity in large parens is uncorrelated with $\alpha^{tr}(y'')$ or it is zero. The latter is the case, and so we have

$$\frac{\partial\alpha(y,t)}{\partial t} - \tfrac{1}{2}\int \Xi(y,y')\omega(y',t)d^3y' = 0. \quad (5.12)$$

These relations connect the flow rates $\dot{\alpha}$ with the applied thermodynamic forces; they are the generalization of the linear flow equations of irreversible thermodynamics. The sources Ξ appear now as "generalized conductances". They are Onsager coefficients with the symmetry property (1.6).

A sufficient condition for microscopic reversibility is thermal equilibrium. For the steady state we cannot say much in general. Clearly, $\Gamma(y,y')$ is symmetrical in y and y', and, as discussed by Balescu,[43] it is of the form $F(|\mathbf{r}-\mathbf{r}'|) + H(\mathbf{r})H(\mathbf{r}')$, where the first term involves correlation on the molecular distance scale, and the second one possible correlations on the hydrodynamic (macroscopic) distance scale. For $H(\mathbf{r}) \neq 0$, Eq. (5.6) is usually not satisfied.

6. SPECTRAL FUNCTIONS

In Ref. 14 the spectra were derived from an intuitive probabilistic approach. We can arrive at these results also following Sec. 2; we shall generalize them to other useful forms.

First we notice that according to Bayes's theorem[44] the two-time probability can be linked to a conditional probability. This is true for finite-dimensional processes, but can be expected to hold for functionals as well [see, however, the paragraph subsequent to Eq. (6.13)]:

$$P_2[n(y,t);n'(y,t')] = P[n(y,t)\,|\,n'(y,t')]P_1[n'(y)]. \tag{6.1}$$

Or, multiplying with $\alpha(y,t)\alpha^{\mathrm{tr}}(y',0)$ and averaging, we obtain

$$\Phi(y,y',t) = \langle\langle \alpha(y,t)\rangle_{\text{cond to }\alpha(y',0)}\alpha^{\mathrm{tr}}(y',0)\rangle, \tag{6.2}$$

whence from (2.10)

$$\begin{aligned}\Phi(y,y',t) &= g_y(t,0)\langle\alpha(y,0)\alpha^{\mathrm{tr}}(y',0)\rangle \\ &= g_y(t,0)\Gamma(y,y'), \qquad t \geqslant 0.\end{aligned} \tag{6.3}$$

For negative t we can interchange y and y' [cf. Eq. (5.3)]:

$$\Phi(y,y',t) = \Phi^{\mathrm{tr}}(y',y,-t) = \Gamma(y,y')g^{\mathrm{tr}}_{y'}(-t,0), \qquad t \leqslant 0. \tag{6.4}$$

The spectra $\Sigma(y,y',\omega)$ are the Fourier transforms of the function Φ. Instead, we break the interval $(-\infty,\infty)$ into two parts and take the Laplace transform. Then, from (6.3) and (6.4):

$$\Sigma(y,y',\omega) = 2G_y(i\omega)\Gamma(y,y') + 2\Gamma(y,y')G^{\mathrm{tr}}_{y'}(-i\omega), \tag{6.5}$$

where G is again the resolvent operator. (The conditions under which a function has a Fourier transform and a Laplace transform are quite different. This is discussed in Appendix B.) The terms on the rhs of (6.5) are Hermitean conjugate to each other; if the process is microscopically reversible, they are complex conjugate to each other [cf. Eq. (5.5)]. Consequently, for such processes

$$\Sigma(y,y',\omega)\,|_{\text{micr rev}} = 4\mathrm{Re}G_y(i\omega)\Gamma(y,y'). \tag{6.6}$$

The spectra can also be expressed in the sources. We obtain, operating on Σ with $\Lambda_y + i\omega$ from the left and with $\Lambda^{\mathrm{tr}}_{y'} - i\omega$ from the right:

$$\begin{aligned}&(\Lambda_y + i\omega)\Sigma(y,y',\omega)(\Lambda^{\mathrm{tr}}_{y'} - i\omega) \\ &\quad = 2\Gamma(y,y')\Lambda^{\mathrm{tr}}_{y'} + 2\Lambda_y\Gamma(y,y') = 2\Xi(y,y'),\end{aligned} \tag{6.7}$$

where we used the Λ theorem. For "Markovian linear" processes the solution of this operator equation is immediate:

$$\Sigma(y,y',\omega) = 2G_y(i\omega)\Xi(y,y')G^{\mathrm{tr}}_{y'}(-i\omega). \tag{6.8}$$

The boundary conditions on $\Sigma(y,y',\omega)$ are the same as those on G_y and $\bar{G}_{y'}$; hence they are automatically fulfilled. Since (6.7) is of higher order in Λ, there could be other solutions, however. In order to compare (6.5) and (6.8) further, we make a spectral decomposition of the resolvent and employ (3.4). Then (6.5) gives

$$\begin{aligned}\Sigma &= 2\sum_m \frac{P_{my}}{\lambda_m + i\omega}\sum_{kl}\frac{P_{ky}\,\Xi\,P^{\mathrm{tr}}_{ly'}}{\lambda_k + \lambda_l} + hcj \\ &= 2\sum_{kl}\frac{P_{ky}\,\Xi\,P^{\mathrm{tr}}_{ly'}}{\lambda_k + \lambda_l}\left(\frac{1}{\lambda_k + i\omega} + \frac{1}{\lambda_l - i\omega}\right)\end{aligned} \tag{6.9}$$

where we used the projector property $P_{my}P_{ky} = \delta_{mk}P_{ky}$ and where *hcj* denotes the Hermitian conjugate of the preceding term. From (6.8) we have

$$\Sigma = 2\sum_{kl}\frac{P_{ky}\,\Xi\,P^{\mathrm{tr}}_{ly'}}{(\lambda_k + i\omega)(\lambda_l - i\omega)}, \tag{6.10}$$

which by partial fractions gives the same result. Further, we easily deduce from this the low- and high-frequency asymptotes (the latter only *if a highest* λ_k *exists*):

$$\Lambda_y\Sigma\Lambda^{\mathrm{tr}}_{y'} = 2\Xi, \qquad \omega \to 0, \tag{6.11}$$

$$\mathrm{Re}\Sigma = 2\Xi/\omega^2, \qquad \omega \text{ large}. \tag{6.12}$$

For a second avenue, we could have started from Eqs. (3.9). Now, Eq. (3.9a), is a convolution of Fourier transforms and Eq. (3.9b) is a convolution of Laplace transforms. We prefer the latter; then, the transform for $u > 0$ is just $G_y(s)\Xi G^{\mathrm{tr}}_{y'}(-s)$ (Sneddon[45]). Thus (6.8) is obtained once more.

Expression (6.8) is much less pleasant to work with than (6.5) since it is quadratic in the resolvent. Often, the covariance function can be found by inspection of the Λ theorem. If by this or other means the covariances are known, the *correlation method*, with the spectra given by (6.5), is much to be preferred over the *response or source method*, with the spectra given by (6.8).

For microscopically reversible processes, a more simple source expression results, from (6.6) and (3.6):

$$\Sigma(y,y',\omega)\,|_{\text{micr rev}} = 2\,\mathrm{Re}G_y(i\omega)G_y(0)\,\Xi\,(y,y'). \tag{6.13}$$

Complications arise if the process has surface sources, but is still "response linear". We know from examples that the spectrum (6.5) in this case is incomplete.[46] The reason is, in our opinion, that (6.1) does not hold [the conditional probability functional is undetermined, unless $v(y,t)$ is specified]. Thus only the second avenue is open. Starting from (3.20), we obtain for Φ an extension of (3.8), involving the surface terms. The Laplace-transformed result yields for the spectra

$$\begin{aligned}\Sigma(y,y',\omega) &= 2G_y(i\omega)\,\Xi\,(y,y')G^{\mathrm{tr}}_{y'}(-i\omega) \\ &\quad + 2H_{Sy}(i\omega)\Upsilon(y_0,y'_0)H^{\mathrm{tr}}_{Sy'}(-i\omega).\end{aligned} \tag{6.14}$$

The bulk term (first term on the rhs) can be reverted to the form (6.5) using the covariance

function $\Gamma'(y,y')$ minus the contribution from surface singularities. The surface terms remain, to our knowledge, always quadratic in the Green's functions. The result analogous to (6.5) is then, with the proper homogeneous bc applied to G,

$$\Sigma(y,y',\omega) = 2G_y(i\omega)\Gamma'(y,y') + 2\Gamma'(y,y')G^{tr}_{y'}(-i\omega) + 2H_{Sy}(i\omega)\Upsilon(y_0,y_0')H^{tr}_{Sy'}(-i\omega) + 2[H_{Sy}(i\omega)\mathrm{ly}\Gamma'(y_0,y')G^{tr}_{y'}(-i\omega) + hcj]. \tag{6.15}$$

Additional spectra. In various applications it is necessary to know the spectra of $\langle Q\alpha(y,t)\alpha^{tr}(y,t)R^{tr}$, where Q and R are linear operators in $\mathfrak{K}$. One finds, denoting these spectra as Σ_{QR},

$$\Sigma_{QR}(y,y',\omega) = Q_y\Sigma(y,y',\omega)R^{tr}_{y'}; \tag{6.16}$$

e.g., in conjunction with (6.5),

$$\Sigma_{QR} = 2Q_yG_y(+i\omega)\Gamma(y,y')R^{tr}_{y'} + hcj = 2\int d^ly''Q_{y''}\mathfrak{G}(y,+i\omega;y'')R^{tr}_{y'} + hcj. \tag{6.16'}$$

This expression must be interpreted with care. The operators Q and R can only be taken inside the integral if the result is interpreted as a Schwartz distribution, possibly involving δ functions, δ' functions, etc. For instance, if we have $Q = d^2/dy^2$ in a one-dimensional problem, the function $d^2\mathfrak{G}/dy^2$ is discontinuous at $y = y''$, represented by the distributional derivative

$$d^2\mathfrak{G}(y,s;y'')/dy^2 = \{d^2\mathfrak{G}/dy^2\}' + [d\mathfrak{G}/dy]^{y''+0}_{y''-0}\,\delta(y-y''),$$

where the curly bracket $\{\}'$ means an expression undefined for $y = y''$. One easily verifies that this result, when integrated over $\varphi(y'')$, is in agreement with the explicit procedure in which the integral is broken up into two parts ($y'' < y, y'' > y$) and in which one obtains terms from differentiation to the limits in the integrals. Likewise, in a three-dimensional diffusion example the singularity at $\mathbf{r} = 0$ must be noted as

$$\nabla^2\mathfrak{G}(\mathbf{r},s;\mathbf{r}'') = \{\nabla^2\mathfrak{G}\}' - 4\pi K\delta(\mathbf{r}-\mathbf{r}''),$$

where $K/|\mathbf{r}-\mathbf{r}''|$ is the limit of $\mathfrak{G}$ for $\mathbf{r} \to \mathbf{r}''$. The contributions from these singularities are quite important.

In some macroscopic problems[46] the cross correlation spectra $\Pi(y,y'\omega)$ of the densities and the sources, $\langle \alpha(y,t)\xi^{tr}(y',t)\rangle$, are of interest. They follow from a definition in accord with (1.10) and (2.19):

$$\Pi(y,y',\omega) = 2\lim_{t\to\infty}\int_{-\infty}^{\infty} e^{i\omega u}\langle\alpha(y,t)\times\xi^{tr}(y',t+u)\rangle_{cond}du' = 2\lim_{t\to\infty}\int_{-\infty}^{\infty} e^{i\omega(u'-t)}\langle\alpha(y,t)\times\xi(y',u')\rangle_{cond}\,du'. \tag{6.17}$$

In this we substitute the solution (2.10) of the Langevin equation. The initial term can be omitted in view of (3.24). Hence we obtain

$$\Pi(y,y',\omega) = 2\lim_{t\to\infty}\int_{-\infty}^{\infty} e^{i\omega(u'-t)}du' \times\int_0^{t+0} dt'\,g_y(t,t')\Xi(y,y')\delta(t'-u'). \tag{6.18}$$

We change the order of integration, so the integral over the δ function can be carried out for any t':

$$\Pi(y,y',\omega) = 2\lim_{t\to\infty}\int_0^t dt'\,e^{-i\omega(t-t')}g_y(t,t')\Xi(y,y'). \tag{6.19}$$

From the series expansion for g we see

$$g_y(t,t') = g_y(T,0), \qquad T = t-t'.$$

Thus we arrive at

$$\Pi(y,y',\omega) = 2\lim_{t\to\infty}\int_0^t dTe^{-i\omega T}g_y(T,0)\Xi(y,y') = 2\int_0^{\infty} dTe^{-i\omega T}g_y(T,0)\Xi(y,y') = 2\,G_y(i\omega)\Xi(y,y'). \tag{6.20}$$

These spectra, like those of (6.5), are linear in the resolvant operator.

II. LINKS WITH THE MASTER-RATE FUNCTIONAL

7. SOURCES AND GENERALIZED FOKKER-PLANCK MOMENTS

We now carry out the other program, mentioned in Sec. 1, and establish the relationships between Λ and Ξ with the "master-rate functional" via generalized FP moments (this section), and find expression for the collisional part of Λ and for Ξ for a number of cases (next section).

The master-rate functional is defined by

$$W[\mathbf{n}(y),\mathbf{n}'(y)] = \lim_{\Delta t\to+0}(1/\Delta t)P[\mathbf{n}'(y,\Delta t)|\mathbf{n}(y,0)]. \tag{7.1}$$

The limit is, however, to be taken with a grain of salt. Actually Δt must be short compared to relaxation times for the densities $\mathbf{n}(y,t)$, but long with respect to the time duration of interaction (as is clear in van Hove's derivation of the ME[19]). We now define the first generalized FP moments as follows[47]:

$$A_{y_1}[\mathbf{n}(y,t)] = \lim_{\Delta t\to+0}(1/\Delta t)\langle\mathbf{n}(y_1,t+\Delta t)-\mathbf{n}(y_1,t)\rangle_{coll} = \int\delta\mathbf{n}'(y)T_{y_1}[\mathbf{n}'(y)-\mathbf{n}(y,t)]\,W[\mathbf{n}(y),\mathbf{n}'(y)], \tag{7.2}$$

$$B_{y_1y_2}[\mathbf{n}(y,t)] = \lim_{\Delta t\to+0}(1/\Delta t)\langle\{\mathbf{n}(y_1,t+\Delta t)-\mathbf{n}(y_1,t)\}$$

$$\times\{\mathbf{n}(y_2, t+\Delta t) - \mathbf{n}(y_2, t)\}^{\mathrm{tr}}\rangle_{\mathrm{coll}}$$
$$= \int \delta\mathbf{n}'(y) T_{y_1}[\mathbf{n}'(y) - \mathbf{n}(y,t)] T_{y_2}[\mathbf{n}'(y) - \mathbf{n}(y,t)]^{\mathrm{tr}}$$
$$\times W[\mathbf{n}(y), \mathbf{n}'(y)]. \quad (7.3)$$

Here T_{y_i} is a distribution which projects the functions at the point y_i. The integrals are over the function space of $\mathbf{n}'(y)$.

In the definition of these moments there is an ambiguity peculiar to transport processes. Changes in the local densities occur both due to ponderomotive forces giving rise to streaming and due to local forces giving rise to collisions. Streaming changes are always of order Δt; hence they contribute possibly to A, but never to B. In order to define both moments consistently, we incorporate only changes due to collisions, whence the subscript coll in (7.2) and (7.3); similarly for the W of equation (7.1). The Langevin equations (2.1) are accordingly written as

$$\left(\frac{\partial \mathbf{n}}{\partial t}\right)_{\mathrm{smooth}} + \Lambda_{\mathrm{str}}\,\mathbf{n}(y,t) - \left(\frac{\partial \mathbf{n}}{\partial t}\right)_{\mathrm{coll}} = \xi(y,t), \quad (7.4)$$

where Λ_{str} refers to the streaming part of Λ. In contrast to our view expressed by (2.1), we shall look upon the first term as the *smooth* part of the local derivative, whereas the *stochastic* part is included in the change due to collisions, i.e., the third term. Averaging this term over a time Δt, of smallness indicated above, so that $\langle\xi\rangle_{\Delta t} = 0$, we find from the definition (7.2)

$$\left\langle\left(\frac{\partial \mathbf{n}}{\partial t}\right)_{\mathrm{coll}}\right\rangle_{\Delta t} \equiv -\Lambda_{\mathrm{coll}}\,\Delta\mathbf{n}(y,t) = A_y[\mathbf{n}(y,t)], \quad (7.5)$$

where the second equality defines the (linearized) collision operator. *The first order* FP *moments are therefore stochastic elements* of $\mathfrak{K}$. Taking another conditional average over an ensemble with fixed $\mathbf{n}(y,o)$, we have for the phenomenological equations from (7.4)

$$\frac{\partial}{\partial t}\langle\mathbf{n}(y,t)\rangle_{\mathrm{cond}} + \Lambda_{\mathrm{str}}\langle\mathbf{n}(y,t)\rangle_{\mathrm{cond}}$$
$$+ \Lambda_{\mathrm{coll}}\langle\Delta\mathbf{n}(y,t)\rangle_{\mathrm{cond}} = 0 \quad (7.6)$$

or

$$\frac{\partial}{\partial t}\langle\mathbf{n}(y,t)\rangle_{\mathrm{cond}} + \Lambda_{\mathrm{str}}\langle\mathbf{n}(y,t)\rangle_{\mathrm{cond}}$$
$$= \langle A_y[\mathbf{n}(y,t)]\rangle_{\mathrm{cond}}. \quad (7.6')$$

To find the connection with the second-order FP moments, we use the hydrodynamic derivative $d/dt = \partial/\partial t + \Lambda_{\mathrm{str}}$ and integrate (7.4) over a time Δt, starting from the stationary state $\langle\mathbf{n}(y,t)\rangle$. The result is

$$\mathbf{n}(y + \dot{y}\Delta t, t+\Delta t) - \langle\mathbf{n}(y,t)\rangle = [\mathbf{n}(y, t+\Delta t)$$
$$- \langle\mathbf{n}(y,t)\rangle]_{\mathrm{coll}} + \int_t^{t+\Delta t} \xi(y,t')dt'. \quad (7.7)$$

With regard to our interpretation of (7.4), the lhs of this result is smooth and of order Δt. Whence, multiplying with the transpose result for y', we get

$$\langle[\mathbf{n}(y, t+\Delta t) - \langle\mathbf{n}(y,t)\rangle][\mathbf{n}(y', t+\Delta t$$
$$- \langle\mathbf{n}(y',t)\rangle]^{\mathrm{tr}}\rangle_{\mathrm{coll}}/\Delta t$$
$$= \frac{1}{\Delta t}\int_0^{\Delta t}\int_0^{\Delta t} dt'dt''\langle\xi(y,t')\xi^{\mathrm{tr}}(y',t'')\rangle + O(\Delta t). \quad (7.8)$$

Or, using as new variables t' and $t' - t''$, we find, observing (1.5),

$$\Xi(y,y') = B_{yy'}[\langle\mathbf{n}(y,t)\rangle], \quad (7.9)$$

a result entirely analogous to that of simple Brownian motion. The second-order FP moments, evaluated as functional of $\langle\mathbf{n}(y)\rangle$ will also be denoted as $B^0_{yy'}$; *these moments are not stochastic, but are simple bivariate functions of* y *and* y'.

8. EXPRESSIONS FOR THE FP MOMENTS

We proceed with the calculation of A and B. Generally, an m-body collision (e.g., in a solid) is characterized by the transition rate $T(y_1^{p_1}y_2^{p_2}\cdots y_m^{p_m}, \hat{y}_1^{q_1}\hat{y}_2^{q_2}\cdots\hat{y}_m^{q_m})$, where m particles of "species" or bands $p_1, \cdots, p_m$ and "states" $y_1^{p_1}\cdots y_m^{p_m}$ are excited or de-excited into species $q_1, \cdots, q_m$ with states $\hat{y}_1^{q_1}\cdots\hat{y}_m^{q_m}$. (For the concepts in quotes, see the Introduction.) We consider first the simple case of one-body collisions, with no interband transitions or change in species. Thus, $T(y^p, y'^q) = Q^p(y,y')\delta^{pq}$. The master-rate functional for this case is

$$W[\mathbf{n}(y), \mathbf{n}'(y)] = \sum_{p,q\neq p}\int\int Q^p(y_1,y_2)dy_1dy_2$$
$$\times\delta[n'^p(y), n^p(y) - \delta(y-y_1) + \delta(y-y_2)]$$
$$\times\delta[n'^q(y), n^q(y)]. \quad (8.1)$$

The functional integrations (7.1) and (7.2) can now be carried out. The result is[48]

$$A^p_y[\mathbf{n}(y,t)] = \int dy'[Q^p(y',y) - Q^p(y,y')], \quad (8.2)$$

$$B^{pq}_{yy'}[\mathbf{n}(y,t)] = -\{Q^p(y',y) + Q^p(y,y')\}\delta^{pq}$$
$$+ \delta(y-y')\int dy''[Q^p(y'',y) + Q^p(y,y'')]\delta^{pq}. \quad (8.3)$$

The case that transitions occur from one species to another, without change in coordinates (macroscopic theory) or change in coordinates and $\mathbf{k}$ vector (microscopic theory) is characterized by $T(y^p, y'^q) = P^{pq}(y)\delta(y-y')$. The situation is the same as in Ref. 10, if we consider a section $\Delta\Omega$ of the y-space. Thus, writing $1/\Delta\Omega \approx \delta(y-y')$, we obtain

$$A^p_y[\mathbf{n}(y,t)] = \sum_s{}'[P^{sp}(y) - P^{ps}(y)], \quad (8.4)$$

$$B^{pq}_{yy'}[\mathbf{n}(y,t)] = -[P^{pq}(y) + P^{qp}(y)]\delta(y-y'), \quad p\neq q, \quad (8.5)$$

$$B^{pp}_{yy'}[\mathbf{n}(y,t)] = -\sum_s{}'[P^{sp}(y) + P^{ps}(y)]\delta(y-y'). \tag{8.6}$$

The dimension of A is Ω^{-1}, that of B, Ω^{-2}.

Finally, we consider a one-component system with two-body collisions. The master-rate functional is

$$\begin{aligned} W[n(y),n'(y)] = \tfrac{1}{2}\iiint Q(y_1y_2,y_3y_4)\,dy_1dy_2dy_3dy_4 \\ \times \delta[n'(y), n(y) - \delta(y-y_1) - \delta(y-y_2) \\ + \delta(y-y_3) + \delta(y-y_4)]. \end{aligned} \tag{8.7}$$

The factor $\frac{1}{2}$ is put in since otherwise collisions between particles at y_1 and y_2 would be counted twice; further we assumed

$$\begin{aligned} Q(y_1y_2,y_3y_4) = Q(y_2y_1,y_3y_4) = Q(y_1y_2,y_4y_3) \\ = Q(y_2y_1,y_4y_3), \end{aligned} \tag{8.8}$$

while $Q = 0$ if any two of the four y's are equal. For the FP moments we find

$$A_y = \iiint dy_2dy_3dy_4[Q(y_3y_2,yy_4) - Q(yy_2,y_3y_4)] \tag{8.9}$$

and

$$\begin{aligned} B_{yy'} = \iint dy_1dy_2[Q(yy',y_1y_2) + Q(y_1y_2,yy') \\ - 2Q(yy_1,y'y_2) - 2Q(y'y_1,yy_2)] \\ + \delta(y-y')\iiint dy_1dy_2dy_3[Q(yy_1,y_2y_3) \\ + Q(y_1y_2,yy_3)]. \end{aligned} \tag{8.10}$$

We note that in all expressions Q depends on the instantaneous values of $\mathbf{n}(y,t)$, at the appropriate points y_1, y_2, etc. The expressions for A [Eqs. (8.2), (8.4), and (8.9)] express properly the collisional part of the phenomenological equations. The expressions for B must be evaluated for $\mathbf{n}(y,t) \to \langle \mathbf{n}(y,t) \rangle$.

9. CONCLUSIONS

In the kinetic approach to statistical mechanics, the basic equations are the Liouville and the von Neumann equation, which under certain conditions reduce to a Markovian master equation. The latter, in turn, leads to a set of Langevin equations, in which a complicated set of interactions is replaced by fluctuating source functions. These equations describe the approach to equilibrium (or the steady state), as well as fluctuations around this state.

We have considered fluctuations in densities $n^p(y,t)$, where y is a continuous variable in a macroscopic or microscopic domain $\mathfrak{D}$ of a space $\mathfrak{R}^l$. We do not generalize, in contrast to earlier papers by Lax[9] and by van Vliet and Fassett,[10] the results of finite-dimensional Markovian processes to the cases considered; instead, mathematical procedures, applicable to the situation, are introduced. In particular, we use a Hilbert space representation for the stochastic densities $n^p(y,t)$ and a spectral decomposition of the resolvent for the Markovian transport operator $\mathsf{L} = \partial/\partial t + \Lambda$. With this procedure, the "Λ theorem" for the two-point covariance functions Γ [Eq. (2.30)] is derived. This is a powerful theorem which permits Γ to be found from a kinetic point of view, i.e. from Λ and Ξ. Several solutions are stated [Eqs. (3.3), (3.4), (3.10)].

The approach to the steady state is treated in a manner similar to Uhlenbeck and Ornstein's original method.[2] However, due to the denumerably infinite or continuous spectrum of eigenvalues of Λ, we do not find the familiar exponentially smoothed path,[49] but a complex result, Eq. (4.7). In thermal equilibrium the same symmetry exists as for finite-dimensional processes, allowing us to solve the Λ theorem directly if the resolvent Λ is known. Generalized Onsager relations are derived [cf. Eq. (5.12)].

For the spectral intensities $\Sigma^{pq}(y,y',\omega)$ or Fourier transforms of the two-point time-displaced covariance functions, two types of expressions are derived. First, *expressions linear in the resolvent operator are obtained* (these are equivalent to the Laplace-transformed Green's function formalism of Ref. 14), Eqs. (6.5) and (6.6). This result is limited, however, to "Markovian linear" processes and excludes stochastic boundary conditions (as was not clear in the treatment of Ref. 14). *Expressions quadratic in the resolvent operator are more complex but have general validity.* [Eqs. (6.8), (6.13), and (6.14)].

Finally, the Langevin sources Ξ are linked to the master-rate functional for the transitions of the over-all system state. The connection with the FP moments A and B, more complex than for finite-dimensional processes (due to streaming terms of Λ), is given in Eqs. (7.6′) and (7.9). These FP moments are indispensable in order to know the correct Λ and Ξ of the Λ theorem and are computed for three cases: transitions which interchange species, Eqs (8.4)–(8.6); one-body collisions, Eqs. (8.2) and (8.3); two-body collisions, Eqs. (8.9) and (8.10). The expressions for A indicate that the *Markovian form of Λ is usually an integral form*, Eqs. (8.2) and (8.9), similar to the Boltzmann collision integral. The results (8.3) and (8.10) for B are new and will be verified in the applications.[28]

ACKNOWLEDGMENTS

I have benefited from discussions and seminars about this work in various places. An earlier version was discussed with Professor C. Th. J. Alkemade and Dr. R. J. J. Zylstra from the University of Utrecht, as well as with others at the Institute for Theoretical Physics in Utrecht during the spring of 1968. I am indebted to Professor L. van Hove for a discussion about the master equation. Further, I thank Professor A. van der Ziel in Minneapolis and several colleagues in Montreal for comments and encouragement.

APPENDIX A: EXISTENCE OF A SOLUTION FOR THE VELOCITY CORRELATION FUNCTION ASSOCIATED WITH THE BOLTZMANN TRANSPORT EQUATION

In order that the Λ theorem have a solution for integral operators, it is necessary and sufficient that the source function [or the second-order FP moment B, Eq. (7.9)] is orthogonal to the solution Θ of the adjoint homogeneous equation [cf. Eq. (3.26)]. Since we speak of integral operators, one may suppose that we ignore the streaming terms of the Boltzmann equation. This is not quite so. The term $\mathbf{v}\cdot\nabla_{\mathbf{r}} n(\mathbf{r},\mathbf{v},t)$ must be absent, since n and α satisfy different bc on the boundary of the domain $\mathfrak{D}(\mathbf{r})$. Consequently, we exclude $\mathbf{r}$ dependence. However, the term $(\mathbf{F}/m)\cdot\nabla_{\mathbf{v}} n(\mathbf{v},t)$ is harmless, since the bc on the surface of the domain in $\mathbf{v}$ space are of a general nature: all functions $\psi(|\mathbf{v}|\to\infty)$ vanish. We thus write for the transport in $\mathbf{v}$ space of a one-component classical gas (see also Ref. 28)

$$\begin{aligned}\frac{\partial n(\mathbf{v},t)}{\partial t} &= -(\mathbf{F}/m)\cdot\nabla_{\mathbf{v}} n(\mathbf{v},t) + \int n(\mathbf{v}'',t)\mathfrak{L}(\mathbf{v}'',\mathbf{v})d^3v'' \\ &\quad - n(\mathbf{v},t)\int \mathfrak{L}(\mathbf{v},\mathbf{v}'')\,d^3v'' \\ &= \int d^3v''\, n(\mathbf{v}'',t)[\mathfrak{L}(\mathbf{v}'',\mathbf{v}) + (\mathbf{F}/m)\cdot\nabla_{\mathbf{v}''}\delta(\mathbf{v}''-\mathbf{v})] \\ &\quad - n(\mathbf{v},t)\int \mathfrak{L}(\mathbf{v},\mathbf{v}'')\,d^3v''. \qquad \text{(A1)}\end{aligned}$$

The terms in the square brackets we denote by $\omega(y'',y)$, the last integral to the right by $q(y)$ and $y \equiv \mathbf{v}$ (or in the quantum analog, $y \equiv \mathbf{k}$). Then, since the equation is linear in $n(y,t)$, the same result holds for the fluctuations; therefore,

$$\Lambda\gamma(y) = -\int dy''\,\omega(y'',y)\gamma(y'') + \gamma(y)q(y). \qquad \text{(A2)}$$

This is satisfied by the steady-state solution

$$\Lambda n(y) = -\int dy''\,\omega(y'',y)n(y'') + n(y)q(y) = 0. \qquad \text{(A3)}$$

Then for any function $\psi(y,y')$ we have

$$\begin{aligned}\Lambda_y\psi + \Lambda_{y'}\psi &= -\int dy''\,\omega(y'',y)\psi(y'',y') + \psi(y,y')q(y) \\ &\quad - \int dy''\,\omega(y'',y')\psi(y,y'') + \psi(y,y')q(y') \\ &= -\iint[\omega(\xi,y)\delta(\eta-y') \\ &\quad + \omega(\eta,y')\delta(\xi-y)]\psi(\xi,\eta)d\xi d\eta \\ &\quad + \psi(y,y')[q(y)+q(y')]. \qquad \text{(A4)}\end{aligned}$$

Now, let Θ be the adjoint homogeneous solution; then this function satisfies

$$\begin{aligned}&\iint[\omega(y,\xi)\delta(\eta-y') + \omega(y',\eta)\delta(\xi-u)]\Theta(\xi,\eta)\,d\xi d\eta \\ &\quad = \Theta(y,y')[q(y)+q(y')]; \qquad \text{(A5)}\end{aligned}$$

in particular, for $y = y'$,

$$\begin{aligned}&\iint[\omega(y,\xi)\delta(\eta-y) + \omega(y,\eta)\delta(\xi-y)]\Theta(\xi,\eta)\,d\xi d\eta \\ &\quad = 2\Theta(y,y)q(y). \qquad \text{(A6)}\end{aligned}$$

We must compute

$$(\Theta,B) = \iint B(y,y')\Theta(y,y')\,dydy'.$$

We take B from Eq. (8.3). Then it follows that

$$\begin{aligned}(\Theta,B) &= -\iint n(y)\omega(y,y')\Theta(y,y')\,dydy' \\ &\quad - \iint n(y')\omega(y',y)\Theta(y,y')\,dydy' \\ &\quad + \iint\Theta(y,y)[n(y)\Theta(y,y') + n(y')\omega(y',y)]\,dydy' \\ &\quad + (\mathbf{F}/m)\cdot\{\iint n(y)\nabla_y\delta(y'-y)\Theta(y,y')\,dydy' \\ &\quad + \iint n(y')\nabla_{y'}\delta(y'-y)\Theta(y,y')\,dydy' \\ &\quad - \iint\Theta(y,y)n(y')\nabla_{y'}\delta(y'-y)\,dydy'\}. \qquad \text{(A7)}\end{aligned}$$

With (A3) we write for the third term

$$2\int dy\;\Theta(y,y)n(y)q(y). \qquad \text{(A8)}$$

For the field terms we have

$$\begin{aligned}&\mathbf{F}/m\cdot\int dy\,\{-\nabla_y[n(y)\Theta(\underline{y},y)] - \nabla_y[n(y)\Theta(y,\underline{y})] \\ &\quad + \Theta(y,y)\nabla_y n(y)\}. \qquad \text{(A9)}\end{aligned}$$

Here the underscoring $\underline{y}$ means that we differentiate only to this part of the argument in Θ. When we add to (A9) the term $\int dy\,\nabla_{\underline{y}}[n(y)\Theta(\underline{y},\underline{y})]$, which vanishes because of the bc for $|\mathbf{v}|\to\infty$, we easily see that the integrand in (A9) is zero. We therefore find

$$\begin{aligned}(\Theta,B) &= -\int n(y)\,dy\,\{\int\omega(y,y')\Theta(y,y')\,dy' \\ &\quad + \int\omega(y,y')\Theta(y',y)\,d\underline{y}' - 2\Theta(y,y)q(y)\}. \qquad \text{(A10)}\end{aligned}$$

But Θ satisfies the homogeneous equation (A6). Consequently, the terms within $\{\}$ in (A10) are zero; hence

$$(\Theta,B) = 0. \qquad \text{QED}$$

What is the physical meaning of Θ? We know the solution of the homogeneous equation corresponding to (A4) is

$$\mathrm{H}(y,y') = n(y)n(y'). \qquad \text{(A11)}$$

Accordingly, we can also write the solution (A5) as

$$\Theta(y,y') = \tilde{n}(y)\tilde{n}(y'), \qquad \text{(A12)}$$

where $\tilde{n}(y)$ is the steady-state solution *with reversed scattering probabilities*. Thus $\tilde{n}(y)$ represents a negative-temperature state with $\mathfrak{L}(\mathbf{k}\to\mathbf{k}')$ replacing $\mathfrak{L}(\mathbf{k}'\to\mathbf{k})$.

APPENDIX B: DIVERGENT SPECTRA AND LAPLACE TRANSFORMS

In the section on the spectral functions, our aim was to obtain an expression linear in the Green's functions via the Wiener-Khintchine theorem. Yet

these spectra are often divergent; i.e., they tend to infinity more slowly than ω^{-1}, and, consequently, the integral $\int \Sigma(\omega)\, d\omega$ does not exist. For instance, in a one-dimensional diffusion problem in a semi-infinite domain with Dirichlet boundary conditions, the following Green's function occurs:

$$g(y,t;y',o) = [1/2(\pi D t)^{1/2}]\{e^{-(y-y')^2/4Dt} - e^{-(y+y')^2/4Dt}\}, \tag{B1}$$

with Laplace transform

$$G(y,s;y') = 1/2(Ds)^{1/2}\{e^{-|y-y'|(s/D)^{1/2}} - e^{-(y+y')(s/D)^{1/2}}\}. \tag{B2}$$

If the spectral expression (6.5) is correct, then Eq. (B2) results in a spectrum going as $\omega^{-1/2}$ for $y = y'$, yielding clearly a divergent spectrum. Curiously, there is seldom a problem with such spectra in the response method: One can always feed white-noise sources into a network and, depending on the transfer function, obtain any behavior for the spectral density of the output fluctuations, both for $\omega \to \infty$ and $\omega \to 0$. In particular, the Fourier-transformed Langevin equation corresponding to (2.1), $(i\omega + \Lambda)\bar{\alpha} = \bar{\xi}$, has a solution if the resolvent $G(s)$ exists along the imaginary axis for most ω. In the resolvent the poles are all in the negative half-plane. Thus $G(s)$ is determined with the appropriate boundary conditions for $\mathrm{Res} > 0$, and the imaginary axis is approached from the right, i.e., $s = \pm i\omega + 0$.

To study in more detail the correlation method and the validity of the use of Laplace transforms, we start from the definition for the spectrum

$$\Sigma(y,y',\omega) = \frac{2}{T}\lim_{T\to\infty}\langle \bar{\alpha}(y,\omega,T)\bar{\alpha}^{\dagger}(y,\omega,T)\rangle, \tag{B3}$$

where $\bar{\alpha}(y,\omega,T)$ is the Fourier transform of a function $\alpha(y,t,T)$ which equals $\alpha(y,t)$ inside $-T/2 \leq t \leq T/2$, and is zero elsewhere; the brackets are an ensemble average, necessary as long as the limit is not actually performed. By the convolution theorem for Fourier transforms, we obtain

$$\Sigma(y,y',\omega) = \lim_{T\to\infty}\frac{2}{T}\int_{-\infty}^{\infty} e^{i\omega\tau}d\tau\int_{-\infty}^{\infty}\langle \alpha(y,t,T) \times \alpha^{\dagger}(y',t+\tau,T)\rangle dt. \tag{B4}$$

If the correlation function goes fast enough to zero, we care very little about the limit and consider $\langle \alpha(y,t,T)\alpha^{\dagger}(y',t+\tau,T)\rangle$ as independent of t, i.e., as stationary. Possibly for $\tau = 0$ the variance or covariance function does not exist for certain (y,y'); omitting these isolated singularities, we then have

$$\begin{aligned}\Sigma(y,y',\omega) &= 2\int_{-\infty}^{\infty} e^{i\omega\tau}d\tau\Phi(y,y',\tau)\\ &= 2\int_0^{\infty} e^{i\omega t}\Phi(y,y',t)dt\\ &\quad + 2\int_0^{\infty} e^{-i\omega t}\Phi^{\mathrm{tr}}(y',y,t)dt.\end{aligned} \tag{B5}$$

If Φ is of negative exponential order $O(e^{-\gamma t})$, $t > 0$, $\gamma > 0$, its Laplace transform $\hat{\Phi}(s)$ exists for $\mathrm{Res} > -\gamma$, so that

$$\Sigma(y,y',\omega) = 2\hat{\Phi}(y,y',-i\omega) + 2\hat{\Phi}^{\mathrm{tr}}(y',y,i\omega). \tag{B6}$$

But, as a rule, we must be more careful. According to generalized harmonic analysis[50] we have, instead of (B4),

$$\begin{aligned}\Sigma(y,y',\omega) &= \lim_{\epsilon\to o}\frac{2}{\epsilon}\int_{-\infty}^{\infty} dt\Phi(y,y',t)\int_{\omega}^{\omega+\epsilon} e^{i\omega' t}d\omega'\\ &= \lim_{\epsilon\to o}\frac{2}{\epsilon}\int_{-\infty}^{\infty} dt\,\Phi(y,y',t)\frac{e^{i(\omega+\epsilon)t} - e^{i\omega t}}{it}.\end{aligned} \tag{B7}$$

Two alternate expressions follow from (B7):

$$\Sigma(y,y',\omega) = \lim_{\epsilon\to o} 2\int_{-\infty}^{\infty} dt\Phi(y,y',t)e^{i\omega t}e^{i\epsilon t/2} \times \frac{\sin(\epsilon t/2)}{\epsilon t/2} \tag{B8a}$$

$$= 2\frac{d}{d\omega}\int_{-\infty}^{\infty} dt\Phi(y,y',t)\frac{e^{i\omega t} - 1}{it}. \tag{B8b}$$

Several cases will be considered (besides the simple case that Φ is of negative exponential order considered above).[51] We split (B8) into two parts and discuss the convergence of Φ for $t > 0$. First, let $\int_0^{\infty} |\Phi(t)|\, dt$ exist for all y and y'. It follows from Weierstrasz's criterion that (B8a) is uniformly convergent for all ϵ, since

$$|\Phi(y,y',t)e^{i\omega t}e^{i\epsilon t/2}\sin(\epsilon t/2)/(\epsilon t/2)| \leq |\Phi|.$$

We can thus take the limit under the integral, finding a normal Fourier integral. Likewise, since we have

$$|e^{-(\alpha - i\omega)t}\Phi(y,y',t)| \leq |\Phi|, \qquad \alpha \geq 0,$$

the Laplace transform of Φ has a limit for $\alpha \to 0$ which can be taken under the integral sign. Thus, (B6) follows.

Secondly, let $\Phi(t)$ be square integrable in $\mathfrak{L}^2(0,\infty)$. Then a Fourier–Plancherel transform exists as a limit in the mean, as follows by application of Lebesgue's theorem[52] to (B8a). Moreover, one can prove that $\hat{\Phi}(s)$ for $\alpha = \mathrm{Res} > 0$ is function of $\mathfrak{K}^2$ space, i.e.,

$$\int_{-\infty}^{\infty} |\hat{\Phi}(\alpha + iy)|^2\, dy \leq M \quad \text{for} \quad \alpha > 0, \tag{B9}$$

with a finite limit for $\alpha \to +0$ which is equal to the Fourier–Plancherel transform

$$\underset{A\to\infty}{\text{l.i.m.}}\int_0^A dt\, e^{i\omega t}\Phi = \lim_{\alpha\to+0}\hat{\Phi}(\alpha - i\omega), \tag{B10}$$

compare Doetsch[53] (l.i.m. stands for "limit in the mean"). Also the observation that Φ is a function of $\mathfrak{K}^2$ space is sufficient for (B9) to hold. Whence,

as a slight extension of (B6), we have

$$\Sigma(y,y',\omega) = 2\hat{\Phi}(y,y',-i\omega+0) + 2\hat{\Phi}^{\mathrm{tr}}(y',y,i\omega+0). \tag{B11}$$

Third, we consider the case that Φ is not square integrable. Such is the case for the one-dimensional diffusion process (B1). The Fourier integral is easily shown to be still conditionally convergent; in addition, the integral (B8) from 0 to ∞) is absolutely convergent, and the same integral with a real part $-\alpha t$ added to the exponent is uniformly convergent in α. Whence, setting for convenience Σ_1 for the first part of (B8b), we arrive at

$$\begin{aligned}\tfrac{1}{2}\Sigma_1(\omega) &= \lim_{\alpha\to 0}\frac{d}{d\omega}\int_0^\infty dt\,\Phi(t)\,\frac{e^{-(\alpha-i\omega)t}-1}{it}\\ &= \lim_{\alpha\to 0}\frac{d}{d\alpha}\int_0^\infty dt\,\Phi(t)\,\frac{e^{-(\alpha-i\omega)t}-1}{-t}\\ &= \int_0^\infty dt\,\Phi(t)\left(\frac{d}{d\alpha}\,\frac{e^{-(\alpha-i\omega)t}-1}{-t}\right)_{\alpha=+0}\\ &= \hat{\Phi}(i\omega+0).\end{aligned} \tag{B12}$$

This proves once more Eq. (B11).

Finally, the pathological case that $\Phi \propto \delta(t)$ for $y = y'$ is not covered by this discussion, though one often verifies that the correct result follows from $S(y,y',\omega)$ computed by (6.5), if we let $y' \to y$, *a posteriori*.

---

* Work started at the University of Minnesota, supported by the National Science Foundation.

1 S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam, 1962).

2 G. E. Uhlenbeck and L. S. Ornstein, Phys. Rev. **36**, 823 (1930).

3 M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. **17**, 323 (1945).

4 S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943). [References 2–4 also occur in *Noise and Stochastic Processes*, edited by N. Wax (Dover, New York, 1954).]

5 Some authors consider the ensemble description to be superfluous in quantum statistics; cf. N. G. van Kampen in *Fundamental Problems in Statistical Mechanics* edited by E. D. G. Cohen (North-Holland, Amsterdam, 1962), Vol. I, p. 173.

6 M. Lax, Phys. Rev. **145**, 110 (1966).

7 A. N. Kolmogorov, Math. Ann. **104**, 415 (1931).

8 R. Stratonovitch, *Topics in the Theory of Random Noise* (Gordon and Breach, New York, 1963).

9 M. Lax, Rev. Mod. Phys. **32**, 25 (1960).

10 K. M. van Vliet and J. R. Fassett, in *Fluctuation Phenomena in Solids*, edited by R. E. Burgess (Academic, New York, 1965), Secs. I–IV, p. 267.

11 H. B. G. Casimir, Rev. Mod. Phys. **17**, 343 (1945).

12 M. Lax, Rev. Mod. Phys. **38**, 541 (1966).

13 (a) L. P. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon, New York, 1960), Chap. XIII.
(b) J. McKenna and H. L. Frisch, Phys. Rev. **145**, 93 (1966).

14 K. M. van Vliet and J. R. Fassett, in Ref. 10, Secs. V and VI.

15 M. Lax, Ref. 9, Secs. 12 and 13.

16 P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. I, Sec. 7.5.

17 The correct procedure employs the isometry of the $\mathfrak{L}^2$ and ℓ^2 Hilbert spaces and transforms the transport equations into a matrix equation via a spectral resolution of the integral or differential operators; the same applies to the Schrödinger equation.

18 The first name applies if $y = \mathbf{r}$ (cf. S. Ichimaru, in Ref. 10, p. 122); the second name applies in the microscopic case, though different names are found with different authors (see also Sec. 3B here).

19 L. van Hove, Physica **21**, 517 (1955); **23**, 441 (1957).

20 I. Prigogine and P. Résibois, Physica **27**, 629 (1961).

21 R. Balescu, *Statistical Mechanics of Charged Particles* (Interscience, New York, 1963).

22 R. W. Zwanzig in *Lectures in Theoretical Physics*, edited by W. E. Britten, B. W. Downs, and J. Downs (Interscience, New York, 1961), Vol. III, p. 113.

23 S. Fujitta, in *Statistical Physics, Vol. 3* edited by N. Ranganathan, H. Leff, and H. Wheeler (Benjamin, New York, 1963), p. 219.

24 L. van Hove, in *La théorie des gaz neutres et ionizés*, edited by C. de Witt and J. F. Detoeuf (Hermann, Paris, 1960), p. 149.

25 For macroscopic variables a master equation can be obtained by integration over the proper range of quantum states. The connection with the phenomenological equation was first shown by N. G. van Kampen, Physica **23**, 707 (1957).

26 G. Severne, Physica **30**, 1365 (1964).

27 B. Leaf and W. C. Schieve, Physica **36**, 589 (1967).

28 K. M. van Vliet, J. Math. Physics **12**, 1998 (1971).

29 *Remarks on notation.* We employ matrix operations for vectors in $\mathcal{S}^s$, rather than tensor calculus, as is more customary in abstract vector spaces. Thus dyadic operators are square matrices and are printed sans serif. Greek lowercase symbols refer to elements in $\mathfrak{K}$ and are column matrices $\alpha(y,t) = \{\alpha^1(y,t),\cdots,\alpha^s(y,t)\}$. The adjoint elements are row matrices $\alpha^\dagger(y,t) = (\alpha^{1*}(y,t),\cdots,\alpha^{s*}(y,t))$. In what follows we also introduce the tensor product space $\mathfrak{K}\otimes\mathfrak{K}$, whose elements are written in Greek capitals. Notice that no Greek symbols are printed boldface even though one symbol represents many variables. Latin symbols are used in the ordinary vector space $\mathfrak{R}^3$, vectors being boldface ($\mathbf{r}$) and tensors being boldface italic ($\boldsymbol{D}$).

30 The tilde is used for adjoint transformations of $\mathfrak{K}$, rather than the dagger; the latter, super†, is reserved to denote Hermitian conjugation of matrices in $\mathcal{S}^s$, whereas super$^{\mathrm{tr}}$ denotes transposition of matrices in $\mathcal{S}^s$.

31 Reference 16, Sec. 7.5.

32 In (2.1) we take the scalar product with $\tilde{g}_\nu(y,t')$ from the right and in (2.8′) we take the scalar product with $\alpha(y,t')$ from the left; then we subtract, integrate from 0 to $t_1 = t' + 0$, and apply (2.5) and (2.9′).

33 F. Riesz and B. Sz. Nagy, *Leçons d'analyse fonctionnelle* (Gauthier-Villars, Paris, 1965), 4th ed., in particular, Secs. 132, 147, and 148.

34 It is to be remembered that Λ is not generally Hermitian, though we assume that sufficient conditions for (2.12) apply, e.g., $\Lambda\tilde{\Lambda} = \tilde{\Lambda}\Lambda$. The φ's are generally not orthogonal, but we have biorthogonality, $(\varphi_k,\psi_l) = \delta_{kl}$. In Dirac notation, with $(\xi,\eta) \to \langle\eta|\xi\rangle$, we can write $\mathsf{P}_k = |\varphi_k\rangle\langle\psi_k|$.

35 For $-t < u \le 0$ the integral over ds'' can still be nonvanishing, but then the range of integration over s' must be restricted to $s' < t + u$. Or, with $u' < u \le 0$, the range for s' is $0 \le s' \le t + u'$. Carrying out the integrations in Eq. (2.22), we arrive directly at the result (2.24b).

36 K. M. van Vliet and J. Blok, Physica **32**, 231 (1956). The form (3.1) was first obtained for coupled harmonic oscillators in Ref. 3.

37 The importance of (3.5) and (3.7) lies in the fact that solely from the properties of the operator Λ itself (i.e., from its eigenvalues and projectors) one can judge whether the process has the simplicity of a thermal equilibrium process.

38 M. S. Green, Physica **24**, 393 (1958).

39 See Ref. 14, p. 329.

40 R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1953), Vol. I, p. 118.

41 See Ref. 40, p. 356.

42 L. Onsager, Phys. Rev. **37**, 405 (1931); **38**, 2265 (1931).

43 Reference 21, pp. 22–26.

44 See, e.g., A. Papoulis, *Probability, Random Variables, and Stochastic Processes* (McGraw-Hill, New York, 1965), pp. 33ff.

45 We need precisely the convolution form as stated in I. Sneddon, *Fourier Transforms* (McGraw-Hill, New York, 1951), p. 31, Eq. (70).

46 Diffusion fluctuations in PN junctions offer an example, studied by M. L. Tarng, Ph.D. Thesis (University of Minnesota, 1969).

47 We use the standard symbols A and B, thereby deviating

from our convention (see Ref. 29).

[48] The first term of (8.3) is found when the functional integral is sampled at $y' = y_1, y = y_2$, whereas the second term results when $y = y_1, y' = y_2$. The third term occurs when we sample over the function space at $y = y' = y_2$; we are then left with the integral $\iint\delta(y - y_2)\delta(y' - y_2)Q^p(\gamma_1, \gamma_2)dy_1 dy_2 = \delta(y - y') \int Q^p(y_1, y)dy_1$; likewise for the fourth term.

[49] L. Tisza and I. Manning, Phys. Rev. **105**, 1695 (1957).

[50] N. Wiener, *The Fourier Integral and Certain of Its Applications* (Cambridge U.P., New York, 1933).

[51] Though in Eq. (2.13) each term is of negative exponential order, this holds not necessarily for the sum or integral, as is shown by the example in Eq. (B1).

[52] Reference 33, p. 290ff.

[53] G. Doetsch, *Handbuch der Laplace Transformation* (Birkhauser, Basel, 1956), Chap. 12, Sec. 2, Satz 1.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Markov Approach to Density Fluctuations Due to Transport and Scattering. II. Applications*

K. M. van Vliet
Centre de Recherches Mathématiques. Université de Montréal, Montréal, Canada.
(Received 5 October 1970)

Applications of a macroscopic and microscopic nature are given of the Markov formalism, developed in the previous paper, for finding the pair-correlation function, two-point covariance function, and spectral intensities from the phenomenological transport equations, transitions, and scattering. As macroscopic examples, we discuss Rayleigh diffusion, Coulomb correlations, and space-charge-limited flow in solids. The diffusion equation is shown to be not strictly Markovian, though correct Langevin diffusion sources are easily found. Dielectric relaxation is shown to be a macroscopic manifestation of Coulomb correlations in a plasma. The Λ theorem of the previous paper yields for the pair-correlation functions the original Debye–Hückel result plus a δ term. The spectra for space-charge-limited flow due to single-carrier injection are treated with the Green's-function procedure. The discrepancies between existing theories are removed since the Coulomb correlations in the steady state are shown to be not of the Debye–Hückel type. As microscopic applications, we consider ideal gases in the presence of streaming due to fields, an extension of Lax's work. The connection with the BBGK two-point equations for one- and two-body collisions is established. Finally, we integrate over the stochastic Boltzmann equation to obtain stochastic hydrodynamic equations. These provide a microscopic basis is for the noise sources associated with electrical conduction, heat conduction, and with the Navier-Stokes equation. Results for the hot-electron Boltzmann gas are compared with those of Price.

1. INTRODUCTION AND SUMMARY OF RESULTS

In the preceding paper[1] (referred to as I) a general formalism was presented for finding the covariance functions and associated spectral intensities of fluctuations in densities, $n^p(y, t)$. The formalism is applicable to fluctuations $\alpha^p \equiv n^p(y, t) - \langle n^p(y, t)\rangle$ around a steady state, characterized by a linear-(ized) set of kinetic equations for the regression to the steady state, of the type $\sum_q (\partial/\partial t + \Lambda^{pq})\alpha^q(y, t) = \xi^p(y, t)$, where the ξ's are source functions in the sense of Langevin, and where Λ is the phenomenological transport operator. The kinetic equations may refer to ordinary transport in position space, i.e., $y = \mathbf{r}$; then p characterizes the various macroscopic densities of interest in a given system. On the other hand, the kinetic equations may be of a microscopic nature and refer to streaming and collision processes in the phase space or its quantum equivalent, i.e., $y = \{\mathbf{v}, \mathbf{r}\}$ or $\{\mathbf{k}, \mathbf{r}\}$; then p refers to the species (e.g., ions and electrons in a plasma) or to discrete quantization of the occupation number states (e.g., band index of Bloch electrons in a solid).

We used a Markovian approach for these processes, based on a generalized Langevin description ("second Brownian motion").

We restate the main definitions and some results of I:

$$F_2^{pq}(y, y') \equiv \langle n^p(y, t)n^q(y', t)\rangle \tag{1.1a}$$

(density–density or pair-correlation functions);

$$\Gamma^{pq}(y, y') \equiv \langle \Delta n^p(y, t)\Delta n^q(y', t)\rangle \tag{1.1b}$$

(density–density or two-point covariance functions);

$$\Sigma^{pq}(y, y', \omega) = 2\int_{-\infty}^{\infty} \langle \Delta n^p(y, t)\Delta n^q(y', 0)\rangle e^{-i\omega t}\, dt \tag{1.2}$$

(spectral intensity functions);

$$\Xi^{pq}(y, y')\delta(t - t') = \langle \xi^p(y, t)\xi^q(y', t')\rangle \tag{1.3}$$

(Langevin source kernels).

For the two-point covariance functions we derived the Λ theorem [Eq. (I 2.30)]:

$$\Lambda_y\Gamma(y, y') + \Gamma(y, y')\Lambda^{tr}_{y'} = \Xi(y, y'), \tag{1.4}$$

where $\Gamma = [\Gamma^{pq}], \Lambda_y = [\Lambda_y^{pq}]$ is a matrix (integro)-differential operator with respect to y, and $\Xi = [\Xi^{pq}]$. In the microscopic case the transport operator consists of two distinct parts, *viz*. Λ_{str}, which expresses the effect of "streaming" due to ponderomotive forces, and Λ_{coll}, which expresses the effect of collisions caused by local forces. The microscopic version of the Λ theorem will only be considered for a one-component gas:

$$(\Lambda_{\text{str}} + \Lambda'_{\text{str}} + \Lambda_{\text{coll}} + \Lambda'_{\text{coll}})\,\Gamma(y, y') = \Xi(y, y'), \tag{1.4'}$$

where the super prime denotes operators acting on y'. The connection between the pair-correlation functions and the two-point covariance func-

from our convention (see Ref. 29).

[48] The first term of (8.3) is found when the functional integral is sampled at $y' = y_1, y = y_2$, whereas the second term results when $y = y_1, y' = y_2$. The third term occurs when we sample over the function space at $y = y' = y_2$; we are then left with the integral $\iint\delta(y - y_2)\delta(y' - y_2)Q^p(\gamma_1, \gamma_2)dy_1 dy_2 = \delta(y - y') \int Q^p(y_1, y)dy_1$; likewise for the fourth term.

[49] L. Tisza and I. Manning, Phys. Rev. **105**, 1695 (1957).

[50] N. Wiener, *The Fourier Integral and Certain of Its Applications* (Cambridge U.P., New York, 1933).

[51] Though in Eq. (2.13) each term is of negative exponential order, this holds not necessarily for the sum or integral, as is shown by the example in Eq. (B1).

[52] Reference 33, p. 290ff.

[53] G. Doetsch, *Handbuch der Laplace Transformation* (Birkhauser, Basel, 1956), Chap. 12, Sec. 2, Satz 1.

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Markov Approach to Density Fluctuations Due to Transport and Scattering. II. Applications*

K. M. van Vliet
Centre de Recherches Mathématiques. Université de Montréal, Montréal, Canada.
(Received 5 October 1970)

Applications of a macroscopic and microscopic nature are given of the Markov formalism, developed in the previous paper, for finding the pair-correlation function, two-point covariance function, and spectral intensities from the phenomenological transport equations, transitions, and scattering. As macroscopic examples, we discuss Rayleigh diffusion, Coulomb correlations, and space-charge-limited flow in solids. The diffusion equation is shown to be not strictly Markovian, though correct Langevin diffusion sources are easily found. Dielectric relaxation is shown to be a macroscopic manifestation of Coulomb correlations in a plasma. The Λ theorem of the previous paper yields for the pair-correlation functions the original Debye–Hückel result plus a δ term. The spectra for space-charge-limited flow due to single-carrier injection are treated with the Green's-function procedure. The discrepancies between existing theories are removed since the Coulomb correlations in the steady state are shown to be not of the Debye–Hückel type. As microscopic applications, we consider ideal gases in the presence of streaming due to fields, an extension of Lax's work. The connection with the BBGK two-point equations for one- and two-body collisions is established. Finally, we integrate over the stochastic Boltzmann equation to obtain stochastic hydrodynamic equations. These provide a microscopic basis is for the noise sources associated with electrical conduction, heat conduction, and with the Navier-Stokes equation. Results for the hot-electron Boltzmann gas are compared with those of Price.

1. INTRODUCTION AND SUMMARY OF RESULTS

In the preceding paper[1] (referred to as I) a general formalism was presented for finding the covariance functions and associated spectral intensities of fluctuations in densities, $n^p(y, t)$. The formalism is applicable to fluctuations $\alpha^p \equiv n^p(y, t) - \langle n^p(y, t)\rangle$ around a steady state, characterized by a linear-(ized) set of kinetic equations for the regression to the steady state, of the type $\sum_q (\partial/\partial t + \Lambda^{pq})\alpha^q(y, t) = \xi^p(y, t)$, where the ξ's are source functions in the sense of Langevin, and where Λ is the phenomenological transport operator. The kinetic equations may refer to ordinary transport in position space, i.e., $y = \mathbf{r}$; then p characterizes the various macroscopic densities of interest in a given system. On the other hand, the kinetic equations may be of a microscopic nature and refer to streaming and collision processes in the phase space or its quantum equivalent, i.e., $y = \{\mathbf{v}, \mathbf{r}\}$ or $\{\mathbf{k}, \mathbf{r}\}$; then p refers to the species (e.g., ions and electrons in a plasma) or to discrete quantization of the occupation number states (e.g., band index of Bloch electrons in a solid).

We used a Markovian approach for these processes, based on a generalized Langevin description ("second Brownian motion").

We restate the main definitions and some results of I:

$$F_2^{pq}(y, y') \equiv \langle n^p(y, t)n^q(y', t)\rangle \tag{1.1a}$$

(density–density or pair-correlation functions);

$$\Gamma^{pq}(y, y') \equiv \langle \Delta n^p(y, t)\Delta n^q(y', t)\rangle \tag{1.1b}$$

(density–density or two-point covariance functions);

$$\Sigma^{pq}(y, y', \omega) = 2\int_{-\infty}^{\infty} \langle \Delta n^p(y, t)\Delta n^q(y', 0)\rangle e^{-i\omega t}\, dt \tag{1.2}$$

(spectral intensity functions);

$$\Xi^{pq}(y, y')\delta(t - t') = \langle \xi^p(y, t)\xi^q(y', t')\rangle \tag{1.3}$$

(Langevin source kernels).

For the two-point covariance functions we derived the Λ theorem [Eq. (I 2.30)]:

$$\Lambda_y\Gamma(y, y') + \Gamma(y, y')\Lambda^{tr}_{y'} = \Xi(y, y'), \tag{1.4}$$

where $\Gamma = [\Gamma^{pq}], \Lambda_y = [\Lambda_y^{pq}]$ is a matrix (integro)-differential operator with respect to y, and $\Xi = [\Xi^{pq}]$. In the microscopic case the transport operator consists of two distinct parts, *viz*. Λ_{str}, which expresses the effect of "streaming" due to ponderomotive forces, and Λ_{coll}, which expresses the effect of collisions caused by local forces. The microscopic version of the Λ theorem will only be considered for a one-component gas:

$$(\Lambda_{\text{str}} + \Lambda'_{\text{str}} + \Lambda_{\text{coll}} + \Lambda'_{\text{coll}})\,\Gamma(y, y') = \Xi(y, y'), \tag{1.4'}$$

where the super prime denotes operators acting on y'. The connection between the pair-correlation functions and the two-point covariance func-

tions is standard [Eq. (I 3.11)]. The connection between Γ and the two-point distribution function f_2 of the Liouville equation is given by [Eq. (I 3.13)]:

$$\Gamma^{pq}(y, y') = f_2^{pq}(y, y') - f_1^p(y) f_1^q(y') + \delta^{pq} f_1^p(y)\delta(y - y'), \tag{1.5}$$

where $f_1^p(y) \equiv \langle n^p(y, t)\rangle$.

For the spectral intensities, a variety of expressions were derived, the most important ones being

$$\Sigma(y, y', \omega) = 2G_y(i\omega)\Gamma(y, y') + hcj, \tag{1.6a}$$

$$\Sigma(y, y', \omega) = 2G_y(i\omega)\Xi(y, y')G^{tr}_{y'}(-i\omega). \tag{1.6b}$$

The first relation expresses Σ in the resolvent G of Λ and the covariance functions Γ, and the second one expresses Σ directly in terms of the source functions Ξ. Again, these are matrix expressions, i.e., $\Sigma = [\Sigma^{pq}]$. The abbreviation *hcj* denotes the Hermitean conjugate of the form given at the right-hand-side (rhs); i.e., it replaces $p \to q$, $y \to y'$, $i\omega \to -i\omega$. The above expressions are incomplete in some cases (cf. I, Secs. 3 and 5).

Various transition and collision processes were considered, and the corresponding generalized first-order and second-order Fokker–Planck (FP) moments, denoted as $[A^p]$ and $[B^{pq}]$ were computed in I, Sec. 8. The main connections with the Langevin and phenomenological equations were obtained in I, Sec. 7; thus, the phenomenological equations can be expressed as [Eq. (I 7.6′)]

$$\frac{\partial}{\partial t}\langle \Delta \mathbf{n}(y, t)\rangle_{cond} + \Lambda_{str}\langle \Delta \mathbf{n}(y, t)\rangle_{cond} = -\Lambda_{coll}\langle \Delta \mathbf{n}(y, t)\rangle_{cond} = \langle A_y[\mathbf{n}]\rangle_{cond'}, \tag{1.7}$$

and the connection with the Langevin kernels is [Eq. (I 7.9)]

$$\Xi(y\, y') = B_{y y'}[\langle \mathbf{n}\rangle] \equiv B^0_{y y'}. \tag{1.8}$$

In the present paper we consider macroscopic applications (Secs. 2–4), as well as microscopic applications (Secs. 5–8) of the foregoing formalism. We shall then be interested in specific forms of the FP moments A^p and B^{pq} and the operators Λ^{pq}. Solutions for Γ and Σ will be obtained for some of these applications, while for others the implications, of the above relations will be discussed.

In Sec. 2 the simple example of macroscopic diffusion is treated. The phenomenological equation is derived from an elementary random-walk procedure which actually goes back to Lord Rayleigh (Ref. 2). The diffusion equation is found to be valid only on a sufficiently coarse scale, which is not surprising in view of earlier studies on Brownian motion by Chandrasekhar and Einstein (see Ref. 3). Thus, a diffusion process is only approximately Markovian. The density–density correlation function in this picture is a simple δ function with Poisonian strength [Eq. (2.11)]. The diffusion source function, however, is correctly found from this simple model [Eq. (2.9)]. This source is of fundamental importance in many macroscopic problems. [It has a peculiar singularity, $\nabla\nabla'[\delta(\mathbf{r} - \mathbf{r}')\langle n(\mathbf{r})\rangle]$, which is explained in the microscopic treatment.] These results remain valid when drift is added, being still exact in thermal equilibrium, and approximately exact in the steady state.

In Sec. 3 we prove the equivalence between dielectric relaxation and the Debye–Hückel theory for Coulomb interaction. Since the latter is based on an average "molecular field," it is clear that a macroscopic reasoning must be applicable. In fact, all that we require are the equations for dielectric relaxation for excess space charge, together with the source (2.9). The complete Debye–Hückel result for a plasma with several kinds of ions is recovered [Eq. (3.13)]. The temperature, prevalent in the statistical-mechanical derivation, enters the result only via the Einstein relation between mobility and diffusivity. Moreover, our result for Γ includes automatically the dimensional singularity for $\mathbf{r} \to \mathbf{r}'$, absent in the original Debye–Hückel procedure.

Section 4 deals with a more device-oriented example, *viz.* fluctuations in space-charge-limited flow in solids, due to single-carrier injection. In this case, there is a net space charge and the current-voltage characteristic is quadratic, as expressed in the standard articles by Lampert and Rose and others. The Λ theorem for the density–density correlation function is complex and is *not* satisfied by the Debye–Hückel function, as assumed by various authors. We have not yet succeeded in solving this integro partial differential equation; however a corresponding theorem for the voltage–voltage correlation function is easily derived and approximately solved. For the spectral intensity of the open-voltage fluctuations we obtain double thermal noise, as was found by others using more elementary techniques.

In Sec. 5 we consider the solutions of the microscopic Λ theorem and the spectral intensity for ideal gases. This is an extension of an earlier treatment by Lax (cf. Ref. 17), in which we incorporate streaming terms stemming from external fields.

In Sec. 6 the microscopic Λ theorem is considered in detail for the Boltzmann gas with one- and two-body collisions. Using relation (1.5), the Λ theorem is converted to a theorem for the two-point distribution function f_2. The resulting equations are compared with results for f_2 from the BBGKY hierarchy.

Finally, in the last two sections we make the connection between the microscopic and the macroscopic results, by starting from a stochastic Boltzmann equation, and integrating over the velocity or $\mathbf{k}$-space variables. However, this procedure takes a rather unexpected turn and is not straight-

forward. When we multiply the stochastic Boltzmann equation with certain functions $\Psi(\mathbf{k},\mathbf{r})$ which are conserved in a scattering process (collisional invariants) and integrate over $\mathbf{k}$ space, both the collision integral and the stochastic source functions vanish from the result. Hence, the conservation theorems have instantaneous validity, as is shown in Sec. 7. The stochastic nature of these theorems shows up, however, in the flow averages, such as the particle current, heat current, pressure tensor, etc. The noise sources of these quantities are easily expressed in the microscopic two-point covariance function; stochastic hydrodynamic equations, which confirm our previous macroscopic transport equations, are derived [Eq. (7.15) for charge transport, Eq. (7.18) for momentum transport, Eq. (7.21) for heat conduction]. The various noise sources must be expressible in the transport coefficients, which for the equilibrium case is born out by the dissipation-fluctuation theorem. In the steady state new microscopic results can be expected. As an example, we compute the current fluctuations for hot electrons in Sec. 8. Comparing our results [Eqs. (8.10) and (8.11)] with those of Price, we notice that Price's method tacitly assumes that the electrons are independent; i.e., that the covariance function is a δ function, a result which is not substantiated by the exact solution of the Λ theorem in several cases (two-carrier collisions, space-charge forces). Price's Kubo-like expressions [Eqs. (8.10′) and (8.11′)] are shown to be ambiguous for the nonequilibrium steady state.

I. MACROSCOPIC APPLICATIONS

2. RAYLEIGH DIFFUSION

Our procedure is perhaps best illustrated by the simple macroscopic example in which deviations from the steady-state density $\langle n(\mathbf{r})\rangle$ of a one-component gas are governed by diffusion. That is, we consider diffusion of the *fluctuations* $\Delta n(\mathbf{r})$. The steady state itself may be nonhomogenous and be maintained by a steady particle flow $\mathbf{J}$ involving drift and diffusion [see Eq. (2.12) below] or thermal equilibrium may prevail in which case $\mathbf{J}=0$.

The simplest model of diffusion was given by Lord Rayleigh in 1899.[2] It involves scattering in position space over distances $\mathbf{a}_i$, and as such is well applicable to ionic diffusion. To apply it to electronic or heat diffusion, one must stretch his imagination and compare $|\mathbf{a}|$ to the mean free path. Let $Q(\mathbf{r},\mathbf{r}')\,d^3r d^3r'$ be the rate of scattering from $\mathbf{r}$ (within d^3r) to $\mathbf{r}'$ within d^3r'). Let further f_i be the probability for scattering per second over a lattice distance $\pm\mathbf{a}_i$ (we assume equal probabilities for forward or backward scattering). Then we obtain

$$Q(\mathbf{r},\mathbf{r}') = n(\mathbf{r})\sum_i f_i[\delta(\mathbf{r}-\mathbf{r}'-\mathbf{a}_i)+\delta(\mathbf{r}-\mathbf{r}'+\mathbf{a}_i)]. \tag{2.1}$$

For the first-order FP moment we find from Eq. (I 8.2)

$$A_{\mathbf{r}} = \sum_i f_i[n(\mathbf{r}+\mathbf{a}_i)+n(\mathbf{r}-\mathbf{a}_i)-2n(\mathbf{r})]; \tag{2.2}$$

likewise, for the second-order FP moment, using Eq. (I 8.3)

$$B_{\mathbf{r}\mathbf{r}'} = -\sum_i f_i\{[n(\mathbf{r})+n(\mathbf{r}')][\delta(\mathbf{r}-\mathbf{r}'-\mathbf{a}_i)+\delta(\mathbf{r}-\mathbf{r}'+\mathbf{a}_i)]-\delta(\mathbf{r}-\mathbf{r}')\times[n(\mathbf{r}+\mathbf{a}_i)+n(r-\mathbf{a}_i)+2n(\mathbf{r})]\}. \tag{2.3}$$

The macroscopic diffusion equation is recovered for lengths $\gg|a_i|$, so that by expansion of (2.2), we obtain

$$A_{\mathbf{r}} \approx \sum_i f_i\,\nabla\nabla n(\mathbf{r}):\mathbf{a}_i\mathbf{a}_i \equiv \boldsymbol{D}:\nabla\nabla n(\mathbf{r}), \tag{2.4}$$

with the diffusion tensor defined as

$$\boldsymbol{D} = \sum_i f_i\mathbf{a}_i\mathbf{a}_i. \tag{2.5}$$

Clearly, the diffusion equation is only an approximation to a Markovian process. This is not surprising, since it is known since the early studies of Brownian motion that fluctuations in position coordinates only defy the construction of an exact FP equation,[3] so that an exact Markovian master description is certainly out of question.

The second-order FP moment remains in the form of a distribution. Its action on any function is obtained by formally expanding the δ function up to second order. In addition we expand $n(\mathbf{r}\pm\mathbf{a}_i)$ and use the rules

$$n(\mathbf{r}')\nabla\delta(\mathbf{r}-\mathbf{r}') = n(\mathbf{r})\nabla\delta(\mathbf{r}-\mathbf{r}')+[\nabla n(\mathbf{r})]\delta(\mathbf{r}-\mathbf{r}'), \tag{2.6a}$$

$$n(\mathbf{r}')\nabla\nabla\,\delta(\mathbf{r}-\mathbf{r}') = n(\mathbf{r})\nabla\nabla\,\delta(\mathbf{r}-\mathbf{r}') + 2[\nabla n(\mathbf{r})]\nabla\delta(\mathbf{r}-\mathbf{r}')+[\nabla\nabla n(\mathbf{r})]\delta(\mathbf{r}-\mathbf{r}'), \tag{2.6b}$$

$$\nabla\delta(\mathbf{r}-\mathbf{r}') = -\nabla'\delta(\mathbf{r}-\mathbf{r}'), \tag{2.6c}$$

(where ∇' refers to the gradient with respect to $\mathbf{r}'$). We now obtain

$$B_{\mathbf{r}\mathbf{r}'} \approx 2\boldsymbol{D}:\nabla\nabla'[n(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')]. \tag{2.7}$$

For an isotropic case $\boldsymbol{D}=D\boldsymbol{I}$, with $\boldsymbol{I}$ being the unit tensor. If drift is added, the phenomenological equation, Eq. (1.7), becomes

$$\frac{\partial\langle\Delta n\rangle_{\text{cond}}}{\partial t}+\mathbf{v}_d\cdot\nabla\langle\Delta n\rangle_{\text{cond}} = D\nabla^2\langle\Delta n\rangle_{\text{cond}}, \tag{2.8}$$

but the source Ξ [Eq. (1.8)] is unaffected:

$$\Xi(\mathbf{r},\mathbf{r}') = 2D\nabla\cdot\nabla'[\langle n(\mathbf{r})\rangle\delta(\mathbf{r}-\mathbf{r}')]. \tag{2.9}$$

This is the source function originally suggested by van der Ziel.[4]

The Λ theorem (1.4) requires the solution of

$$[\mathbf{v}_d\cdot\nabla+\mathbf{v}_d\cdot\nabla'-\boldsymbol{D}:\nabla\nabla-\boldsymbol{D}:\nabla'\nabla']\Gamma(\mathbf{r},\mathbf{r}') = 2\boldsymbol{D}:\nabla\nabla'[\langle n(\mathbf{r})\rangle\delta(\mathbf{r}-\mathbf{r}')]. \tag{2.10}$$

By inspection we see that a solution with the required symmetry is

$$\Gamma(\mathbf{r}, \mathbf{r}') = \langle n(\mathbf{r})\rangle \delta(\mathbf{r} - \mathbf{r}'), \tag{2.11}$$

provided

$$[\mathbf{v}_d \cdot \nabla - D : \nabla\nabla]\langle n(r)\rangle = 0. \tag{2.12}$$

The latter condition means $\nabla \cdot \langle \mathbf{J}(\mathbf{r})\rangle = 0$, where $\mathbf{J}$ is the current density. Clearly, (2.12) is satisfied in thermal equilibrium ($\mathbf{J} = 0$) or in the steady state of an election gas when displacement current is negligible.

The diffusion source is derived here for a crude model involving macroscopic scattering, $\mathbf{r} \rightarrow \mathbf{r}'$. In a microscopic picture *the scattering is in* k *space,* $\mathbf{k} \rightarrow \mathbf{k}'$, *with no change in position.* The first-order FP moment is found to yield the collision integral of the Boltzmann equation. Curiously, when the sources are incorporated into this equation and an integration over k space is carried out, the source density (2.9) is recovered for $\omega\tau_{\text{coll}} \ll 1$, appearing this time in conjunction with flow averages such as the current and the viscous pressure tensor; we consider this in Sec. 7.

Ambipolar diffusion, involving two coupled diffusion equations with the assumption of quasi-neutrality (i.e., near-zero dielectric relaxation time) can be treated likewise. As an extension of the source function (2.9), one obtains

$$\Xi_{\text{amb diff}}(\mathbf{r}, \mathbf{r}') = 2\nabla \cdot \nabla'[D_a(\mathbf{r}) \frac{n_0(\mathbf{r})p_0(\mathbf{r})}{n_0(\mathbf{r}) + p_0(\mathbf{r})} \times \delta(\mathbf{r} - \mathbf{r}')]. \tag{2.13}$$

where $D_a(\mathbf{r})$ is the ambipolar diffusivity, and where the subscript zero denotes average values.[5]

3. DIELECTRIC RELAXATION, EQUIVALENCE WITH THE DEBYE–HÜCKEL THEORY

The Debye–Hückel theory for density correlations caused by Coulomb interaction is essentially a "molecular field" theory. In the original theory this is clear since an average potential $\Phi(\mathbf{r})$ is assigned to the collection of charges surrounding a given ion.[6] In the more sophisticated approach of Landau and Lifshitz,[7] Bogolyubov's two-point equation is solved; this equation follows from the canonical ensemble with *a priori* integration over the velocity space, so that again exact dynamical effects are excluded. We can therefore expect that the same correlations can be found entirely macroscopically, by use of the simple equations for current flow in the presence of space charge, i.e., dielectric relaxation.

We consider a plasma of ionized gases (or electrons and holes), which is neutral on the average $\Sigma\langle n^p\rangle q^p = 0$. Here n^p is the density and q^p the charge of ions of species p. For the currents we write

$$\frac{\partial n^p}{\partial t} + \frac{1}{q^p} \operatorname{div}\mathbf{J}^p = 0, \tag{3.1}$$

$$\mathbf{J}^p = \mu^p n^p q^p \mathbf{E} - q^p D^p \operatorname{grad} n^p + q^p \boldsymbol{\eta}(\mathbf{r}, t), \tag{3.2}$$

where $\boldsymbol{\eta}(\mathbf{r}, t)$ is a source term.

The second equation is substituted into the first one and linearized in Δn^p and $\Delta\mathbf{E}$. We assume (near) equilibrium, with $\langle \mathbf{E}\rangle \approx 0, \langle \nabla n^p\rangle \approx 0$. By Poisson's equation the fluctuations in the field and the ion densities are related:

$$\nabla \cdot \Delta\mathbf{E} = \sum_s q^s \Delta n^s / \epsilon\epsilon_0. \tag{3.3}$$

The result is

$$\frac{\partial \Delta n^p}{\partial t} - D^p \nabla^2 \Delta n^p + \sum_s \frac{q^s}{q^p} \frac{\Delta n^s}{\tau_\Omega^p} = \nabla \cdot \boldsymbol{\eta}(\mathbf{r}, t) \equiv \xi^p(\mathbf{r}, t), \tag{3.4}$$

where $\tau_\Omega^p = \epsilon\epsilon_0/\mu^p n_0^p q^p$ is the dielectric relaxation time due to charges q^p and where $n_0^p \equiv \langle n^p\rangle$. The operator matrix Λ is

$$\Lambda^{pp'} = -\delta^{pp'} D^p \nabla^2 + (q^{p'}/q^p)(1/\tau_\Omega^p). \tag{3.5}$$

Using the Einstein relation, we write alternately[8]

$$\Lambda^{pp'} = -\delta^{pp'} D^p \nabla^2 + q^p q^{p'} D^p n_0^p / kT\epsilon\epsilon_0. \tag{3.5'}$$

The density correlations satisfy the Λ theorem, with the source function (2.9)

$$\sum_s [\Lambda_{\mathbf{r}}^{ps} \Gamma^{sq}(\mathbf{r}, \mathbf{r}') + \Lambda_{\mathbf{r}'}^{qs} \Gamma^{ps}(\mathbf{r}, \mathbf{r}')] = 2D^p \nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{r}'} [n_0^p(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}')]\delta^{pq}. \tag{3.6}$$

We make the ansatz

$$\Gamma^{pq} = n_0^p(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}')\delta^{pq} + \hat{\Gamma}^{pq}. \tag{3.7}$$

With this substituted into (3.6), the resulting equation for $\hat{\Gamma}^{pq}$ is

$$\sum_s \left[\Lambda_{\mathbf{r}}^{ps} \hat{\Gamma}^{sq}(\mathbf{r}, \mathbf{r}') + \Lambda_{\mathbf{r}'}^{qs} \hat{\Gamma}^{ps}(\mathbf{r}, \mathbf{r}')\right] = -\left[\left(\frac{D^p D^q}{kT\epsilon\epsilon_0}\right) q^p q^q n_0^p(\mathbf{r}) n_0^q(\mathbf{r}) - \delta^{pq} D^p \nabla^2 n_0^p(\mathbf{r})\right] \times \delta(\mathbf{r} - \mathbf{r}'). \tag{3.8}$$

This set is only solved easily in thermal equilibrium, i.e., when n_0^p and n_0^q do not depend on position. We write then further:

$$\hat{\Gamma}^{pq} = n_0^p n_0^q q^p q^q \omega(\mathbf{r}, \mathbf{r}'). \tag{3.9}$$

The set (3.8) is then satisfied identically if

$$\nabla^2\omega - \varkappa^2\omega = \nabla'^2\omega - \varkappa^2\omega = [\varkappa^2/\textstyle\sum_s n_0^s (q^s)^2]\delta(\mathbf{r} - \mathbf{r}'), \tag{3.10}$$

where $\varkappa^{-1}$ is the Debye length defined by

$$\varkappa^2 = \textstyle\sum_s n_0^s (q^s)^2 / kT\epsilon\epsilon_0. \tag{3.11}$$

Equation (3.10) is the defining equation for the Helmholtz Green's function. The result is

$$\omega(\mathbf{r},\mathbf{r}') = -\frac{\varkappa^2}{\sum n_0^s (q^s)^2}\,\frac{e^{-\varkappa|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\quad . \tag{3.12}$$

The full set of covariance functions is found to be

$$\Gamma^{pq}(\mathbf{r},\mathbf{r}') \equiv \langle \Delta n^p(\mathbf{r})\Delta n^q(\mathbf{r}')\rangle = n_0^p(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\delta^{pq} - \frac{n_0^p n_0^q q^p q^q}{\sum n_0^s (q^s)^2}\,\frac{\varkappa^2 e^{-\varkappa|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\,. \tag{3.13}$$

For electrons and holes in semiconductors we find the Coulomb correlations in the form given by Lax and Mengert[9]:

$$\langle \Delta n(\mathbf{r})\Delta n(\mathbf{r}')\rangle = n_0\delta(\mathbf{r}-\mathbf{r}') - [n_0^2/(n_0+p_0)] \times D(\mathbf{r}-\mathbf{r}'), \tag{3.14a}$$

$$\langle \Delta p(r)\Delta p(\mathbf{r}')\rangle = p_0\delta(\mathbf{r}-\mathbf{r}') - [p_0^2/(n_0+p_0)] \times D(\mathbf{r}-\mathbf{r}'), \tag{3.14b}$$

$$\langle \Delta n(\mathbf{r})\Delta p(\mathbf{r})\rangle = [n_0 p_0/(n_0+p_0)]D(\mathbf{r}-\mathbf{r}'), \tag{3.14c}$$

where D is the Helmholtz factor of (3.13). For $\varkappa\to\infty$, $D(\mathbf{r})\to\delta(\mathbf{r})$. The expressions (3.14) then reduce to $[n_0p_0/(n_0+p_0)]\delta(\mathbf{r}-\mathbf{r}')$, which is the standard result for a system of *constrained* charges without interaction. The charge constraint follows indeed from (3.3) if $\nabla\cdot\Delta\mathbf{E}\to 0$.

Equation (3.13) is the standard result, *including the dimensional singularity for* $\mathbf{r}-\mathbf{r}'$, the origin of which was discussed in I, Sec. 3B. The method presented here is entirely a nonequilibrium method; the factor kT enters only into the result via the Einstein relation. We have not *a priori* used the equality of both parts of the Λ theorem, Eq. (I 5.6), in order to see where nonequilibrium effects would come in. Close to equilibrium, the neglect of the term with $\langle\nabla n^p\rangle$ in (3.4) is still reasonable, so (3.8) follows. The solution (3.13) still has approximate validity, with $n_0^p(\mathbf{r})$ being the local value. Far from equilibrium, the operator Λ of (3.5) must be amended with a field term and correlations of hydrodynamic range occur (cf. I, Sec. 5, last paragraph). Some steady-state solutions of the Λ theorem have been obtained.[10]

Generally, the results are quite complex. For another example, see the next section.

In connection with the next section we still mention the one-dimensional infinite-domain solution of (3.10): $\omega\propto D(x-x')$, with

$$D(x) = \tfrac{1}{2}\varkappa e^{-\varkappa|x|}. \tag{3.15}$$

The formulae (3.14) are changed correspondingly.

4. FLUCTUATIONS IN SPACE-CHARGE-LIMITED FLOW

The spectra for fluctuations in space-charge-limited currents due to injection of either electrons or holes (single injection) were derived by van der Ziel and van Vliet[11] via the Fourier method and the spectra of the sources [this method is in principle similar to that of Eq. (I 6.8)], and by Sergescu and Friedman[12] via the Green's-function method of van Vliet and Fassett[13] [which is equivalent to using Eq. (I 6.5)]. The results of both theories are quite different and have little in common in appearance. According to I, Sec. 6 the two methods must be equivalent, however. The discrepancy is due to the fact that the method of Ref. 13 is incomplete, unless the covariance function is obtained consistently from the same equations, i.e., from the Λ theorem. Sergescu and Friedman assume *ad hoc* that the correlations are of the Debye–Hückel type [Eq. (3.15), which is incorrect], as we show presently

The equations for single injection (of electrons) are

$$\frac{\partial n}{\partial t} = \frac{1}{e}\,\nabla\cdot\mathbf{J}, \tag{4.1}$$

$$\mathbf{J} = e\,\mu n\mathbf{E} + eD\,\nabla n + e\eta(\mathbf{r},t), \tag{4.2}$$

$$\nabla\cdot\mathbf{E} = -\,en/\epsilon\epsilon_0. \tag{4.3}$$

The last equation relates now the average space charge (which is not zero as in the preceding section) as well as the fluctuations to the self-consistent field. Substituting (4.3) and (4.2) into (4.1) we have the transport equation

$$\frac{\partial n}{\partial t} + \frac{en^2\mu}{\epsilon\epsilon_0}\,\nabla\cdot\mathbf{E} - \mu\mathbf{E}\cdot\nabla n - D\nabla^2 n = \nabla\cdot\eta(\mathbf{r},t) \equiv \xi(\mathbf{r},t). \tag{4.4}$$

Linearizing, $n = n_0 + n_1$, $\mathbf{E} = \mathbf{E}_0 + \mathbf{E}_1$, we have

$$\frac{\partial n_1}{\partial t} + \frac{2\mu e n_0 n_1}{\epsilon\epsilon_0} - \mu\,\mathbf{E}_1(n_1)\cdot\nabla n_0 - \mu\mathbf{E}_0\cdot\nabla n_1 - D\nabla^2 n_1 = \xi(\mathbf{r},t). \tag{4.5}$$

We confine ourselves further to a one-dimensional geometry. The approximate dc field solution is well known for that case (cf. Ref. 11).

We write $u = (x/l)^{1/2}$, where l is the length of the specimen, whereas the cross section will be taken to be unity:

$$V_0 \approx V_a(x/l)^{3/2} = V_a u^3, \tag{4.6a}$$

$$E_0 = -\nabla V_0 \approx \tfrac{3}{2}(V_a/l)u, \tag{4.6b}$$

$$n_0 = -(\epsilon\epsilon_0/e)\nabla\cdot E_0 \approx \tfrac{3}{4}(\epsilon\epsilon_0/e)(V_a/l^2)u^{-1}, \tag{4.6c}$$

$$\nabla n_0 \approx -\tfrac{3}{8}(\epsilon\epsilon_0/e)(V_a/l^3)u^{-3}, \tag{4.6d}$$

(V_a is the average voltage across the sample). We also introduce the standard symbols for the conductance, capacitance, and relaxation time:

$$g_0 = \tfrac{9}{4}\,\mu\,\epsilon\epsilon_0\,V_a/l^3, \tag{4.7a}$$

$$C_0 = \epsilon\epsilon_0/l, \tag{4.7b}$$

$$\tau = 3C_0/g_0 = 4l^2/3\mu V_a. \tag{4.7c}$$

Equation (4.5) now takes the form

$$\frac{\partial n_1}{\partial t} + \frac{2}{\tau}\frac{n_1}{u} - \frac{1}{\tau}\frac{1}{u^3}\int_0^u u' n_1(u')\,du' + \frac{1}{\tau}\frac{\partial n_1}{\partial u} - \frac{D}{4l^2}\frac{1}{u}\frac{\partial}{\partial u}\left(\frac{1}{u}\frac{\partial n_1}{\partial u}\right) = \xi(u,t). \quad (4.8)$$

For the operator Λ we have[14]

$$\Lambda = \frac{2}{\tau u} - \frac{1}{\tau u^3}\int_0^u u'du' + \frac{1}{\tau}\frac{\partial}{\partial u} - \frac{D}{4l^2}\left(\frac{1}{u}\frac{\partial}{\partial u}\right)^2. \quad (4.9)$$

The Λ theorem can now be applied. Using the source given by (2.9), we have

$$\Lambda_u\Gamma + \Lambda_{u'}\Gamma = \frac{D}{2l^2}\frac{1}{uu'}\frac{\partial^2}{\partial u\,\partial u'}\left(\frac{n_0(u)\delta(u-u')}{2lu}\right). \quad (4.10)$$

As was shown in other papers, the fluctuating voltage over a stretch $(0,x)$ is a better variable in these problems. The connection is

$$v_1 = \gamma\int_0^u u_1 du_1 \int_0^{u_1} u_2 n_1(u_2)du_2, \quad (4.11)$$

where $\gamma \equiv 4l^2e/\epsilon\epsilon_0$, with inversion:

$$n_1 = \frac{1}{\gamma u}\frac{\partial}{\partial u}\left(\frac{1}{u}\frac{\partial v_1}{\partial u}\right). \quad (4.12)$$

In terms of v_1 the transport equation (4.8) becomes[14]

$$\frac{1}{\gamma u}\frac{\partial}{\partial u}\left[\frac{1}{u}\frac{\partial^2 v_1}{\partial u\partial t} + \frac{1}{u\tau}\frac{\partial^2 v_1}{\partial u^2} - \frac{D}{4l^2}\left(\frac{1}{u}\frac{\partial}{\partial u}\right)^3 v_1\right] = \xi(u,t) = \frac{1}{\gamma u}\frac{\partial}{\partial u}\frac{6e}{g_0\tau}\eta(u,t), \quad (4.13)$$

where we used $\xi = \partial\eta/\partial x$. This equation can immediately be integrated once:

$$\frac{1}{u}\frac{\partial^2 v_1}{\partial u\partial t} + \frac{1}{u\tau}\frac{\partial^2 v_1}{\partial u^2} - \frac{D}{4l^2}\left(\frac{1}{u}\frac{\partial}{\partial u}\right)^3 v_1 - \frac{6e}{g_0\tau}\eta(u,t) = C(t). \quad (4.14)$$

The integration constant is easily identified. We split the current of Eq. (4.2) into $J_0 + j_1(t)$ and calculate the latter in terms of the same variables. Adding to this the displacement current and setting

$$\hat{j}_1(t) = j_1(t) + \epsilon\epsilon_0\frac{\partial E_1}{\partial t},$$

we find $\hat{j}_1(t) \propto C(t)$. It is therefore easiest (though not necessary) to consider an open-circuited device driven by a constant current. Then $C(t)$ vanishes identically. Eq. (3.14) is then a new Langevin-type equation.

A. Equations for the Correlation Functions

Besides the density–density covariance function Γ we introduce the voltage–density covariance function $\Omega(u,u') = \langle v_1(u)n_1(u')\rangle$ and the voltage–voltage covariance function $\mathcal{U}(u,u') = \langle v_1(u)v_1(u')\rangle$. The connections are

$$\Omega(u,u') = \gamma\int_0^u u_1 du_1 \int_0^{u_1} u_2\Gamma(u_2,u')du_2, \quad (4.15)$$

$$\mathcal{U}(u,u') = \gamma\int_0^{u'} u_1 du_1 \int_0^{u_1} u_2\Omega(u,u_2)du_2. \quad (4.16)$$

The equations for Ω and $\mathcal{U}$ are found to be from (4.10):

$$\frac{1}{\gamma\tau}\frac{1}{u}\frac{\partial}{\partial u}\left[\frac{1}{u}\frac{\partial^2\Omega(u,u')}{\partial u^2} - \frac{D\tau}{4l^2}\left(\frac{1}{u}\frac{\partial}{\partial u}\right)^3\Omega(u,u')\right] + \frac{1}{\gamma\tau}\frac{1}{u'}\frac{\partial}{\partial u'}\left[\frac{1}{u'}\frac{\partial^2\Omega(u',u)}{\partial u'^2} - \frac{D\tau}{4l^2}\left(\frac{1}{u'}\frac{\partial}{\partial u'}\right)^3\Omega(u'u)\right] = \frac{D}{4l^3}\frac{1}{uu'}\frac{\partial^2}{\partial u\partial u'}\left(\frac{n_0(u)}{u}\delta(u-u')\right), \quad (4.17)$$

and also,

$$\left(\frac{1}{u}\frac{\partial}{\partial u}\right)^2\left(\frac{1}{u'}\frac{\partial}{\partial u'}\right)^2\left[\frac{\partial\mathcal{U}}{\partial u} - \frac{D\tau}{4l^2}\left(\frac{1}{u}\frac{\partial}{\partial u}\right)^2\mathcal{U} + \frac{\partial\mathcal{U}}{\partial u'} - \frac{D\tau}{4l^2}\left(\frac{1}{u'}\frac{\partial}{\partial u'}\right)^2\mathcal{U}\right] = \frac{\gamma^2 D\tau}{4l^3}\left(\frac{1}{u}\frac{\partial}{\partial u}\right)\left(\frac{1}{u'}\frac{\partial}{\partial u'}\right)\left[\frac{n_0(u)}{u}\delta(u-u')\right]. \quad (4.18)$$

We have immediately a particular integral of (4.18) by integrating twice over the area $0 \leq \hat{u} \leq u$, $0 \leq \hat{u}' \leq u'$. The result is, using (4.6c) and the Einstein relation for D:

$$\frac{\partial\mathcal{U}}{\partial u} + \frac{\partial\mathcal{U}}{\partial u'} - \frac{D\tau}{4l^2}\left[\left(\frac{1}{u}\frac{\partial}{\partial u}\right)^2 + \left(\frac{1}{u'}\frac{\partial}{\partial u'}\right)^2\right]\mathcal{U} = \frac{4lkT}{\epsilon\epsilon_0}[u'H(u-u') + uH(u'-u)], \quad (4.19)$$

where $H(u)$ is the Heavyside unit step function.

It is not immediately clear what boundary conditions should be satisfied, except that by grounding the conductor at $u = 0$ we have

$$\mathcal{U}(0,u') = \mathcal{U}(u,0) = 0. \tag{4.20}$$

Though we assumed that the dc potential minimum caused by the space charge occurs at $u = \varepsilon \approx 0$, this can certainly not hold at all times for the fluctuations. In fact, this minimum shifts stochastically in position, so that at the location of the dc minimum $\partial\mathcal{U}/\partial u \neq 0$. The finite magnitude is accounted for by the ac diffusion around the dc potential minimum. For the purpose of finding the voltage fluctuations we can neglect, however, the diffusion terms in (4.19) if $D\tau = \varkappa^2 \ll l^2$ (as will be verified *a posteriori*), where $\varkappa$ is an average Debye length for the interval $(0,1)$. We are then left with the simple first-order partial differential equation

$$\frac{\partial\mathcal{U}}{\partial u} + \frac{\partial\mathcal{U}}{\partial u'} \approx \frac{4lkT}{\epsilon\epsilon_0}\,[u'H(u-u') + uH(u'-u)]; \tag{4.21}$$

from (4.20) it follows that this equation implies

$$\left(\frac{\partial\mathcal{U}}{\partial u}\right)_{u=0} \approx \left(\frac{\partial\mathcal{U}}{\partial u'}\right)_{u'=0} \approx 0. \tag{4.22}$$

The solution of (4.21) subject to (4.20) is

$$\mathcal{U}(u,u') \approx (4lkT/\epsilon\epsilon_0)[\tfrac{1}{2}u'^2H(u-u') + \tfrac{1}{2}u^2H(u'-u)]. \tag{4.23}$$

This solution is quite good, but fails for very small u or u' and very-short-range correlations, $u \approx u'$, as can be deduced by substituting into the full equation (4.19). In fact, up to first-order perturbation, we have $\mathcal{U} = \mathcal{U}_0 + \mathcal{U}_1$; we then find[15]

$$\mathcal{U}(u,u') = \frac{4lkT}{\epsilon\epsilon_0}\left(\tfrac{1}{2}u'^2H(u-u') + \tfrac{1}{2}u^2H(u'-u) - \frac{\varkappa^2}{2l^2}\,\delta(u-u')\,\log u\right). \tag{4.23'}$$

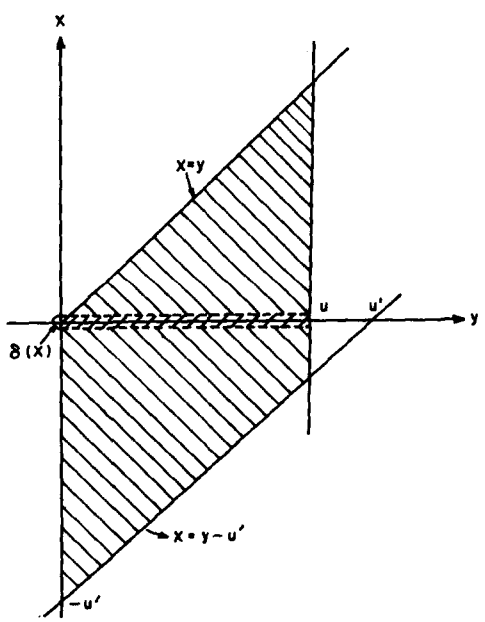

FIG. 1. Pertaining to the integral of Eq. (4.27).

The second term is of course only small in the sense of a distribution for suitable test functions $\varphi(u)$. The correctness of (4.23) will be further substantiated under 4B below.

Unfortunately, no similar useful approximation holds for Ω and Γ since (4.23), when differentiated, produces only spike terms. The full equation (4.19) is needed in this case. Though the solution for the density-density correlations is expected to be a short-range function, it may be inferred that the simple Debye function of (3.15) does not satisfy Eq. (4.10).

B. Spectral Intensity of Voltage Fluctuations

The Fourier method was already employed in Ref. 11. We can easily dress up this method with Green's functions. We start directly with the Langevin equation (4.14), with $C(t) \equiv 0$, which has as source strength

$$H(u,u') = \frac{27e\epsilon\epsilon_0 V_a D}{g_0^2\tau^2 l^3}\,\frac{\delta(u-u')}{u^2}. \tag{4.24}$$

The Laplace-transformed Green's function pertaining to (4.14) satisfies, with the diffusion term again neglected,

$$\frac{s}{u}\frac{\partial\mathcal{G}}{\partial u} + \frac{1}{u\tau}\frac{\partial^2\mathcal{G}}{\partial u^2} = \delta(u-u'); \tag{4.25}$$

as in (4.20) and (4.22) we require $\mathcal{G} = 0$ and $\partial\mathcal{G}/\partial u = 0$ for $u = 0$, so that

$$\mathcal{G}(u,u') = (u'/s)(1 - e^{-s\tau(u-u')})H(u-u'), \tag{4.26}$$

with u' being an internal point $0 < u' \leq l$. From (1.6b) and (4.24) we find for the spectrum, with $s = i\omega$:

$$\Sigma(u,u',\omega) = \int_0^u du'' \int_0^{u'} du'''(1 - e^{-s\tau(u-u'')}) \times (1 - e^{s\tau(u'-u''')})\,\frac{54e\epsilon\epsilon_0 V_a D}{s^2 g_0^2\tau^2 l^3}\,\delta(u''-u'''). \tag{4.27}$$

We introduce as new variables $u'' - u''' = x$ and $u'' = y$. The path of integration is then for $u < u'$ as in Fig. 1. (For $u > u'$, set $u''' - u'' = x$ and $u''' = y$). One finds

$$\Sigma(u,u',\omega) = \frac{54e\epsilon\epsilon_0 V_a D}{g_0^2 l^3}\left(-\frac{u}{s^2\tau^2}(1 + e^{s\tau(u'-u)}) + \frac{1}{s^3\tau^3}(1 - e^{s\tau(u'-u)} - e^{-s\tau u} + e^{s\tau u'})\right)H(u'-u) + hcj, \tag{4.28}$$

where hcj means in the present context, $u \to u'$, $u' \to u$, $s \to -s$. Further,

$$\mathrm{Re}\,\Sigma(u,u',\omega) = \frac{54e\epsilon\epsilon_0 V_a D}{g_0^2 l^3\omega^3\tau^3}\{u\omega\tau[1 + \cos\omega\tau(u'-u)] + [\sin\omega\tau(u'-u) - \sin\omega\tau u - \sin\omega\tau u']\} \times H(u'-u) + hcj. \tag{4.29}$$

We now shall obtain the same result by using Eq. (1.6a) and the result for the covariance function (4.23). In this approach we must use the Green's function pertaining to the Markovian form of the transport equation [*cf.* Eq (I 1.2)]; hence we write (4.14) in the form

$$\frac{\partial v_1}{\partial t} + \frac{\tau^{-1}\partial v_1}{\partial u} = \vartheta(u,t),$$

where ϑ has still a $\delta(t)$ correlation behavior in the time (which is all that is required for this approach to hold). Thus the "Markovian Green's function" satisfies

$$sG(u,u',s) + \tau^{-1}\partial\,\frac{G(u,u',s)}{\partial u} = \delta(u-u'), \qquad (4.30)$$

which has as solution

$$G(u,u',s) = \tau e^{-s\tau(u-u')}H(u-u'). \qquad (4.31)$$

Whence, for the spectrum, we obtain

$$\begin{aligned}\Sigma(u,u',\omega) &= \frac{4lkT\tau}{\epsilon\epsilon_0}\left(\int_0^u e^{-s\tau(u-u'')}[u'^2H(u''-u')+u''^2H(u'-u'')]du''+\int_0^{u'} e^{s\tau(u'-u'')}[u''^2H(u-u'')+u^2H(u''-u)]du''\right)\\ &= \frac{8lkT\tau}{\epsilon\epsilon_0}\left(\frac{-u}{s^2\tau^2}(1+e^{s\tau(u'-u)})+\frac{1}{s^3\tau^3}(1-e^{s\tau(u'-u)}+e^{s\tau u'}-e^{-s\tau u})\right)H(u'-u)+hcj.\end{aligned} \qquad (4.32)$$

This is identical with (4.28): the equivalence of the factors in front follows directly from Eqs. (4.7).

Finally, for the total open voltage noise across the specimen ($u' = 1$, $u = 1 - 0$) we find from both methods

$$\Sigma_{\text{total}}(\omega) = \frac{16lkT\tau}{\epsilon\epsilon_0}\frac{1}{\omega^3\tau^3}(\omega\tau - \sin\omega\tau). \qquad (4.33)$$

The impedance was calculated by van der Ziel from an equation similar to (4.14), with the result[16]

$$Z(\omega) = (2l\tau/\epsilon\epsilon_0)(1 - e^{-i\omega\tau} - \tfrac{1}{2}\omega^2\tau^2 - i\omega\tau)/(i\omega\tau)^3. \qquad (4.34)$$

One sees that (4.33) amounts to the, by now, familiar *double* thermal noise, $8kT\,\mathrm{Re}Z(\omega)$. Besides the fact that two different procedures have been reconciled, this section has illustrated the correctness of the Markovian approach for density fluctuations in a nonequilibrium situation.

II. SOME MICROSCOPIC APPLICATIONS

5. IDEAL GASES IN AN EXTERNAL FIELD

For sufficiently dilute gases the Boltzmann equation serves as phenomenological equation and the associated Λ theorem determines the covariance function up to the neglect of triple correlations. The procedure is entirely exact only for ideal gases with one-body collisions as was already shown by Lax[17]; we shall amend his treatment here by allowing for the streaming terms in an external field. In this and the next section we consider external fields only. If space-charge fields are included, Eqs. (5.8) and (6.8) are no longer correct since these fields are integrals over the particle densities (compare Delcroix[18]). True physical correlations occur when there are two-body collisions, on which we comment in the next section.

For a one-component gas with one-body collisions we have a scattering kernel

$$Q(y,y') = Q(\mathbf{rk},\mathbf{k}')\delta(\mathbf{r}-\mathbf{r}'). \qquad (5.1)$$

The phenomenological equation follows from (1.7), with A given by Eq. (I 8.2):

$$A_{\mathbf{k}} = \int d^3k'\,[Q(\mathbf{rk}',\mathbf{k}) - Q(\mathbf{rk},\mathbf{k}')], \qquad (5.2)$$

whereas

$$\Lambda_{\text{str}} = \mathbf{v}_{\mathbf{k}}\cdot\nabla_{\mathbf{r}} + (\mathbf{F}/\hbar)\cdot\nabla_{\mathbf{k}}, \qquad (5.3)$$

where $\mathbf{F}(\mathbf{r})$ is the force field. We write further

$$Q(\mathbf{rk},\mathbf{k}')\,d^3r d^3k d^3k' = \nu(\mathbf{rk})[1+\epsilon\nu(\mathbf{rk}')]\mathfrak{Q}(\mathbf{k},\mathbf{k}'), \qquad (5.4)$$

where $\nu(\mathbf{rk})$ is the number of particles in the state $(\mathbf{rk})$; $\epsilon = 0$ for Boltzmann statistics, + 1 for Bose–Einstein statistics and − 1 for Fermi–Dirac statistics. There is a bit of a problem with FD and BE statistics when using densities rather than occupancies. The connection is of course $n(\mathbf{rk}) = \nu(\mathbf{rk})\rho(\mathbf{k})\sigma(\mathbf{r})$, where $\rho(\mathbf{k})$ is the density of states in $\mathbf{k}$ space and $\sigma(\mathbf{r})$ is the density in $\mathbf{r}$ space. The former arises naturally from the quantization in $\mathbf{k}$ space, but the latter artificially by associating some environment with a point in $\mathbf{r}$ space.[19] Accordingly (5.4) will also be written as

$$Q(\mathbf{rk},\mathbf{k}') = n(\mathbf{rk})[1+\epsilon\nu(\mathbf{rk}')]\mathfrak{Q}(\mathbf{k},\mathbf{k}')\rho(\mathbf{k}'). \qquad (5.4')$$

For the BE and FD case (5.4′) must be linearized to find Λ_{coll} as defined in Eq. (I 7.5). The B moment, following from (5.1), (5.4′), and Eq. (I, 8.3), is

$$B^0_{\mathbf{rk},\mathbf{k}'} = -\delta(\mathbf{r}-\mathbf{r}')\{\langle n(\mathbf{rk})\rangle[1+\epsilon\langle\nu(\mathbf{rk}')\rangle]\mathfrak{L}(\mathbf{k},\mathbf{k}')\rho(\mathbf{k}') + \langle n(\mathbf{rk}')\rangle[1+\epsilon\langle\nu(\mathbf{rk})\rangle]\mathfrak{L}(\mathbf{k}',\mathbf{k})\rho(\mathbf{k})\}$$
$$+\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}')\int d^3k''\rho(\mathbf{k}'')\{\langle n(\mathbf{rk})\rangle[1+\epsilon\langle\nu(\mathbf{rk}'')\rangle]\mathfrak{L}(\mathbf{k},\mathbf{k}'') + \langle n(\mathbf{rk}')\rangle[1+\epsilon\langle\nu(\mathbf{rk}'')\rangle]\mathfrak{L}(\mathbf{k}',\mathbf{k}'')\}. \quad (5.5)$$

The microscopic Λ theorem (1.4′) now reads

$$[\mathbf{v}_\mathbf{k}\cdot\nabla_\mathbf{r} + \mathbf{v}_{\mathbf{k}'}\cdot\nabla_{\mathbf{r}'} + \mathbf{F}(\mathbf{r})\hbar^{-1}\cdot\nabla_\mathbf{k} + \mathbf{F}(\mathbf{r}')\hbar^{-1}\cdot\nabla_{\mathbf{k}'}]\Gamma(\mathbf{rk},\mathbf{r}'\mathbf{k}')$$
$$+\int d^3k''\,\mathfrak{L}(\mathbf{k},\mathbf{k}'')\{\rho(\mathbf{k}'')[1+\epsilon\langle\nu(\mathbf{rk}'')\rangle]\Gamma(\mathbf{rk},\mathbf{r}'\mathbf{k}') + \epsilon\rho(\mathbf{k})\langle\nu(\mathbf{rk})\rangle\Gamma(\mathbf{rk}'',\mathbf{r}'\mathbf{k}')\}$$
$$-\int d^3k''\,\mathfrak{L}(\mathbf{k}'',\mathbf{k})\{\rho(\mathbf{k})[1+\epsilon\langle\nu(\mathbf{rk})\rangle]\Gamma(\mathbf{rk}'',\mathbf{r}'\mathbf{k}') + \epsilon\rho(\mathbf{k}'')\langle\nu(\mathbf{rk}'')\rangle\Gamma(\mathbf{rk},\mathbf{r}',\mathbf{k}')\}$$
$$+\int d^3k''\,\mathfrak{L}(\mathbf{k}',\mathbf{k}'')\{\rho(\mathbf{k}'')[1+\epsilon\langle\nu(\mathbf{r}'\mathbf{k}'')\rangle]\Gamma(\mathbf{rk},\mathbf{r}'\mathbf{k}') + \epsilon\rho(\mathbf{k}')\langle\nu(\mathbf{r}'\mathbf{k}')\rangle\Gamma(\mathbf{rk},\mathbf{r}'\mathbf{k}'')\}$$
$$-\int d^3k''\,\mathfrak{L}(\mathbf{k}'',\mathbf{k}')\{\rho(\mathbf{k}')[1+\epsilon\langle\nu(\mathbf{r}'\mathbf{k}')\rangle]\Gamma(\mathbf{rk},\mathbf{r}'\mathbf{k}'') + \epsilon\rho(\mathbf{k}'')\langle\nu(\mathbf{r}'\mathbf{k}'')\rangle\Gamma(\mathbf{rk},\mathbf{r}'\mathbf{k}')\} = B^0_{\mathbf{rk},\mathbf{k}'}. \quad (5.6)$$

We first consider the Boltzmann case. The usual ansatz

$$\Gamma = \delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}')\langle n(\mathbf{rk})\rangle + \hat{\Gamma} \quad (5.7)$$

is succesful, with $\hat{\Gamma}\equiv 0$ both for thermal equilibrium and the steady state. [For two-body collisions, $\hat{\Gamma}\not\equiv 0$ in the steady state (see Sec. 6).] The reason is that in the Λ theorem the collision terms, operating on the δ part, cancel the functional B, except for a difference $\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}')\Lambda_{\text{coll}}\langle n(\mathbf{rk})\rangle$. The streaming terms under our presumed conditions yield

$$(\Lambda_{\text{str}}+\Lambda'_{\text{str}})[\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}')\langle n(\mathbf{rk})\rangle]$$
$$=\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}')\Lambda_{\text{str}}\langle n(\mathbf{rk})\rangle, \quad (5.8)$$

as is easily verified. Since for a Boltzmann gas $\langle n\rangle$ satisfies the regression equation for Δn, the result (5.7) with $\hat{\Gamma}\equiv 0$ follows. Results in the presence of space-charge forces we hope to consider in future work.

For the FD and BE cases we can try likewise

$$\Gamma_{\text{BE or FD}} = \delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}')\langle n(\mathbf{rk})\rangle^0$$
$$\times[1+\epsilon\langle\nu(\mathbf{rk})\rangle^0] + \hat{\Gamma}, \quad (5.9)$$

where detailed balancing applies to the local equilibrium solution $\langle\nu(\mathbf{rk})\rangle^0 \equiv f^0$ of the Boltzmann transport equation, i.e.,

$$f^0(\mathbf{rk})[1+\epsilon f^0(\mathbf{rk}')]\,\mathfrak{L}(\mathbf{k},\mathbf{k}')$$
$$= f^0(\mathbf{rk}')[1+\epsilon f^0(\mathbf{rk})]\,\mathfrak{L}(\mathbf{k}',\mathbf{k}). \quad (5.10)$$

When this is substituted into (5.6) one finds indeed that all terms in zero-order cancel, with the result for $\hat{\Gamma}$

$$(\Lambda_{\text{str}}+\Lambda'_{\text{str}}+\Lambda_{\text{coll}}+\Lambda'_{\text{coll}})\hat{\Gamma}$$
$$=\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}')\Lambda_{\text{str}}f^0(1+\epsilon f^0)$$
$$+\delta(\mathbf{r}-\mathbf{r}')[\Omega_\mathbf{k} f^1(\mathbf{k}) + \Omega_{\mathbf{k}'} f^1(\mathbf{k}')], \quad (5.11)$$

where Ω is complex integral operator. The solution has not been further pursued.

The spectral density of the covariance function can be found from our previous equations. If only an external electrical field in the z direction is present, the Green's function satisfies, with $\boldsymbol{\alpha} = q\mathbf{E}/\hbar$,

$$s\,\mathfrak{G} + \boldsymbol{\alpha}\cdot\nabla_\mathbf{k}\mathfrak{G} + \mathfrak{G}/\tau = \delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}'); \quad (5.12)$$

whence

$$\mathfrak{G} = (1/\alpha)\delta(\mathbf{r}-\mathbf{r}')\delta(k_x-k'_x)\delta(k_y-k'_y)H(k_z-k'_z)$$
$$\times\exp[-(s\tau+1)(k_z-k'_z)/\alpha\tau]. \quad (5.13)$$

Since we are only interested in the Green's operator

$$G_{\mathbf{kr}}(s)\varphi(\mathbf{kr}) = \int\mathfrak{G}(\mathbf{kr},s;\mathbf{k}'\mathbf{r}')\varphi(\mathbf{k}'\mathbf{r}')d\Omega$$

we find for $\alpha\tau \ll k_z$, from integration by parts,

$$G_{\mathbf{kr}}(s) \approx [\tau/(1+s\tau)]\mathsf{I}, \quad (5.14)$$

where I is the idem operator. For the spectrum, Eq. (1.6a) yields

$$\Sigma(\mathbf{kr},\mathbf{k}'\mathbf{r}',\omega) = 2\langle n(\mathbf{kr})\rangle^0[1+\epsilon\langle\nu(\mathbf{kr})\rangle^0$$
$$\times\delta(\mathbf{k}-\mathbf{k}')\delta(\mathbf{r}-\mathbf{r}')\tau/(1+i\omega\tau) + hcj$$
$$+\text{terms in }\hat{\Gamma}. \quad (5.15)$$

Restricting ourselves to FD statistics and small fields, we have for the current fluctuations

$$\Sigma_{\Delta J\Delta J}(\mathbf{r},\mathbf{r}',\omega) = 2q^2\int\int\mathbf{v}_\mathbf{k}\mathbf{v}_{\mathbf{k}'}\,\Sigma(\mathbf{kr},\mathbf{k}'\mathbf{r}',\omega)d^3kd^3k'$$
$$=\delta(\mathbf{r}'-\mathbf{r})\frac{q^2}{\pi^3}\int\!\!\!\!\!\!\diint\mathbf{v}_\mathbf{k}\mathbf{v}_\mathbf{k}f^0(1-f^0)$$
$$\times\frac{\tau}{1+\omega^2\tau^2}\frac{d\mathcal{E}dS_\mathbf{k}}{\hbar|\mathbf{v}_\mathbf{k}|}$$
$$\approx\delta(\mathbf{r}-\mathbf{r}')\frac{q^2kT}{\pi^3\hbar}\!\!\!\!\!\!\diint\mathbf{v}(\mathbf{k}_F)\mathbf{v}(\mathbf{k}_F)\frac{dS_F}{v(\mathbf{k}_F)}$$
$$\times\frac{\tau_F}{1+\omega^2\tau_F^2}$$
$$=4\delta(\mathbf{r}-\mathbf{r}')kT\sigma, \quad (5.16)$$

where we used $f^0(1-f^0) = -kT\partial f^0/\partial \mathcal{E} \approx \delta(\mathcal{E}-\mathcal{E}_F)$, with $\mathcal{E}_F$ being the Fermi energy; σ is the conductivity tensor of a Fermi gas. A more general route to obtain the equivalent of the Nyquist formula in the presence of arbitrary external fields will be followed in Secs. 7 and 8.

6. CONNECTION WITH THE BBGKY TWO-POINT EQUATION

We substitute Eq. (1.5) into the microscopic Λ theorem. The steady-state one-point distribution is also denoted by $n^0(\mathbf{rk}) \equiv \langle n(\mathbf{rk})\rangle$. We consider only a one-component Boltzmann gas. Observing that n^0 satisfies the regression equation, the Λ theorem yields the following result for the two-point distribution f_2:

$$\begin{aligned}[\mathbf{v}_\mathbf{k}\cdot\nabla_\mathbf{r} + \mathbf{v}_{\mathbf{k}'}\cdot\nabla_{\mathbf{r}'} + (\mathbf{F}/\hbar)\cdot\nabla_\mathbf{k} + (\mathbf{F}'/\hbar)\cdot\nabla_{\mathbf{k}'}]f_2(y,y') \\ = -(\Lambda_{\text{coll}} + \Lambda'_{\text{coll}})f_2(y,y') \\ - \delta(y-y')\Lambda_{\text{str}}n^0(y) \\ + B_{yy'}[n^0(y)] - (\Lambda_{\text{coll}} + \Lambda'_{\text{coll}}) \\ [n^0(y)\delta(y-y')].\end{aligned} \tag{6.1}$$

(We wrote y for $\mathbf{k}, \mathbf{r}$.)

For one-body collisions the results of the previous sections apply. The collision integral is given by Eqs. (5.2) and (5.4′), and the collision operator is

$$\Lambda^{\text{I}}_{\text{coll},\mathbf{k}}\varphi(y) = \int d^3k_1[\bar{\mathcal{Q}}(\mathbf{k},\mathbf{k}_1)\varphi(\mathbf{k}) - \bar{\mathcal{Q}}(\mathbf{k}_1,\mathbf{k})\varphi(\mathbf{k}_1)]; \tag{6.2}$$

the bar above the scattering probability indicates that the density of states has been absorbed, i.e., $\bar{\mathcal{Q}}(\mathbf{k},\mathbf{k}_1) = \mathcal{Q}(\mathbf{k},\mathbf{k}_1)\rho(\mathbf{k}_1)$. As shown in the previous section, the last three terms of the rhs of Eq. (6.1) cancel exactly for any steady state, whence, the two-point distribution satisfies

$$\begin{aligned}[\mathbf{v}_\mathbf{k}\cdot\nabla_\mathbf{r} + \mathbf{v}_{\mathbf{k}'}\cdot\nabla_{\mathbf{r}'} + (\mathbf{F}/\hbar)\cdot\nabla_\mathbf{k} + (\mathbf{F}'/\hbar)\cdot\nabla_{\mathbf{k}'}]f_2(y,y') \\ = -(\Lambda^{\text{I}}_{\text{coll},\mathbf{k}} + \Lambda^{\text{I}}_{\text{coll},\mathbf{k}'})f_2(y,y').\end{aligned} \tag{6.3}$$

More important, and in line with standard treatments, we consider the case in which two-body collisions occur. We introduce the two-body scattering operator:

$$\begin{aligned}\mathcal{T}_\mathbf{k}[\phi,\psi] = \int\int\int d^3k_1d^3k_2d^3k_3[-\bar{\mathcal{Q}}(\mathbf{kk}_1,\mathbf{k}_2\mathbf{k}_3) \\ \times \phi(\mathbf{k})\psi(\mathbf{k}_1) + \bar{\mathcal{Q}}(\mathbf{k}_2\mathbf{k}_3,\mathbf{kk}_1)\phi(\mathbf{k}_2)\psi(\mathbf{k}_3)],\end{aligned} \tag{6.4}$$

where the $\bar{\mathcal{Q}}$'s satisfy some symmetry rules [Eq (I 8.8)]. The two-body collision integral is then

$$A_\mathbf{k}[n(y,t)] = \mathcal{T}_\mathbf{k}[n,n], \tag{6.5}$$

and the two-body collision operator is found to be

$$\Lambda^{\text{II}}_{\text{coll},\mathbf{k}}\phi(y) = -\mathcal{T}_\mathbf{k}[n^0,\phi] - \mathcal{T}_\mathbf{k}[\phi,n^0]. \tag{6.6}$$

We calculated the last term on the rhs of (6.1). The result is

$$\begin{aligned}\delta(\mathbf{r}-\mathbf{r}')\{-2\int\int d^3k_1d^3k_2[\bar{\mathcal{Q}}(\mathbf{kk}',\mathbf{k}_1\mathbf{k}_2)n^0(\mathbf{k})n^0(\mathbf{k}') \\ - \bar{\mathcal{Q}}(\mathbf{k}'\mathbf{k}_1,\mathbf{kk}_2)n^0(\mathbf{k}')n^0(\mathbf{k}_1) \\ - \bar{\mathcal{Q}}(\mathbf{kk}_1,\mathbf{k}'\mathbf{k}_2)n^0(\mathbf{k})n^0(\mathbf{k}_1)] \\ - \delta(\mathbf{k}-\mathbf{k}')\int\int\int d^3k_1d^3k_2d^3k_3 \\ \times [\bar{\mathcal{Q}}(\mathbf{kk}_1,\mathbf{k}_2\mathbf{k}_3)n^0(\mathbf{k})n^0(\mathbf{k}_1) \\ + \bar{\mathcal{Q}}(\mathbf{k}'\mathbf{k}_1,\mathbf{k}_2\mathbf{k}_3)n^0(\mathbf{k}')n^0(\mathbf{k}_1)]\}.\end{aligned} \tag{6.7}$$

This is to be compared with the functional $B_{yy'}$, given in Eq. (I 8.10). If detailed balancing applies, (6.7) is identical with (I 8.10), and a two-point equation entirely similar to (6.3) results. Thus the equilibrium result is simple. In a steady state the triple integrals leave a term $\delta(y-y')A_\mathbf{k}[n^0(y)]$, which cancels the second term on the rhs of (6.1) by virtue of Eq. (1.7)! The final result is therefore

$$\begin{aligned}[\mathbf{v}_\mathbf{k}\cdot\nabla_\mathbf{r} + \mathbf{v}_{\mathbf{k}'}\cdot\nabla_{\mathbf{r}'} + (\mathbf{F}/\hbar)\cdot\nabla_\mathbf{k} + (\mathbf{F}'/\hbar)\cdot\nabla_{\mathbf{k}'}]f_2(y,y') \\ = -(\Lambda^{\text{II}}_{\text{coll},\mathbf{k}} + \Lambda^{\text{II}}_{\text{coll},\mathbf{k}'})f_2(y,y') \\ + \delta(\mathbf{r}-\mathbf{r}')\int\int d^3k_1d^3k_2 \\ \times [\bar{\mathcal{Q}}(\mathbf{k}_1\mathbf{k}_2,\mathbf{kk}')n^0(\mathbf{k}_1)n^0(\mathbf{k}_2) \\ - \bar{\mathcal{Q}}(\mathbf{kk}',\mathbf{k}_1\mathbf{k}_2)n^0(\mathbf{k})n^0(\mathbf{k}')],\end{aligned} \tag{6.8}$$

with Λ^{II} expressible as in (6.6).

Some authors introduce the Boltzmann operator $\mathcal{J}_\mathbf{k}$ as $\int d\mathbf{k}\,\bar{\mathcal{Q}}$, where the integration is over the test particle and scattered $\mathbf{k}$ vectors. Then the first term on the rhs of (6.8) is

$$\begin{aligned}\mathcal{J}_\mathbf{k}[f_2(\mathbf{k}_3,\mathbf{k}')n^0(\mathbf{k}_2) - f_2(\mathbf{k}_1,\mathbf{k}')n^0(\mathbf{k}) \\ + f_2(\mathbf{k}_2\mathbf{k}')n^0(\mathbf{k}_3) - f_2(\mathbf{k},\mathbf{k}')n^0(\mathbf{k}_1)] \\ + \mathcal{J}_{\mathbf{k}'}[\text{same},\mathbf{k}\leftrightarrow\mathbf{k}'].\end{aligned}$$

The result (6.8) in this form corresponds with a form of the BBGKY two-point equation given by Tsugé,[20] except for the inhomogeneous δ term, which provides a "boundary condition" in case of confluence of $\mathbf{r}$ and $\mathbf{r}'$.

7. NOISE SOURCES ASSOCIATED WITH THE CONSERVATION THEOREMS OF THE BOLTZMANN EQUATION AND THE HYDRODYNAMIC EQUATIONS

Conservation theorems are obtained by multiplying the Boltzmann equation with summational invariants $\Psi(\mathbf{rk})$, integrating over all $\mathbf{k}$ space, and summing over all species. We first show that these conservation theorems have instantaneous validity.

The stochastic Boltzmann equation for species p is

$$\begin{aligned}\left(\frac{\partial}{\partial t} + \mathbf{v}_\mathbf{k}\cdot\nabla_\mathbf{r} + \hbar^{-1}\mathbf{F}^p\cdot\nabla_\mathbf{k}\right)n^p(\mathbf{rk},t) \\ = A^p[n(\mathbf{rk},t)] + \xi^p(\mathbf{rk},t).\end{aligned} \tag{7.1}$$

We assume that $\mathbf{F}^p$ is the Lorentz force $q^p(\mathbf{E} + \mathbf{v}_k \times \mathbf{B})$. With integration by parts we obtain

$$\frac{\partial}{\partial t}\int \Psi(\mathbf{rk})\, n^p d^3k + \nabla_r \cdot \int \Psi(\mathbf{rk})\mathbf{v}_k n^p d^3k - \int \nabla_r \Psi \cdot \mathbf{v}_k n^p d^3k - \hbar^{-1}\int \nabla_k \Psi \cdot \mathbf{F}^p n^p d^3k = \int \Psi(\mathbf{rk}) A^p[n^p] d^3k + \int \Psi(\mathbf{rk})\xi^p d^3k. \quad (7.2)$$

Let a bar denote an average over $\mathbf{k}$ space:

$$\overline{\Psi^p(\mathbf{rt})} n^p(\mathbf{r},t) = \int d^3k \Psi n^p(\mathbf{rk},t), \quad (7.3a)$$

$$\overline{\Psi^p \mathbf{v}_k} n^p(\mathbf{r},t) = \mathbf{J}^p_\Psi(\mathbf{r},t) = \int d^3k \Psi \mathbf{v}_k n^p(\mathbf{rk},t). \quad (7.3b)$$

The lhs of Eq. (7.2) can then be written in terms of these quantities. The first term on the rhs yields zero if Ψ is a summational invariant:

$$\sum_p \int \Psi A^p d^3k = 0. \quad (7.4)$$

The proof for one-body collisions [(I 8.2)] or two-body collisions [(I 8.9)] is standard.[21] The stochastic term on the rhs can likewise be ignored, since its second moment is zero, as we now show. For one-body collisions [(I 8.3)]:

$$\sum_{pq}\int\int \Psi(\mathbf{rk})\Psi(\mathbf{r'k'}) B^{pq}(\mathbf{rk},\mathbf{r'k'}) d^3k d^3k' = \delta(\mathbf{r}-\mathbf{r'})\sum_p \{-\int\int d^3k d^3k' \Psi(\mathbf{rk})\Psi(\mathbf{r'k'})[Q^p(\mathbf{rk},\mathbf{k'}) + Q^p(\mathbf{rk'k})] + \int\int d^3k d^3k'' \Psi(\mathbf{rk})\Psi(\mathbf{rk})[Q^p(\mathbf{rk},\mathbf{k''}) + Q^p(\mathbf{rk''},\mathbf{k})]\} = \delta(\mathbf{r}-\mathbf{r'})\sum_p \int d^3k \psi(\mathbf{rk}) \int d^3k' [Q^p(\mathbf{rk},\mathbf{k'}) + Q^p(\mathbf{rk'},\mathbf{k})][\Psi(\mathbf{rk}) - \Psi(\mathbf{rk'})] = 0, \quad (7.5)$$

since the last square-bracketed expression is zero for any scattering $\mathbf{k} \to \mathbf{k'}$. The proof for two-body collisions [(I 8.10)] is left to the reader[22]; whence, the result (7.2) becomes

$$\sum_p \left(\frac{\partial}{\partial t}(\overline{\Psi^p} n^p) + \nabla_r \cdot \mathbf{J}^p_\Psi - J^p_{\nabla_r \Psi} - \hbar^{-1}\overline{\nabla_k \Psi^p} n^p \cdot \mathbf{F}^p\right) = 0. \quad (7.6)$$

We stress that the $\mathbf{k}$ space averages here are still stochastic quantities, since the distributions $n^p(\mathbf{rk},t)$ fluctuate. Sometimes it is said that the collision terms have disappeared from the conservation theorems, and one might think that also the stochastic terms have vanished. Neither is true, however, since the full stochastic Boltzmann equation is still needed for the calculation of the flow averages.

We now discuss the fluctuations. In the flow averages fluctuations are only meaningful for frequencies much less than the collision time (we look for hydrodynamic effects only). Also, the local changes are slow for most values of $\mathbf{k}$; whence, $\partial/\partial t \to i\omega \approx 0$ and $\Lambda_{str} \approx \Lambda_{force}$ only. Instead of (7.1) we consider therefore the solutions of

$$(\Lambda_{force,k} \times \Lambda_{coll,k})\Delta \mathbf{n}(\mathbf{rk},t) \approx \xi(\mathbf{rk},t), \quad (7.7)$$

in which $\mathbf{r}$ is just a parameter. A special solution is then $G_k(0)\,\xi(\mathbf{rk},t)$; to this we can add a solution of the homogeneous equation if it exists. Such is the case for the Boltzmann gas in any steady state and for FD and BE gases close enough to thermal equilibrium. We assume that the boundary conditions are what Lax terms "fictitious bc"; i.e., we are interested in the fluctuations in a subdomain $\mathfrak{D}(r)$ of an infinite system with free exchange across the boundary. In this case, the distributions $n^p(\mathbf{rk},t)$ fluctuate, as well as the total densities $n^p(\mathbf{r},t)$.

We consider a steady state Boltzmann gas. [For the near-equilibrium FD or BE gases, the results (7.11)ff are also valid, providing the bar signifies a $\mathbf{k}$-space average over the normalized distribution $\propto n^p(\mathbf{rk},t)[1 + \epsilon\nu^p(\mathbf{rk},t)].$] The required solution of (7.7) is

$$\Delta n^p(\mathbf{rk},t) \approx \frac{\langle n^p(\mathbf{rk})\rangle}{\langle n^p(\mathbf{r})\rangle}\Delta n^p(\mathbf{r},t) + [G_k(0)\xi(\mathbf{rk},t)]^p. \quad (7.8)$$

The first term, which satisfies the homogeneous equation corresponding to (7.7), expresses the fluctuations of the distribution over $\mathbf{k}$ which are fully correlated; the second term stems from scattering, not correlated with the fluctuations in total density. (See also I, Sec. 3D.) Substituting into (7.3b), we find

$$\mathbf{J}^p_\Psi = \langle \mathbf{J}^p_\Psi\rangle + \langle\overline{\Psi^p \mathbf{v}_k}\rangle \Delta n^p(\mathbf{r},t) + \mu^p_\Psi(\mathbf{r},t), \quad (7.9)$$

with current sources

$$\mu^p_\Psi = \int d^3k \Psi \mathbf{v}_k \sum_q G^{pq}_k(0)\xi^q(\mathbf{rk},t). \quad (7.10a)$$

The other relevant sources are

$$\zeta^p_\Psi = \int d^3k \nabla_r \Psi \cdot \mathbf{v}_k \sum_q G^{pq}_k(0)\xi^q(\mathbf{rk},t), \quad (7.10b)$$

$$\mathfrak{s}^p_\Psi = \int d^3k \nabla_k \Psi \sum_q G^{pq}_k(0)\xi^q(\mathbf{rk},t). \quad (7.10c)$$

The conservation theorems (7.6) thus yield the stochastic hydrodynamic equations[23]

$$\langle\overline{\Psi^p(\mathbf{r})}\rangle \frac{\partial \Delta n^p(\mathbf{r},t)}{\partial t} + \nabla_r \cdot [\langle\overline{\Psi^p \mathbf{v}_k}\rangle \Delta n^p(\mathbf{r},t)] - \langle\overline{\nabla_r \Psi^p \cdot \mathbf{v}_k}\rangle \Delta n^p(\mathbf{r},t) - \hbar^{-1}\mathbf{F}^p \cdot \langle\overline{\nabla_k \Psi}\rangle \Delta n^p(\mathbf{r},t) = \zeta^p_\Psi - \nabla_r \cdot \mu^p_\Psi + \hbar^{-1}\mathbf{F}^p \cdot \mathfrak{s}^p_\Psi. \quad (7.11)$$

The sources are correlated. Using the results of

I, Sec. 6, and setting $\langle \mu^p(t)\mu^q(0)\rangle = M^{pq}\delta(t)$ we have, e.g.,

$$M_\Psi^{pq}(\mathbf{r},\mathbf{r}') = \int\int d^3k d^3k' \Psi(\mathbf{rk})\Psi(\mathbf{r}'\mathbf{k}')\mathbf{v}_\mathbf{k}\mathbf{v}_{\mathbf{k}'} \times \sum_{rs} G_\mathbf{k}^{pr}(0)\, G_{\mathbf{k}'}^{qs}(0)\, \Xi(\mathbf{rk},\mathbf{r}'\mathbf{k}')$$
$$= \int\int d^3k d^3k' \Psi(\mathbf{rk})\Psi(\mathbf{r}'\mathbf{k}')\mathbf{v}_\mathbf{k}\mathbf{v}_{\mathbf{k}'} \times \Big(\sum_r G_\mathbf{k}^{pr}(0)\,\Gamma^{rq}(\mathbf{rk},\mathbf{r}'\mathbf{k}') + \text{conj.}\Big)$$
$$= \int_0^\infty dt I(\mathbf{k}) I(\mathbf{k}') I(\mathbf{k}'')\Psi\Psi'\mathbf{V}_\mathbf{k}\mathbf{V}_{\mathbf{k}'}\{[g(\mathbf{k},t;\mathbf{k}'',0) \times \Gamma(\mathbf{rk}'',\mathbf{r}'\mathbf{k}')]^{pq} + \text{conj}\}, \tag{7.12}$$

where conj means $p \to q$, $\mathbf{k} \to \mathbf{k}'$, $\mathbf{r} \to \mathbf{r}'$, and where $I(\mathbf{k})$ stands for $\int d^3k$.

The three cases of common interest arise from setting Ψ equal to the charge q^p, the momentum $\hbar\mathbf{k}^p$, and the energy $\frac{1}{2}m^p(\mathbf{v}^p - \mathbf{w})^2$; here $\mathbf{w}$ is the barycentric velocity defined by

$$\rho\mathbf{w} = \sum_p \rho^p \overline{\langle \mathbf{v}^p\rangle} \equiv \sum_p \rho^p \mathbf{v}_d^p, \tag{7.13}$$

$$\rho^p(\mathbf{r},t) = m^p n^p(\mathbf{r},t), \rho = \sum\rho^p \tag{7.14}$$

($\mathbf{v}_d^p$ is the drift velocity for species p).

A. Charge Transport.

The hydrodynamic equation for charge transport corroborates the macroscopic equations of Sec. 3 and 4. With $\Psi = q^p$ and $\mu_\Psi^p = q^p\eta^p$, we obtain

$$q^p\frac{\partial \Delta n^p}{\partial t} + q^p\nabla\cdot[\mathbf{v}_d^p(\mathbf{r})\Delta n^p(\mathbf{r},t)] = -q^p\nabla\cdot\eta^p(r,t). \tag{7.15}$$

The middle term will also be denoted by $\Delta\mathbf{J}^{*p}$ where the asterisk indicates that this fluctuation is "coarse grained in time", i.e., excludes the sources of (7.9). Then,

$$q^p\frac{\partial \Delta n^p}{\partial t} + \nabla\cdot(\Delta\mathbf{J}^{*p}) = -q^p\nabla\cdot\eta^p(r,t). \tag{7.15'}$$

The current source is from (7.12):

$$H(\mathbf{r},\mathbf{r}') = \int_0^\infty dt\, \mathcal{g}(\mathbf{k})\mathcal{g}(\mathbf{k}')\mathcal{g}(\mathbf{k}'')\mathbf{v}_\mathbf{k}\mathbf{v}_{\mathbf{k}'} \times [g(\mathbf{k},t;\mathbf{k}'',0)\Gamma(\mathbf{rk}'',\mathbf{r}'\mathbf{k}') + \text{conj}], \tag{7.16}$$

where $\mathcal{g}(\mathbf{k})$ means $\sum_p \int d^3k^p$. In case the Boltzmann equations for the various species are not coupled, $\mathcal{g}(k)$ reduces to $I(k)$, and only the diagonal elements $H^{pp}(\mathbf{r},\mathbf{r}')$ are of importance. When we compare (7.15) and (7.15') with (3.4) or (4.4), we see that the source H implies for the source Ξ of those sections

$$\Xi(\mathbf{r},\mathbf{r}') = \nabla_\mathbf{r}\nabla_{\mathbf{r}'}: \int_0^\infty dt I(\mathbf{k})I(\mathbf{k}')I(\mathbf{k}'')\mathbf{v}_\mathbf{k}\mathbf{v}_{\mathbf{k}'} \times [g(\mathbf{k},t;\mathbf{k}'',0)\Gamma(\mathbf{rk}'',\mathbf{r}'\mathbf{k}') + \text{conj}]. \tag{7.17}$$

In Sec. 5 we have seen that near thermal equilibrium $\Gamma(\mathbf{rk},\mathbf{r}'\mathbf{k}') \propto \delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{k}-\mathbf{k}')$. The $\mathbf{k}\,\delta$ function is integrated out, but the $\mathbf{r}\,\delta$ function remains. Thus, the source Ξ becomes of the form (2.9). The detailed result depends on the model employed to evaluate the remaining integrals in (7.17), as is discussed in the next section.

B. Momentum Transport

We sum the equations for all species and assume that the energy surfaces are spherical, $\hbar\mathbf{k}^p = m^p\mathbf{v}_\mathbf{k}$. Then writing

$$\mathbf{v}^p\mathbf{v}^p = (\mathbf{v}^p - \langle\mathbf{w}\rangle)(\mathbf{v}^p - \langle\mathbf{w}\rangle) + \mathbf{v}^p\langle\mathbf{w}\rangle + \langle\mathbf{w}\rangle\mathbf{v}^p - \langle\mathbf{w}\rangle\langle\mathbf{w}\rangle,$$

we obtain

$$\frac{\partial}{\partial t}[\Delta(\rho\mathbf{w})] + \nabla\cdot[\Delta(\rho\mathbf{w}\mathbf{w}) + \sum_p \overline{(\mathbf{v}^p - \langle\mathbf{w}\rangle)(\mathbf{v}^p - \langle\mathbf{w}\rangle)}\,\Delta\rho^p] - \sum_p \mathbf{F}^p\Delta\rho^p/m^p = \sum_p[-\nabla\cdot\boldsymbol{\pi}^p + \mathbf{F}^p\nu^p], \tag{7.18}$$

where $\boldsymbol{\pi}$ describe the pressure fluctuations and ν the particle fluctuations. The bar term can also be written as $\nabla\cdot\Delta P^*$, where P is the pressure tensor. In the absence of external fields, the noise sources are $\nabla\nabla'$: Π with the fourth-order tensor Π given by

$$\Pi(\mathbf{r},\mathbf{r}') = \int_0^\infty dt\, \mathcal{g}(\mathbf{v})\mathcal{g}(\mathbf{v}')\mathcal{g}(\mathbf{v}'')\mathbf{v}\mathbf{v}\mathbf{v}'\mathbf{v}'mm' \times [g(\mathbf{v}t;\mathbf{v}'',0)\Gamma(\mathbf{r}\mathbf{v}'',\mathbf{r}'\mathbf{v}') + \text{conj}]. \tag{7.19}$$

From Eq. (7.18) a stochastic Navier–Stokes equation can be derived. This will not be further pursued.

C. Heat Transport

With $\Psi = u^p = \frac{1}{2}m^p(\mathbf{v}^p - \mathbf{w})^2$ we can obtain a stochastic heat transport equation for a classical system with barycentric flow. The result is quite complex. We shall instead consider the heat flow in a one-component FD gas, such as for electrons in a metal. Let $\Psi = \mathcal{E}(\mathbf{k}) - q\Phi(\mathbf{r}) - \hat{\mu} = \mathcal{E}(\mathbf{k}) - \kappa(\mathbf{r})$, where $\Phi(\mathbf{r})$ is the electrical potential, $\kappa(\mathbf{r})$ is the chemical potential, and $\hat{\mu}$ is the electrochemical potential. The heat flux will be defined by[24]

$$\mathbf{K}(\mathbf{r},t) = \int d^3k[\mathcal{E}(k) - \kappa]\mathbf{v}_\mathbf{k}\, n(\mathbf{rk},t) = \overline{[\mathcal{E}(\mathbf{k}) - \kappa]\mathbf{v}_\mathbf{k}}\, n(\mathbf{r},t). \tag{7.20}$$

With the same notation as before, we obtain from (7.11)

$$\frac{\partial}{\partial t}[\overline{(\mathcal{E}-\kappa)}\,\Delta n] + \nabla\cdot\Delta\mathbf{K}^*(\mathbf{r},t) + \frac{\nabla\mu}{q}\cdot\Delta\mathbf{J}^* = -\nabla\cdot\epsilon - \nabla\hat{\mu}\cdot\eta, \tag{7.21}$$

where ϵ describes the energy flow fluctuations, and η the particle flow fluctuations as given by

(7.16). [We used here $\nabla_{\mathbf{k}}\mathcal{E} = \hbar\mathbf{v}_{\mathbf{k}}$ and $\hat{\mu} = \kappa + q\Phi$.] The last term in (7.21) stems from the Joule heating. We write again

$$\langle \epsilon(\mathbf{r},t)\epsilon(\mathbf{r}',t')\rangle = E(\mathbf{r},\mathbf{r}')\delta(t-t'),$$
$$\langle \epsilon(\mathbf{r},t)\eta(\mathbf{r}',t')\rangle = Z(\mathbf{r},\mathbf{r}')\delta(t-t'),$$

where

$$E(\mathbf{r},\mathbf{r}') = \int_0^\infty dt I(\mathbf{k})I(\mathbf{k}')I(\mathbf{k}'')(\mathcal{E}(\mathbf{k}) - \kappa(\mathbf{r})) \times (\mathcal{E}(\mathbf{k}') - \kappa(\mathbf{r}'))\mathbf{v}_{\mathbf{k}}\mathbf{v}_{\mathbf{k}'} \times [g(\mathbf{k},t;\mathbf{k}'',0)\Gamma(\mathbf{r}\mathbf{k}'',\mathbf{r}'\mathbf{k}') + \text{conj}], \quad (7.22)$$

$$Z(\mathbf{r},\mathbf{r}') = q\int_0^\infty dt I(\mathbf{k})I(\mathbf{k}')I(\mathbf{k}'')(\mathcal{E}(\mathbf{k}) - \kappa(\mathbf{r}))\mathbf{v}_{\mathbf{k}}\mathbf{v}_{\mathbf{k}'} \times [g(\mathbf{k},t;\mathbf{k}'',0)\Gamma(\mathbf{r}\mathbf{k}'',\mathbf{r}'\mathbf{k}') + \text{conj}]. \quad (7.23)$$

The total spectrum of the sources is now immediately found. Writing $\Delta\mathbf{K}^*$ and $\Delta\mathbf{J}^*$ in terms of grad $\hat{\mu}$ and grad T, we arrive at a stochastic heat conduction equation.

8. NOISE SOURCES AND TRANSPORT COEFFICIENTS

The various noise sources introduced are closely related to the transport coefficients. In a near-equilibrium state this is of course already borne out by the fluctuation–dissipation theorem. The results of this section then merely provide a microscopic basis for the validity of this theorem. In a steady state, new information can be obtained, not available from equilibrium statistical mechanics or near-equilibrium irreversible thermodynamics.

A. Hot-Electron Boltzmann Gas

In a steady state, far from equilibrium, it is expedient to consider the "differential transport coefficients" (cf. Price[25]). Thus, let there be a steady transport characterized by $\Lambda_{\text{force}} = (q/\hbar)(\mathbf{E}_0 + \mathbf{v}_{\mathbf{k}} \times \mathbf{B})\cdot\nabla_{\mathbf{k}}$, whereas there will be a position-dependent small perturbation

$$\Lambda' = (q\mathbf{E}'/\hbar)\cdot\nabla_{\mathbf{k}} + \mathbf{v}_{\mathbf{k}}\cdot\nabla_{\mathbf{r}}. \quad (8.1)$$

We write further

$$\langle n(\mathbf{r}\mathbf{k},t)\rangle = \phi^s(\mathbf{r}\mathbf{k}) + \phi'(\mathbf{r}\mathbf{k}). \quad (8.2)$$

As usual, the steady part ϕ^s must be reinterpreted as a *local* distribution; i.e., the integration constants of the steady-state solution are allowed to be position dependent. We assume that the perturbation is proportional to $e^{i\omega t}$. For $\mathbf{E}'$ this is easy to realize. A periodic diffusion is hypothetical in that we must vary some parameter of the local distribution (e.g., the electrochemical potential $\nabla_{\mathbf{r}} \to (\partial/\partial\hat{\mu})\nabla_{\mathbf{r}}\hat{\mu}^0 e^{i\omega t}$). Then, for the first-order perturbations, we have

$$(i\omega + \Lambda_{\text{force}} + \Lambda_{\text{coll}})\,\phi'(\mathbf{r}\mathbf{k}) = -\Lambda'\phi^s(\mathbf{r}\mathbf{k}). \quad (8.3)$$

The distribution $\phi'(\mathbf{r}\mathbf{k})$ may be further expanded according to powers of the magnetic field:

$$\phi' = \phi_0' + \phi_1' + \phi_2' + \cdots; \quad (8.4)$$

Eq. (8.3) then generates a series of equations, connecting functions of certain order to others which are one order lower (cf. Price[26]). We shall omit these refinements.

The solution of (8.3) and similar equations of Price are, in our notation,

$$\phi'(\mathbf{r}\mathbf{k}) = -(\Lambda + i\omega)^{-1}\Lambda'\phi^s(\mathbf{r}\mathbf{k}) = -\int_0^\infty e^{-i\omega t}dt I(\mathbf{k}')g(\mathbf{k},t;\mathbf{k}',0)\Lambda'\phi^s(\mathbf{r}\mathbf{k}'); \quad (8.5)$$

whence also,

$$\bar{\bar{\Psi}} \equiv \frac{1}{\phi^s(\mathbf{r})}\int \Psi(\mathbf{r}\mathbf{k})\phi'(\mathbf{r}\mathbf{k})d^3k = -\frac{1}{\phi^s(\mathbf{r})}\int_0^\infty e^{-i\omega t}dt I(\mathbf{k})I(\mathbf{k}')\Psi(\mathbf{r}\mathbf{k}) \times g[\mathbf{k},t;\mathbf{k}',0)\Lambda'\phi^s(\mathbf{r}\mathbf{k}'), \quad (8.6)$$

where the double bar denotes a $\mathbf{k}$-space average over the differential distribution $\phi'/\phi^s(\mathbf{r})$. In Price's notation we should introduce

$$\langle\Psi;t\rangle_{\text{cond}} = I(\mathbf{k})\Psi(\mathbf{r}\mathbf{k})g(\mathbf{k},t;\mathbf{k}',0); \quad (8.7)$$

this is kind of a "probability after effect" whereby the Green's function is interpreted as a conditional probability while the particle $\mathbf{k}$ vector undergoes Brownian motion (compare I, Sec. 1 for criticism on this view). From the last two equations we arrive at

$$\bar{\bar{\Psi}} = -\int_0^\infty e^{-i\omega t}dt I(\mathbf{k})\langle\Psi;t\rangle_{\text{cond}}\frac{\Lambda'\phi^s(\mathbf{r}\mathbf{k})}{\phi^s(\mathbf{r})} \doteq -\int_0^\infty e^{-i\omega t}dt I(\mathbf{k})\tilde{\Lambda}'\langle\Psi;t\rangle_{\text{cond}}\frac{\phi^s(\mathbf{r}\mathbf{k})}{\phi^s(\mathbf{r})}, \quad (8.8)$$

where $\tilde{\Lambda}'$ is the operator adjoint to Λ' [the last expression is only correct if Λ' does not work on the normalization function $\phi^s(\mathbf{r})$]. This is Price's result, obtained in a simple way, without the use of the conjugate quantities $\Psi^\dagger$ and the "integral method" introduced in his articles.[27, 28] Finally, using again the single bar to signify space averages over the stationary distribution $\phi^s/\phi^s(\mathbf{r})$,

$$\bar{\bar{\Psi}} \doteq -\int_0^\infty e^{-i\omega t}dt\,\overline{\tilde{\Lambda}'\langle\Psi;t\rangle}_{\text{cond}}. \quad (8.9)$$

The differential current $\mathbf{J}' = q\mathbf{v}'\phi^s(\mathbf{r})$ has a diffusion part $-q\nabla\cdot D^*\phi^s(\mathbf{r})$ and a conduction part $\sigma^*\cdot\mathbf{E}'$ according to the terms of Λ' in (8.1), where $D^*(\omega)$ and $\sigma^*(\omega)$ denote the differential diffusivity and conductivity. From (8.6) we find in a straightforward fashion

$$D^* = \int_0^\infty e^{-i\omega t} dt I(\mathbf{k}) I(\mathbf{k}') \mathbf{v}_\mathbf{k} \mathbf{v}_{\mathbf{k}'} g(\mathbf{k}, t; \mathbf{k}', 0) \frac{\phi^s(\mathbf{rk}')}{\phi^s(\mathbf{r})}, \tag{8.10}$$

$$\sigma^* = -q \int_0^\infty e^{-i\omega t} dt I(\mathbf{k}) I(\mathbf{k}') \mathbf{v}_\mathbf{k} g(\mathbf{k}; t; \mathbf{k}', 0) \hbar^{-1} \times \nabla_{\mathbf{k}'} \phi^s(\mathbf{rk}'). \tag{8.11}$$

Using Price's quantities (8.7), we obtain results that take a slightly different form:

$$D^* = \int_0^\infty e^{-i\omega t} dt \, \overline{\mathbf{v}\langle \mathbf{v}; t\rangle}_{\text{cond}}, \tag{8.10'}$$

$$\sigma^* = q\langle n^s(\mathbf{r})\rangle \int_0^\infty e^{-i\omega t} dt \, \hbar^{-1} \overline{\nabla_\mathbf{k} \langle \mathbf{v}_\mathbf{k}; t\rangle}_{\text{cond}}. \tag{8.11'}$$

For most frequencies of interest (up to Ghz range) the factor $e^{-i\omega t} \approx 1$; then $\int_0^\infty dt \langle \mathbf{v}; t\rangle_{\text{cond}}$ defines a vector mean free path $\mathbf{l}(\mathbf{k})$. Further, we let $\phi' \to 0$ and $\phi^s(\mathbf{rk}) \to \langle n(\mathbf{rk})\rangle$ *a posteriori*.

Price's formulas are particularly simple; it is tempting to interpret (8.10′) as the correlation function of the velocity fluctuations. Then, by the Wiener-Khintchine theorem the velocity fluctuation spectrum is $4D^*$ and the corresponding current fluctuation spectrum is $4D^*\langle n(\mathbf{r})\rangle\delta(\mathbf{r} - \mathbf{r}')$. According to Price, this is an *exact* result.

We believe, however, that this is incorrect. *By interpreting the Green's function as the conditional probability for changes in* $\mathbf{k}$, *independence of the carriers is tacitly assumed.*

Formulas (8.10′) and (8.11′) place the time dependence in the operators $\mathbf{v}(t)$, a sort of Heisenberg form, whereas formulas (8.10) and (8.11) vest the time dependence in the distribution function $\phi(\mathbf{rk}, t)$, a sort of Schrödinger form. In the quantum-statistical equilibrium treatment, the equivalence of these pictures is well founded and the Kubo formula, of which (8.10′) and (8.11′) are reminescent, results. In the steady state, as applicable to a hot-electron gas, the equivalence requires the validity of

$$\Gamma(\mathbf{rk}; \mathbf{r}'\mathbf{k}') = \langle n(\mathbf{rk})\rangle\delta(\mathbf{r} - \mathbf{r}')\delta(\mathbf{k} - \mathbf{k}'),$$

which can only be verified if the noise sources enter explicitly into the theory. We have seen that the above result is exact only if (a) electron–electron scattering is absent, (b) space-charge forces in the streaming terms are absent.

Under the above conditions, Price's results follow more directly from our expression (8.10). Comparison with (7.16) yields

$$\Sigma_g = 2H(\mathbf{r}, \mathbf{r}') = 4D^*\langle n(\mathbf{r})\rangle\delta(\mathbf{r} - \mathbf{r}'). \tag{8.12}$$

The equivalent noise temperature is found by setting

$$k\theta_i = q^2\langle n\rangle \mathrm{Re}D^*_{ii}/\mathrm{Re}\sigma^*_{ii}. \tag{8.13}$$

The calculation, involving the evaluation of the vector mean free path $\mathbf{l}(\mathbf{k})$ and its derivative $\partial\mathbf{l}/\partial\mathbf{k}$, was carried out by Price[25] and was compared with experiments by Erlbach and Gunn.[29] In thermal equilibrium Eq. (8.12) holds *a fortiori*, with $D^* \to D$ and $\theta_i = T$.

B. Heat Conductivity and Seebeck Effect in near Equilibrium

The general formulas for other transport coefficients in a near-equilibrium state are well known. In order to compare with the elementary treatments, we write also

$$g(\mathbf{k}'') \int_0^\infty dt \, g(\mathbf{k}, t; \mathbf{k}'', 0) \to \tau_{\text{op}}(\mathbf{k}), \tag{8.14}$$

where τ_{op} is a "relaxation time operator." Using (5.9) for a FD gas, with $\hat{\Gamma} \to 0$ for a near-equilibrium state, one easily finds for the noise sources (7.22) and (7.23):

$$E(\mathbf{r}, \mathbf{r}') = 2kT^2\boldsymbol{\lambda}\delta(\mathbf{r} - \mathbf{r}'), \tag{8.15}$$

$$Z(\mathbf{r}, \mathbf{r}') = 2kT^2\boldsymbol{\sigma}\cdot\boldsymbol{\theta}\delta(\mathbf{r} - \mathbf{r}'), \tag{8.16}$$

where $\boldsymbol{\lambda}$ is the heat conductivity, $\boldsymbol{\sigma}$ the electrical conductivity, and $\boldsymbol{\theta}$ is the Seebeck tensor. The last result can also be expressed in the Peltier tensor $\boldsymbol{\pi}$ noticing $\boldsymbol{\pi}(\mathbf{B}) = T\boldsymbol{\theta}^{\text{tr}}(-\mathbf{B})$. In all instances, generalized Nyquist relations are obtained.

ACKNOWLEDGMENTS

The original stimulus to this paper and the previous one came from unresolved problems of noise in solid-state devices, suggested to me by Professor A. van der Ziel at the University of Minnesota. I have also benefitted from discussions on space-charge-limited flow with Dr. J. J. Zijlstra of the University of Utrecht. I am indebted to Professor M. Kac, who, after the completion of this paper brought to my attention recent work by R. F. Fox at Rockefeller University, also dealing with a stochastic Boltzmann equation.[30]

[1] K. M. van Vliet, preceeding paper, J. Math. Phys. **12**, 1981 (1971).
[2] Lord Rayleigh, Phil. Mag. **47**, 246 (1899).
[3] G. Uhlenbeck and L. S. Ornstein, Phys. Rev. **36**, 823 (1930); S. Chandrasekhar, Rev. Mod. Phys. **17**, 323 (1945).
[4] A. van der Ziel, Proc. IRE **43**, 1639 (1955).
[5] K. M. van Vliet, Solid-State Electron. **13**, 649 (1970).
[6] P. Debye and G. Hückel, Physik. Zeitschrift **24**, 305 (1923).
[7] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley, Reading, Mass., 1958), Sec. 74; see also N. N. Bogolyubov, J. Phys. USSR **10**, 256 (1946).
[8] For a Fermi gas we should have used the generalized Einstein relation

$$qD = \mu kT[\mathfrak{F}_{1/2}(\mathcal{E}_F/kT)/\mathfrak{F}_{1/2}(\mathcal{E}_F/kT)] \equiv \mu kT\theta,$$

where $\mathcal{E}_F$ is the Fermi level and $\mathfrak{F}_\eta$ is a Fermi integral. The

result for the Debye length $\varkappa^{-1}$ is changed accordingly, and is found in accord with the result from statistical mechanics (Ref. 7, Landau and Lifshitz, Eq. (74. 16)).

[9] M. Lax and P. Mengert, J. Phys. Chem. Solids **14**, 248 (1960), Appendix C.

[10] M. L. Tarng, "Fluctuations in PN Junctions at High Injection Levels", Ph. D. Thesis (Univ. of Minnesota, 1969).

[11] A. van der Ziel and K. M. van Vliet, Solid-State Electron. **11**, 508 (1968).

[12] V. Sergescu and A. Friedman, Brit. J. Appl. Phys. **18**, 124 (1967); Rev. Roumanium Phys. **12**, 457 (1967); Phys. Status Solidi **28**, 385 (1968).

[13] K. M. van Vliet and J. R. Fassett, in *Fluctuation Phenomena in Solids*, edited by R. E. Burgess (Academic, New York, 1965), p. 267, in particular, Secs. V and VI.

[14] By the operator $[(1/u)(\partial/\partial u)]^2$ we mean

$$\frac{1}{u}\frac{\partial}{\partial u}\left[\frac{1}{u}\frac{\partial}{\partial u}(\cdots)\right];$$

similar for higher powers.

[15] We assumed that at the far end from the space-charge minimum, $u = 1$, the effect of $\mathfrak{V}_1$ is zero.

[16] A. van der Ziel, Solid-State Electron. **9**, 1139 (1966).

[17] M. Lax, Rev. Mod. Phys. **32**, 25 (1960), Sec. 12.

[18] J. L. Delcroix, in *La théorie des Gaz Neutres et Ionisés*, edited by C. de Witt and J. F. Detoeuf (Hermann, Paris, 1960).

[19] The δ function in (5. 1) can of course not be exact since we must take into account the size of the scatterers. More important, however, use of the quantum-mechanical picture on a local scale, as it follows from Wannier's theorem, cannot be strictly justified; see J. C. Slater, Phys. Rev. **76**, 1592 (1949).

[20] S. Tsugé, J. Phys. Soc. Japan **26**, Suppl. 246 (1969), Phys. Letters **26A**, 236 (1968).

[21] S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam, 1962), Chap. IX.

[22] For two-body collisions between unlike particles the scattering function is $\mathfrak{L}(k^p k^q, k'^p k'^q)$ and the double sum of the lhs of (7. 5) is essential.

[23] The source term of $\partial(\mathfrak{Vn})/\partial t$ is neglected again for sufficiently small ω.

[24] The "heat flux" used here is actually the entropy flux times T; this is correct for our choice of forces ∇T and $\nabla\hat{\mu}$ [cf. Ref. 21 and J. M. Ziman, *Phonons and Electrons* (Oxford U. P., New York, 1960)].

[25] P. J. Price, in Ref. 13, p. 355.

[26] P. J. Price, IBM J 1, 239, (1957).

[27] P. J. Price, IBM J 2, 200 (1958).

[28] P. J. Price, J. Phys. Chem. Solids **8**, 136 (1959)

[29] E. Erlbach and J. B. Gunn, in *Proceedings of the International Conference of the Physics of Semiconductors*, 1962 (Institute of Physics and the Physical Society, London, 1962), p. 128.

[30] R. F. Fox, "Contributions to the Theory of Non-equilibrium Thermodynamics," Ph.D. Thesis (Rockefeller University, New York, 1969); R. F. Fox and G. E. Uhlenbeck, Phys. Fluids **13**, 2881 (1970).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Double Laplace Transformation in Mixed Boundary-Initial Value Problems

Kenneth Evans, Jr., and E. Atlee Jackson
Department of Physics and Coordinated Science Laboratory, University of Illinois, Urbana, Illinois
(Received 11 May, 1970; Revised Manuscript Received 4 January 1971)

A comprehensive treatment of the application of the double Laplace transform to the combined boundary-initial value problem for systems of linear, hyperbolic, partial differential equations with constant coefficients is given. The treatment is restricted to two independent variables x and t. A discussion of the relations among the boundary and initial conditions necessary for a well-formulated problem is given, and it is shown that the solution subject to these restrictions does satisfy the boundary and initial conditions. An extensive examination of the solution in different regions of space-time is given, and the connection between this solution and the more common "normal-mode" solution proportional to $\exp[ikx - i\omega_l(k)t]$ or $\exp[ik_l(\omega)x - i\omega t]$ is discussed. A generalized wave equation is used throughout the paper for illustration.

1. INTRODUCTION

In this paper various aspects of the mixed boundary-initial value problem for systems of linear, hyperbolic, partial differential equations of two variables x, t are discussed. Such systems of equations arise in linearized treatments of the dynamical properties of many physical systems, especially in connection with the stability properties of prescribed states. A natural method for obtaining the solutions of these types of equations in the region $x \geq 0, t \geq 0$ is to use double Laplace transformation. This paper gives a comprehensive treatment of the application of this method to the mixed boundary-initial value problem.

Depending on the characteristics of the system of differential equations, the inverse Laplace transformation is not always defined for arbitrary boundary and initial conditions. A prescription for treating this difficulty has been proposed by several authors.[1-3] In this paper the content of this prescription is clarified, and it is proved that the prescription leads to a solution satisfying the prescribed boundary and initial conditions. A well-formulated expression for the general solution is obtained, and the character of this expression in different regions of space-time as well as its relationship to more common expressions, is extensively discussed.

In the usual treatments of the equations described above, the initial and boundary value problems are treated separately. A method commonly used is to assume a solution proportional to e^{ikx} (for initial value problems) or $e^{-i\omega t}$ (for boundary value problems) and to Laplace or Fourier transform in the remaining variable. In this way one obtains "normal-mode" solutions which are proportional to $\exp[ikx - i\omega_l(k)t]$ or $\exp[ik_l(\omega)x - i\omega t]$, where $\omega_l(k)$ and $k_l(\omega)$ are roots of a dispersion relation $D(k, \omega) = 0$. Such solutions, of course, are not valid in all parts of the space-time region $x \geq 0$, $t \geq 0$ if the system is bounded at $x = 0$ and subject to initial conditions at $t = 0$. One of the objectives of the present paper is to clarify the relationship between the general solutions and these normal-

result for the Debye length $\varkappa^{-1}$ is changed accordingly, and is found in accord with the result from statistical mechanics (Ref. 7, Landau and Lifshitz, Eq. (74. 16)).

[9] M. Lax and P. Mengert, J. Phys. Chem. Solids **14**, 248 (1960), Appendix C.

[10] M. L. Tarng, "Fluctuations in PN Junctions at High Injection Levels", Ph. D. Thesis (Univ. of Minnesota, 1969).

[11] A. van der Ziel and K. M. van Vliet, Solid-State Electron. **11**, 508 (1968).

[12] V. Sergescu and A. Friedman, Brit. J. Appl. Phys. **18**, 124 (1967); Rev. Roumanium Phys. **12**, 457 (1967); Phys. Status Solidi **28**, 385 (1968).

[13] K. M. van Vliet and J. R. Fassett, in *Fluctuation Phenomena in Solids*, edited by R. E. Burgess (Academic, New York, 1965), p. 267, in particular, Secs. V and VI.

[14] By the operator $[(1/u)(\partial/\partial u)]^2$ we mean

$$\frac{1}{u}\frac{\partial}{\partial u}\left[\frac{1}{u}\frac{\partial}{\partial u}(\cdots)\right];$$

similar for higher powers.

[15] We assumed that at the far end from the space-charge minimum, $u = 1$, the effect of $\mathfrak{V}_1$ is zero.

[16] A. van der Ziel, Solid-State Electron. **9**, 1139 (1966).

[17] M. Lax, Rev. Mod. Phys. **32**, 25 (1960), Sec. 12.

[18] J. L. Delcroix, in *La théorie des Gaz Neutres et Ionisés*, edited by C. de Witt and J. F. Detoeuf (Hermann, Paris, 1960).

[19] The δ function in (5. 1) can of course not be exact since we must take into account the size of the scatterers. More important, however, use of the quantum-mechanical picture on a local scale, as it follows from Wannier's theorem, cannot be strictly justified; see J. C. Slater, Phys. Rev. **76**, 1592 (1949).

[20] S. Tsugé, J. Phys. Soc. Japan **26**, Suppl. 246 (1969), Phys. Letters **26A**, 236 (1968).

[21] S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam, 1962), Chap. IX.

[22] For two-body collisions between unlike particles the scattering function is $\mathfrak{L}(k^p k^q, k'^p k'^q)$ and the double sum of the lhs of (7. 5) is essential.

[23] The source term of $\partial(\mathfrak{Vn})/\partial t$ is neglected again for sufficiently small ω.

[24] The "heat flux" used here is actually the entropy flux times T; this is correct for our choice of forces ∇T and $\nabla\hat{\mu}$ [cf. Ref. 21 and J. M. Ziman, *Phonons and Electrons* (Oxford U. P., New York, 1960)].

[25] P. J. Price, in Ref. 13, p. 355.

[26] P. J. Price, IBM J 1, 239, (1957).

[27] P. J. Price, IBM J 2, 200 (1958).

[28] P. J. Price, J. Phys. Chem. Solids **8**, 136 (1959)

[29] E. Erlbach and J. B. Gunn, in *Proceedings of the International Conference of the Physics of Semiconductors*, 1962 (Institute of Physics and the Physical Society, London, 1962), p. 128.

[30] R. F. Fox, "Contributions to the Theory of Non-equilibrium Thermodynamics," Ph.D. Thesis (Rockefeller University, New York, 1969); R. F. Fox and G. E. Uhlenbeck, Phys. Fluids **13**, 2881 (1970).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Double Laplace Transformation in Mixed Boundary-Initial Value Problems

Kenneth Evans, Jr., and E. Atlee Jackson
Department of Physics and Coordinated Science Laboratory, University of Illinois, Urbana, Illinois
(Received 11 May, 1970; Revised Manuscript Received 4 January 1971)

A comprehensive treatment of the application of the double Laplace transform to the combined boundary-initial value problem for systems of linear, hyperbolic, partial differential equations with constant coefficients is given. The treatment is restricted to two independent variables x and t. A discussion of the relations among the boundary and initial conditions necessary for a well-formulated problem is given, and it is shown that the solution subject to these restrictions does satisfy the boundary and initial conditions. An extensive examination of the solution in different regions of space-time is given, and the connection between this solution and the more common "normal-mode" solution proportional to $\exp[ikx - i\omega_l(k)t]$ or $\exp[ik_l(\omega)x - i\omega t]$ is discussed. A generalized wave equation is used throughout the paper for illustration.

1. INTRODUCTION

In this paper various aspects of the mixed boundary-initial value problem for systems of linear, hyperbolic, partial differential equations of two variables x, t are discussed. Such systems of equations arise in linearized treatments of the dynamical properties of many physical systems, especially in connection with the stability properties of prescribed states. A natural method for obtaining the solutions of these types of equations in the region $x \geq 0, t \geq 0$ is to use double Laplace transformation. This paper gives a comprehensive treatment of the application of this method to the mixed boundary-initial value problem.

Depending on the characteristics of the system of differential equations, the inverse Laplace transformation is not always defined for arbitrary boundary and initial conditions. A prescription for treating this difficulty has been proposed by several authors.[1-3] In this paper the content of this prescription is clarified, and it is proved that the prescription leads to a solution satisfying the prescribed boundary and initial conditions. A well-formulated expression for the general solution is obtained, and the character of this expression in different regions of space-time as well as its relationship to more common expressions, is extensively discussed.

In the usual treatments of the equations described above, the initial and boundary value problems are treated separately. A method commonly used is to assume a solution proportional to e^{ikx} (for initial value problems) or $e^{-i\omega t}$ (for boundary value problems) and to Laplace or Fourier transform in the remaining variable. In this way one obtains "normal-mode" solutions which are proportional to $\exp[ikx - i\omega_l(k)t]$ or $\exp[ik_l(\omega)x - i\omega t]$, where $\omega_l(k)$ and $k_l(\omega)$ are roots of a dispersion relation $D(k, \omega) = 0$. Such solutions, of course, are not valid in all parts of the space-time region $x \geq 0$, $t \geq 0$ if the system is bounded at $x = 0$ and subject to initial conditions at $t = 0$. One of the objectives of the present paper is to clarify the relationship between the general solutions and these normal-

mode solutions. It is shown that the normal modes $\exp[ikx - i\omega_l(k)t]$ are valid in general only for $x > ct$, whereas the modes $\exp[ik_l(\omega)x - i\omega t]$ are valid in general only if $c't > x$, where c and c' are non negative constants related to the characteristic velocities of the system. Moreover, when the normal-mode solution is not valid, it becomes clear in what manner complicated transient behavior takes its place. Even if transient effects are not of primary interest, there is a considerable conceptual advantage in understanding how these normal-mode solutions fit into the general solutions. There are, in fact, situations in which non-normal-mode solutions may persist for all $t > x/c$, a fact easily understood from the general analysis.

To illustrate many of the points in the following sections, the generalized wave equation (GWE):

$$\left[\left(\frac{\partial}{\partial t} + c_1\frac{\partial}{\partial x}\right)\left(\frac{\partial}{\partial t} + c_2\frac{\partial}{\partial x}\right) - b_1b_2\right] f(x,t) = 0 \tag{1.1}$$

is employed. This equation is equivalent to the following system of equations:

$$\frac{\partial f_1}{\partial t} + c_1\frac{\partial f_1}{\partial x} + b_1 f_2 = 0, \tag{1.2}$$

$$\frac{\partial f_2}{\partial t} + c_2\frac{\partial f_2}{\partial x} + b_2 f_1 = 0. \tag{1.3}$$

These equations reduce to the usual wave equation if $c_1 = -c_2$ and $b_1 = b_2 = 0$. Depending on the values of c_1, c_2, b_1, and b_2, this system can exhibit various types of instabilities or propagating properties.

The organization of the paper is as follows: Section 2 deals with the equations to be treated and the known existence–uniqueness theorems. The double Laplace transformation is discussed in Sec. 3. Section 4 contains a review of the definition of characteristics for systems of equations and their relationship to the dispersion relation. Sections 5 and 6 treat the restrictions among the boundary and initial conditions necessary for a well-formulated problem. The demonstration that the solution does satisfy the boundary and initial conditions is given in Sec. 7. Section 8 contains a discussion of the solution in the various regions of space–time. Finally, Sec. 9 gives the relationship between the general solutions and the normal-mode solutions. The reader interested in only the mechanics of the method, which is fairly straightforward, might omit the discussion on the definition of hyperbolic systems and the related existence–uniqueness theorems in Sec. 2, all of Sec. 7, and possibly Sec. 9.

2. FORM OF THE EQUATIONS

This paper treats systems of first-order, linear, homogeneous, partial differential equations with real, constant coefficients. The method is applicable, however, to single higher-order equations with constant coefficients since they can be equivalently written as systems of first-order equations.[4] For the sake of transparency, only two independent variables, x and t, are considered. Only systems with the same number N of unknowns and equations are treated. The equations to be considered are then of the form:

$$a_{ij}\frac{\partial f_j}{\partial t} + b_{ij}\frac{\partial f_j}{\partial x} + c_{ij}f_j = 0, \qquad i,j = 1,\cdots,N. \tag{2.1}$$

Summation with respect to repeated indices is understood throughout this paper, the $f_i = f_i(x,t)$ are the N unknown functions, and a_{ij}, b_{ij}, and c_{ij} are elements of real, constant $N \times N$ matrices.

In addition, only those systems of the above form which are hyperbolic as defined by Gelfand and Shilov[5] are considered. This definition, paraphrased slightly, is as follows: First, $\det|a_{ij}|$ is assumed nonzero. The roots of the polynomial

$$D(p,q) = \det|a_{ij}p + b_{ij}q + c_{ij}| \tag{2.2}$$

are denoted by $p_l(q), l = 1,\cdots,N$, and the function $P(q)$ is defined as follows:

$$P(q) = \max\{\mathrm{Re}\,p_i(q) \mid i = 1,\cdots,N\}. \tag{2.3}$$

The system (2.1) is then hyperbolic if $P(q)$ is bounded by a linear function of $|q|$:

$$P(q) \le A|q| + B, \tag{2.4}$$

and for purely imaginary $q = ik$, $P(q)$ is bounded:

$$P(ik) \le C. \tag{2.5}$$

Systems which are hyperbolic in this sense are precisely those for which the Cauchy problem [determination of a solution which satisfies $f_i(x,0) = \phi_i(x), i = 1,\cdots,N$ for given initial conditions $\phi_i(x)$ specified for all x] is well posed in the region $t \ge 0$, $|x| < \infty$ for sufficiently smooth initial conditions; that is, the solution exists, is unique, and depends continuously on the initial conditions.[6–8]

While the preceding definition of hyperbolicity is the most useful in consideration of the Cauchy problem, another, more restrictive definition seems to be more appropriate for the mixed problem (determination of a solution which satisfies specified initial conditions at $t = 0$ and boundary conditions at $x = 0$). This definition, due to Courant and Hilbert[9] and also slightly paraphrased, is as follows: It is assumed that $\det|a_{ij}| \neq 0$. The system (2.1) is hyperbolic (in this sense) if the roots $c_i, i = 1,\cdots,N$ of the equation

$$Q = \det|-ca_{ij} + b_{ij}| = 0 \tag{2.6}$$

are real, and in addition the matrix $A^{-1}B$ has N linearly independent eigenvectors $l_i, i = 1,\cdots,N$.

(A is the matrix with elements a_{ij}, and B, the matrix with elements b_{ij}.) Equations which are hyperbolic according to the second definition are linearly equivalent to a system

$$\frac{\partial F_i}{\partial t} + c_i \frac{\partial F_i}{\partial x} + c'_{ij} F_j = 0, \quad i,j = 1, \cdots, N, \tag{2.7}$$

where the $F_i = F_i(x,t)$ are linear combinations of the $f_i(x,t)$, and the c'_{ij} are the elements of a constant matrix. [The index i is not summed in Eq. (2.7).] The form (2.7) is called the normal form of Eq. (2.1) when it exists. This second definition has the advantage that for systems of this type the problem of finding a solution for the following specification of initial and boundary conditions is well posed in the region $x \geq 0, t \geq 0$.[10] The functions $f_i(x,0) = \phi_i(x)$ are specified at $t = 0$ for $x \geq 0$, and if there are M of the c_i which satisfy $c_i > 0$, then M of the functions $f_i(0,t) = \psi_i(t)$ are specified at $x = 0$ for $t \geq 0$. The M functions $f_i(0,t)$ which are specified must be chosen so the remaining $N - M$ functions can be expressed linearly in terms of them. The converse of this theorem, that is, that only those systems which are hyperbolic according to the second definition have solutions to the problem described, is not proved to the best of the authors' knowledge, as was the converse of the corresponding theorem applicable to the Cauchy problem.

The rationale for using the first definition in this work is simply that there are systems of physical interest which are hyperbolic according to the first definition but not according to the second definition. The discussion of this paper seems to apply to at least some of these systems. The distinction between the two definitions lies in systems in which two or more of the c_i are equal. (If all the c_i are distinct, there always exist N linearly independent eigenvectors l_i of the matrix $A^{-1}B$.) The lack of a converse to the existence–uniqueness theorem for the mixed problem leads one to hope that an existence–uniqueness theorem in some form also exists for those equations to be considered which are not hyperbolic according to the second definition.

3. DOUBLE LAPLACE TRANSFORMATION OF THE EQUATIONS

As stated in the Introduction, the method of solution of the equations defined in Sec. 2 is to be double Laplace transformation. This method is especially appropriate for the mixed boundary–initial value problem in the region $x \geq 0, t \geq 0$. The transforms are defined as follows:

$$F_i(p,q) = \int_0^\infty dt \int_0^\infty dx\, e^{-pt-qx} f_i(x,t), \tag{3.1}$$

$$f_i^I(p) = \int_0^\infty dt\, e^{-pt} f_i(0,t), \tag{3.2}$$

$$f_i^{II}(q) = \int_0^\infty dx\, e^{-qx} f_i(x,0). \tag{3.3}$$

$F_i(p,q)$ is the double transform of $f_i(x,t)$, and $f_i^I(p)$ and $f_i^{II}(q)$ are the single transforms of $f_i(0,t)$ and $f_i(x,0)$, respectively. The boundary and initial conditions are assumed to be Laplace transformable. The inverses are given by[1,11]

$$f_i(x,t) = (2\pi i)^{-2} \int_{C_p} dp \int_{C_q} dp\, e^{pt+qx} F_i(p,q), \tag{3.4}$$

$$f_i(0,t) = (2\pi i)^{-1} \int_{C_p} dp\, e^{pt} f_i^I(p), \tag{3.5}$$

$$f_i(x,0) = (2\pi i)^{-1} \int_{C_q} dq\, e^{pt} f_i^{II}(q). \tag{3.6}$$

The contours C_p and C_q are the usual Bromwich contours, which are straight lines $p = p_0 + i\sigma$ and $q = q_0 + i\tau$, where σ and τ vary from $-\infty$ to $+\infty$, and p_0 and q_0 must be chosen so that the contours lie to the right of all singularities in the p and q planes, respectively. It is seen in Secs. 5 and 6 that this procedure is not defined in some cases unless the transforms $f_i^I(p)$ and $f_i^{II}(q)$ are suitably restricted.

To find the Laplace transformed solution to Eqs. (2.1), the equations are multipled by $\exp(-pt - qx)$ and integrated over t and x from 0 to ∞. After integrating by parts,[1,11] the equations become

$$[a_{ij}p + b_{ij}q + c_{ij}]F_j(p,q) = a_{ij} f_j^{II}(q) + b_{ij} f_j^I(p). \tag{3.7}$$

These equations form an algebraic system of equations whose solution is

$$F_i(p,q) = [a_{jk} f_k^{II}(q) + b_{jk} f_k^I(p)]\, d_{ji}(p,q)/D(p,q), \tag{3.8}$$

where

$$\Delta_{ij} = \Delta_{ij}(p,q) = a_{ij}p + b_{ij}q + c_{ij}, \tag{3.9}$$

$$D = D(p,q) = \det|\Delta_{ij}|, \tag{3.10}$$

$$d_{ij} = d_{ij}(p,q) = \text{cofactor of } \Delta_{ij}. \tag{3.11}$$

The unknown functions $f_i(x,t)$ are then given by Eq. (3.4) along with Eq. (3.8).

If one had treated Eqs. (2.1) by Fourier transformation, the exponential factor in the integral (3.4) would have been $\exp(ikx - i\omega t)$ instead of $\exp(pt + qx)$. The relationship between (k,ω) and (p,q) is then $p = -i\omega$ and $q = ik$.

4. CHARACTERISTICS

Characteristics are widely known to play an important part in the theory of partial differential equations. In many physical treatments, however, the emphasis is placed on the dispersion relationship, and the characteristics are slighted. In this paper the important role played by the characteristics is emphasized.

The characteristic determinant of the system of equations (2.1) is defined by

$$Q\left(\frac{\partial \phi}{\partial t}, \frac{\partial \phi}{\partial x}\right) = \det\left| a_{ij} \frac{\partial \phi}{\partial t} + b_{ij} \frac{\partial \phi}{\partial x} \right|, \qquad (4.1)$$

and the characteristics are given in terms of the solutions $\phi_l = \phi_l(x,t), l = 1, \cdots, N$ of $Q = 0$ by $\phi_l(x,t) = \text{const.}$[12] For the case of constant a_{ij} and b_{ij} the ϕ_l are in the form $\phi_l(x,t) = x - c_l t$. The $c_l, l = 1, \cdots, N$, which are called the characteristic velocities, are the same quantities which appeared in the second definition of hyperbolicity. For equations of the type considered here, the c_l are real and constant.

The equation $D(p,q) = 0$ is the dispersion relation for the system (2.1). [$D(p,q)$ is defined in Eq. (3.10).] There is a simple but important relation between the roots $p_l(q), l = 1, \cdots, N$ of the dispersion relation and the characteristic velocities $c_l(q)$.[13,14] Since

$$D(p,q) = \det|a_{ij}p + b_{ij}q + c_{ij}| \xrightarrow[|p|,|q|\to\infty]{} Q(p,q), \qquad (4.2)$$

the roots $p_l(q)$ are asymptotically equal to $-c_l q$. Thus each root $p_l(q)$ can be associated with the characteristic velocity c_l. (This association is not necessarily unique. See Sec. 6.)

It is common to represent the roots of the dispersion relation on a dispersion diagram. This diagram shows $\omega_l(k)$, when $\omega_l(k)$ and k are real ($p = -i\omega, q = ik$). Such a diagram is shown in Fig. 1 for the GWE for various choices of the characteristic velocities and the quantity $b_1 b_2$. (The four diagrams shown represent the four basic types of instability, which are distinguished in part by the slope of the characteristics. This is another example of the physical importance of characteristics and has been discussed by Akhiezer *et al.*[13])

5. RELATIONS AMONG THE BOUNDARY CONDITIONS

As was noted in Sec. 2, the expression (3.4) does not always represent a solution unless the boundary and initial conditions are suitably restricted. There are essentially two kinds of restrictions, and these are treated in this and the following sections. The type of restriction treated in this section occurs if one or more families of characteristics lie parallel to the boundary $x = 0$,[12] that is, if some of the c_i are zero. [No families of characteristics lie parallel to the boundary $t = 0$ corresponding to $c_i = \infty$, for if this were the case, the system (2.1) would not be hyperbolic.[15]]

If there are L families of characteristics parallel to the boundary $x = 0$, then L of the $\phi_i(x,t)$ must be of the form $\phi_i(x,t) = x$. In that case, the characteristic determinant, Eq. (4.1), becomes $Q = \det|b_{ij}| = 0$. Thus there are characteristics parallel to the boundary $x = 0$ if and only if $\det|b_{ij}| = 0$. (Similarly there are characteristics parallel to the line $t = 0$ if and only if $\det|a_{ij}| = 0$. It has been assumed that $\det|a_{ij}| \neq 0$, so there cannot be characteristics along $t = 0$.)

It follows that if there are characteristics on the boundary $x = 0$, the rank R of the matrix with elements b_{ij} must be less than N. (It is *not* necessary that $R = N - L$, only that $R \geq N - L$.) In this case there are $N - R$ linearly independent solutions $l_i^{(k)}$, $k = 1, \cdots, N - R$ and $i = 1, \cdots, N$ of the equations $l_i^{(k)} b_{ij} = 0$ for $j = 1, \cdots, N$. If Eqs. (2.1) are multiplied by $l_i^{(k)}$ and summed and x is set equal to zero, the result is

$$l_i^{(k)}\left(a_{ij} \frac{\partial f_j}{\partial t}(0,t) + c_{ij} f_{ij}(0,t)\right) = 0. \qquad (5.1)$$

These equations can be seen to be $N - R$ relations that must be satisfied by the boundary conditions $f_i(0,t)$ as a consequence of characteristics lying on the boundary $x = 0$. This result is not so recondite, in that it merely states that the boundary conditions must be chosen to satisfy the system of equations (2.1) when $x = 0$. If Eqs. (5.1) are Laplace transformed, corresponding relations among the $f_i^I(p)$ are obtained:

$$l_i^{(k)}[(a_{ij}p + c_{ij}) f_j^I(p)] = l_i^{(k)} a_{ij} f_j(0,0). \qquad (5.2)$$

As an example of this type of restriction one may take the GWE with $b_1 = b_2 = 0$, and $c_2 > 0$. Such an equation describes wave motion in a medium moving with a velocity equal to the wave velocity in the medium when the latter is at rest. The velocity c_2 is twice this velocity. Equation (5.1) gives the relation among the boundary conditions to be $\partial f_1(x = 0, t)/\partial t = 0$. The known general solution of these equations is

$$f_1(x,t) = f(x - c_1 t) = f(x), \qquad (5.3)$$

$$f_2(x,t) = g(x - c_2 t), \qquad (5.4)$$

where f and g are arbitrary, sufficiently differentiable functions. Since $f_1(x = 0, t) = f(0) = \text{const}$, the relation is satisfied by this solution.

6. RELATIONS AMONG THE BOUNDARY AND INITIAL CONDITIONS

The restrictions on the boundary conditions treated in the last section occur if some of the c_i are zero. The restrictions treated in this section

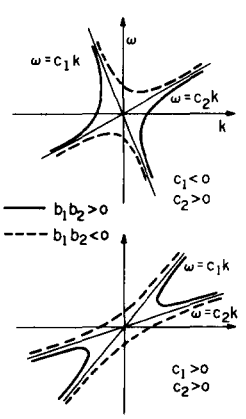

Fig. 1. Relationship between the characteristics and the asymptotes of the dispersion diagram for the generalized wave equation.

occur if some of the c_i are negative. Figure 2 demonstrates how information specified at $t = 0$ is carried throughout the system. If, as is shown in this figure, there are characteristics with $c_i < 0$, then some of this information is transmitted back to the boundary $x = 0$. It is to be expected, then, that any additional information specified at $x = 0$ must be comptatible with the information which is propagated to $x = 0$ from conditions specified at $t = 0$.

To see how this restriction occurs mathematically, it should be recalled that the contours C_p and C_q for the inversion integral (3.4) must lie to the right of all singularities in their respective planes.

Now if there are some $c_i < 0$, then the corresponding roots of the dispersion relation $p_i(q) \to |c_i| q$ as $q \to \infty$. Since $D(p, q) = 0$ at $p = p_i(q)$, the integrand in (3.4) has a pole at $p = p_i(q)$. There is a corresponding pole in the q plane at $q_i(p) \to |c_i|^{-1} p$. For roots of this type ($c_i < 0$), there is no way to choose the contours C_p and C_q both to the right of singularities in their respective planes. To see how this comes about, assume q_0 is chosen so that C_q lies to the right of $q_i(p_0)$. See Fig. 3. It is then necessary that $p_i(q_0)$ lie to the right of C_p in the p plane, a prohibited situation. The effect of such a situation would be to make the integral (3.4) divergent. The corresponding case for $c_i > 0$, for which there is no such problem, is also shown in Fig. 3.

The most obvious solution to this problem is to set the residues of these poles equal to zero, that is,

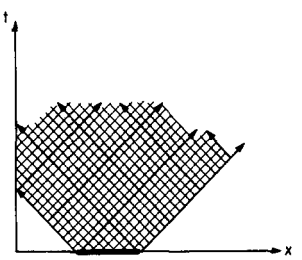

Fig. 2. A schematic illustration of how information specified at $t = 0$ is transmitted through the system along the characteristics.

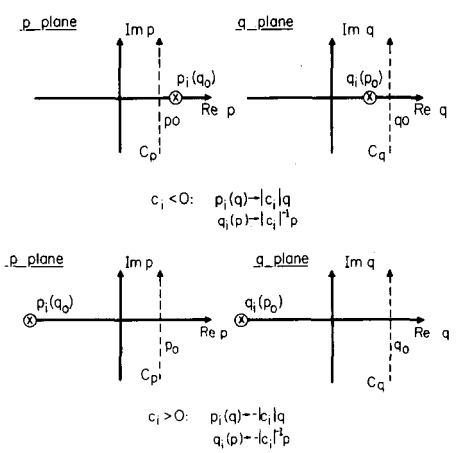

Fig. 3. Impossibility of constructing Bromwich contours C_p and C_q when there are negative characteristic velocities. The corresponding case for positive-characteristic velocities is also shown.

to eliminate the poles. This is the approach taken by several authors.[1-3] None of these authors has, however, examined the consequences of this approach, apart from particular examples. In fact, it is not generally the case that the above prescription is unique, although the lack of uniqueness is of no real consequence.

The question of uniqueness is treated first. It is usually the case that two roots $p_i(q)$ and $p_j(q)$, $i \neq j$ correspond to two Riemann sheets of the same function. If the cut between the two sheets is taken differently, the roots have different values for some values of q. There is no reason to specify that the cuts be made in a particular way, and in fact, it is convenient to be able to choose them in different ways for different purposes. If the $p_i(q)$ are not unique, then setting a residue equal to zero at $p = p_i(q)$ is not a unique prescription. This difficulty is resolved by noting that it is only necessary to set the residue equal to zero for p and q on and to the right of C_p and C_q, respectively. In this region the roots $p_i(q)$ are uniquely specified by their asymptotic values. (C_p and C_q are to the right of any branch points.) For the integration in (3.4) it is only necessary to know the integrand for values of p and q on their respective contours C_p and C_q. Changing the cuts does not change the value of the integrand on the contour. If it is desired to know the integrand in the region to the left of the contours, it may be obtained by analytic continuation. It can be seen, then, that even though the prescription is not unique, the results when inverted to (x, t) space are unique.

The next problem is to find what restrictions on the boundary and initial conditions are obtained from this prescription. If it is assumed that the roots $p_i(q)$ which are connected with negative characteristic velocities are all distinct,[16] then it is sufficient to set

$$[a_{jk} f_k^{II}(q) + b_{jk} f_k^{I}(p)] d_{ji}(p, q) = 0 \qquad (6.1)$$

at each of the roots $p_i(q)$ [or $q_i(p)$] which are associated with negative characteristic velocities. Equation (6.1) is a restriction among the boundary and initial conditions. It appears, however, that there are, in fact, N restrictions [one for each value of i in Eq. (6.1)] for each root associated with a negative characteristic velocity. There is , in fact, only one restriction. In order to see this, it is convenient to consider the equation for expanding a determinant in terms of its cofactors:

$$\delta_{ik} D = \Delta_{ij} d_{kj} = \Delta_{ji} d_{jk}. \qquad (6.2)$$

The symbol δ_{ik} is the Kronecker δ symbol. For $p = p_i(q)$ the expression becomes $\Delta_{ij} d_{kj} = 0$. This is a system of algebraic equations for d_{kj} for given, fixed k. Since the matrix with elements Δ_{ij} has rank $N - 1$ (at least one d_{ij} must be nonzero or there would be no pole in the first place), there is only one linearly independent solution to this

equation. Thus d_{kj} must be proportional to d_{nj} for $j, n = 1, \cdots, N$. In other words, all the rows of the matrix with elements d_{ij} are proportional at any root of $D = 0$. Similarly, using the second part of Eq. (6.2), all the columns are proportional. It follows that there is only one independent relation (6.1) for each $c_i < 0$.

As an example of this type of restriction, one may take the wave equation (the GWE with $b_1 = b_2 = 0$ and $-c_1 = c_2 = c$). The restriction corresponding to Eq. (6.1) is

$$f_1^{II}(q) - cf_1^{I}(cq) = 0, \tag{6.3}$$

which can be inverted to give

$$f_1(x, t = 0) - f_1(x = 0,\ t = x/c) = 0. \tag{6.4}$$

Equation (6.4) is consistent with the known general solution

$$f_1 = f(x - c_1 t) = f(x + ct), \tag{6.5}$$

$$f_2 = g(x - c_2 t) = g(x - ct), \tag{6.6}$$

where f and g are arbitrary, sufficiently differentiable functions. It should be noted that if the terms b_1 and b_2 are not taken to be zero, then there are still relations among the boundary and initial conditions analogous to those obtained in this and the preceeding sections. (The b_1 and b_2 terms do not affect the characteristics.) In this case, however, the general solution is no longer a simply expressible form, and the relations obtained are consequently more useful.

7. SATISFACTION OF THE BOUNDARY AND INITIAL CONDITIONS

If one wishes to apply the uniqueness–existence theorems discussed in Sec. 2, it is necessary to verify that the solution (3.4), subject to the restrictions (5.1) and (6.1), indeed approaches the initial (or boundary) conditions as t (or x) approaches zero. An outline of the proof for the satisfaction of the initial conditions is as follows. If the transform $F_i(p, q)$ in Eq. (3.4) is expanded in a power series in p^{-1}, those terms involving $(p^{-1})^n$ for $n > 1$ do not contribute as $t \to 0$. In other words, it is sufficient to replace $F_i(p, q)$ in Eq. (3.4) by its limit for large p in order to find $f_i(x, t \to 0)$. The bulk of the proof consists in finding this asymptotic limit of $F_i(p, q)$. A similar procedure can be carried out for the boundary conditions, in which case the limit as $q \to \infty$ is desired.

It is necessary to know the large-argument expansion of the transforms $f_i^I(p)$ of the initial conditions $f_i(0, t)$. It is assumed that these initial conditions are such that, in a neighborhood of $t = 0$, they can be expanded in a Taylor's series:

$$f_i(0, t) = f_i(0, 0) + \frac{tf_i(0, 0)}{t\ \partial t} + \cdots. \tag{7.1}$$

Further, it is assumed that, as long as t is restricted to the above neighborhood, the function $f_i(0, t)$ may be replaced by the function whose expansion is (7.1) for *all* t. This fact should be kept in mind since no distinction will be made between the two functions in the following, because only small t is considered. A similar statement applies to $f_i(x, 0)$ in the limit $x \to 0$.

If Eq. (7.1) is transformed, the result is the desired expansion in p^{-1}:

$$f_i^I(p) = p^{-1} f_i(0, 0) + p^{-2} \frac{\partial f_i(0, 0)}{\partial t} + \cdots. \tag{7.2}$$

Two cases will be considered—case A: $\det|b_{ij}| \neq 0$ and case B: $\det|b_{ij}| = 0$. It should be recalled that $\det|a_{ij}|$ is always nonzero.

Case A is treated first, and satisfaction of the initial conditions will be the first consideration in this case. As $p \to \infty$, the leading terms of the following functions are

$$D(p, q) \to \det|a_{ij}p| = p^N \det|a_{ij}|, \tag{7.3}$$

$$d_{ij}(p, q) \to A_{ij} p^{N-1}, \tag{7.4}$$

where A_{ij} is the cofactor of a_{ij}. In other words, $D(p, q)$ is a polynomial of order N in p, and d_{ij} is a polynomial of order $N - 1$ or less in p. Keeping the leading terms as $p \to \infty$ as discussed above, the solution (3.4) becomes

$$f_i(x, t \to 0) = (2\pi i)^{-2} \int dp dq\, e^{pt + qx} \times \left(a_{jk} f_k^{II}(q) + \frac{b_{jk} f_k(0, 0)}{p}\right) \frac{A_{ji} p^{N-1}}{\det|a_{ij}| p^N} \tag{7.5}$$

plus higher-order terms in p^{-1}. This integral can be integrated by residues. The result is

$$\begin{aligned} f_i(x, t \to 0) &= (2\pi i)^{-1} \int dq\, e^{qx} a_{jk} f_k^{II}(q) A_{ji} / \det|a_{ij}| \\ &= (2\pi i)^{-1} \int dq\, e^{qx} f_i^{II}(q) \\ &= f_i(x, 0). \end{aligned} \tag{7.6}$$

The higher-order terms integrate to zero for $t \to 0$, and the second step is a consequence of $\delta_{ik} \det|a_{ij}| = a_{jk} A_{ji}$. According to Eq. (7.6), the solution (3.4) satisfies the initial conditions. A similar argument indicates that the solution satisfies the boundary conditions.

A remark should be made about this proof when there are negative characteristics. Since some of the boundary and initial conditions are determined in terms of the others, there is no *a priori* guarantee that if the given conditions are sufficiently well behaved to be expanded as in Eq. (7.1), that the determined ones are also sufficiently well behaved. To see that, in fact, the latter *are* well behaved, one may examine the relation (6.1), which determines them in the limit $p \to \infty$ so that $p_i(q) \to c_i q$:

$$[a_{jk} f_k^{II}(q) + b_{jk} f_k^{I}(-c_i q)]\, d_{ji}(-c_i q, q) = 0. \tag{7.7}$$

It can be seen that if the given functions $f_i^I(p)$ and $f_i^{II}(q)$ can be represented as a power series in p^{-1} or q^{-1}, then the unknown functions can also be represented by such a power series.

Case B is treated next. Since $\det|a_{ij}| \neq 0$, the argument used in case A will suffice to show that the initial conditions are satisfied. There are restrictions, Eq. (5.1) or (5.2), however, on the boundary conditions, and it is shown in the following that the boundary conditions are satisfied only if these restrictions are taken into account.

If the contour C_q is moved to the right so that $q \to \infty$, Eq. (3.4) becomes

$$f_i(x \to 0, t) = (2\pi i)^{-2} \int dp\,dq\; e^{pt+qx} [a_{jk} f_k(0,0)/q + b_{jk} f_k^I(p)]\, d_{ji}(q \to \infty)/D(q \to \infty). \tag{7.8}$$

Let $D(p, q)$ be of order q^J $(J < N)$ as $q \to \infty$, and let $J + I_i$ be the highest order of d_{ji} for fixed i with $j = 1, \cdots, N$. (It is shown in Sec. 8 that J is in fact equal to $N - L$, where L is the number of characteristics with $c_i = 0$). Consider the equation for the expansion of D by cofactors:

$$\delta_{ik} D = \Delta_{jk} d_{ji} = (a_{jk} p + b_{jk} q + c_{jk}) d_{ji}. \tag{7.9}$$

Then, as $q \to \infty$,

case (i): $\delta_{ik} = q b_{jk} d_{ji}(q \to \infty)/D(q \to \infty)$,

$$I_i = J - 1; \tag{7.10}$$

case (ii): $0 = q b_{jk} d_{ji}(q \to \infty)/D(q \to \infty)$,

$$I_i \geq J. \tag{7.11}$$

In case (i) $a_{jk} d_{ji}(q \to \infty)/D(q \to \infty) = 0(q^{-1})$, so the terms involving $f_k(0, 0)$ in Eq. (7.8) integrate to zero. The remaining terms are, according to Eq. (7.10),

$$\begin{aligned} f_i(x \to 0, t) &= (2\pi i)^{-2} \int dp\,dq\; e^{pt+qx}\, \delta_{ik} f_k^I(p)/q \\ &= (2\pi i)^{-1} \int dp\; e^{pt} f_i^I(p) \\ &= f_i(0, t). \end{aligned} \tag{7.12}$$

In case (ii) it can be seen that $d_{ji}(q \to \infty)/D(q \to \infty)$ for fixed i with $j = 1, \cdots, N$ is a valid choice for one of the linearly independent solutions $l_j^{(k)}$. Therefore, Eq. (5.2), the conditions on the boundary conditions, give

$$\begin{aligned} &d_{ji}(q \to \infty) a_{jk} f_k(0,0)/D(q \to \infty) \\ &\quad = d_{ji}(q \to \infty)[(a_{jk} p + c_{jk}) f_k^I(p)]/D(q \to \infty). \end{aligned} \tag{7.13}$$

Using this relation in Eq. (7.8) results in

$$\begin{aligned} f_i(x \to 0, t) &= (2\pi i)^{-2} \int dp\,dq\; e^{pt+qx} (a_{jk} p + b_{jk} q + c_{jk}) \\ &\quad \times \frac{f_k^I(p) d_{jk}(q \to \infty)}{q D(q \to \infty)} = (2\pi i)^{-2} \int dp\,dq\; e^{pt+qx} f_i^I(p)/q \\ &= f_i(0, t). \end{aligned} \tag{7.14}$$

8. FEATURES OF THE SOLUTION

In this section some of the features which typically appear in the integration in Eq. (3.4) are discussed. Although the results may appear complicated in such a general presentation, in any particular example it should be clear how these features appear. It is shown in this section that the solution $f_i(x, t)$ consists of different types of terms in different regions of space–time. These regions are bounded by characteristics, for it is known that discontinuities of the solution can occur only along characteristics.[17] There is, in particular, one important type of discontinuity that may arise in mixed boundary–initial value problems. Since the equations are known to have a continuous solution when continuous initial conditions are specified for all x,[6–8] specification of initial conditions only for $x \geq 0$ creates a possible discontinuity at the origin. This discontinuity propagates along the characteristics passing through the origin. These characteristics divide the (x, t) space into regions in which the solutions may have different functional forms. If the boundary and initial conditions have discontinuities, these discontinuites are propagated through the system along the characteristics which pass through the points on the x or t axis where the discontinuities occur. Although this latter type of discontinuity is not treated, the mechanism by which it appears in the integrals is similar to the mechanism for the ones which are treated.

It is assumed in this section that the transforms $f_i^I(q)$ and $f_i^{II}(q)$ are such that they go to zero at least as fast as p^{-1} and q^{-1} as p and $q \to \infty$. This means that the contours C_p and C_q can be closed by an infinite semicircle to the right or left (depending on the behavior of e^{pt+qx}) with no extra contribution to the integral (3.4). This property follows from Jordan's lemma.[18] [For Jordan's lemma to apply, the integrand apart from the exponential factor must fall off faster than p^{-1} or q^{-1}. The analysis of the last section shows this will be the case provided $f_i^I(p)$ and $f_i^{II}(q)$ fall off this fast.]

For the moment it is assumed that all the c_i are distinct and that none is zero. Let the characteristic velocities be labeled in increasing order, that is, let them be labeled so that $i > j$ implies $c_i > c_j$. Let the regions in (x, t) space be labeled so that region (i) is just to the left of the characteristic corresponding to c_i. See Fig. 4.

In order to investigate the solution, it is divided into two parts, $f_i^I(x, t)$ and $f_i^{II}(x, t)$, and each part is considered separately. The function $f_i^I(x, t)$, which involves the boundary conditions, is treated first:

$$f_i^I(x, t) = (2\pi i)^{-2} \int dp\,dq\; e^{pt+qx} \frac{b_{jk} f_k^I(p) d_{ji}(p, q)}{D(p, q)}. \tag{8.1}$$

This expression is first integrated by extending the contour C_p to the left and integrating over p:

$$f_i^I(x,t) = (2\pi i)^{-1} \sum_{m=1}^{N} \int_{C_q} dq\, e^{p_m(q)t+qx} \times \frac{b_{jk} f_k^I(p_m(q)) d_{ji}(p_m(q),q)}{\partial D/\partial p(p_m(q),q)} + (2\pi i)^{-2} \int_{C_q} dp \times \int_{C_{p'}} dp\, e^{pt+qx} \frac{b_{jk} f_k^I(p) d_{ji}(p,q)}{D(p,q)}, \quad (8.2)$$

where the contour $C_{p'}$ encloses only the singularities of the $f_k^I(p)$. See Fig. 5. [It is assumed that all the roots of $D(p,q)$ are distinct.] The second integral can be integrated over q by closing the contour C_q to the left. The result is

$$f_i^I(x,t) = (2\pi i)^{-1} \sum_{m=1}^{N} \int_{C_q} dq\, e^{p_m(q)t+qx} \times \frac{b_{jk} f_k^I(p_m(q))\, d_{ji}(p_m(q),q)}{\partial D/\partial p(p_m(q),q)} + (2\pi i)^{-1} \sum_{m=1}^{N} \int_{C_{p'}} dp\, e^{pt+q_m(p)x} \frac{b_{jk} f_k^I(p)\, d_{ji}(p,q_m(p))}{\partial D/\partial q(p,q_m(p))}. \quad (8.3)$$

In region (1) the first integral is zero as the exponential part is

$$\exp[p_m(q)t + qx] \to \exp[q(x - |c_m|t)], \text{ as } q \to \infty \quad m = 1, \cdots, N, \quad (8.4)$$

and the contour C_q may be closed to the right where it encloses no singularities.

In region (2) the only term of the first integral which contributes is that for $m = 1$. The integrand of this term has singularities at:

(A) singularities of $f_k^I(p_1(q))$ apart from (C),

(B) zeros of $\frac{\partial D}{\partial p}(p_1(q), q)$,

(C) singularities of $p_1(q)$.

Since one can write

$$\frac{\partial D}{\partial p}(p_1(q),q) = \det|a_{ij}| \prod_{k=2}^{N} [p_1(q) - p_k(q)], \quad (8.5)$$

the singularities (B) are the points at which $p_1(q) = p_k(q), k = 2, \cdots, N$. If $p_1(q)$ has cuts, these points include the branch points. The singularities (C) are the cuts of $p_1(q)$ (if there are any), as the roots $p_i(q)$ can have no poles according to Eq. (2.4). Consider the contribution to the first integral due to the singularities (A). [It is assumed that these are distinct from the singularities (B) and (C).] This term is

$$(2\pi i)^{-1} \int_{C_q'} dq\, e^{P_1(q)t+qx} \frac{b_{jk} f_k^I(p_1(q),q)\, d_{ji}(p_1(q),q)}{\partial D/\partial p(p_1(q),q)}, \quad (8.6)$$

where the contour C_q' includes only the singularities of the $f_k^I(p_1(q))$ apart from the singularities (C). Next, let the roots $p_i(q)$ and $q_i(p)$ be labeled (uniquely or not) so there is a one-to-one correspondence between $p_i(q)$ and $q_i(p)$ for a given i. This correspondence is given by $p = -c_i q$ for p and $q \to \infty$ and by the analytic continuation of this relation for other values of p and q. (See the discussion in Sec. 6.) One can then change variables from q to $p = p_1(q)$. The term (8.6) becomes

$$(2\pi i)^{-1} \int_{C_p'} dp\, \frac{dq}{dp} e^{pt+q_1(p)x} \frac{b_{jk} f_k^I(p)\, d_{ji}(p,q_1(p))}{\partial D/\partial p(p,q_1(p))}. \quad (8.7)$$

However

$$\frac{dq}{dp} = \left(\frac{dp_1(q)}{dq}\right)^{-1} = -\frac{\partial D/\partial p(p_1(q),q)}{\partial D/\partial q(p_1(q),q)} = -\frac{\partial D/\partial p(p,q_1(p))}{\partial D/\partial q(p,q_1(p))}, \quad (8.8)$$

so that (8.6) becomes

$$-(2\pi i)^{-1} \int_{C_p'} dp\, e^{pt+q_1(p)x} \frac{b_{jk} f_k^I(p)\, d_{ji}(p,q_1(p))}{\partial D/\partial q(p,q_1(p))}. \quad (8.9)$$

Obviously, term (8.9) cancels the $m = 1$ term of the second integral in Eq. (8.3). Similarly in region (3) the singularities due to the boundary conditions in the new term which enters the first integral cancel the $m = 2$ term, and so on. Finally, in region $(N + 1)$, the second integral is entirely canceled.

A similar argument can be carried out for $f_i^{II}(x,t)$,

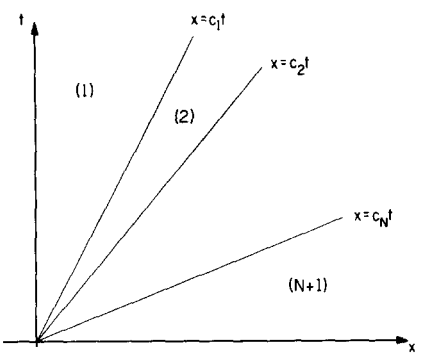

Fig. 4. Division of space-time into regions when all the characteristic velocities are positive.

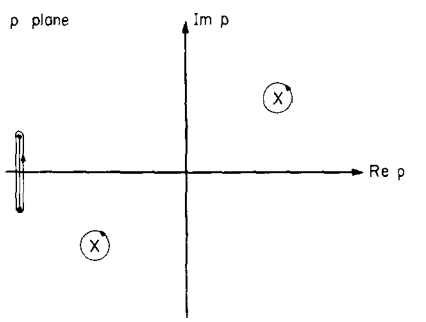

Fig. 5. The contour C_p' appearing in the second integral of Eq. (8.3).

TABLE I. Terms which neither vanish nor are canceled in the integration for $f_i^I(x,t)$ and $f_i^{II}(x,t)$ in Eqs. (8.3) and (8.10).

	$f_i^I(x,t)$		$f_i^{II}(x,t)$	
Region	First integral	Second integral	First integral	Second integral
(1)	0	$m = 1, \cdots, N$	$m = 1, \cdots, N$	0
(2)	$m = 1$	$m = 2, \cdots, N$	$m = 2, \cdots, N$	$m = 1$
(3)	$m = 1, 2$	$m = 3, \cdots, N$	$m = 3, \cdots, N$	$m = 1, 2$
(P)	$m = 1, \cdots, P-1$	$m = P, \cdots, N$	$m = P, \cdots, N$	$m = 1, \cdots, P-1$
(N)	$m = 1, \cdots, N-1$	$m = N$	$m = N$	$m = 1, \cdots, N-1$
$(N+1)$	$m = 1, \cdots, N$	0	0	$m = 1, \cdots, N$

TABLE II. Terms which neither vanish nor are canceled in the integration for $f_i^I(x,t)$ and $f_i^{II}(x,t)$ in Eqs. (8.11) and (8.12).

Region	$f_i^I(x,t)$	$f_i^{II}(x,t)$
(1)	$l = 1, \cdots, N$	0
(2)	$l = 2, \cdots, N$	$l = 1$
(3)	$l = 3, \cdots, N$	$l = 1, 2$
(P)	$l = P, \cdots, N$	$l = 1, \cdots, P-1$
(N)	$l = N$	$l = 1, \cdots, N-1$
$(N+1)$	0	$l = 1, \cdots, N$

which is the part of $f_i(x,t)$ involving the initial conditions

$$f_i^{II}(x,t) = (2\pi i)^{-1} \sum_{m=1}^{N} \int_{C_p} dp\ e^{pt+q_m(p)x} \times \frac{a_{jk} f_k^{II}(q_m(p))\, d_{ji}(p, q_m(p))}{\partial D/\partial q(p, q_m(p))} + (2\pi i)^{-1} \sum_{m=1}^{N} \times \int_{C_q'} dq\ e^{p_m(q)t+qx} \frac{a_{jk} f_k^{II}(q)\, d_{ji}(p_m(q), q)}{\partial D/\partial p(p_m(q), q)} . \tag{8.10}$$

In this expression the first integral is zero in the region $(N+1)$ with a new term appearing and part of it cancelling a term in the second integral in each new region proceeding back to region (1). In region (1) the second integral is entirely canceled.

These results are summarized in Table I. This table shows which terms appear in each of the integrals in Eq. (8.3) and (8.10), that is, it shows the terms which are neither zero nor canceled. Even when the singularities (A) are not distinct from (B) and (C), there may be cancellation. (See the example at the end of this section.) The cancellation occurs in much the same way as for the case shown, and a separate derivation is not given here.

At this point it should be noted that it is not necessary to do the integrations in the order they were done in Eq. (8.3) and (8.10). It would be just as appropriate to integrate $f_i^I(x,t)$ over q first or to integrate $f_i^{II}(x,t)$ over p first:

$$f_i^I(x,t) = (2\pi i)^{-1} \sum_{l=1}^{N} \int_{C_p} dp\ e^{pt+q_l(p)x} \times \frac{b_{jk} f_k^I(p)\, d_{ji}(p, q_l(p))}{\partial D/\partial q(p, q_l(p))} , \tag{8.11}$$

$$f_i^{II}(x,t) = (2\pi i)^{-1} \sum_{l=1}^{N} \int_{C_q} dq\ e^{p_l(q)t+qx} \times \frac{a_{jk} f_k^{II}(q)\, d_{ji}(p_l(q), q)}{\partial D/\partial p(p, q_l(p))} . \tag{8.12}$$

Examination of the factor $e^{pt+q_l(p)x}$ or $e^{p_l(q)t+qx}$ determines whether the lth term appears in any given region. The results are summarized in Table II.

The case for which not all of the c_i are distinct can be considered now. If Q of the c_i are equal, say for $i = R+1, \cdots, R+Q$, then Q new terms appear or are canceled as the characteristic corresponding to these c_i is crossed. The result is the same as if regions $(R+2), \cdots, (R+Q)$ were squeezed down to a line (the characteristic itself).

The case for which some of the c_i are zero is more difficult. Let $c_i = 0, i = 1, \cdots, L$ and let the other characteristics be labeled as in the first of the section. Let the regions be labeled so that region (i) is just above the characteristic corresponding to c_i. The region adjacent to $x = 0$ is $(L+1)$. The form of $D(p,q)$ for large p and q is then

$$D(p,q) \to \det|a_{ij}|\, p^L (p - p_{L+1}(q)) \cdots (p - p_N(q)). \tag{8.13}$$

It can be seen that the highest order of q in $D(p,q)$ is q^J, where $J = N - L$. (That $J < N$ is a consequence of $\det|b_{ij}| = 0$.) There are then only J roots $q_i(p), i = L+1, \cdots, N$. There are no additional terms in the second integral of $f_i^I(x,t)$ in Eq. (8.3), the first integral of $f_i^{II}(x,t)$ in Eq. (8.10), or in $f_i^I(x,t)$ in Eq. (8.11) no matter whether there are characteristics on the boundary or not. There are, however, additional terms in the other integrals. The net result is that Tables I and II can be used for regions $(L+1), \cdots, (N)$ if some minor differences for terms which are associated with characteristics on the boundary are noted: The integrand in the first integral in Eq. (8.3) for $f_i^I(x,t)$ contains singularities in region (P) due to the singularities of $f_k^I(p_m(q))$ for $m = 1, \cdots, L$ but not for $m = L+1, \cdots, P$. (These terms for $m = L+1, \cdots, P$ were used to cancel terms in the second integral.) Also, since the coefficient of q^J in $D(p,q)$ is a function of p for $\det|b_{ij}| = 0$, the roots $q_i(p)$ may be infinite at finite values of p, and $\partial D/\partial q\,(p, q_i(p))$ may have zeros at these values

of p. These types of singularities appear in the first integral of $f_i^{II}(x,t)$ in Eq. (8.10) and in $f_i^{I}(x,t)$ in Eq. (8.11).

Finally, the case where some, say M, of the c_i are negative is considered. Again let the c_i be labeled in ascending order, and let region (i) lie to the left of $x = c_i t$. See Fig. 6. In this case, the integral in $f_i(x,t)$ cannot in general be separated into the two parts $f_i^{I}(x,t)$ amd $f_i^{II}(x,t)$. The restrictions among the boundary and initial conditions discussed in Sec. 6 ensure only that the integrand of both of these terms taken together has no poles corresponding to negative characteristic velocities. Separately, they may have such poles and hence be undefined. The separation may be made, however, if it is understood (1) that the expressions for both $f_i^{I}(x,t)$ and $f_i^{II}(x,t)$ must be integrated over the *same* variable first and (2) that there are no terms corresponding to the zeros of $D(p,q)$ which are associated with c_i for $i = 1, \cdots, M$ in the first integrals of Eqs. (8.3) and (8.10) and in Eqs. (8.11) and (8.12). The second integrals of Eqs. (8.3) and (8.10) *do* have terms corresponding to $m = 1, \cdots, M$. The second integrals are not divergent since the contour C_p' does not have to lie to the right of all singularities of the integrand as did the contour C_p. With these differences, Tables I and II can still be used for those regions which lie in the quadrant $x \geq 0$, $t \geq 0$.

To illustrate the results of this section, the GWE with $b_1 b_2 > 0$ will be used. The characteristic velocity c_2 is taken to be positive, and the three cases for which the characteristic velocity c_1 is positive, zero, or negative are considered. The roots of the dispersion relation are

$$p_{1,2}(q) = -\tfrac{1}{2}(c_1 + c_2)q \pm \tfrac{1}{2}[(c_2 - c_1)^2 q^2 + 4b_1 b_2]^{1/2}, \tag{8.14}$$

$$c_1 c_2 q_{1,2}(p) = -\tfrac{1}{2}(c_1 + c_2)p \pm \tfrac{1}{2}[(c_2 - c_1)^2 p^2 + 4c_1 c_2 b_1 b_2]^{1/2}. \tag{8.15}$$

The dispersion diagrams are shown in Fig. 1. The initial values are taken as follows:

$$f_1(x, t=0) = n a^n x^{-1} J_n(ax), \tag{8.16}$$

$$f_2(x, t=0) = 0, \tag{8.17}$$

where $a = 2(b_1 b_2)^{1/2}/(c_2 - c_1)$ and n is a positive integer. For this choice of a, the branch points of the initial value correspond with the branch points of the dispersion relation so that Table I cannot be used. Equation (8.12) for the initial value part $f_i^{II}(x,t)$ of the solution can be evaluated, however, via Eq. (8.12) and standard Laplace transform tables. The solution is

$$f_i^{II}(x,t) = \begin{cases} 0 & \text{region (1)}, \\ \phi_1 & \text{region (2)}, \\ \phi_1 + \phi_2 & \text{region (3)}, \end{cases} \tag{8.18}$$

where

$$\phi_1 = \tfrac{1}{2} a^{n+1} (\xi_1/\xi_2)^{(n-1)/2} J_{n-1}(a \xi_1^{1/2} \xi_2^{1/2}), \tag{8.19}$$

$$\phi_2 = \tfrac{1}{2} a^{n+1} (\xi_2/\xi_1)^{(n+1)/2} J_{n+1}(a \xi_1^{1/2} \xi_2^{1/2}), \tag{8.20}$$

$$\xi_i = x - c_i t, \quad i = 1, 2. \tag{8.21}$$

The ϕ_1 terms come from the root $p_1(q)$ and the ϕ_2 terms come from the root $p_2(q)$. The results are in accordance with Table II.

Case 1. $c_1 > 0$: For this case the boundary and initial value problems are essentially independent. If one takes the boundary conditions to be zero, the total solution $f_1(x,t)$ is given by $f_i^{II}(x,t)$. From the asymptotic values of the Bessel functions, one can see that the solution tends to die out along a line $x = vt$ in region (3). Inside region (2), however, the Bessel functions have an imaginary argument, and the solution grows along a line $x = vt$. In region (1) the solution is zero, so that for long times the solution dies out at a fixed x. This system is predicted to be convectively unstable[13]; that is, an initial disturbance would grow and move through the system so that at any fixed x, the disturbance would eventually die out. Although the definition of convective instability is based on an infinite system and does not include boundary effects,[19] it is seen that the behavior of the semi-infinite system treated here (with the given boundary and initial conditions) does indeed behave similarly to the infinite system.

Case 2. $c_1 = 0$: For this case the boundary and initial condition problems are also separate. Even though there is a relation among the boundary conditions:

$$\frac{\partial f_1(x=0,t)}{\partial t} + b_1 f_2(x=0,t) = 0, \tag{8.22}$$

it can be satisfied by taking the boundary conditions to be zero, so that the total solution $f_1(x,t)$ is again given by $f_1^{II}(x,t)$. Regions (2) and (3) constitute all of the region $x \geq 0$, $t \geq 0$, in accordance with the remarks made in this section on zero characteristic velocities.

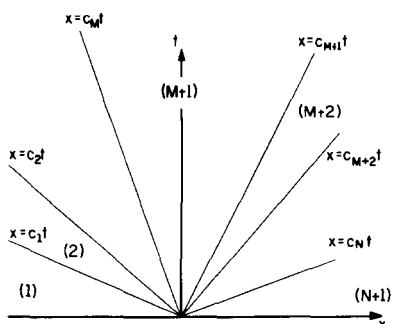

Fig. 6. Division of space–time into regions when some of the characteristic velocities are negative.

This system is on the borderline between convective and absolute (see case 3) instability. Such borderline systems can exhibit either growth or decay for fixed x and large t.[20,21] The given solution grows proportional to $\exp[a(c_2xt)^{1/2}]$ for fixed x and large t. This growth should be compared to that for the "normal-mode" solution. (See Sec. 9.) The latter growth is proportional to $e^{\Gamma t}$, where Γ is the largest imaginary part of $\omega_i(k)$, $i = 1, 2$, and is independent of x and t.

Case 3. $c_1 < 0$: In this case the boundary and initial condition problems are not independent. The boundary and initial values are related by

$$[f_1^{II}(q) + c_1 f_1^I(p)](p + c_2 q) - [f_2^{II}(q) + c_2 f_2^I(p)]b_1 = 0 \tag{8.23}$$

at $p = p_1(q)$ or $q = q_1(p)$. Moreover, in this case if the solution is divided into two parts, $f_1^I(x, t)$ and $f_1^{II}(x, t)$, then $f_1^{II}(x, t)$ does not contain terms due to $p_1(q)$. The part $f_1^{II}(x, t)$ for this case is given by Eq. (8.18) except that the ϕ_1 terms are missing.

If, as in the previous cases, it is desired to make the total solution $f_1(x, t)$ be given by (8.18) (including the ϕ_1 terms), it is necessary to choose the boundary conditions appropriately. They must, in fact, be given by Eq. (8.18) evaluated by $x = 0$ for $f_1(x = 0, t)$ and by the corresponding expression for $f_2(x = 0, t)$. These boundary conditions are

$$f_1(x = 0, t) = \tfrac{1}{2}a^{n+1}(c_1/c_2)^{(n-1)/2}(-)^{n-1} \times J_{n-1}(a(c_1c_2)^{1/2}t), \tag{8.24}$$

$$f_2(x = 0, t) = -\tfrac{1}{2}(c_2 - c_1)a^{n+2}b_1^{-1} \times (c_1/c_2)^{n/2}(-)^n J_n(a(c_1c_2)^{1/2}t). \tag{8.25}$$

It can be verified that their transforms satisfy Eq. (8.23). Since the expression for $f_1^{II}(x, t)$ was evaluated by integrating over p first, the expression for $f_1^I(x, t)$ must also be integrated over p first. This expression is given by Eq. (8.3), except that only the $m = 2$ term in the first integral contributes, while both terms contribute in the second integral. It can be shown that the $m = 2$ terms in the two integrals cancel. The remaining term can easily be shown to give

$$f_1^I(x, t) = \phi_1, \quad x \geq 0, \quad t \geq 0. \tag{8.26}$$

For the given choice of boundary conditions, then, the terms that were lost in $f_1^{II}(x, t)$ are regained in $f_1^I(x, t)$, and the total solution $f_1(x, t) = f_1^I(x, t) + f_1^{II}(x, t)$ is given by the expression in Eq. (8.18) as desired.

For this case the infinite system is predicted to be absolutely unstable[13]; that is, an unstable initial disturbance continues to grow for all time at a fixed x. The solution obtained for the semi-infinite system also exhibits this behavior as it grows along any line $x = vt$ in that part of region (2) which is in the region of interest. Case 3 has been studied in detail by Bobroff and Haus.[22]

9. THE "NORMAL-MODE" SOLUTION VS THE ACTUAL SOLUTION

A common method of solving systems of linear partial differential equations such as are treated in this paper is to assume a solution proportional to $\exp[ikx - i\omega_m(k)t]$ or $\exp[ik_m(\omega)x - i\omega t]$, where $\omega_m(k)$ and $k_m(\omega)$ are the roots of the dispersion relation corresponding to $p_m(q)$ and $q_m(p)$. ($\omega = ip$ and $k = -iq$.) Solutions of this type are called the "normal-mode" solutions. These solutions *are* solutions of the equations. The question that arises is to what boundary and initial conditions do they pertain? The answer is that in general it takes a very special boundary or initial condition to give rise to a solution consisting of only one normal mode, and in some cases it is even impossible.[23,24] It is possible, however, to see what role these normal modes do play in the solution obtained in this paper.

Only the case where all the c_i are distinct and positive is considered here. The necessary information is available in Sec. 8, however, to apply the reasoning used here to the other cases. It is assumed that the transforms of the boundary conditions $f_i^I(p)$ have a simple pole at $-i\omega_0$ and that the transforms of the initial conditions $f_i^{II}(q)$ have a simple pole at ik_0. Under this assumption the second integral of $f_i^I(x, t)$, Eq. (8.3), can be integrated to give

$$\sum_{m=1}^{N} e^{-i\omega_0 t + q_m(-i\omega_0)x} \times \frac{b_{jk}\,\mathrm{Res} f_k^I(-i\omega_0) d_{ji}(-i\omega_0, q_m(-i\omega_0))}{\partial D/\partial \mathrm{q}(-i\omega_0, q_m(-i\omega_0))}, \tag{9.1}$$

and the second integral of $f_i^{II}(x, t)$, Eq. (8.10), can be integrated to give

$$\sum_{m=1}^{N} e^{p_m(ik_0)t + ik_0 x} \times \frac{a_{jk}\,\mathrm{Res} f_k^{II}(ik_0) d_{ji}(p_m(ik_0), ik_0)}{\cdot \partial D/\partial q(p_m(ik_0), ik_0)}, \tag{9.2}$$

where $\mathrm{Res} f_k^I(-i\omega_0)$ and $\mathrm{Res} f_k^{II}(ik_0)$ denote the residues of $f_k^I(p)$ and $f_k^{II}(q)$ at the poles $-i\omega_0$ and ik_0, respectively.

It can be seen, then, that the second integrals of $f_i^I(x, t)$ and $f_i^{II}(x, t)$ in Eq. (8.3) and (8.10) are the normal-mode terms. The first integrals will in general give a more complicated contribution to the solution. Moreover, the results of Sec. 8 indicate that these normal-mode terms are canceled in some regions of (x, t) space. In particular, the normal-mode terms from the boundary conditions do not appear in the region adjacent to the x

axis, whereas all the normal modes from the initial conditions (those proportional to $\exp[ik_0x - i\omega_m(k_0)t)]$ can appear. In this region the system behaves as an infinite system; that is, the effect of the boundary is not felt in this region. Similarly, in the region adjacent to the t axis, none of the normal modes from the initial conditions appear, but all of the normal modes from the boundary conditions {those proportional to $\exp[ik_m(\omega_0) - i\omega_0 t]$} can appear. The long-time behavior of the system is found in this region, and it should be noted that the normal-mode solution for the initial conditions is not, in general, valid here. (It should also be noted that there can be additional terms in each of these regions which are not normal-mode terms at all, in general.)

10. SUMMARY

If the double Laplace transformation method is used to treat systems of linear, partial differential equations such as those given in Eq. (2.1), the solution (in terms of an integral) is given by Eq. (3.4) along with Eqs. (3.8)–(3.11). This expression will only be meaningful if the boundary and initial conditions are suitably restricted. The two major types of restrictions are given in Eqs. (5.1) and (6.1). Those in Eq. (5.1) arise if there are characteristics parallel to the boundary $x = 0$, and those in Eq. (6.1) arise if there are characteristics associated with negative characteristic velocities. It should be noted that these restrictions are necessary for a well-formulated, mixed boundary–initial value problem and would appear in any treatment of the equations. The solution in (x, t) space can be found by performing the integration in Eq. (3.4) by the usual methods for complex integration. A few of the kinds of problems that arise in this integration have been discussed in Sec. 8.

The importance of the characteristics to the physical problem described by the equations has been emphasized. By knowing the connection of the characteristics to the dispersion relation and to the features of the integration, it is possible to understand a great deal about the physical solution without actually performing the integrals.

ACKNOWLEDGMENTS

The material in this paper is based on a thesis for the doctoral degree at the University of Illinois. One of the authors (A. J.) would like to express his sincere appreciation for the hospitality and financial assistance of the FOM-Instituut voor Plasma-Fysica, Rijnhuizen, Jutphaas, Netherlands. This work was supported in part by the Joint Services Electronics Program (U.S. Army, U.S. Navy, and U.S. Air Force), under Contract No. DAAB-07-67-C-0199.

1 J. C. Jaeger, Bull. Am. Math. Soc. **46**, 687 (1940).
2 P. Rolland, Phys. Rev. **140**, B776 (1965).
3 A. M. Fedorchenko, Zh. Techn. Fiz. **36**, 1323 (1966) [Sov. Phys. Tech. Phys. **11**, 989 (1967)].
4 R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience, New York, 1962), Vol. II, p. 58.
5 I. M. Gel'fand and G. E. Shilov, *Generalized Functions* (Academic, New York, 1967), Vol. 3, p. 126.
6 Ref. 5, pp. 126, 129, 132.
7 L. Garding, Acta Math. **85**, 1 (1951).
8 L. Hormander, *Linear Partial Differential Operators* (Springer-Verlag, Berlin, 1963), p. 137.
9 Ref. 4, p. 425.
10 Ref. 4, pp. 472–4.
11 I. N. Sneddon, *Fourier Transforms* (McGraw-Hill, New York, 1951), p. 45 ff.
12 Ref. 4, pp. 407–8.
13 A. I. Akhiezer, I. A. Akhiezer, R. V. Polovin, A. G. Sitenko, and K. N. Stepanov, *Collective Oscillations in a Plasma* (M.I.T. Press, Cambridge, Mass., 1967), Chap. II, Sec. 13.
14 P. A. Sturrock, Phys. Rev. **117**, 1426 (1960).
15 Ref. 4, pp. 407–8.
16 The case for which the roots are not distinct can also be treated. The analysis is algebraically more complicated, and it has not been included to avoid clouding the presentation. It is doubtful if the importance of this case would warrant its inclusion in any event.
17 Ref. 4, p. 486 ff.
18 E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge U. P., New York, 1963), p. 115.
19 P. A. Sturrock, Phys. Rev. **112**, 1488 (1958).
20 J. A. Davis and A. Bers, *Proceedings of the Symposium on Turbulence of Fluids and Plasmas* (Polytechnic Institute of Brooklyn Press, Brooklyn, New York, 1969), pp. 87–108.
21 K. Evans and E. A. Jackson, Phys. Fluids **13**, 1885 (1970).
22 D. L. Bobroff and H. A. Haus, J. Appl. Phys. **38**, 390 (1967).
23 L. A. Peletier, "On a Class of Wave Equations" (Thesis, Technische Hogeschool, Eindhoven, Netherlands, 1967), Chap. IV (unpublished).
24 R. Q. Twiss, Phys. Rev. **88**, 1392 (1952).

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 12, NUMBER 9 SEPTEMBER 1971

Approximate Solution of a Sturm-Liouville System Using Nonorthogonal Expansions: Application to a-a Nuclear Scattering*

R. A. Chatwin† and J. E. Purcell‡
Department of Physics, Florida State University, Tallahassee, Florida

A stationary principle for the Sturm–Liouville system with inhomogeneous boundary conditions leads to an approximate solution in which nonorthogonal expansions are used. It is shown that if the nonorthogonal functions are chosen to be the eigenfunctions of a similar Sturm–Liouville equation, then the numerical solution of the boundary value problem no longer involves an integration of a second derivative, but only the more simple integration of a function. As an illustration, formulas for calculating the nuclear phase shifts of a Schrödinger equation with a long-range Coulomb potential are presented in the notation of R-matrix theory. The numerical convergence of the method is investigated for $\alpha-\alpha$ nuclear scattering from real potentials that have a repulsive core followed by a short-range attraction (Ali and Bodmer). Generalizations of the method have been applied in nuclear physics to coupled differential equations and to eigenvalue problems.

I. INTRODUCTION

This work is part of a program developing the R-matrix theory of nuclear reactions.[1,2] R-matrix methods were first developed by analogies with waveguide systems and with circuit theory and, although their use appears to have been solely in low energy nuclear physics, and lately in atomic and molecular physics, we hope that what we have found useful in nuclear reaction theory may interest other physicists in other fields. Therefore, the theory will first be developed in a general and simple form, and only towards the end specialized to a nuclear physics application.

The essence of systems to which R-matrix methods can be applied is that there exists some differential operator which is simple in some "asymptotic" region of space and more complicated in some "interaction" region. In the asymptotic region one already knows the complete solution of the differential equation. As will be seen below, one can then replace the whole of this simple region by some boundary condition on the surface of the interaction region, and then look for solutions of the reformulated problem. For instance, the nuclear interaction between a proton and a target nucleus may be quite complicated, with spin interactions, absorptive terms, inelastic couplings, and so on; but one reasonably assumes all of these terms to be zero outside of some separation radius R, and from R to infinity one may assume a simple Coulomb interaction between two charges.

We can also think of possible examples in reactor physics and waveguide theory. The core of a reactor is often some complicated array of fuel elements, cooling circuits, and moderating rods, and the neutron transport equation would have to be solved numerically in this region. However the core is surrounded perhaps by some uniform steel container, itself shielded by a more or less uniform thickness of concrete. In these regions one may know already the simple solutions of the transport equation, and thus be able to replace them with a boundary condition on the core. Some development of the approximation to be described in this article may well be useful for such problems, particularly since we have found the method more rapid than conventional codes, and since one may vary certain parameters in the initial equation without having to recalculate everything. As another example, let us imagine some uniform waveguide with a complicated obstacle somewhere inside it. To solve the Helmholtz equation for a propagating wave, we would enclose the obstacle in some convenient surface and solve numerically the resulting problem, just as in R-matrix theory.

The approximation is discussed below for the simple case of an ordinary differential equation. But coupled equations may be solved as easily and directly, with no iteration (see Purcell's work in Ref. 1). Vincent has pointed out to us that wave equations with a nonlocal potential may also be solved without iteration in this method.

A second-order differential equation has two independent solutions. Let us suppose that we know two such solutions in the interval $x \in [a, \infty)$ to be the functions $I(x)$ and $O(x)$. Then we can represent any solution of the differential equation as a linear combination of I and O on the range $[a, \infty)$:

$$u(x) = c_1 I(x) + c_2 O(x),$$
$$u'(x) = c_1 I'(x) + c_2 O'(x).$$

One may eliminate the constant c_2 from these equations and find that

$$u' - uO'O^{-1} = -c_1 W(I, O, r)O^{-1}$$

for $x \in [a, \infty)$, where W is the Wronskian $\{IO' - I'O\}$. It is a property of the Wronskian that it is nonzero when the two arguments I and O are independent solutions of a differential equation. Now the problem has been simplified for computation, because the external region may be replaced by an inhomogeneous boundary condition

$$u'(a) + \alpha u(a) = \gamma,$$

where α and γ are given by $[-O'(a)/O(a)]$ and $[-c_1 W(I, O, a)/O(a)]$, respectively.

In Sec. II we derive an approximation method for solving differential problems of this type, a method which uses expansions in arbitrary independent functions. The differential equation is taken to be of the form

$$K[u] + \lambda\rho(x)u = 0,$$

where K is the second-order differential operator,

λ is some complex constant, and ρ is a real-valued function. In the derivation of the approximation, we shall need to use a differential identity of the form

$$uK[v] - vK[u] = [p(x)(uv' - vu')]',$$

where p is a real-valued function of x. One can easily show that the general operator which satisfies such an identity is of the form[3]

$$K[u] = [p(x)u'(x)]' - q(x)u(x).$$

When q is a real-valued function, this is a Sturm-Liouville operator, and hence the class of differential systems that we shall discuss are the Sturm–Liouville systems with inhomogeneous boundary conditions.

In Sec. III, we illustrate the method by presenting formulas for calculating the phase shifts of a Schrödinger equation with a long-range Coulomb potential and a short-range nuclear potential. In this section the notation used is that of R-matrix theory; it is in this framework originally that the method has been developed and applied.[1,2]

In Sec. IV, the numerical convergence of the method is investigated, because this is the most straightforward way of estimating the accuracy of the approximation.

The accuracy of the method is taken for granted in the present paper. (In fact, checks were made.) Purcell, in his technical report,[1] investigated a variety of simple cases of potential scattering, e.g., square well plus Coulomb potential. The results were indistinguishable from the algebraic solutions, even when only *four* basis functions were used in the approximation. The results were also so stable against changes in various parameters that certain properties and difficulties of the method could not be seen by analyzing such systems. For example, the error is not minimized in the approximation, and the result may not be the *best* approximation possible in whatever trial space is being used. These properties of the method are brought out in Sec. IV, by analyzing a much more awkward potential. Where there is comparison with previously published results, the present calculations are, we feel, more accurate; but these comparisons are included for honesty and completeness, they are not the point of the numerical discussion.

At about the same time as Lane and Robson[2] suggested their stationary functional as the origin of this approximation, a similar functional was discussed by Koroza[4] in solving a class of waveguide problems.

II. THE APPROXIMATION

A. Definitions

Let u_0 be the solution of the Sturm–Liouville system with the inhomogeneous end point conditions: for $x \in [a,b]$

$$[p(x)u']' + [\lambda\rho(x) - q(x)]u = 0, \tag{1}$$

$$u'(a) + \alpha u(a) = \gamma, \qquad u'(b) + \beta u(b) = \delta. \tag{2}$$

In an operational notation with $K = D[p(x)D] - q(x)$, one may rewrite (1) in the form

$$K[u] + \lambda\rho(x)u = 0.$$

The functions p, q, and ρ are real valued, and λ is a complex parameter.

We show in this section that the functional

$$M[u] = \int_a^b dx u[K - L + \lambda\rho(x)]u - 2[\gamma p(a)u(a) - \delta p(b)u(b)] \tag{3}$$

is stationary for weak variations around the function u_0, where L is used as a convenient shorthand for the homogeneous terms in the end point conditions: By definition

$$\int_a^b dx f(x)L[g(x)] = [fp(g' + \beta g)]_{x=b} - [fp(g' + \alpha g)]_{x=a}. \tag{4}$$

Using this stationary principle and expansions in terms of nonorthogonal functions, we derive an approximate solution of the Sturm–Liouville system, a solution which has convenient properties for numerical computation.

B. Equivalent Variational Problem

Consider weak variations[5] of the function u in the space of functions that are continuous and have continuous first derivatives on $[a,b]$. Then, if κ is the real parameter of a variation κv,

$$M[u + \kappa v] - M[u] = \kappa I_1 + \kappa^2 I_2,$$

where I_2 is a functional only of v and v'.

From (3), the first variation is given by

$$I_1 = \int_a^b dx[v(K - L + \lambda\rho)u + u(K - L + \lambda\rho)v] - 2\gamma(pv)_{x=a} + 2\delta(pv)_{x=b}. \tag{5}$$

The Sturm–Liouville operator is self-adjoint, and therefore satisfies a Lagrange identity of the form[3]

$$uK[v] = vK[u] + [p\{uv' - vu'\}]'. \tag{6}$$

This is easily verified by direct differentiation, but we have stated it in this way to clarify the problem of generalizing the theory to systems which are not of the Sturm–Liouville class.

Now the terms in v' may be removed from Eq. (5), and

$$I_1 = 2\int_a^b dx v[K + \lambda\rho(x)]u + 2[pv(u' + \alpha u - \gamma)]_{x=a} - 2[pv(u' + \beta u - \delta)]_{x=b}. \tag{7}$$

For arbitrary v, $I_1 = 0$ if u satisfies the Euler

equation for all $x \in [a,b]$:

$$[K + \lambda\rho(x)]u = 0$$

and the end point conditions

$$u'(a) + \alpha u(a) = \gamma, \qquad u'(b) + \beta u(b) = \delta.$$

Hence the stationary problem has the unique solution u_0, which is just the solution of Eqs. (1) and (2).[6]

C. Approximate Solution

Let us look for an approximate solution of Eqs. (1) – (3) in the form $M[\hat{u}_0]$, where

$$\hat{u}_0 = \sum_{i=1}^{N} d_i v_i \tag{8}$$

is a function in some space $\mathcal{T}$ of functions continuous, with continuous first derivatives on the interval $[a,b]$, and where $\mathcal{T}$ is spanned by the ordered, independent set $\{v_n\}, n = 1, \cdots, N'(N' \geq N)$. These functions need not be orthogonal in any sense. By substituting the expressions for $\hat{u}_0$ into the functional $M[u]$ to be made stationary in the space $\mathcal{T}$, followed by differentiation in each of the parameters d_i, one expects to minimize the error $|M[\hat{u}_0] - M[u_0]|$ in the approximation. This will not prove that the result is a good approximation to the true solution, but a repetition of the process with larger N and with different trial spaces $\mathcal{T}$ indicates the size of the error remaining, and also helps eliminate situations in which one has found a saddle point in the error, or even a maximum.

From Eq. (3) and the stationary condition on the function $M[\hat{u}_0] = M(d)$, that

$$\frac{\partial M[\hat{u}_0]}{\partial d_i} = 0, \qquad i = 1, \cdots, N, \tag{9}$$

it follows that

$$2\mathbf{g} = (\mathbf{A} + \tilde{\mathbf{A}}) \cdot \mathbf{d}, \tag{10}$$

where

$$g_i = \gamma(pv_i)_{x=a}, \; -\delta(pv_i)_{x=b}, \tag{11}$$

$$A_{ij} = \int_a^b dx v_i[K - L + \lambda\rho]v_j. \tag{12}$$

Using Eq. (6) again, one finds that $\mathbf{A}$ is a symmetric matrix. Substitute Eq. (10) into the expression for $M[u]$, Eq. (3):

$$M[\hat{u}_0] = \mathbf{d} \cdot \mathbf{A} \cdot \mathbf{d} - 2\mathbf{d} \cdot \mathbf{g} = -\mathbf{g} \cdot \mathbf{A}^{-1} \cdot \mathbf{g}. \tag{13}$$

If one has found a good approximation to $M[u_0]$, this does not mean that $\hat{u}_0$ given by Eq. (8) is good too; the approximation is rather to the value and derivative of u_0 at the end points. This will become apparent in the specific application of Sec. III.

D. Choice of Trial Functions

One may choose the trial functions to replace the integration of a differential operator in Eq. (12) with the integration of a function. One way is to take the trial functions as solutions of a similar differential equation

$$[p(x)v_i']' = t_i(x)v_i, \qquad i = 1, \cdots, N', \tag{14}$$

where $t_i(x)$ is some arbitrary integrable function. Then the only integrals involved are in Eq. (12):

$$A_{ij} = \int_a^b dx v_i(t_j - q - L + \lambda\rho)v_j. \tag{15}$$

E. End Point Condition $u(a) = 0$

If either of the end point conditions in Eq. (2) is replaced by one of the form $u(a) = 0$, then a corresponding adjustment must be made in the approximation method: The corresponding term in the L operator is dropped:

$$\int_a^b dx f(x)L[g(x)] = [fp(g' + \beta g)]_{x=b}. \tag{4'}$$

The stationary functional is now a direct generalization of that described in Ref. 2,

$$M[u] = \int_a^b dx u[K - L + \lambda\rho(x)]u + 2\delta p(b)u(b). \tag{3'}$$

The first variation in the stationary problem Eq. (7) now has as an end point condition at $x = a$

$$[p(vu' - uv')]_{x=a} = 0,$$

and, hence, this end point condition will be satisfied by

$$u(a) = 0, \qquad v(a) = 0. \tag{16}$$

Therefore the trial functions in II C must be restricted to $v_i(a) = 0$. The Schrödinger equation of the following section is of this type.

Of course, one must also rewrite Eq. (11):

$$g_i = -\delta(pv_i)_{x=b}. \tag{11'}$$

If neither end point condition is covered by Eq. (2), but

$$u(a) = u(b) = 0,$$

then it is interesting to note that the method is reduced to the eigenvalue problem

$$\mathbf{A} \cdot \mathbf{d} = 0,$$

with

$$A_{ij} = \int_a^b dx v_i[K + \lambda\rho]v_j.$$

III. SOLUTION OF THE SCHRÖDINGER EQUATION

Let u_0 be the solution of the radial Schrödinger equation

$$u'' + [E - V(r)]u = 0, \tag{17}$$

$$u(0) = 0, \tag{18}$$

and $u(r)$ bounded on $[0, \infty)$. The differential equation (17) for each E has only two independent solutions: If $I(r)$ and $O(r)$ are some known independent solutions for $r > a$, then, without loss of generality, where U is a complex parameter,

$$u_0 = I - UO, \quad r \geq a. \tag{19}$$

Equation (17) is defined on the space $\mathfrak{D}^{(1)}$ of continuous functions with continuous first derivatives. Therefore, from (19), the external part ($r > a$) of the system above may be replaced by the boundary condition

$$uO' - u'O = W, \quad r = a, \tag{20}$$

where W is the Wronskian $W(I, O; a) = [IO' - OI']_{r=a}$. If I and O are each normalized to unit flux in a problem of quantum mechanical scattering, then U is the scattering "matrix" $e^{2i\delta}$; it is not necessary to normalize u_0 separately.

With $M[u]$ defined by (3'), a functional

$$U[u] = (I/O)_{r=a} + [M[u]/W] \tag{21}$$

has the property $U[u_0] = U$. Therefore, the approximation procedure for M given by Eq. (13) leads to an approximation for the quantity U which has physical interest. (The interval $x \in [a, b]$ has now been replaced by $r \in [0, a]$.)

Henceforth, we shall write simply I for $I(a)$, and O for $O(a)$. Equation (21) together with (13) gives the approximation $U[\hat{u}_0]$.

A. Energy Dependence of the Solution

Let us call E the energy. Since the external solution $O(r)$ is energy dependent, from (2), (4'), and (20), one sees that the matrix $\mathbf{A}$, which is to be inverted, does not have a simple energy dependence. However, let us define a symmetric function matrix $\mathbf{B}(\varphi)$ with elements

$$B_{ij}(\varphi) = \int_0^a dr v_i(K - L_\varphi + E)v_j', \tag{22}$$

where L_φ is given by Eq. (4') and φ is treated as a variable:

$$\int_0^a dr f(r) L_\varphi[g(r)] = [f(g' + \varphi g)]_{r=\alpha}.$$

Then the actual boundary condition is for $\varphi = -O'/O$, and

$$\mathbf{B}(-O'/O) = \mathbf{A}. \tag{23}$$

If one defines the function[7]

$$R(\varphi) = -a^{-1}\mathbf{v}\cdot\mathbf{B}^{-1}\cdot\mathbf{v}, \tag{24}$$

where $v_i = v_i(a) = (O/W)g_i$, then

$$-a\frac{\partial R}{\partial \varphi} = \mathbf{v}\cdot\frac{\partial \mathbf{B}^{-1}}{\partial \varphi}\cdot\mathbf{v} = -\mathbf{v}\cdot\mathbf{B}^{-1}\cdot\frac{\partial \mathbf{B}}{\partial \varphi}\cdot\mathbf{B}^{-1}\cdot\mathbf{v} = \mathbf{v}\cdot\mathbf{B}^{-1}\cdot(\mathbf{vv})\cdot\mathbf{B}^{-1}\cdot\mathbf{v} = a^2R^2. \tag{25}$$

By integration, therefore

$$R(\varphi) = R(0)/[1 + a\varphi R(0)]. \tag{26}$$

With $\varphi = -O'/O$, one may use Eqs. (13), (21) – (23), and (26) to find that

$$U[\hat{u}_0] = \frac{I}{O}\,\frac{1 - (I'/I)aR(0)}{1 - (O'/O)aR(0)}. \tag{27}$$

This is a standard form in R-matrix theory. The other simplification is that the calculation of $R(0)$ now involves inverting the matrix

$$\mathbf{B}(0) = \mathbf{Y} + E\mathbf{Z},$$

where $\mathbf{Y}$ and $\mathbf{Z}$ are both *energy independent*. The symmetric elements of these matrices are

$$Y_{ij} = \int_0^a dr(v_i v_j'' - v_i v_j V) - (v_i v_j')_{r=a},$$
$$Z_{ij} = \int_0^a dr v_i v_j. \tag{28}$$

B. Schrödinger Equation with Coulomb Potentials

As an example, let us solve the three-dimensional Schrödinger equation for the *scattering phase shifts*, when the potential is central and is equal to a repulsive Coulomb potential for $r > a$. The partial wave separation reduces the system to the radial equations

$$\frac{d^2u_l}{dr^2} - \frac{l(l+1)}{r^2}u_l + \frac{2\mu}{\hbar^2}\left[E_{\rm cm} - U_{\rm nuc} - \frac{Z_1Z_2e^2}{r}\right]u_l = 0, \tag{29}$$

for $l = 0, 1, \cdots, \infty$, and the usual boundary conditions (18). The short-range part is called the nuclear potential

$$U_{\rm nuc}(r) = 0, \quad r > a.$$

When $E_{\rm cm} > 0$ there is a continuum of scattering solutions.

The nuclear phase shifts δ_l are defined by (19) and

$$U = \exp[2i(\delta_l + \omega_l)], \tag{30}$$

where I and O in (19) are the ingoing and outgoing Coulomb waves

$$I_l \sim \exp[-i(\rho - \eta \log 2\rho - 1/2l\pi + \sigma_0),$$
$$O_l = I_l^*,$$

$$\rho = kr \equiv (2\mu E_{cm}/\hbar^2)^{1/2} r,$$
$$\eta = \mu Z_1 Z_2 e^2/k\hbar^2,$$
$$\sigma_l = \arg \Gamma(1 + l + i\eta), \quad l = 0, 1, \cdots, \infty.$$

Two alternative, independent solutions of the Coulomb equation are $F_l(r)$ and $G_l(r)$, the regular and irregular Coulomb functions, where

$$I_l = O_l^* = [G_l - iF_l] \exp(i\omega_l),$$

and

$$\omega_l = \sigma_l - \sigma_0.$$

Now (27) is just Eq. (IV. 1. 13) of Lane and Thomas,[5] and

$$\delta_l = \arctan \frac{R_l P_l}{1 - R_l S_l} - \varphi_l, \tag{31}$$

where R_l is the R function $R(0)$ calculated with (24) for each radial equation, P_l is the *penetrability*, and S_l is the *shift factor:*

$$P_l = ak/(F_l^2 + G_l^2),$$
$$S_l = a(F_l F_l' + G_l G_l')/(F_l^2 + G_l^2)$$

(the functions F and G are evaluated at a, as are their derivatives), and φ_l is the *hard-sphere phase shift*

$$\varphi_l = \arctan (F_l/G_l).$$

IV. NUMERICAL CALCULATION OF $\alpha-\alpha$ POTENTIAL SCATTERING

Previous calculations[1] have shown that, with a suitable choice of $\mathcal{T}$, this method gives a good approximation with N equal to just 3, 4, or 5, for (a) scattering from a square well, (b) scattering from a square well plus a Coulomb potential, (c) scattering into coupled channels with square well and with harmonic oscillator interactions, and (d) the bound-state eigenvalue problem in certain attractive wells.

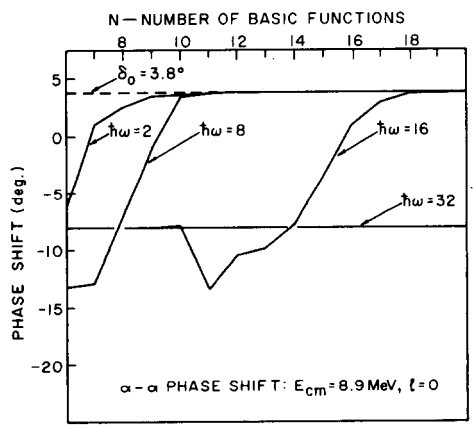

FIG. 1. Convergence of the approximation method for different oscillator strengths $\hbar\omega$ (in MeV) of the trial functions. The convergence for $\hbar\omega = 1$ MeV is not shown, but it is very poor, reaching only 2.1° by $N = 20$. We consider $\hbar\omega = 8$ MeV to give the best results, since it has the steepest rise to a good approximation.

TABLE I. Parameters of the $\alpha-\alpha$ nuclear potential.

	MeV		fm^{-1}	
	U_r	U_a	μ_r	μ_a
$l = 0$	500	130	0.7	0.475
$l = 2$	320	130	0.7	0.475
$l = 4$	0	130	···	0.475

TABLE II. Values of the nuclear and the Coulomb potentials for $\alpha-\alpha$ scattering ($l = 0$). The nuclear term is negligible at a radius of 8 fm.

Radius (fm)	2	4	6	8	10
Potentials (MeV)					
Nuclear	17.7	−3.32	−0.04	$\sim -10^{-4}$	$\sim -10^{-8}$
Coulomb	2.9	1.44	0.96	0.72	0.58

In this section, we shall use a physically interesting potential, the $\alpha-\alpha$ potential of Ali and Bodmer,[8] to demonstrate the convergence properties of this approximation method. We shall show that a good choice of trial space is not just desirable, but necessary; the choice can be made quite simply, and once made is good over a large range of energies. The $\alpha-\alpha$ scattering is described by (29) with $Z_1 = Z_2 = 2$, $\mu = \frac{1}{2} \times 4.003\ 88$ amu, $e^2 = 1.439\ 87$ MeV fm, $(2/\hbar^2) = 0.0478\ 33$ MeV^{-1} amu^{-1} fm^{-2}; and a nuclear potential with a repulsive core followed by an attractive region:

$$U_{\text{nuc}}(r) = U_r \exp(-\mu_r{}^2 r^2) - U_a \exp(-\mu_a{}^2 r^2). \tag{32}$$

The parameters of this potential are given in Table I.

The nuclear potential is very small at $r = 8$ fm (Table II). Therefore, we shall present calculations with $a = 8$ fm, and shall not report the convergence of the results as a is changed.[9]

As trial functions, we used the eigenfunctions of a harmonic oscillator equation, $v_n(r) = \hat{v}_n(r, \hat{l})$, which satisfy

$$\frac{d^2}{dr^2}\hat{v}_n(r, l) + \left[\lambda_{nl} - \frac{l(l+1)}{r^2} + \left(\frac{\mu\omega}{\hbar}\right)^2 r^2\right]\hat{v}_n(r, l) = 0, \tag{33}$$

$$\lambda_{nl} = 2(\mu\omega/\hbar)(2n + l - \tfrac{1}{2}), \quad n = 1, \cdots, \infty,$$

and

$$v_n(0) = 0.$$

Although the trial functions $v_n(r)$ are not orthogonal on $[0, a]$, they are independent (see Appendix). The approximation is defined by the two parameters ω and N, and we must not only look at the convergence of the approximation for increasing N, but also at the results of changing ω.

For easy comparison, we give the published phase shifts[8] (Table III) calculated by Ali and Bodmer from the potential given by (32). In our first calculations, we have used $l = \hat{l}$. The convergence of the calculations for $l = 0$ is shown in Fig. 1, at an

TABLE III. Comparison of phase shifts for $\alpha-\alpha$ scattering calculated using nonorthogonal expansions with published calculations of Ali and Bodmer. The results shown are representative of the range of energies investigated. The approximation used $\hbar\omega = 8$ MeV.

Source of phase shifts (deg)	l	Energy in c.m. (MeV) 1	3	6.15	8.9	11.45	59.93
Ali and Bodmer (Ref. 8)	0	148.6	87.0	35.0	5.4	−15.7	−170.9
	2	0.5	a	114.1	103.1	92.5	−4.3
	4	a	a	2.5	13.9	70.0	152.5
Approximation of present paper		**14**[b]	**12**	**10**	**12**	**12**	**14**
	0	146.8	84.8	33.1	3.8	−17.1	−171.6
		12	**12**	**10**	**12**	**12**	**14**
	2	0.5	64.9	112.7	101.9	91.5	−4.9
		10	**10**	**10**	**10**	**12**	**12**
	4	0.0	0.1	2.0	12.5	63.8	151.

a No value reported.

b Boldface numerals are the earliest even value of N for which the calculations have converged to an accuracy of the decimal place in the phase shift.

energy 8.9 MeV (in the middle of the range to be investigated). Convergence for $l = 2, 4$ was better, but it had a similar pattern, and in particular it was good for $\hbar\omega = 8$ MeV. One sees that a good choice of ω is easy to make. However, if one did not check what happens when the trial functions themselves are changed, one might achieve not only poor convergence or no convergence at all, but even an incorrect answer. Also with a bad choice of ω the procedure may not even give the best approximation within the trial space. With $\hbar\omega = 16$ MeV for example, the approximation to δ_0 (or to U) is better at $N = 10$ than at $N = 11$. This would be presumably a saddle point in the error, rather than a minimum (see Sec. II B). Even though this difficulty appears to be easy to deal with numerically, it shows that the sort of procedure applied here is not a best approximation as has sometimes been stated.

A good trial space ($\hbar\omega = 8$ MeV) chosen at $E = 8.9$ MeV is good for all energies from 1–60 MeV (see Table III). There is a small, consistent difference between our calculations and those of Ali and Bodmer, which is not due to inaccuracies in our calculations, nor to a failing in the method; we made an independent calculation of two phase shifts using a conventional scattering code, in which the Schrödinger equation is integrated numerically, and the difference between the results of the conventional method and our method using nonorthogonal expansions was less than 0.1°.

Because the $\alpha-\alpha$ potential for $l = 0$ has a large repulsive core, the solution u_0 will be flat and near zero around the origin, and will not begin to oscillate until beyond the repulsive region. Therefore, we were interested to see whether a better convergence could be had if $\hat{l} > l = 0$, i.e., if a centrifugal barrier were imposed on the trial functions. The results are shown in Table IV. We varied $\hbar\omega$ for each choice of $\hat{l}$, and we found that $\hbar\omega = 8$ MeV was a best choice each time. With $\hat{l} = 6$, there is good convergence by $N = 7-9$, a small improvement over $\hat{l} = 0$, when we needed $N = 10-12$ basis functions. However, with $\hat{l} = 7$ greater, we could no longer claim a reliable approximation had been found for any value of $\hbar\omega$.

TABLE IV. Use of basis functions with different l values to get better convergence to the $l = 0$ $\alpha-\alpha$ scattering; $E_{cm} = 8.9$ MeV, $\hbar\omega = 8$ MeV. N is the number of basis functions used in each approximation.

N	Harmonic oscillator l value $\hat{l}$ 0	2	4	5	6	7	8
2	−8.0	−8.0	−8.0	−7.7	−6.9	−5.7	−3.9
3	−8.0	−8.0	−6.9	−5.0	−2.8	−0.2	+3.2
4	−8.0	−6.6	−14.4	−13.9	−17.0	−23.5	−34.2
5	−6.4	−13.4	−14.2	−11.3	−7.1	−8.9	−19.4
6	−13.2	−13.3	−7.1	−4.8	−5.0	−8.8	−17.6
7	−13.0	−7.0	−2.2	−0.8	3.3	1.7	−5.4
8	−6.9	−1.3	3.3	3.6	3.6	2.1	−2.5
9	−0.9	3.3	3.6	3.6	3.8	3.3	0.6
10	3.3	3.6	3.8	3.8	3.8	3.5	2.0
11	3.6	3.8	3.8	3.8	3.8	3.7	2.8
12	3.8	3.8	3.8	3.8	3.8	3.7	3.2
13	3.8	3.8	3.8	3.8	3.8	3.7	3.5
14	3.8	3.8	3.8	3.8	3.8	4.3	3.4
15	3.8	3.8	3.8	3.8	3.8	3.8	3.6
16	3.8	3.8	3.8	3.8	3.8	3.8	3.6
17	3.8	3.8	3.8	3.8	3.8	3.8	2.9
18	3.8	3.8	3.8	3.8	3.8	3.8	3.6
19	3.8	3.8	3.8	3.8	3.8	3.8	4.0
20	3.8	3.8	3.8	3.8	3.8	3.8	4.0

ACKNOWLEDGMENTS

We wish to thank Dr. D. Robson for his constant help and interest and Dr. C. M. Vincent for his critical reading of the manuscript and particularly for pointing out the importance of being able to deal with nonlocal potentials.

APPENDIX

In this Appendix, a criticism of the method is answered: The criticism is that the basis functions of the trial space form a (linearly) dependent set when N' is infinite, and, therefore, the expansion coefficients $\{d_i\}$ in (8) and (10) cannot be determined uniquely (**A** would be singular) for some finite value of N, and the approximation will break down.[10]

Here we shall show only that the harmonic oscillator functions are independent on any finite interval. This property does *not* follow from the orthogonality of $\{v_i\}$ on $[0, \infty)$; a set of functions may be independent on a certain interval, and yet dependent on a subinterval. For example, the two functions $|\sin x|$, and $\sin x$, are independent on $[0, 2\pi]$, yet dependent (and identical) on $[0, \pi]$.

Definition: An arbitrary set is independent if and only if every finite subset is independent.

The harmonic oscillator functions are a polynomial multiplied by a certain constant function, viz., for an $l \geq 0$ in (331)

$$v_n = \hat{v}_n(r, l) = C_{nl} r^{l+1} \exp(-\tfrac{1}{2}\alpha^2 r^2) \times L_{n-1}^{(l+1/2)}(\alpha^2 r^2), \quad \text{(A1)}$$

where $\alpha = (\mu\omega/\hbar)^{1/2}$. The standard that we use for the generalized Laguerre polynomial is that of the Bateman Manuscript Project[11]; the leading term of $L_{n-1}^{(l+1/2)}(x)$ is $(-)^{n-1}x^{n-1}/(n-1)!$

Therefore, the maximum number of points on which the functions $\{v_i\}$, $i = 1, \cdots, N$, can be dependent ($r \geq 0$) is the greatest number of real roots of a polynomial of degree $N + 1$ (the point $r = 0$). In other words a finite set of N harmonic oscillator functions cannot be dependent on a set of more than $(N + 1)$ distinct points, and, in particular, *the infinite set of harmonic oscillator functions is independent on a finite interval [0, a].*

It follows that the expansion of any function on $[0, a]$ is unique and, in particular, that all the expansion coefficients of the zero function are zero [compare Eq. (8, 13. 4b) of Ref. 10].

Because the harmonic oscillator functions have proven useful as a nonorthogonal basis,[1] we take this opportunity to give some computational properties for easy reference.

A standard normalization is

$$C_{nl} = [2\alpha(n-1)!/\Gamma(n + l + 1/2)]^{1/2}. \tag{A2}$$

In numerical integrals, one may use

$$\int_0^a dr\hat{v}_m(r, l)\hat{v}_n(r, l) = [\hat{v}_m(a, l)\hat{v}_n'(a, l) - \hat{v}_n(a, l)\hat{v}_m'(a,l)]/4(m-n)\alpha^2 \tag{A3}$$

and

$$\hat{v}_n'(r, l)/\hat{v}_n(r, l) = 1/r\{l + 1 - \alpha^2r^2[1 + 2L_{n-2}^{(l+3/2)}(\alpha^2r^2)/L_{n-1}^{(l+1/2)}(\alpha^2r^2)]\}. \tag{A4}$$

The starting values, when a potential $\sim r^{-2}$ at the origin must be integrated, are given by

$$\lim_{r\to 0} \frac{\hat{v}_m(r, l)\hat{v}_n(r, l)}{r^2} = 2\alpha^3[\Gamma(n + \tfrac{1}{2})\Gamma(m + \tfrac{1}{2})/(n-1)!(m-1)!]^{1/2}, \quad l = 0,$$
$$= 0, \quad l > 0. \tag{A5}$$

The polynomials are computed by upward recurrence on degree:

$$kL_k^{(\beta)} + (x - \beta - 2k + 1)L_{k-1}^{(\beta)} + (k + \beta - 1)L_{k-2}^{(\beta)} = 0, \quad L_0^{(\beta)}(x) = 1, L_1^{(\beta)}(x) = 1 + \beta - x.$$

---

* Research supported in part by the Air Force Office of Scientific Research, Office of Aerospace Research, AF-AFOSR-69-1674, and the National Science Foundation NSF-GP-7901 and NSF-GJ-367.

† Present address: CERN Theory Division, Geneva.

‡ Present address: Department of Physics, Georgia State University, Atlanta, Georgia.

1 J. L. Adams, Ph. D. Dissertation, The Florida State University, 1967 (unpublished); J. E. Purcell, Florida State University Technical Report No. 1 (1969); Phys. Rev. 185, 1279 (1969).

2 A. M. Lane and D. Robson, Phys. Rev. **178**, 1715 (1969); R. A. Chatwin, Phys. Rev. C 2, 1167 (1970).

3 G. Birkhoff and G.-C. Rota, *Ordinary Differential Equations* (Blaisdell, Waltham, Mass., 1969), 2nd ed.

4 V. I. Koroza, Dokl. Akad. Nauk SSSR **186**, 795 (1969)[Sov. Phys. Dokl. **14**, 526 (1969)].

5 A. R. Forsyth, *Calculus of Variations* (Cambridge U.P., London, 1927), Chap. 3.

6 We have supposed that u_0 is the unique solution of a differential system: For certain values of the end point conditions there may be no unique solution, or even no solution at all. However, the variational problem is completely equivalent, and the method to be described may still be used [see Eq. (10) below], except that one would look for solutions of a matrix equation without using a matrix inverse.

7 It is obviously unnecessary to define the R function, because the properties we shall require are already those of the matrix **B**. However, we prefer at this point to use the standard terms of R-matrix theory: A. M. Lane and R. G. Thomas, Rev. Mod. Phys. 30, 257 (1958).

8 S. Ali and A. R. Bodmer, Nucl. Phys. 80, 99 (1969).

9 The matching radius a was varied in certain test calculations reported by one of the authors (J.E.P.) in a technical report (Ref. 1)

10 C. Mahaux and H. A. Weidenmuller, *Shell-Model Approach to Nuclear Reactions* (North Holland, Amsterdam, 1969), Chap. 8.

11 *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill, New York, 1953), Vol. 2., Chap. 10.

Erratum: Linear Random Operator Equations in Mathematical Physics. I

[J. Math. Phys. **11,** 1069 (1970)]

G. Adomian
Department of Mathematics, University of Georgia, Athens, Georgia 30601
(Received 28 May 1971)

On page 1076, starting with Eq. (4.6), we correct as follows.

By substituting (4.6), we can rearrange (4.5) as follows, at least for the perturbation case:

$$\langle u(t)\rangle = L^{-1}\langle g\rangle\,[1 + L^{-1}\langle \alpha(t)L_t^{-1}\,\alpha(t)\rangle]$$

$$= \int_0^t l(t-\tau)\,\langle g(\tau)\rangle\,[1 + \int_0^\tau l(\tau-\gamma)\,\langle \alpha(\gamma)$$

$$\times \int_0^\gamma l(\gamma-\sigma)\,\alpha\,(\sigma)\rangle d\sigma\,d\gamma]d\tau$$

$$= \int_0^t l(t-\tau)\,\langle g(\tau)\rangle\,[1 + \int_0^\tau l(\tau-\gamma)$$

$$\times \int_0^\gamma l(\gamma-\sigma)R_\alpha(\gamma,\sigma)d\sigma\,d\gamma]d\tau,$$

where R_α is the correlation for α. We observe that we have $\langle u\rangle$ in terms of $\langle g\rangle$ and an integral kernel or "stochastic Green's function"

$$l(t-\tau)\,[1 + \int_0^\tau l(\tau-\gamma)\,\int_0^\gamma l(\gamma-\sigma)R_\alpha(\gamma,\sigma)d\sigma\,d\gamma],$$

where l and R_α are given.

The author apologizes for the omission of the L^{-1} operator which was pointed out by a student, A. I. Dale. Insufficient care was exercised since this section is well known and was included finally only for correlation with the other results. The errors involved in the averaging procedure here have been discussed more fully in a paper by this author [J. Stat. Phys. 3, 127 (1971)]. There are, of course, many procedures for establishing closure, but the basic errors become clear and can now be compared. (This will be done in a forthcoming paper.)